Full wwPDB EM Validation Report

Mar 19, 2024 – 09:38 PM JST

PDB ID	:	6JGZ
EMDB ID	:	EMD-9824
Title	:	Structure of RyR2 (F/P/Ca2+ dataset)
Authors	:	Chi, X.M.; Gong, D.S.; Ren, K.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Zhou, Q.; Yan, N.
Deposited on	:	2019-02-16
Resolution	:	4.60 Å(reported)

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

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

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

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

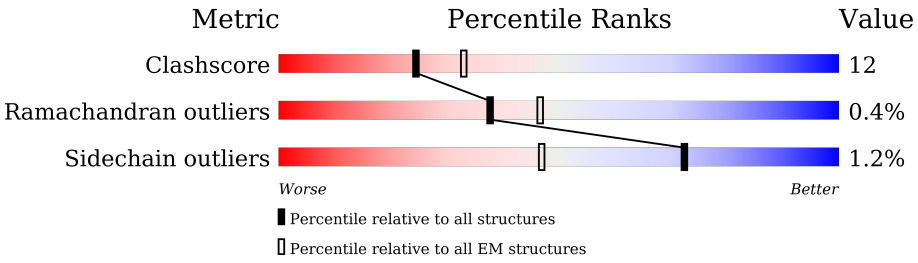
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	67% 32%
1	C	108	67% 32%
1	E	108	65% 34%
1	G	108	68% 31%
2	B	4968	6% 52% 18% 30%
2	D	4968	6% 52% 18% 30%
2	F	4968	6% 52% 18% 30%
2	H	4968	5% 51% 18% 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 109824 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
			819	516	144	155	4		
1	C	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	D	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	F	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	H	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		

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

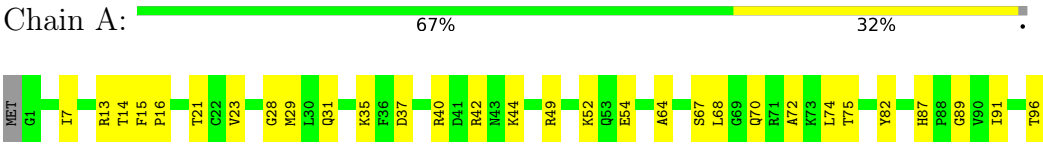
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	H	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

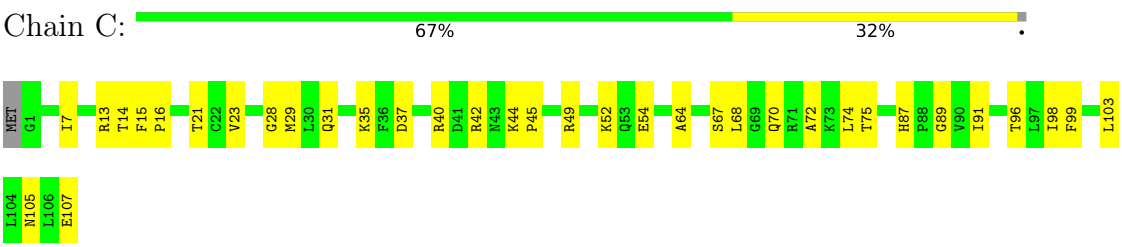
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



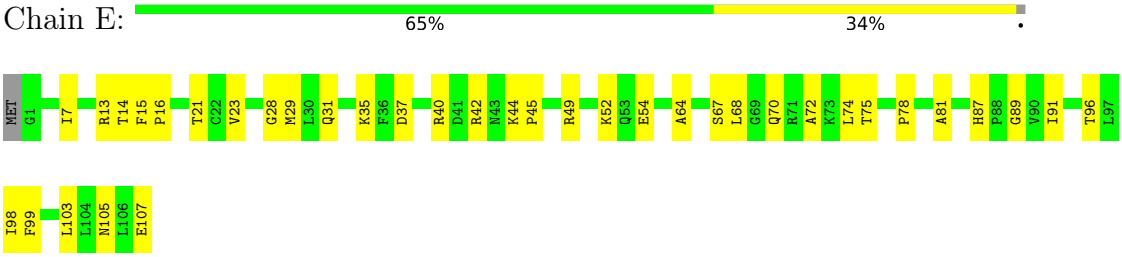
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C:



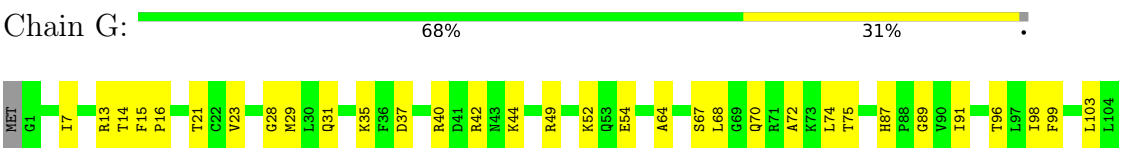
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



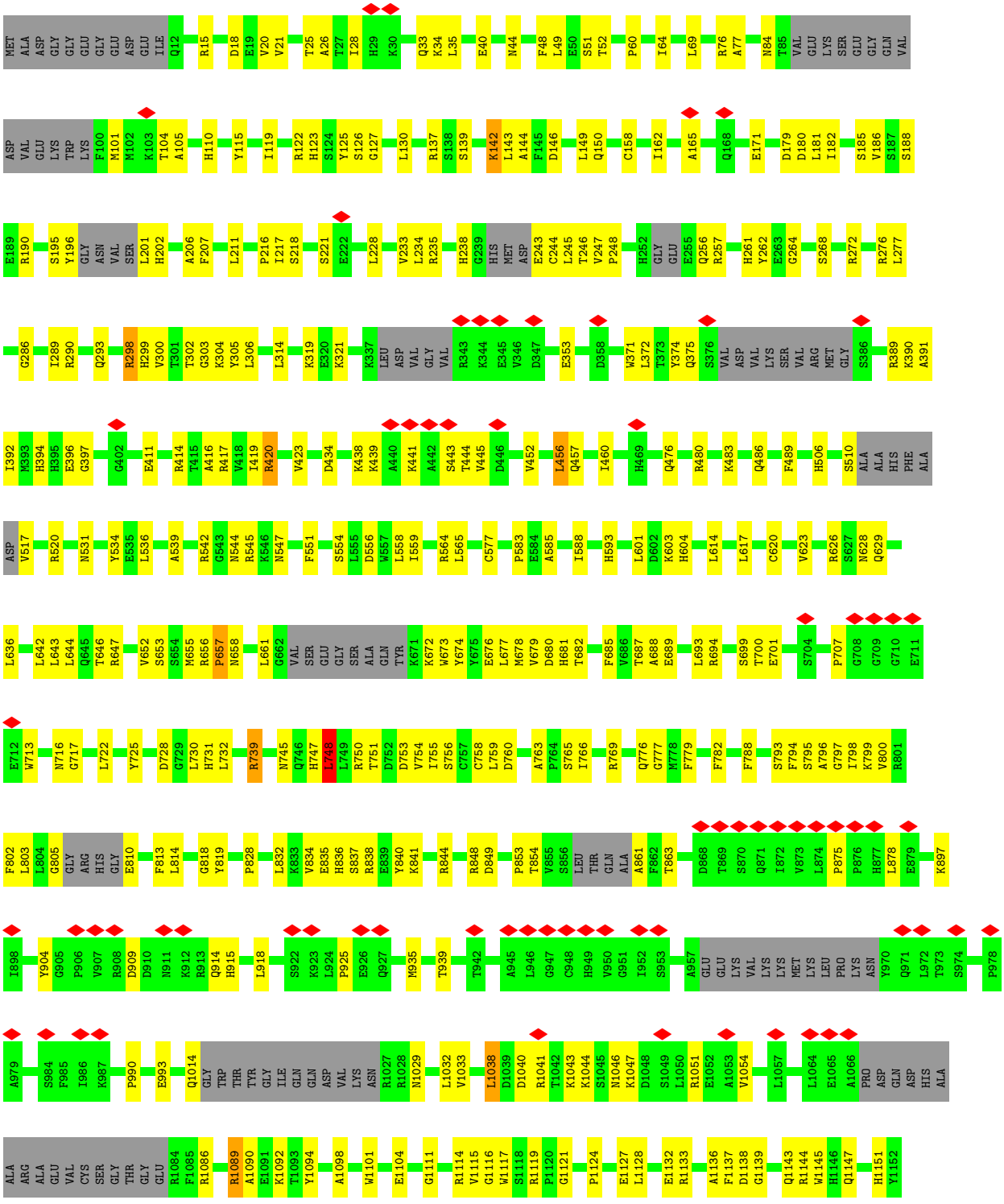
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

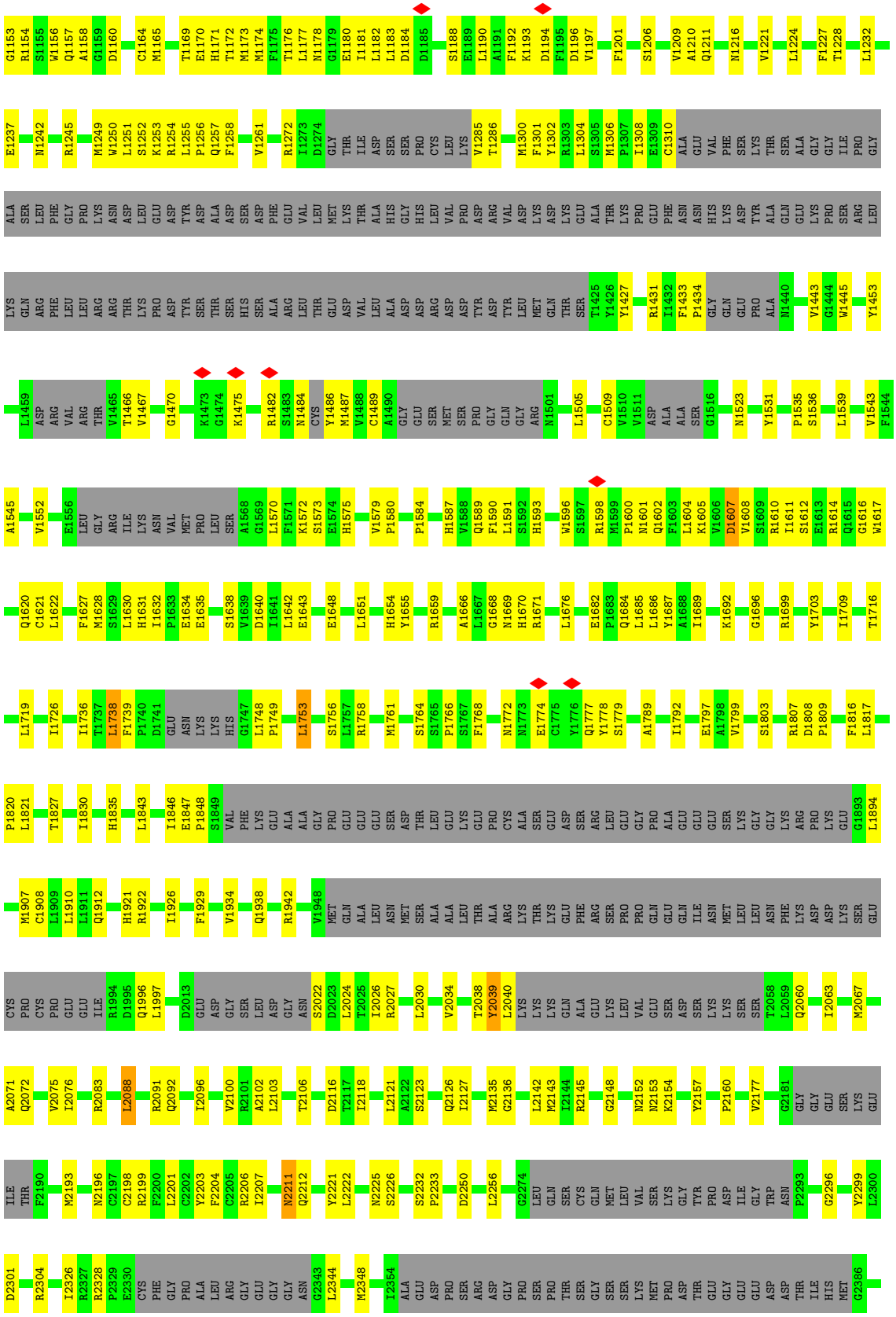
Chain G:

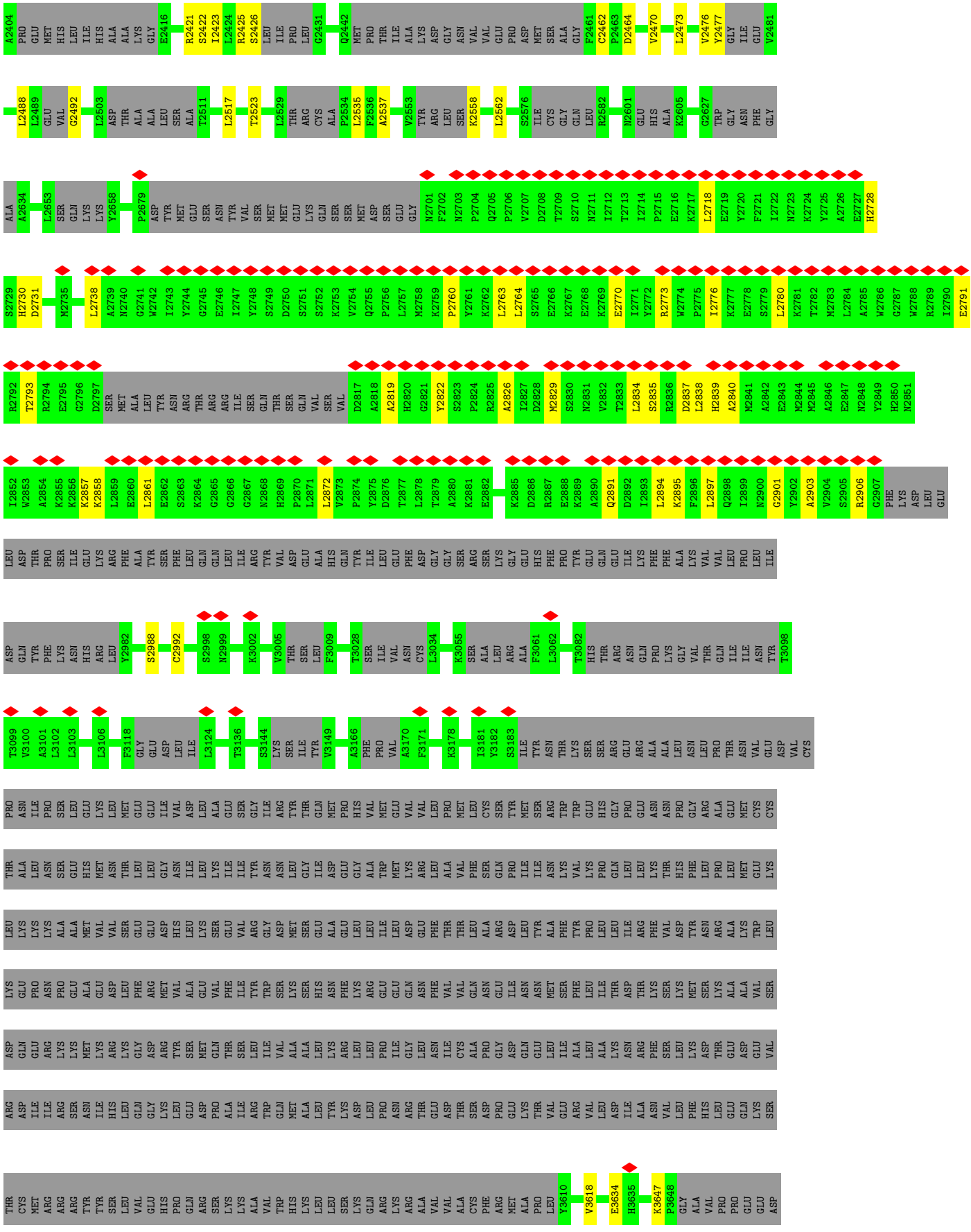


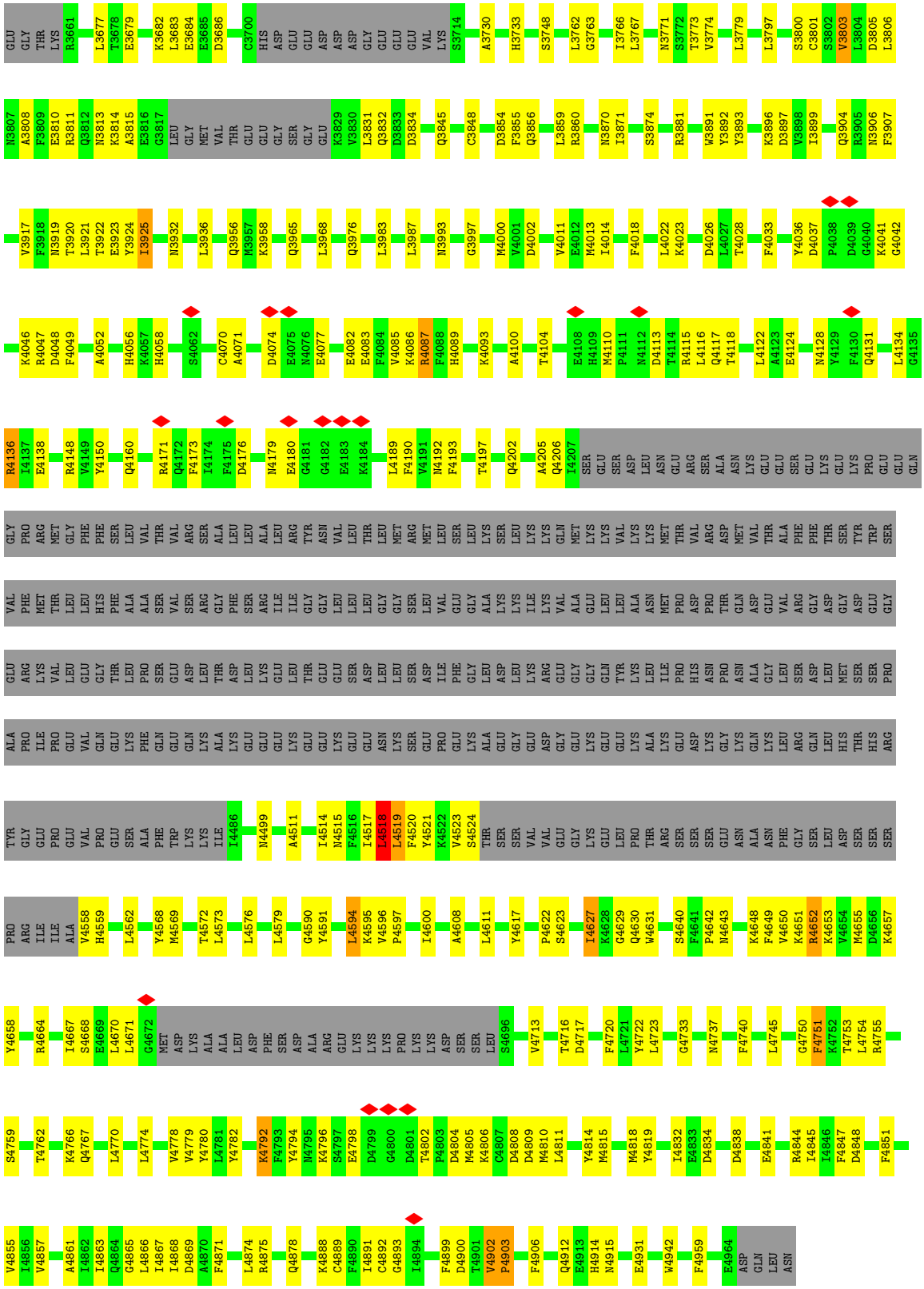
• Molecule 2: RyR2

Chain B:

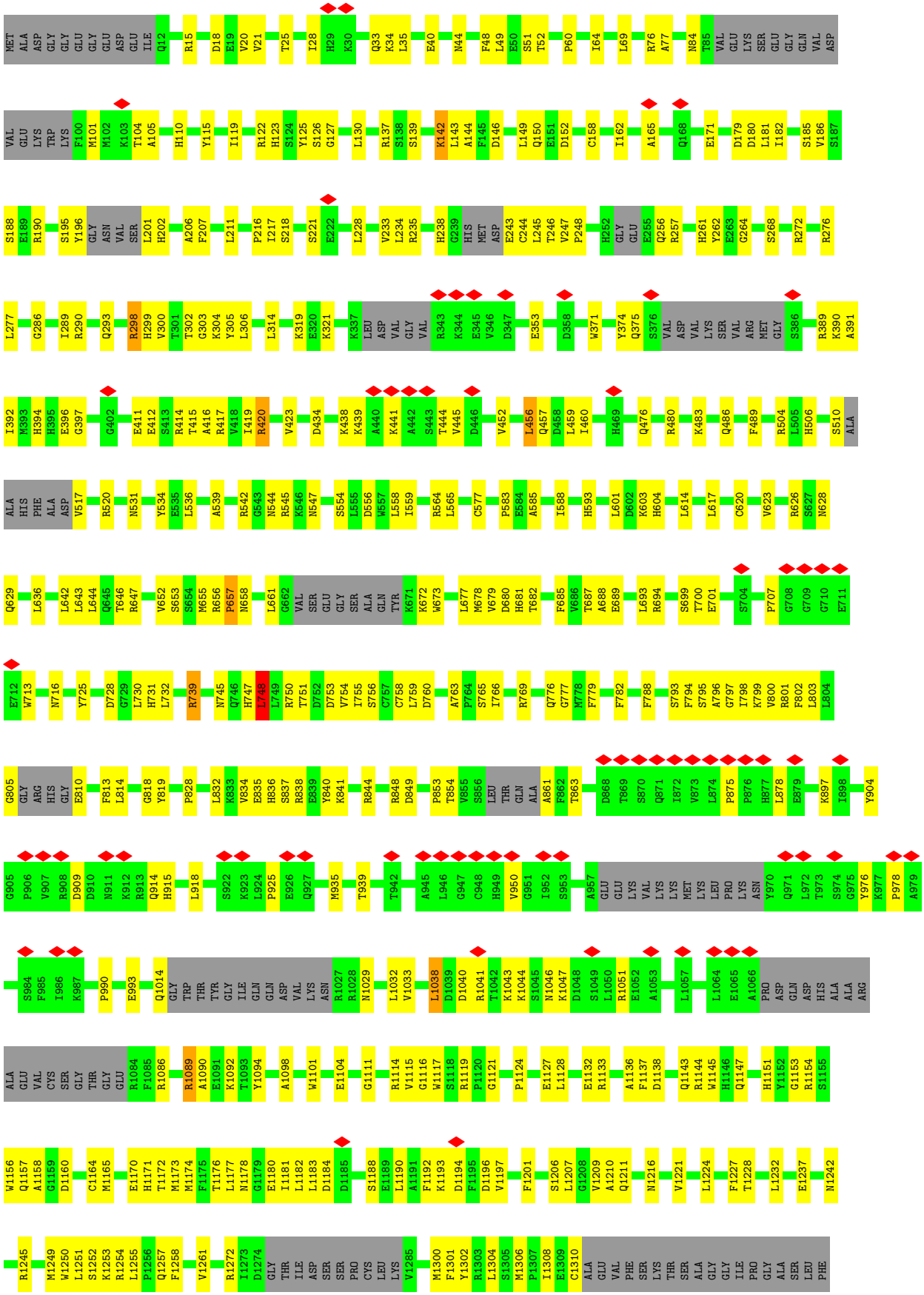


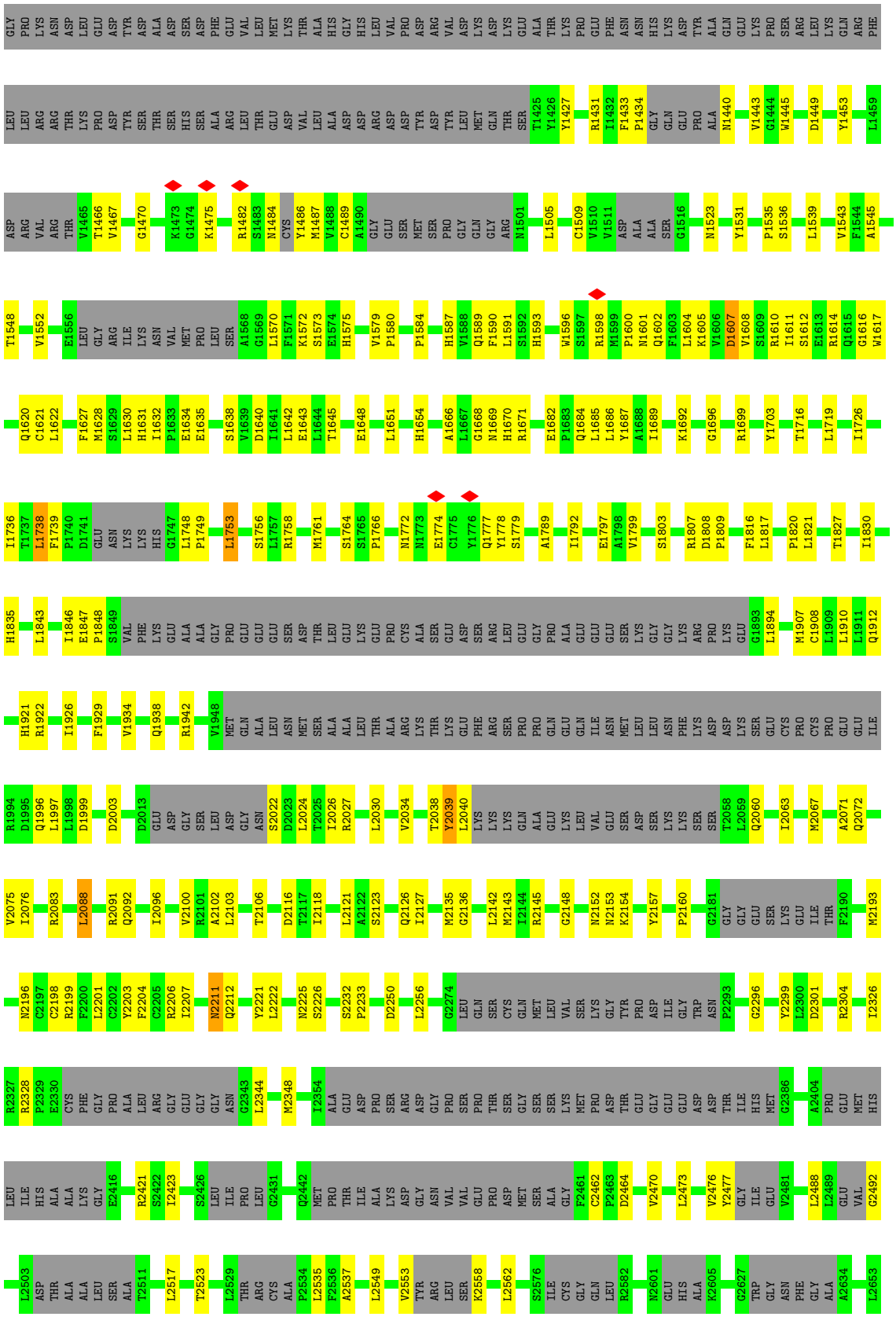


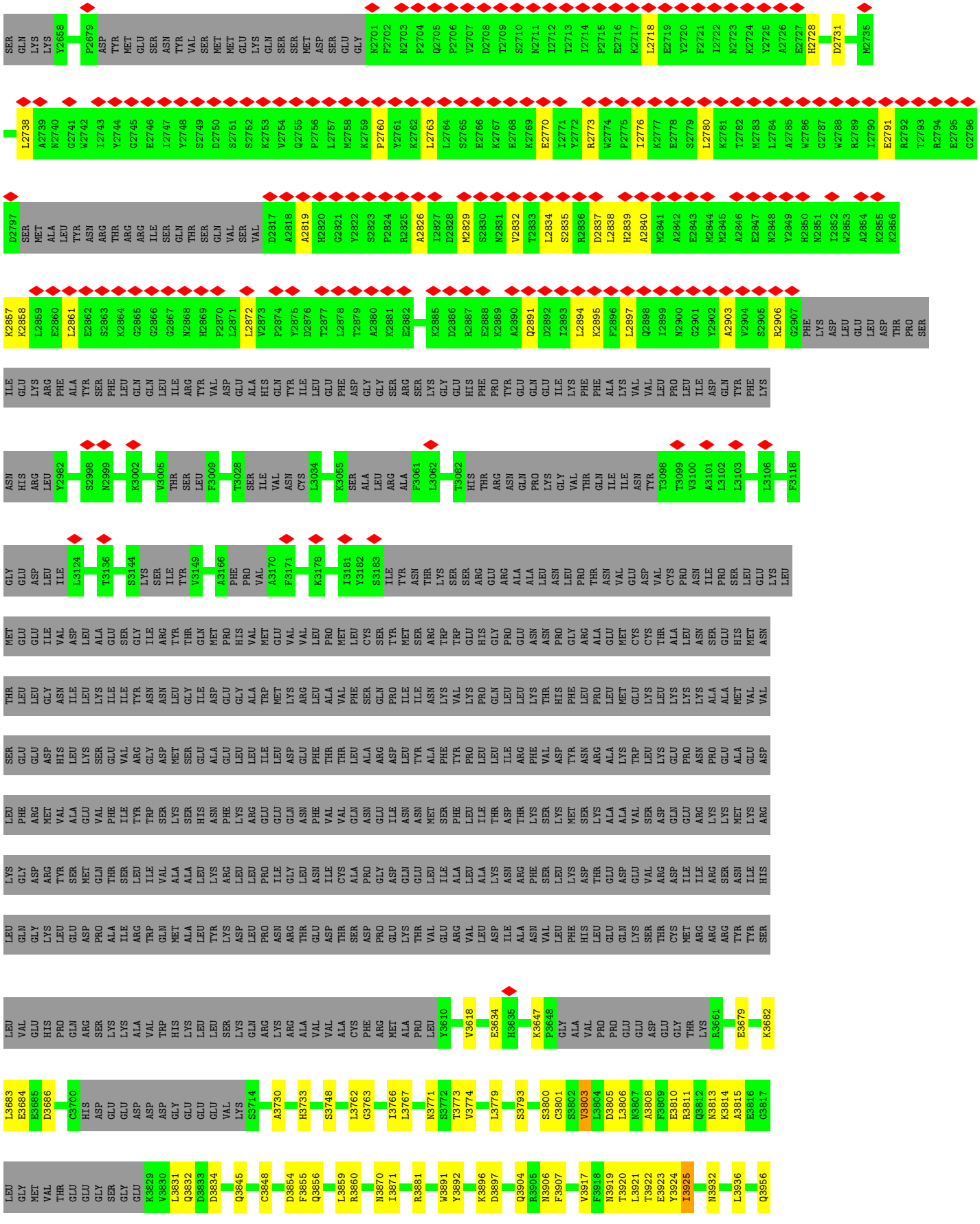

A2404 PRO GLU MET HIS LEU ILE HIS ALA ALA LYS GLY E2416
R2421 S2422 I2423 L2424 R2425 S2426 LEU ILE PRO LEU G2431
G2442 MET PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 C2462 P2463 D2464 V2470 L2473 V2476 Y2477 GLY ILE GLU V2481
L2488 L2489 GLU VAL G2492 L2503 ASP THR ALA ALA LEU SER ALA T2511 L2517 T2523 L2529 THR ARG CYS ALA P2534 L2535 F2536 A2537 V2553 TYR ARG LEU SER K2558 L2562 S2576 ILE CYS GLY GLN LEU R2582 N2601 GLU HIS ALA K2605 G2627 TRP GLY ASN PHE GLY
ALA A2634 L2653 SER GLN LYS LYS Y2658 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725 A2726 E2727 H2728
S2729 H2730 D2731 M2735 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 W2788 R2789 I2790 E2791
R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL D2817 A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851
I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 V2873 P2874 Y2875 D2876 T2877 L2878 T2879 A2880 K2881 E2882 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU GLU
LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU LEU PRO LEU ILE
ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 S2988 C2992 S2998 N2999 K3002 V3005 THR SER LEU F3009 T3028 SER ILE VAL ASN CYS L3034 K3055 SER ALA LEU ARG ALA F3061 L3062 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098
T3099 V3100 A3101 L3102 L3103 L3106 F3118 GLY GLU ASP LEU ILE L3124 T3136 S3144 LYS SER ILE TYR V3149 A3166 PHE PRO VAL A3170 F3171 K3178 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS
PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ARG GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS
THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU LEU GLY ASN ILE LEU LEU ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS THR HIS PHE LEU PRO LEU MET GLU LYS
LEU LYS LYS LYS ALA MET VAL SER GLU GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU ASP GLU PHE THR LEU ALA ARG ASP LEU TYR ALA PHE PHE TYR PRO LEU LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU
LYS GLU PRO ASN PRO GLU ALA ASP GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL ALA GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER
ASP GLN GLU ARG LYS LYS MET LYS ARG GLY LYS TYR SER MET GLN THR SER LEU ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU LEU PHE HIS LEU GLU GLN LYS SER
THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU Y3610 V3618 E3634 H3635 K3647 P3648 GLY ALA VAL PRO PRO GLU GLU ASP

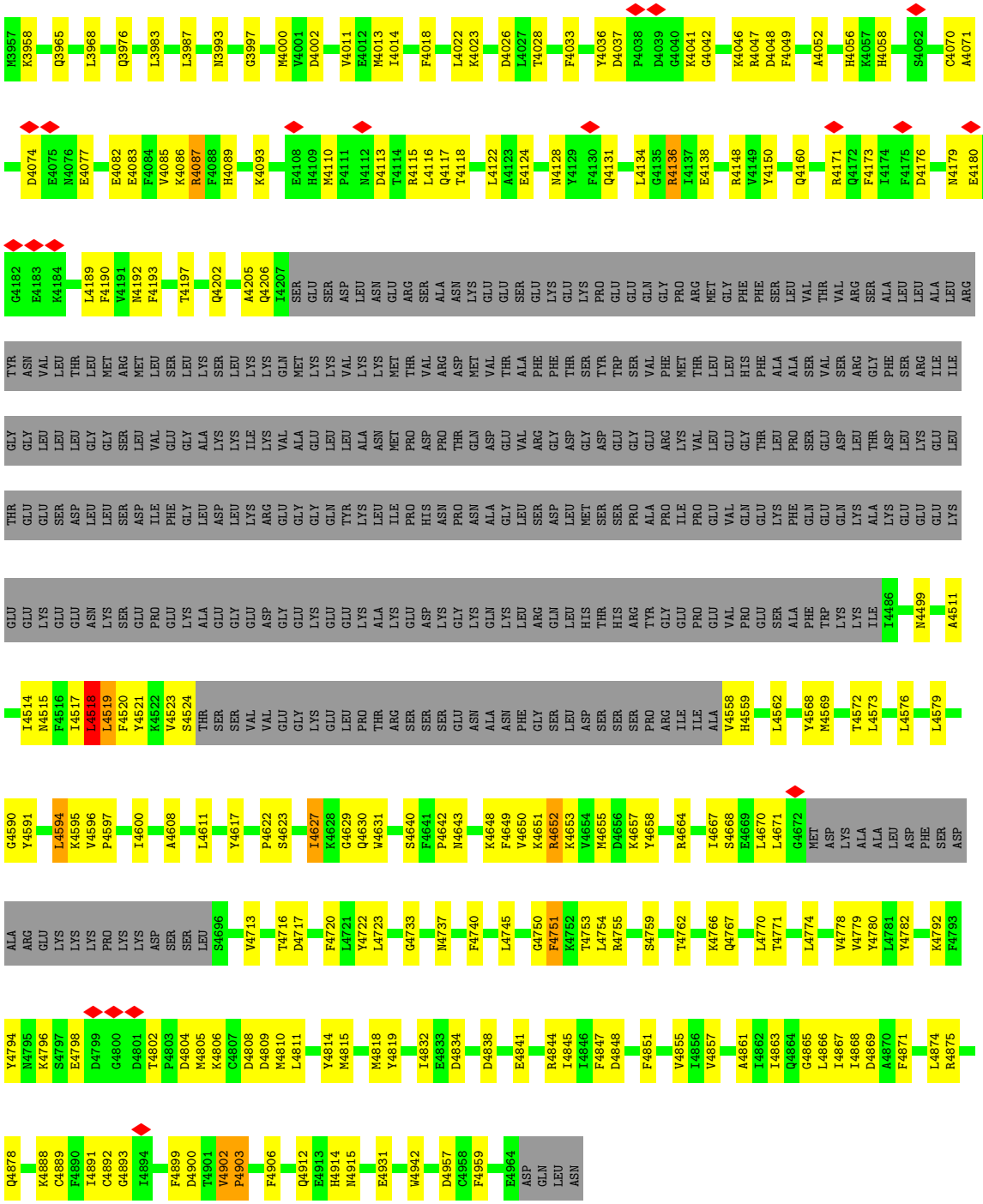


• Molecule 2: RyR2



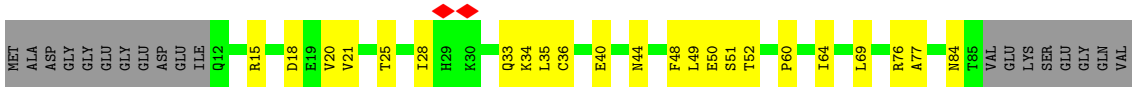


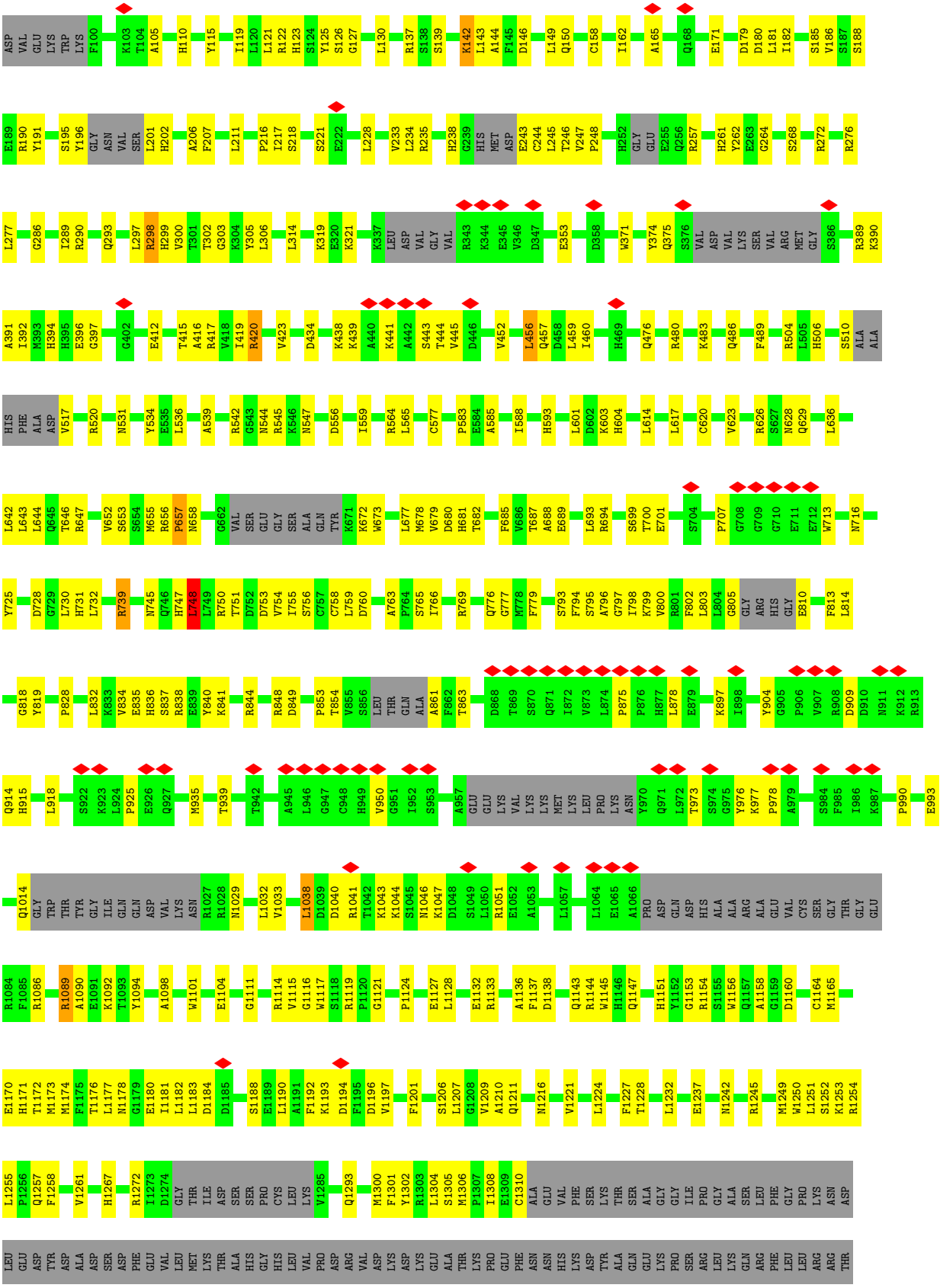


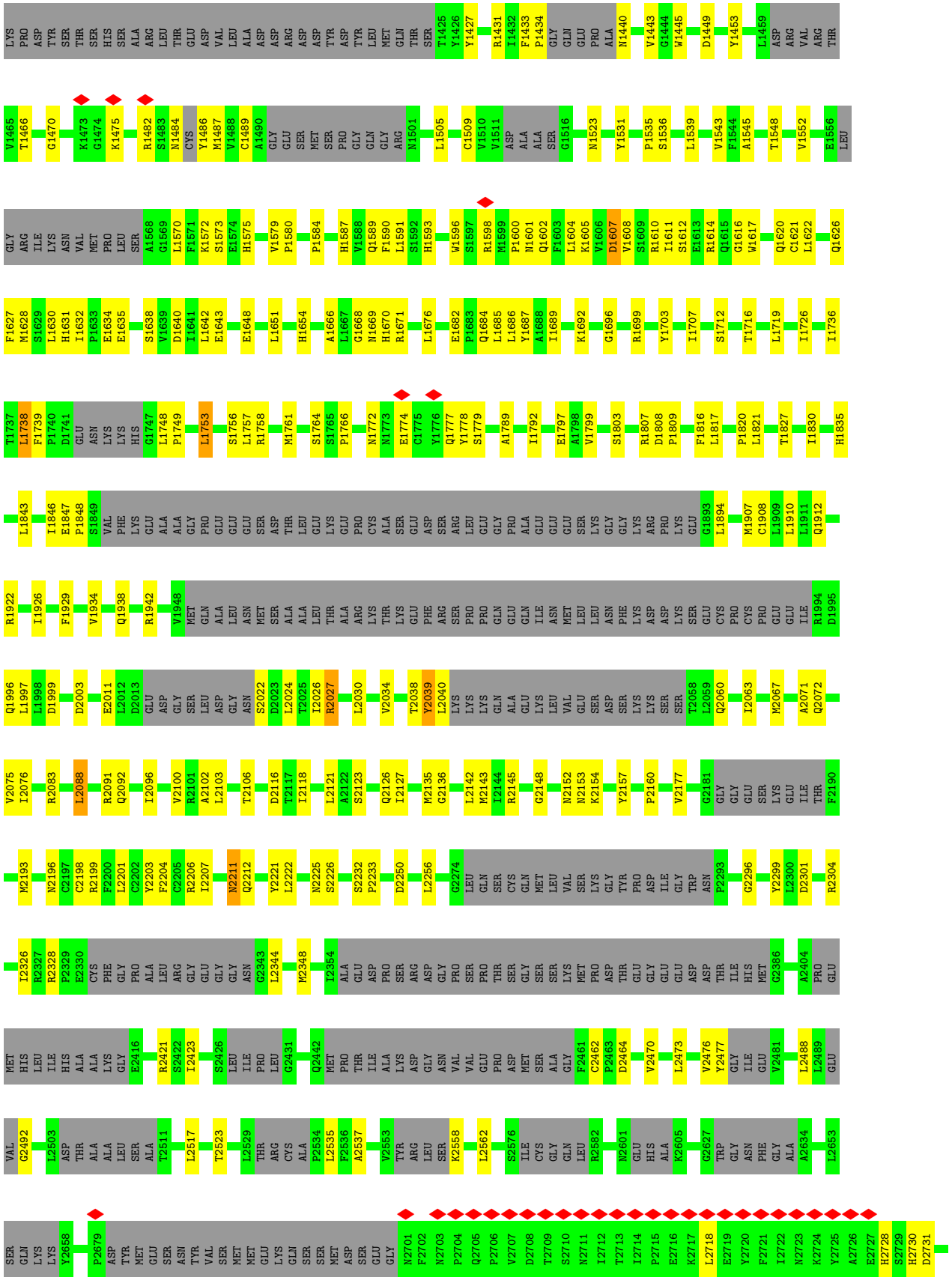


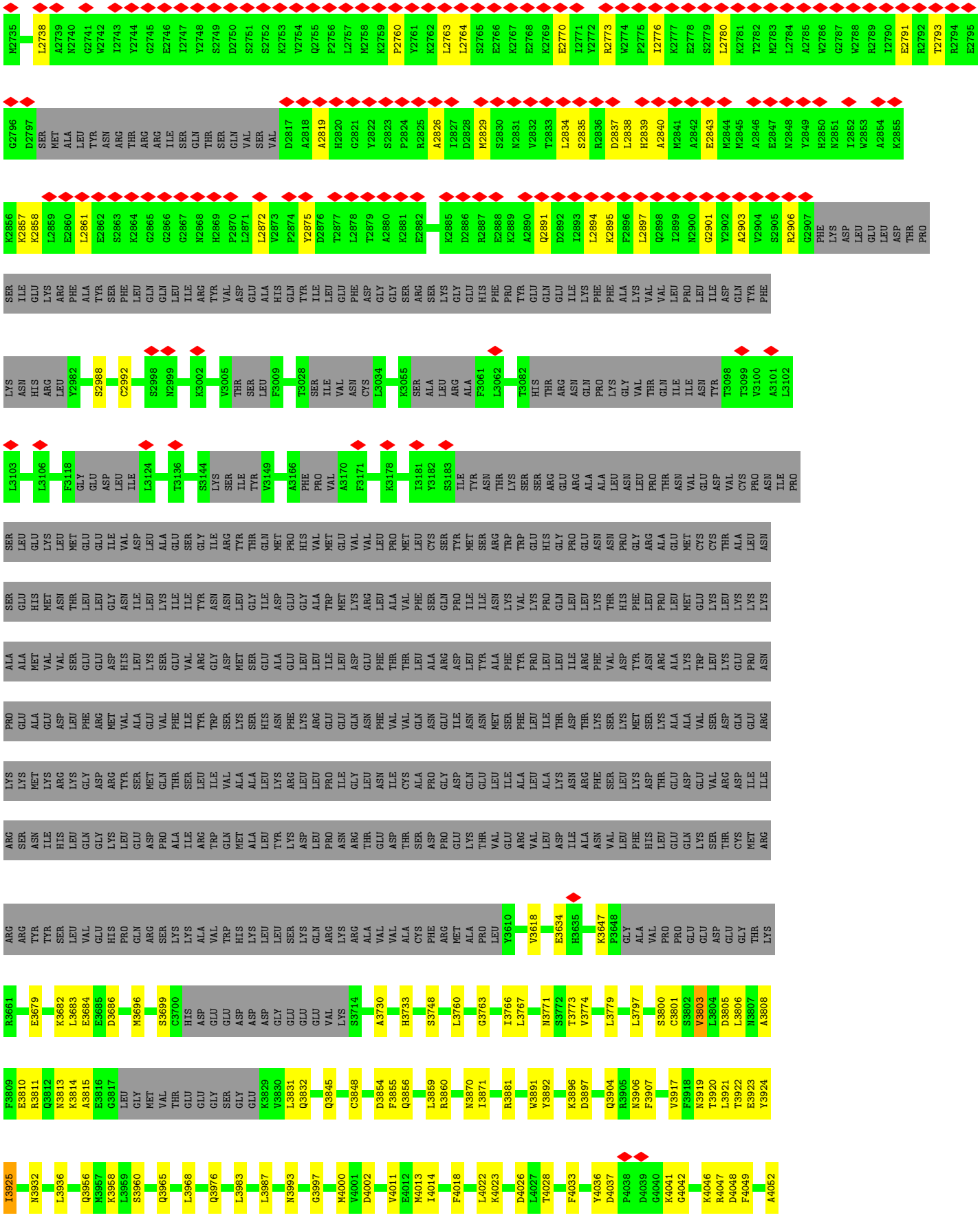
• Molecule 2: RyR2

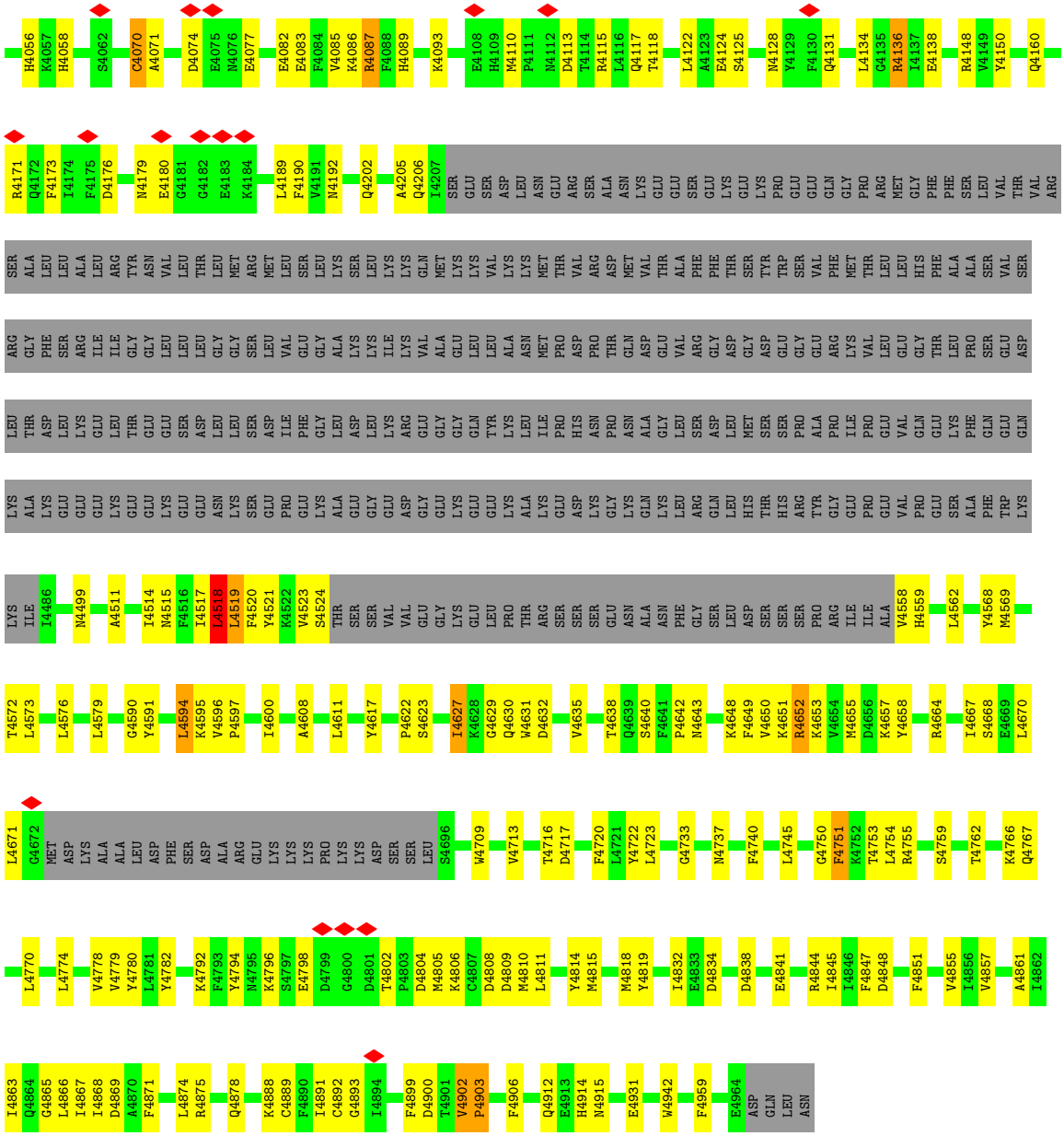
Chain F:





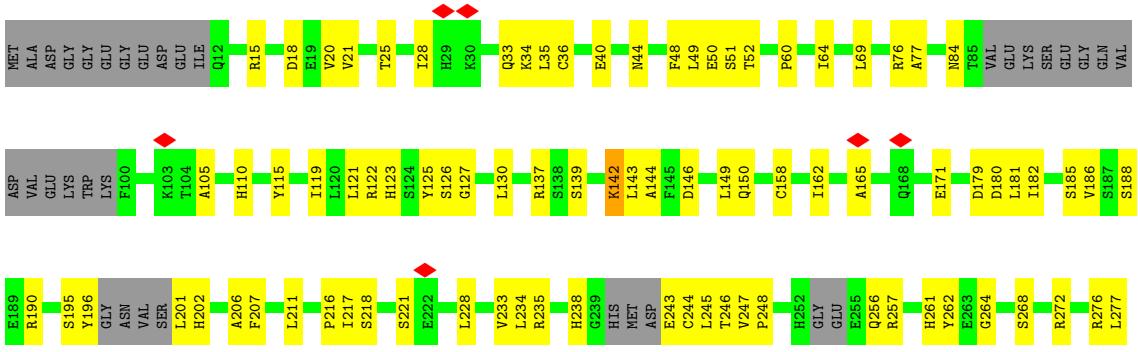


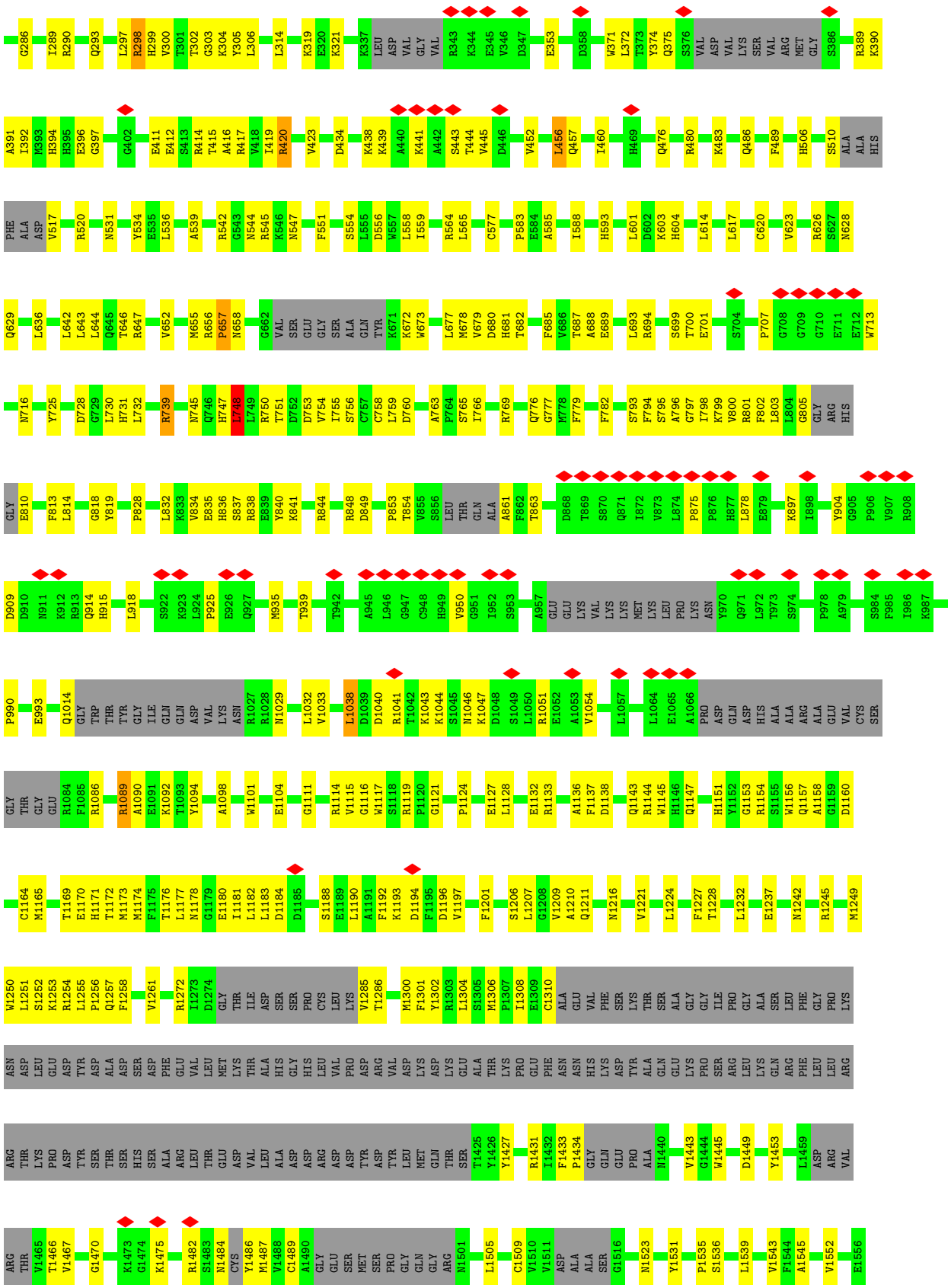


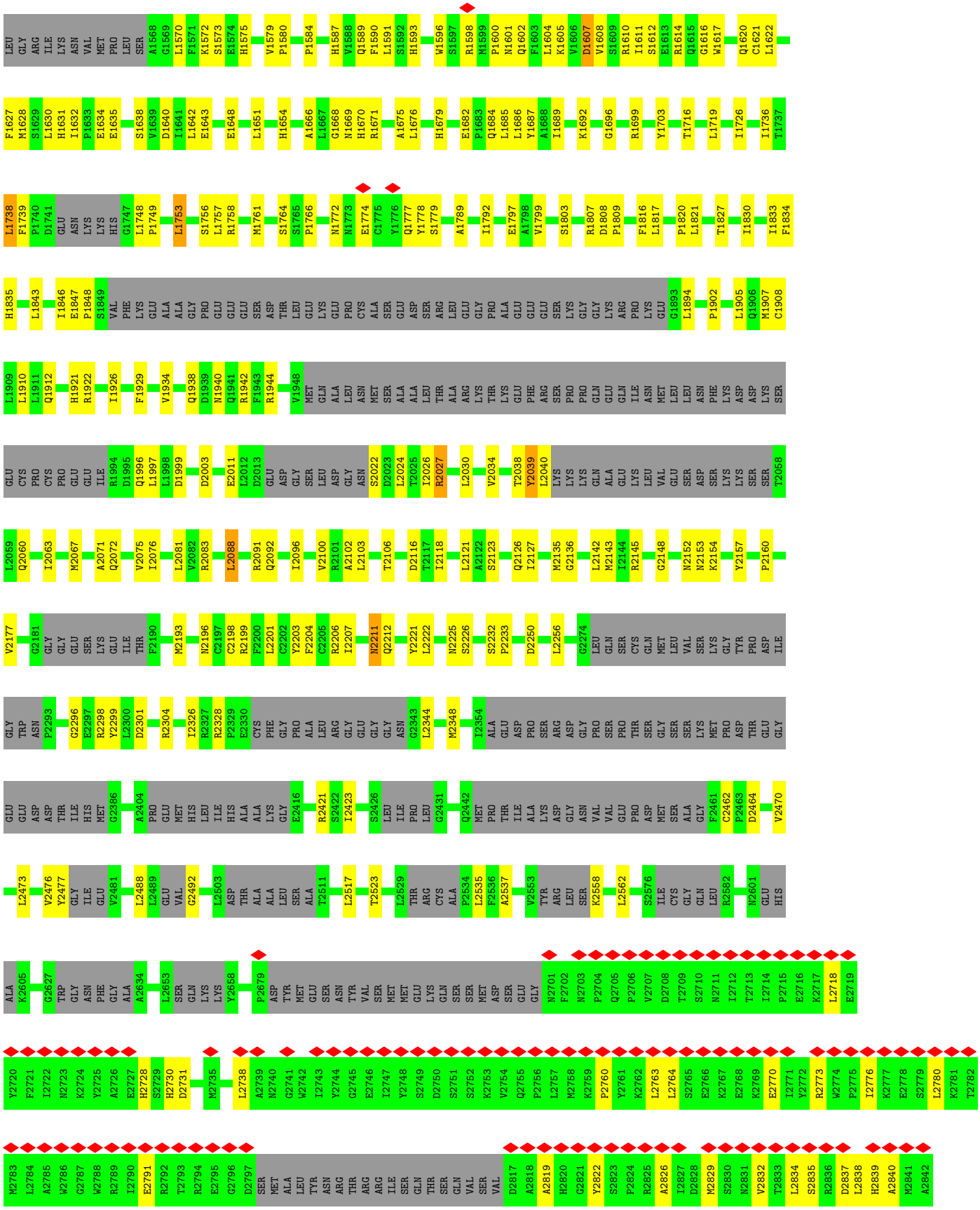


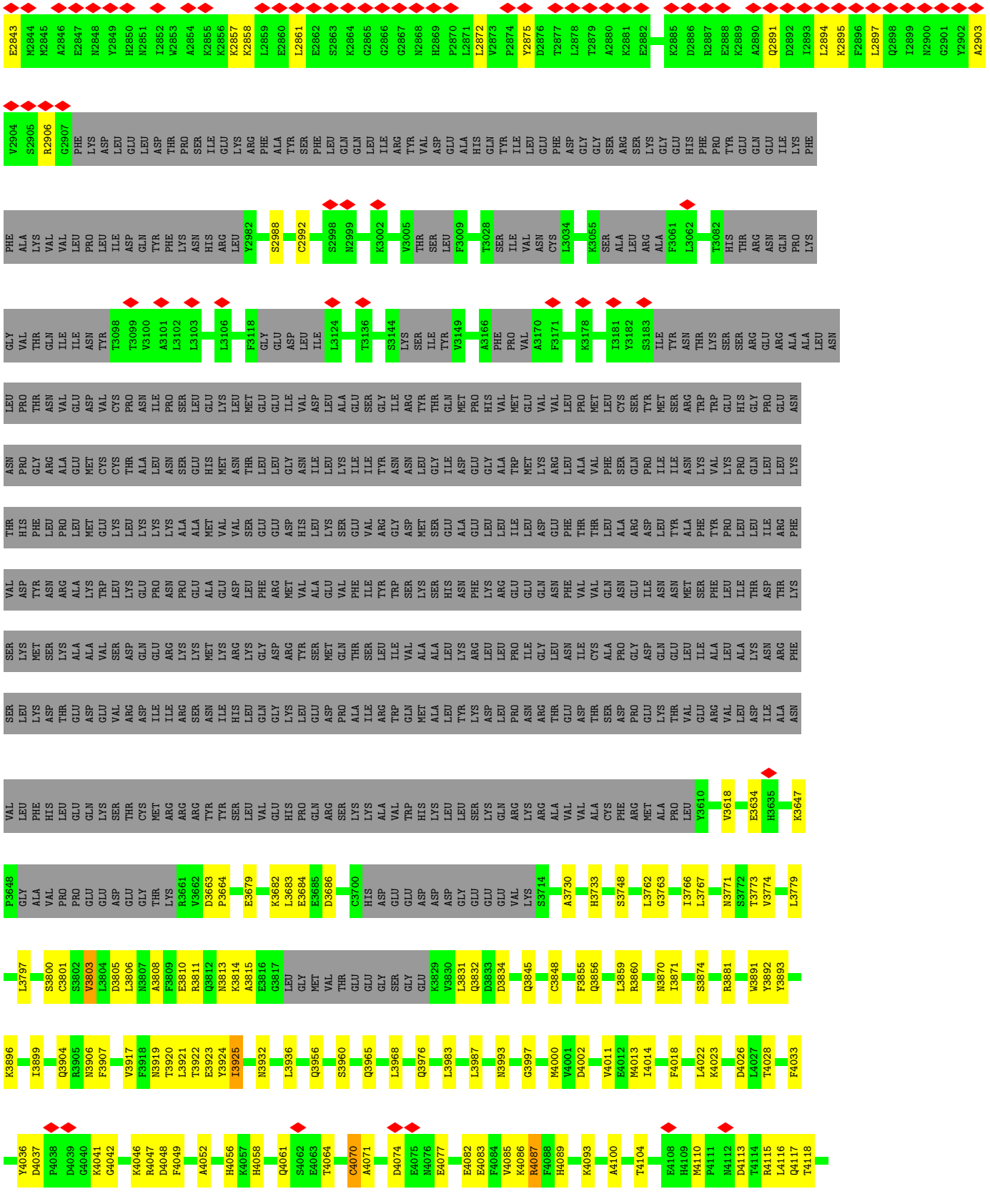
• Molecule 2: RyR2

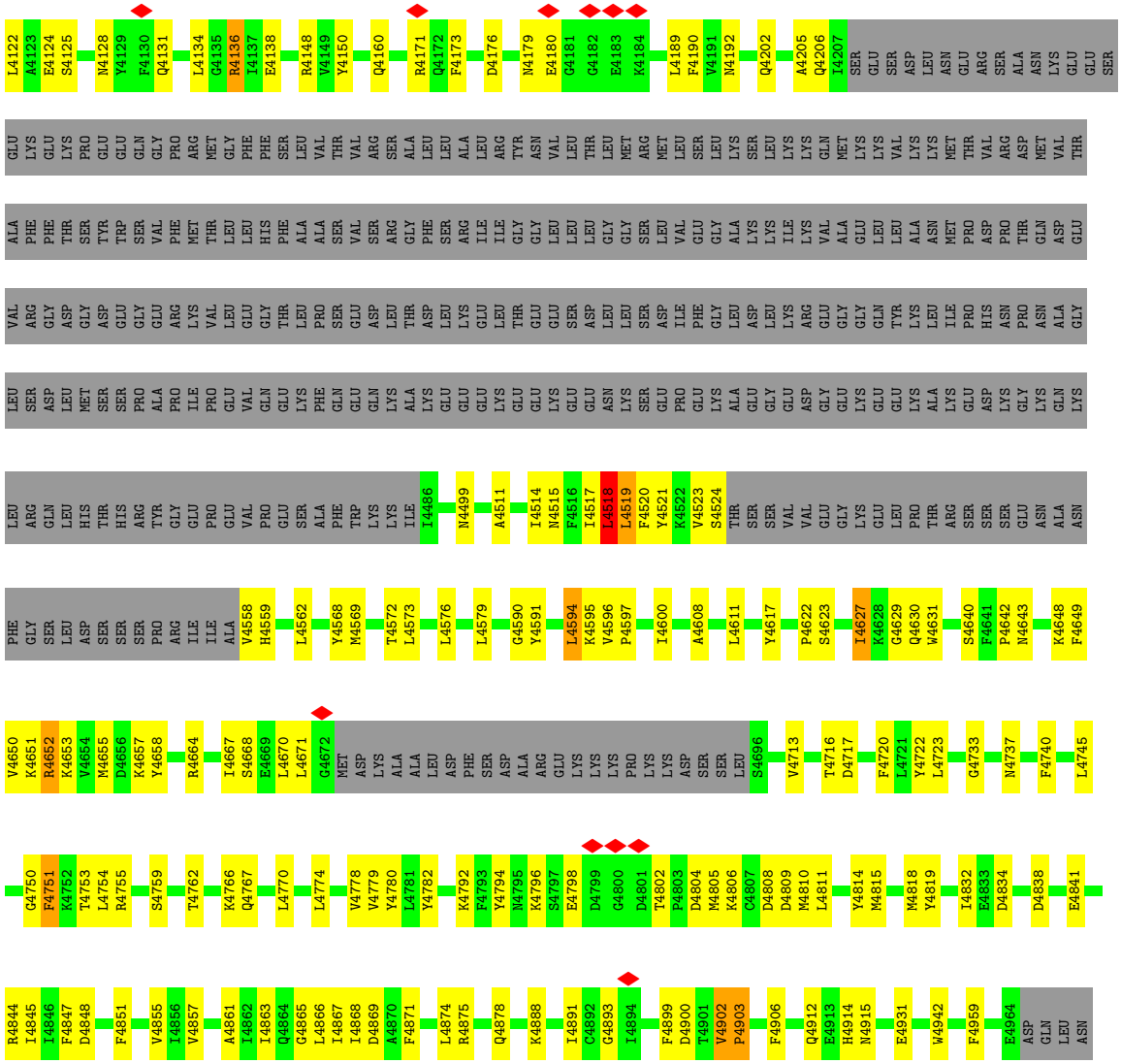
Chain H:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	60287	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.6	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	0.085	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	522.616, 522.616, 522.616	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	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

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	0.35	0/835	0.58	0/1123
1	C	0.35	0/835	0.58	0/1123
1	E	0.35	0/835	0.58	0/1123
1	G	0.35	0/835	0.58	0/1123
2	B	0.38	0/27132	0.62	12/36687 (0.0%)
2	D	0.38	0/27132	0.62	12/36687 (0.0%)
2	F	0.38	0/27132	0.62	12/36687 (0.0%)
2	H	0.38	0/27132	0.62	12/36687 (0.0%)
All	All	0.38	0/111868	0.61	48/151240 (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	29
2	D	0	29
2	F	0	29
2	H	0	29
All	All	0	116

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1753	LEU	CA-CB-CG	6.30	129.80	115.30
2	B	1753	LEU	CA-CB-CG	6.30	129.79	115.30
2	D	1753	LEU	CA-CB-CG	6.30	129.78	115.30
2	F	1753	LEU	CA-CB-CG	6.29	129.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	814	LEU	CA-CB-CG	5.94	128.97	115.30
2	F	814	LEU	CA-CB-CG	5.94	128.96	115.30
2	B	814	LEU	CA-CB-CG	5.92	128.92	115.30
2	D	814	LEU	CA-CB-CG	5.92	128.92	115.30
2	D	2517	LEU	CA-CB-CG	5.47	127.88	115.30
2	B	2517	LEU	CA-CB-CG	5.45	127.84	115.30
2	F	2517	LEU	CA-CB-CG	5.45	127.84	115.30
2	H	2517	LEU	CA-CB-CG	5.45	127.84	115.30
2	H	1738	LEU	CA-CB-CG	5.40	127.72	115.30
2	F	1738	LEU	CA-CB-CG	5.39	127.69	115.30
2	B	1738	LEU	CA-CB-CG	5.38	127.67	115.30
2	D	1738	LEU	CA-CB-CG	5.37	127.65	115.30
2	B	1038	LEU	CA-CB-CG	5.32	127.54	115.30
2	H	1038	LEU	CA-CB-CG	5.32	127.54	115.30
2	D	1038	LEU	CA-CB-CG	5.32	127.54	115.30
2	F	1038	LEU	CA-CB-CG	5.31	127.52	115.30
2	H	3925	ILE	CG1-CB-CG2	-5.27	99.80	111.40
2	B	3925	ILE	CG1-CB-CG2	-5.27	99.81	111.40
2	D	3925	ILE	CG1-CB-CG2	-5.27	99.81	111.40
2	F	3925	ILE	CG1-CB-CG2	-5.25	99.84	111.40
2	B	2088	LEU	CA-CB-CG	5.20	127.26	115.30
2	F	2088	LEU	CA-CB-CG	5.20	127.26	115.30
2	D	2039	TYR	C-N-CA	5.20	134.69	121.70
2	D	2088	LEU	CA-CB-CG	5.19	127.24	115.30
2	F	2039	TYR	C-N-CA	5.19	134.66	121.70
2	H	2088	LEU	CA-CB-CG	5.19	127.23	115.30
2	B	2039	TYR	C-N-CA	5.18	134.66	121.70
2	D	748	LEU	CA-CB-CG	5.18	127.21	115.30
2	F	2022	SER	C-N-CA	5.17	134.64	121.70
2	F	748	LEU	CA-CB-CG	5.17	127.20	115.30
2	B	748	LEU	CA-CB-CG	5.17	127.19	115.30
2	H	748	LEU	CA-CB-CG	5.17	127.19	115.30
2	D	2022	SER	C-N-CA	5.17	134.62	121.70
2	B	2022	SER	C-N-CA	5.16	134.60	121.70
2	H	2022	SER	C-N-CA	5.16	134.60	121.70
2	H	2039	TYR	C-N-CA	5.16	134.59	121.70
2	D	139	SER	C-N-CA	5.15	134.56	121.70
2	B	456	LEU	CA-CB-CG	5.14	127.13	115.30
2	F	456	LEU	CA-CB-CG	5.14	127.13	115.30
2	B	139	SER	C-N-CA	5.14	134.54	121.70
2	D	456	LEU	CA-CB-CG	5.14	127.11	115.30
2	H	139	SER	C-N-CA	5.13	134.54	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	456	LEU	CA-CB-CG	5.13	127.11	115.30
2	F	139	SER	C-N-CA	5.12	134.51	121.70

There are no chirality outliers.

All (116) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	105	ALA	Peptide
2	B	142	LYS	Peptide
2	B	1475	LYS	Peptide
2	B	1579	VAL	Peptide
2	B	1607	ASP	Peptide
2	B	1635	GLU	Peptide
2	B	1756	SER	Peptide
2	B	1758	ARG	Peptide
2	B	1777	GLN	Peptide
2	B	1835	HIS	Peptide
2	B	1847	GLU	Peptide
2	B	2075	VAL	Peptide
2	B	221	SER	Peptide
2	B	2232	SER	Peptide
2	B	2462	CYS	Peptide
2	B	321	LYS	Peptide
2	B	4070	CYS	Peptide
2	B	4074	ASP	Peptide
2	B	4594	LEU	Peptide
2	B	4627	ILE	Peptide
2	B	4751	PHE	Peptide
2	B	657	PRO	Peptide
2	B	728	ASP	Peptide
2	B	739	ARG	Peptide
2	B	748	LEU	Peptide
2	B	777	GLY	Peptide
2	B	818	GLY	Peptide
2	B	819	TYR	Peptide
2	B	838	ARG	Peptide
2	D	105	ALA	Peptide
2	D	142	LYS	Peptide
2	D	1475	LYS	Peptide
2	D	1579	VAL	Peptide
2	D	1607	ASP	Peptide
2	D	1635	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	D	1756	SER	Peptide
2	D	1758	ARG	Peptide
2	D	1777	GLN	Peptide
2	D	1835	HIS	Peptide
2	D	1847	GLU	Peptide
2	D	2075	VAL	Peptide
2	D	221	SER	Peptide
2	D	2232	SER	Peptide
2	D	2462	CYS	Peptide
2	D	321	LYS	Peptide
2	D	4070	CYS	Peptide
2	D	4074	ASP	Peptide
2	D	4594	LEU	Peptide
2	D	4627	ILE	Peptide
2	D	4751	PHE	Peptide
2	D	657	PRO	Peptide
2	D	728	ASP	Peptide
2	D	739	ARG	Peptide
2	D	748	LEU	Peptide
2	D	777	GLY	Peptide
2	D	818	GLY	Peptide
2	D	819	TYR	Peptide
2	D	838	ARG	Peptide
2	F	105	ALA	Peptide
2	F	142	LYS	Peptide
2	F	1475	LYS	Peptide
2	F	1579	VAL	Peptide
2	F	1607	ASP	Peptide
2	F	1635	GLU	Peptide
2	F	1756	SER	Peptide
2	F	1758	ARG	Peptide
2	F	1777	GLN	Peptide
2	F	1835	HIS	Peptide
2	F	1847	GLU	Peptide
2	F	2075	VAL	Peptide
2	F	221	SER	Peptide
2	F	2232	SER	Peptide
2	F	2462	CYS	Peptide
2	F	321	LYS	Peptide
2	F	4070	CYS	Peptide
2	F	4074	ASP	Peptide
2	F	4594	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	F	4627	ILE	Peptide
2	F	4751	PHE	Peptide
2	F	657	PRO	Peptide
2	F	728	ASP	Peptide
2	F	739	ARG	Peptide
2	F	748	LEU	Peptide
2	F	777	GLY	Peptide
2	F	818	GLY	Peptide
2	F	819	TYR	Peptide
2	F	838	ARG	Peptide
2	H	105	ALA	Peptide
2	H	142	LYS	Peptide
2	H	1475	LYS	Peptide
2	H	1579	VAL	Peptide
2	H	1607	ASP	Peptide
2	H	1635	GLU	Peptide
2	H	1756	SER	Peptide
2	H	1758	ARG	Peptide
2	H	1777	GLN	Peptide
2	H	1835	HIS	Peptide
2	H	1847	GLU	Peptide
2	H	2075	VAL	Peptide
2	H	221	SER	Peptide
2	H	2232	SER	Peptide
2	H	2462	CYS	Peptide
2	H	321	LYS	Peptide
2	H	4070	CYS	Peptide
2	H	4074	ASP	Peptide
2	H	4594	LEU	Peptide
2	H	4627	ILE	Peptide
2	H	4751	PHE	Peptide
2	H	657	PRO	Peptide
2	H	728	ASP	Peptide
2	H	739	ARG	Peptide
2	H	748	LEU	Peptide
2	H	777	GLY	Peptide
2	H	818	GLY	Peptide
2	H	819	TYR	Peptide
2	H	838	ARG	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	819	0	824	25	0
1	C	819	0	824	25	0
1	E	819	0	824	26	0
1	G	819	0	824	24	0
2	B	26636	0	25174	673	0
2	D	26636	0	25174	667	0
2	F	26636	0	25174	671	0
2	H	26636	0	25174	682	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	109824	0	103992	2512	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 12.

All (2512) 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:F:4520:PHE:CD1	2:F:4562:LEU:HD21	1.50	1.47
2:B:4520:PHE:CD1	2:B:4562:LEU:HD21	1.50	1.47
2:D:4520:PHE:CD1	2:D:4562:LEU:HD21	1.50	1.46
2:H:4520:PHE:CD1	2:H:4562:LEU:HD21	1.50	1.44
2:B:4808:ASP:HB3	2:D:4523:VAL:CG2	1.55	1.36
2:F:207:PHE:CZ	2:H:2326:ILE:HG23	1.60	1.35
2:D:4808:ASP:HB3	2:F:4523:VAL:CG2	1.54	1.35
2:B:2326:ILE:HG23	2:H:207:PHE:CZ	1.61	1.34
2:D:207:PHE:CZ	2:F:2326:ILE:HG23	1.60	1.34
2:B:4523:VAL:CG2	2:H:4808:ASP:HB3	1.57	1.34
2:B:207:PHE:CZ	2:D:2326:ILE:HG23	1.61	1.33
2:F:4808:ASP:HB3	2:H:4523:VAL:CG2	1.58	1.30
2:B:4902:VAL:HG12	2:B:4903:PRO:CD	1.65	1.27
2:H:4902:VAL:HG12	2:H:4903:PRO:CD	1.64	1.25
2:F:4902:VAL:HG12	2:F:4903:PRO:CD	1.64	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4902:VAL:HG12	2:D:4903:PRO:CD	1.67	1.25
2:H:4779:VAL:HG11	2:H:4818:MET:SD	1.86	1.16
2:B:4779:VAL:HG11	2:B:4818:MET:SD	1.86	1.15
2:F:4779:VAL:HG11	2:F:4818:MET:SD	1.86	1.14
2:F:4808:ASP:HB3	2:H:4523:VAL:HG23	1.23	1.14
2:B:4523:VAL:HG23	2:H:4808:ASP:HB3	1.19	1.14
2:D:4779:VAL:HG11	2:D:4818:MET:SD	1.86	1.13
2:B:4808:ASP:HB3	2:D:4523:VAL:HG23	1.18	1.12
2:B:4808:ASP:CB	2:D:4523:VAL:HG21	1.79	1.12
2:D:4808:ASP:CB	2:F:4523:VAL:HG21	1.79	1.12
2:D:4808:ASP:HB3	2:F:4523:VAL:HG23	1.19	1.11
2:B:4808:ASP:CG	2:D:4523:VAL:HG21	1.72	1.10
2:D:207:PHE:CE2	2:F:2326:ILE:HG23	1.86	1.10
2:F:207:PHE:CE2	2:H:2326:ILE:HG23	1.85	1.10
2:B:4523:VAL:HG21	2:H:4808:ASP:CB	1.82	1.09
2:D:207:PHE:CE1	2:F:2326:ILE:HG23	1.86	1.09
2:F:207:PHE:CE1	2:H:2326:ILE:HG23	1.87	1.09
2:B:4523:VAL:HG21	2:H:4808:ASP:CG	1.73	1.09
2:D:4808:ASP:CG	2:F:4523:VAL:HG21	1.73	1.09
2:B:2326:ILE:HG23	2:H:207:PHE:CE1	1.87	1.08
2:B:207:PHE:CE2	2:D:2326:ILE:HG23	1.89	1.07
2:B:2326:ILE:HG23	2:H:207:PHE:CE2	1.87	1.07
2:B:207:PHE:CE1	2:D:2326:ILE:HG23	1.87	1.07
2:F:4808:ASP:CB	2:H:4523:VAL:HG21	1.83	1.06
2:D:4808:ASP:CB	2:F:4523:VAL:CG2	2.34	1.05
2:B:4774:LEU:CD2	2:D:4754:LEU:HD21	1.86	1.05
2:B:4808:ASP:CB	2:D:4523:VAL:CG2	2.34	1.05
2:B:4754:LEU:HD21	2:H:4774:LEU:CD2	1.87	1.04
2:B:4523:VAL:CG2	2:H:4808:ASP:CB	2.36	1.03
2:D:4774:LEU:CD2	2:F:4754:LEU:HD21	1.89	1.03
2:F:4774:LEU:CD2	2:H:4754:LEU:HD21	1.88	1.03
2:F:4808:ASP:CG	2:H:4523:VAL:HG21	1.76	1.03
2:D:4902:VAL:CG1	2:D:4903:PRO:HD2	1.89	1.03
2:H:4902:VAL:CG1	2:H:4903:PRO:HD2	1.89	1.02
2:D:207:PHE:CE1	2:F:2326:ILE:CG2	2.42	1.02
2:B:4902:VAL:CG1	2:B:4903:PRO:HD2	1.89	1.02
2:D:4808:ASP:HB3	2:F:4523:VAL:HG21	1.37	1.02
2:B:2326:ILE:CG2	2:H:207:PHE:CE1	2.43	1.01
2:F:4902:VAL:CG1	2:F:4903:PRO:HD2	1.89	1.01
2:B:207:PHE:CE1	2:D:2326:ILE:CG2	2.44	1.01
2:F:207:PHE:CE1	2:H:2326:ILE:CG2	2.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4902:VAL:HG12	2:H:4903:PRO:HD2	1.00	0.99
2:F:4902:VAL:HG12	2:F:4903:PRO:HD2	0.99	0.99
2:F:4808:ASP:CB	2:H:4523:VAL:CG2	2.38	0.98
2:B:4902:VAL:HG12	2:B:4903:PRO:HD2	0.99	0.98
2:F:4520:PHE:HD1	2:F:4562:LEU:CD2	1.76	0.98
2:B:4774:LEU:HD22	2:D:4754:LEU:CD2	1.93	0.98
2:H:4520:PHE:CD1	2:H:4562:LEU:CD2	2.46	0.98
2:H:4520:PHE:HD1	2:H:4562:LEU:CD2	1.76	0.98
2:B:4520:PHE:HB3	2:B:4562:LEU:HD23	1.45	0.98
2:B:4754:LEU:CD2	2:H:4774:LEU:HD22	1.93	0.98
2:D:4520:PHE:CD1	2:D:4562:LEU:CD2	2.46	0.98
2:D:4520:PHE:HD1	2:D:4562:LEU:CD2	1.76	0.98
2:D:4774:LEU:HD22	2:F:4754:LEU:HD21	0.99	0.98
2:F:4774:LEU:HD22	2:H:4754:LEU:CD2	1.94	0.97
2:B:4520:PHE:CD1	2:B:4562:LEU:CD2	2.46	0.97
2:D:4902:VAL:HG12	2:D:4903:PRO:HD2	0.97	0.97
2:F:4520:PHE:HB3	2:F:4562:LEU:HD23	1.45	0.97
2:D:207:PHE:CZ	2:F:2326:ILE:HD12	2.00	0.97
2:F:4520:PHE:CD1	2:F:4562:LEU:CD2	2.46	0.97
2:F:4774:LEU:HD22	2:H:4754:LEU:HD21	0.97	0.97
2:H:4520:PHE:HB3	2:H:4562:LEU:HD23	1.45	0.97
2:B:4520:PHE:HD1	2:B:4562:LEU:CD2	1.76	0.97
2:D:207:PHE:CZ	2:F:2326:ILE:CG2	2.48	0.96
2:F:207:PHE:CZ	2:H:2326:ILE:CG2	2.48	0.96
2:F:4808:ASP:HB3	2:H:4523:VAL:HG21	1.40	0.96
2:F:207:PHE:CZ	2:H:2326:ILE:HD12	2.01	0.95
2:B:4754:LEU:HD21	2:H:4774:LEU:HD22	0.96	0.95
2:B:4808:ASP:HB3	2:D:4523:VAL:HG21	1.39	0.95
2:B:2326:ILE:HD12	2:H:207:PHE:CZ	2.02	0.95
2:D:4520:PHE:HB3	2:D:4562:LEU:HD23	1.45	0.95
2:B:207:PHE:CZ	2:D:2326:ILE:CG2	2.50	0.94
2:B:2326:ILE:CG2	2:H:207:PHE:CZ	2.50	0.94
2:B:207:PHE:CZ	2:D:2326:ILE:HD12	2.03	0.94
2:B:4774:LEU:HD22	2:D:4754:LEU:HD21	0.96	0.92
2:D:4865:GLY:HA2	2:F:4868:ILE:HG12	1.54	0.90
2:F:4857:VAL:HG22	2:H:4863:ILE:HG21	1.53	0.90
2:B:4863:ILE:HG21	2:H:4857:VAL:HG22	1.55	0.89
2:B:4865:GLY:HA2	2:D:4868:ILE:HG12	1.55	0.89
2:D:4774:LEU:HD22	2:F:4754:LEU:CD2	1.96	0.89
2:F:4865:GLY:HA2	2:H:4868:ILE:HG12	1.55	0.88
2:B:4868:ILE:HG12	2:H:4865:GLY:HA2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4857:VAL:HG22	2:D:4863:ILE:HG21	1.53	0.88
2:D:4857:VAL:HG22	2:F:4863:ILE:HG21	1.54	0.87
2:F:4902:VAL:CG1	2:F:4903:PRO:CD	2.52	0.86
2:F:4857:VAL:HG13	2:H:4863:ILE:CG2	2.07	0.85
2:B:4902:VAL:CG1	2:B:4903:PRO:CD	2.52	0.85
2:D:4857:VAL:HG13	2:F:4863:ILE:CG2	2.07	0.84
2:H:4902:VAL:CG1	2:H:4903:PRO:CD	2.51	0.84
2:D:76:ARG:CB	2:F:3891:TRP:HB3	2.08	0.83
2:F:76:ARG:CB	2:H:3891:TRP:HB3	2.08	0.83
2:B:4857:VAL:HG13	2:D:4863:ILE:CG2	2.09	0.82
2:B:4863:ILE:CG2	2:H:4857:VAL:HG13	2.10	0.82
2:B:3891:TRP:HB3	2:H:76:ARG:CB	2.10	0.81
2:D:207:PHE:CE2	2:F:2326:ILE:HD12	2.15	0.81
2:F:207:PHE:CE2	2:H:2326:ILE:HD12	2.16	0.80
2:F:4520:PHE:HB3	2:F:4562:LEU:CD2	2.12	0.80
2:H:4520:PHE:HB3	2:H:4562:LEU:CD2	2.12	0.80
2:B:76:ARG:CB	2:D:3891:TRP:HB3	2.11	0.80
2:D:4520:PHE:HB3	2:D:4562:LEU:CD2	2.12	0.79
2:B:4520:PHE:HB3	2:B:4562:LEU:CD2	2.12	0.79
2:F:4779:VAL:CG1	2:F:4818:MET:SD	2.71	0.79
2:B:207:PHE:CE2	2:D:2326:ILE:HD12	2.19	0.78
2:H:4627:ILE:O	2:H:4631:TRP:HB2	1.84	0.78
2:B:4627:ILE:O	2:B:4631:TRP:HB2	1.84	0.78
2:F:4520:PHE:CG	2:F:4562:LEU:HD21	2.17	0.78
2:B:2326:ILE:HD12	2:H:207:PHE:CE2	2.17	0.78
2:H:4520:PHE:CG	2:H:4562:LEU:HD21	2.17	0.78
2:D:4902:VAL:CG1	2:D:4903:PRO:CD	2.54	0.77
2:F:4857:VAL:CG2	2:H:4863:ILE:HG21	2.14	0.77
2:B:4857:VAL:CG2	2:D:4863:ILE:HG21	2.15	0.77
2:F:4627:ILE:O	2:F:4631:TRP:HB2	1.84	0.77
2:H:4779:VAL:CG1	2:H:4818:MET:SD	2.71	0.77
2:F:4857:VAL:HG13	2:H:4863:ILE:HB	1.67	0.77
2:B:4779:VAL:CG1	2:B:4818:MET:SD	2.71	0.76
2:D:4520:PHE:CG	2:D:4562:LEU:HD21	2.17	0.76
2:D:4810:MET:HG2	2:F:4521:TYR:HB2	1.65	0.76
2:B:4810:MET:HG2	2:D:4521:TYR:HB2	1.66	0.76
2:D:4627:ILE:O	2:D:4631:TRP:HB2	1.84	0.76
2:H:4902:VAL:HG12	2:H:4903:PRO:HD3	1.66	0.76
2:D:207:PHE:CD1	2:F:2326:ILE:CG2	2.69	0.75
2:B:4520:PHE:CG	2:B:4562:LEU:HD21	2.17	0.75
2:D:4779:VAL:CG1	2:D:4818:MET:SD	2.71	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4521:TYR:HB2	2:H:4810:MET:HG2	1.68	0.75
2:D:4857:VAL:CG2	2:F:4863:ILE:HG21	2.16	0.75
2:B:4863:ILE:HG21	2:H:4857:VAL:CG2	2.16	0.74
2:B:4863:ILE:HB	2:H:4857:VAL:HG13	1.70	0.74
2:F:4810:MET:HG2	2:H:4521:TYR:HB2	1.69	0.74
2:B:2326:ILE:CG2	2:H:207:PHE:CD1	2.71	0.73
2:F:76:ARG:CB	2:H:3891:TRP:CB	2.66	0.73
2:B:4857:VAL:HG13	2:D:4863:ILE:HB	1.69	0.73
2:F:4848:ASP:HB3	2:H:4819:TYR:HE1	1.53	0.73
2:F:4902:VAL:HG12	2:F:4903:PRO:HD3	1.67	0.73
2:D:4046:LYS:H	2:D:4077:GLU:HB3	1.54	0.73
2:F:207:PHE:CD1	2:H:2326:ILE:CG2	2.70	0.73
2:B:4515:ASN:ND2	2:H:4780:TYR:CE2	2.56	0.73
2:D:190:ARG:NH1	2:F:2423:ILE:HG23	2.04	0.73
2:F:4857:VAL:HG13	2:H:4863:ILE:CB	2.19	0.73
2:B:4902:VAL:HG12	2:B:4903:PRO:HD3	1.68	0.73
2:B:4780:TYR:CE2	2:D:4515:ASN:ND2	2.56	0.73
2:D:76:ARG:CB	2:F:3891:TRP:CB	2.66	0.72
2:F:4046:LYS:H	2:F:4077:GLU:HB3	1.54	0.72
2:D:4857:VAL:HG13	2:F:4863:ILE:HB	1.71	0.72
2:F:190:ARG:NH1	2:H:2423:ILE:HG23	2.04	0.72
2:H:4046:LYS:H	2:H:4077:GLU:HB3	1.54	0.72
2:D:4848:ASP:HB3	2:F:4819:TYR:HE1	1.55	0.72
2:B:3891:TRP:CB	2:H:76:ARG:CB	2.68	0.71
2:B:207:PHE:CD1	2:D:2326:ILE:CG2	2.72	0.71
2:B:4046:LYS:H	2:B:4077:GLU:HB3	1.54	0.71
2:B:4848:ASP:HB3	2:D:4819:TYR:HE1	1.56	0.71
2:D:4851:PHE:O	2:D:4855:VAL:HB	1.91	0.71
2:F:77:ALA:HB2	2:H:3891:TRP:CZ2	2.26	0.71
2:D:77:ALA:HB2	2:F:3891:TRP:CZ2	2.25	0.71
2:F:4851:PHE:O	2:F:4855:VAL:HB	1.91	0.71
2:D:1111:GLY:HA3	2:D:1211:GLN:HE21	1.56	0.71
2:B:76:ARG:CB	2:D:3891:TRP:CB	2.69	0.71
2:D:4865:GLY:HA2	2:F:4868:ILE:CG1	2.20	0.71
2:F:1138:ASP:HB2	2:F:1145:TRP:HE1	1.56	0.71
2:B:2344:LEU:O	2:B:2348:MET:HB2	1.91	0.70
2:B:1111:GLY:HA3	2:B:1211:GLN:HE21	1.56	0.70
2:F:4814:TYR:HE2	2:F:4815:MET:HE1	1.56	0.70
2:B:4851:PHE:O	2:B:4855:VAL:HB	1.91	0.70
2:H:1138:ASP:HB2	2:H:1145:TRP:HE1	1.56	0.70
2:B:2423:ILE:HG23	2:H:190:ARG:NH1	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4857:VAL:HG13	2:F:4863:ILE:CB	2.22	0.70
2:H:4851:PHE:O	2:H:4855:VAL:HB	1.91	0.70
2:B:4857:VAL:HG13	2:D:4863:ILE:CB	2.21	0.70
2:H:1111:GLY:HA3	2:H:1211:GLN:HE21	1.56	0.70
2:F:4865:GLY:HA2	2:H:4868:ILE:CG1	2.21	0.70
2:B:4863:ILE:CB	2:H:4857:VAL:HG13	2.22	0.70
2:F:4780:TYR:CE2	2:H:4515:ASN:ND2	2.59	0.70
2:B:190:ARG:NH1	2:D:2423:ILE:HG23	2.06	0.70
2:D:4780:TYR:CE2	2:F:4515:ASN:ND2	2.58	0.70
2:F:2344:LEU:O	2:F:2348:MET:HB2	1.91	0.70
2:B:3891:TRP:CZ2	2:H:77:ALA:HB2	2.27	0.69
2:F:1242:ASN:HB3	2:F:1807:ARG:HB2	1.75	0.69
2:D:1138:ASP:HB2	2:D:1145:TRP:HE1	1.56	0.69
2:D:2344:LEU:O	2:D:2348:MET:HB2	1.91	0.69
2:B:1138:ASP:HB2	2:B:1145:TRP:HE1	1.56	0.69
2:H:1242:ASN:HB3	2:H:1807:ARG:HB2	1.74	0.69
2:H:2344:LEU:O	2:H:2348:MET:HB2	1.91	0.69
2:B:4819:TYR:HE1	2:H:4848:ASP:HB3	1.57	0.69
2:B:4861:ALA:HB1	2:D:4867:ILE:HG21	1.75	0.69
2:B:4868:ILE:CG1	2:H:4865:GLY:HA2	2.23	0.69
2:B:77:ALA:HB2	2:D:3891:TRP:CZ2	2.28	0.69
2:F:1111:GLY:HA3	2:F:1211:GLN:HE21	1.56	0.68
2:D:1242:ASN:HB3	2:D:1807:ARG:HB2	1.74	0.68
2:B:1242:ASN:HB3	2:B:1807:ARG:HB2	1.74	0.68
2:F:4857:VAL:CG1	2:H:4863:ILE:CG2	2.70	0.68
2:F:4861:ALA:HB1	2:H:4867:ILE:HG21	1.75	0.68
2:B:4865:GLY:HA2	2:D:4868:ILE:CG1	2.22	0.68
2:B:545:ARG:HH21	2:B:583:PRO:HG3	1.60	0.67
2:D:4857:VAL:CG1	2:F:4863:ILE:CG2	2.72	0.67
2:F:394:HIS:HD2	2:F:397:GLY:H	1.43	0.67
2:B:4867:ILE:HG21	2:H:4861:ALA:HB1	1.77	0.67
2:D:207:PHE:CD2	2:F:2326:ILE:HG23	2.30	0.67
2:D:545:ARG:HH21	2:D:583:PRO:HG3	1.60	0.67
2:B:4857:VAL:CG1	2:D:4863:ILE:CG2	2.73	0.67
2:D:4861:ALA:HB1	2:F:4867:ILE:HG21	1.76	0.67
2:B:262:TYR:HB2	2:B:389:ARG:HB3	1.77	0.67
2:D:394:HIS:HD2	2:D:397:GLY:H	1.43	0.67
2:D:4767:GLN:HG2	2:F:4753:THR:OG1	1.95	0.66
2:H:545:ARG:HH21	2:H:583:PRO:HG3	1.60	0.66
2:B:4863:ILE:CG2	2:H:4857:VAL:CG1	2.73	0.66
2:B:244:CYS:SG	2:B:245:LEU:N	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4865:GLY:CA	2:D:4868:ILE:HG12	2.26	0.66
2:D:244:CYS:SG	2:D:245:LEU:N	2.69	0.66
2:D:4902:VAL:HG12	2:D:4903:PRO:HD3	1.75	0.66
2:H:748:LEU:HD13	2:H:750:ARG:HE	1.61	0.66
2:F:545:ARG:HH21	2:F:583:PRO:HG3	1.60	0.66
2:D:4518:LEU:HD13	2:D:4521:TYR:CE2	2.31	0.66
2:F:207:PHE:CD2	2:H:2326:ILE:HG23	2.30	0.66
2:B:1431:ARG:HE	2:B:1505:LEU:HD21	1.60	0.66
2:D:1431:ARG:HE	2:D:1505:LEU:HD21	1.60	0.66
2:F:4518:LEU:HD13	2:F:4521:TYR:CE2	2.31	0.66
2:B:394:HIS:HD2	2:B:397:GLY:H	1.43	0.66
2:B:748:LEU:HD13	2:B:750:ARG:HE	1.61	0.66
2:D:262:TYR:HB2	2:D:389:ARG:HB3	1.77	0.66
2:H:244:CYS:SG	2:H:245:LEU:N	2.69	0.66
2:F:1431:ARG:HE	2:F:1505:LEU:HD21	1.60	0.66
2:F:244:CYS:SG	2:F:245:LEU:N	2.69	0.65
2:B:4767:GLN:HG2	2:D:4753:THR:OG1	1.96	0.65
2:H:262:TYR:HB2	2:H:389:ARG:HB3	1.77	0.65
2:H:1445:TRP:H	2:H:1487:MET:HB2	1.62	0.65
2:B:1445:TRP:H	2:B:1487:MET:HB2	1.62	0.65
2:D:144:ALA:HB1	2:D:206:ALA:HA	1.78	0.65
2:H:1431:ARG:HE	2:H:1505:LEU:HD21	1.60	0.65
2:D:1445:TRP:H	2:D:1487:MET:HB2	1.61	0.65
2:D:1482:ARG:HH11	2:D:1531:TYR:HA	1.61	0.65
2:F:1482:ARG:HH11	2:F:1531:TYR:HA	1.61	0.65
2:H:1117:TRP:HE1	2:H:1164:CYS:HB3	1.62	0.65
2:B:144:ALA:HB1	2:B:206:ALA:HA	1.78	0.65
2:F:1445:TRP:H	2:F:1487:MET:HB2	1.62	0.65
2:D:2891:GLN:HB3	2:D:2895:LYS:HE2	1.79	0.65
2:F:262:TYR:HB2	2:F:389:ARG:HB3	1.77	0.65
2:F:748:LEU:HD13	2:F:750:ARG:HE	1.61	0.65
2:F:144:ALA:HB1	2:F:206:ALA:HA	1.78	0.64
2:D:4810:MET:CG	2:F:4521:TYR:HB2	2.26	0.64
2:H:1703:TYR:HD2	2:H:1820:PRO:HB2	1.63	0.64
2:H:4518:LEU:HD13	2:H:4521:TYR:CE2	2.31	0.64
2:B:4518:LEU:HD13	2:B:4521:TYR:CE2	2.31	0.64
2:B:4753:THR:OG1	2:H:4767:GLN:HG2	1.98	0.64
2:F:4767:GLN:HG2	2:H:4753:THR:OG1	1.98	0.64
2:B:2891:GLN:HB3	2:B:2895:LYS:HE2	1.79	0.64
2:F:1117:TRP:HE1	2:F:1164:CYS:HB3	1.62	0.64
1:G:40:ARG:HH12	2:H:685:PHE:HB3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4511:ALA:HA	2:D:4514:ILE:HD12	1.80	0.64
2:H:1482:ARG:HH11	2:H:1531:TYR:HA	1.61	0.64
2:D:1117:TRP:HE1	2:D:1164:CYS:HB3	1.62	0.64
1:E:40:ARG:HH12	2:F:685:PHE:HB3	1.63	0.64
2:F:374:TYR:HA	2:F:391:ALA:HA	1.80	0.64
2:B:2770:GLU:HA	2:B:2773:ARG:HB2	1.80	0.64
2:D:748:LEU:HD13	2:D:750:ARG:HE	1.61	0.64
2:F:4511:ALA:HA	2:F:4514:ILE:HD12	1.80	0.64
2:H:144:ALA:HB1	2:H:206:ALA:HA	1.78	0.64
2:D:300:VAL:O	2:D:420:ARG:NH1	2.31	0.64
2:D:2770:GLU:HA	2:D:2773:ARG:HB2	1.80	0.64
2:H:374:TYR:HA	2:H:391:ALA:HA	1.80	0.64
2:B:2326:ILE:HG23	2:H:207:PHE:CD2	2.32	0.63
2:B:4511:ALA:HA	2:B:4514:ILE:HD12	1.80	0.63
2:B:4810:MET:CG	2:D:4521:TYR:HB2	2.28	0.63
2:H:394:HIS:HD2	2:H:397:GLY:H	1.43	0.63
2:B:1165:MET:HB2	2:B:1174:MET:HB2	1.81	0.63
2:B:1482:ARG:HH11	2:B:1531:TYR:HA	1.61	0.63
2:B:1703:TYR:HD2	2:B:1820:PRO:HB2	1.63	0.63
2:F:207:PHE:CD1	2:H:2326:ILE:HG23	2.32	0.63
2:B:4868:ILE:HG12	2:H:4865:GLY:CA	2.27	0.63
2:F:2891:GLN:HB3	2:F:2895:LYS:HE2	1.79	0.63
2:H:1165:MET:HB2	2:H:1174:MET:HB2	1.81	0.63
2:F:1114:ARG:HB2	2:F:1206:SER:HB3	1.81	0.63
2:H:2891:GLN:HB3	2:H:2895:LYS:HE2	1.79	0.63
2:F:1703:TYR:HD2	2:F:1820:PRO:HB2	1.63	0.63
2:H:2770:GLU:HA	2:H:2773:ARG:HB2	1.80	0.63
2:H:4511:ALA:HA	2:H:4514:ILE:HD12	1.80	0.63
1:A:40:ARG:HH12	2:B:685:PHE:HB3	1.63	0.63
1:C:87:HIS:H	1:C:91:ILE:HB	1.64	0.63
2:D:207:PHE:CD1	2:F:2326:ILE:HG23	2.30	0.63
1:G:31:GLN:HB2	1:G:96:THR:HB	1.81	0.63
2:H:4520:PHE:CB	2:H:4562:LEU:CD2	2.77	0.63
2:D:1165:MET:HB2	2:D:1174:MET:HB2	1.81	0.63
2:B:207:PHE:CD2	2:D:2326:ILE:HG23	2.34	0.63
2:B:1117:TRP:HE1	2:B:1164:CYS:HB3	1.62	0.63
1:C:40:ARG:HH12	2:D:685:PHE:HB3	1.63	0.63
2:F:2770:GLU:HA	2:F:2773:ARG:HB2	1.80	0.63
2:F:4520:PHE:CB	2:F:4562:LEU:CD2	2.77	0.63
2:H:300:VAL:O	2:H:420:ARG:NH1	2.31	0.63
2:H:1610:ARG:NH1	2:H:1612:SER:OG	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HB2	1:A:96:THR:HB	1.81	0.62
2:B:374:TYR:HA	2:B:391:ALA:HA	1.80	0.62
2:B:1114:ARG:HB2	2:B:1206:SER:HB3	1.81	0.62
2:D:4848:ASP:OD2	2:F:4819:TYR:CE1	2.52	0.62
2:F:4865:GLY:CA	2:H:4868:ILE:HG12	2.25	0.62
1:A:87:HIS:H	1:A:91:ILE:HB	1.64	0.62
2:F:4047:ARG:NH1	2:F:4077:GLU:OE2	2.33	0.62
2:B:300:VAL:O	2:B:420:ARG:NH1	2.31	0.62
2:B:4047:ARG:NH1	2:B:4077:GLU:OE2	2.33	0.62
2:D:374:TYR:HA	2:D:391:ALA:HA	1.80	0.62
2:B:1610:ARG:NH1	2:B:1612:SER:OG	2.32	0.62
1:E:87:HIS:H	1:E:91:ILE:HB	1.64	0.62
2:F:1165:MET:HB2	2:F:1174:MET:HB2	1.81	0.62
2:D:4865:GLY:CA	2:F:4868:ILE:HG12	2.25	0.62
2:F:1137:PHE:HA	2:F:1144:ARG:HA	1.82	0.62
2:D:1137:PHE:HA	2:D:1144:ARG:HA	1.82	0.62
2:H:4047:ARG:NH1	2:H:4077:GLU:OE2	2.33	0.62
2:D:1114:ARG:HB2	2:D:1206:SER:HB3	1.81	0.62
2:B:4521:TYR:HB2	2:H:4810:MET:CG	2.29	0.62
1:C:31:GLN:HB2	1:C:96:THR:HB	1.81	0.62
2:D:1703:TYR:HD2	2:D:1820:PRO:HB2	1.63	0.62
1:E:31:GLN:HB2	1:E:96:THR:HB	1.81	0.62
2:H:1114:ARG:HB2	2:H:1206:SER:HB3	1.81	0.62
2:H:1137:PHE:HA	2:H:1144:ARG:HA	1.82	0.62
2:D:1153:GLY:HA3	2:D:1182:LEU:HB3	1.82	0.62
2:D:4520:PHE:CB	2:D:4562:LEU:CD2	2.77	0.62
2:F:677:LEU:HB2	2:F:755:ILE:HB	1.82	0.62
2:F:1610:ARG:NH1	2:F:1612:SER:OG	2.32	0.62
2:F:4810:MET:CG	2:H:4521:TYR:HB2	2.30	0.62
2:F:1153:GLY:HA3	2:F:1182:LEU:HB3	1.82	0.61
2:D:677:LEU:HB2	2:D:755:ILE:HB	1.82	0.61
2:D:4047:ARG:NH1	2:D:4077:GLU:OE2	2.33	0.61
2:D:4874:LEU:O	2:D:4878:GLN:NE2	2.33	0.61
2:B:1153:GLY:HA3	2:B:1182:LEU:HB3	1.82	0.61
2:D:1250:TRP:HE1	2:D:1643:GLU:HG3	1.65	0.61
2:F:1670:HIS:ND1	2:F:1778:TYR:O	2.34	0.61
2:F:4148:ARG:NH2	2:F:4150:TYR:OH	2.33	0.61
2:F:4874:LEU:O	2:F:4878:GLN:NE2	2.33	0.61
2:H:1153:GLY:HA3	2:H:1182:LEU:HB3	1.82	0.61
2:D:4148:ARG:NH2	2:D:4150:TYR:OH	2.33	0.61
2:B:1101:TRP:HA	2:B:1237:GLU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1670:HIS:ND1	2:D:1778:TYR:O	2.33	0.61
2:H:2127:ILE:HD11	2:H:2143:MET:HG3	1.83	0.61
2:B:1137:PHE:HA	2:B:1144:ARG:HA	1.82	0.61
2:B:2326:ILE:HG23	2:H:207:PHE:CD1	2.32	0.61
1:G:87:HIS:H	1:G:91:ILE:HB	1.64	0.61
2:B:1761:MET:SD	2:B:1761:MET:N	2.73	0.61
2:B:4520:PHE:CB	2:B:4562:LEU:CD2	2.77	0.61
2:D:1610:ARG:NH1	2:D:1612:SER:OG	2.32	0.61
2:F:300:VAL:O	2:F:420:ARG:NH1	2.31	0.61
2:B:4874:LEU:O	2:B:4878:GLN:NE2	2.33	0.61
2:H:677:LEU:HB2	2:H:755:ILE:HB	1.82	0.61
2:H:1250:TRP:HE1	2:H:1643:GLU:HG3	1.65	0.61
2:B:2127:ILE:HD11	2:B:2143:MET:HG3	1.83	0.61
2:F:4848:ASP:OD2	2:H:4819:TYR:CE1	2.54	0.61
2:B:1427:TYR:HA	2:B:1509:CYS:HA	1.83	0.61
2:H:4874:LEU:O	2:H:4878:GLN:NE2	2.33	0.61
2:D:1427:TYR:HA	2:D:1509:CYS:HA	1.83	0.60
2:F:1250:TRP:HE1	2:F:1643:GLU:HG3	1.65	0.60
2:B:1250:TRP:HE1	2:B:1643:GLU:HG3	1.65	0.60
2:B:4517:ILE:O	2:B:4519:LEU:N	2.32	0.60
2:F:1427:TYR:HA	2:F:1509:CYS:HA	1.83	0.60
2:B:1670:HIS:ND1	2:B:1778:TYR:O	2.34	0.60
2:D:1258:PHE:HB2	2:D:1593:HIS:HB3	1.83	0.60
2:H:1116:GLY:HA3	2:H:1136:ALA:HA	1.84	0.60
2:D:1101:TRP:HA	2:D:1237:GLU:HB2	1.83	0.60
2:B:1116:GLY:HA3	2:B:1136:ALA:HA	1.84	0.60
2:D:188:SER:HB2	2:D:190:ARG:HH21	1.67	0.60
2:F:1258:PHE:HB2	2:F:1593:HIS:HB3	1.83	0.60
2:H:1670:HIS:ND1	2:H:1778:TYR:O	2.34	0.60
2:B:677:LEU:HB2	2:B:755:ILE:HB	1.82	0.60
2:B:4148:ARG:NH2	2:B:4150:TYR:OH	2.33	0.60
2:D:1116:GLY:HA3	2:D:1136:ALA:HA	1.84	0.60
2:D:1726:ILE:HD11	2:D:2121:LEU:HD11	1.84	0.60
2:F:1124:PRO:HB2	2:F:1252:SER:HB3	1.83	0.60
2:H:1258:PHE:HB2	2:H:1593:HIS:HB3	1.83	0.60
2:H:1427:TYR:HA	2:H:1509:CYS:HA	1.83	0.60
2:H:1761:MET:SD	2:H:1761:MET:N	2.73	0.60
1:E:21:THR:H	1:E:107:GLU:HB2	1.67	0.60
2:F:2127:ILE:HD11	2:F:2143:MET:HG3	1.83	0.60
2:B:4848:ASP:OD2	2:D:4819:TYR:CE1	2.55	0.60
2:D:629:GLN:OE1	2:D:1669:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1124:PRO:HB2	2:D:1252:SER:HB3	1.83	0.60
2:H:1101:TRP:HA	2:H:1237:GLU:HB2	1.82	0.60
2:B:1726:ILE:HD11	2:B:2121:LEU:HD11	1.84	0.60
2:B:188:SER:HB2	2:B:190:ARG:HH21	1.67	0.59
2:D:2470:VAL:HG11	2:D:2523:THR:HG23	1.84	0.59
2:F:1116:GLY:HA3	2:F:1136:ALA:HA	1.84	0.59
1:G:21:THR:H	1:G:107:GLU:HB2	1.67	0.59
2:B:1258:PHE:HB2	2:B:1593:HIS:HB3	1.83	0.59
2:F:756:SER:HB3	2:F:769:ARG:HB2	1.84	0.59
2:D:2127:ILE:HD11	2:D:2143:MET:HG3	1.83	0.59
2:F:298:ARG:HE	2:F:303:GLY:HA2	1.68	0.59
2:F:1809:PRO:HB3	2:F:1817:LEU:HB2	1.84	0.59
2:F:2470:VAL:HG11	2:F:2523:THR:HG23	1.85	0.59
2:H:4517:ILE:O	2:H:4519:LEU:N	2.32	0.59
2:B:2470:VAL:HG11	2:B:2523:THR:HG23	1.85	0.59
2:F:636:LEU:HD21	2:F:643:LEU:HD21	1.85	0.59
2:F:4517:ILE:O	2:F:4519:LEU:N	2.32	0.59
2:H:4148:ARG:NH2	2:H:4150:TYR:OH	2.33	0.59
2:D:4608:ALA:HB1	2:D:4650:VAL:HG11	1.84	0.59
2:H:629:GLN:OE1	2:H:1669:ASN:ND2	2.35	0.59
2:H:2470:VAL:HG11	2:H:2523:THR:HG23	1.84	0.59
2:H:4608:ALA:HB1	2:H:4650:VAL:HG11	1.84	0.59
2:B:4608:ALA:HB1	2:B:4650:VAL:HG11	1.84	0.59
2:F:4751:PHE:O	2:F:4755:ARG:NH1	2.36	0.59
2:D:4814:TYR:HE2	2:D:4815:MET:HE1	1.67	0.59
2:F:247:VAL:O	2:F:272:ARG:NH1	2.36	0.59
2:F:1726:ILE:HD11	2:F:2121:LEU:HD11	1.84	0.59
2:H:247:VAL:O	2:H:272:ARG:NH1	2.36	0.59
2:H:1124:PRO:HB2	2:H:1252:SER:HB3	1.83	0.59
2:D:4866:LEU:HD12	2:F:4871:PHE:HE2	1.68	0.59
2:F:629:GLN:OE1	2:F:1669:ASN:ND2	2.35	0.59
2:F:1101:TRP:HA	2:F:1237:GLU:HB2	1.83	0.59
2:B:247:VAL:O	2:B:272:ARG:NH1	2.36	0.59
2:B:4819:TYR:CE1	2:H:4848:ASP:OD2	2.56	0.59
2:D:832:LEU:O	2:D:1614:ARG:NH1	2.36	0.59
2:D:1809:PRO:HB3	2:D:1817:LEU:HB2	1.84	0.59
2:F:4608:ALA:HB1	2:F:4650:VAL:HG11	1.84	0.59
2:F:4845:ILE:HG23	2:H:4819:TYR:CD1	2.38	0.59
2:H:756:SER:HB3	2:H:769:ARG:HB2	1.84	0.59
2:H:1726:ILE:HD11	2:H:2121:LEU:HD11	1.84	0.59
2:B:1124:PRO:HB2	2:B:1252:SER:HB3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:VAL:O	2:D:272:ARG:NH1	2.36	0.58
2:D:636:LEU:HD21	2:D:643:LEU:HD21	1.85	0.58
2:H:188:SER:HB2	2:H:190:ARG:HH21	1.67	0.58
2:H:298:ARG:HE	2:H:303:GLY:HA2	1.67	0.58
2:H:636:LEU:HD21	2:H:643:LEU:HD21	1.85	0.58
2:H:1809:PRO:HB3	2:H:1817:LEU:HB2	1.84	0.58
2:B:832:LEU:O	2:B:1614:ARG:NH1	2.36	0.58
1:C:21:THR:H	1:C:107:GLU:HB2	1.67	0.58
2:D:4751:PHE:O	2:D:4755:ARG:NH1	2.36	0.58
2:F:188:SER:HB2	2:F:190:ARG:HH21	1.67	0.58
2:H:4751:PHE:O	2:H:4755:ARG:NH1	2.36	0.58
2:B:150:GLN:NE2	2:B:158:CYS:SG	2.76	0.58
2:D:298:ARG:HE	2:D:303:GLY:HA2	1.68	0.58
2:F:832:LEU:O	2:F:1614:ARG:NH1	2.36	0.58
2:B:693:LEU:HD21	2:B:798:ILE:HG21	1.86	0.58
2:F:1121:GLY:O	2:F:1133:ARG:NH1	2.36	0.58
2:H:1589:GLN:NE2	2:H:1634:GLU:OE1	2.37	0.58
2:B:298:ARG:HE	2:B:303:GLY:HA2	1.68	0.58
2:B:629:GLN:OE1	2:B:1669:ASN:ND2	2.35	0.58
2:F:1589:GLN:NE2	2:F:1634:GLU:OE1	2.37	0.58
2:H:832:LEU:O	2:H:1614:ARG:NH1	2.36	0.58
2:H:248:PRO:O	2:H:257:ARG:NH2	2.37	0.58
1:A:21:THR:H	1:A:107:GLU:HB2	1.67	0.58
2:B:1809:PRO:HB3	2:B:1817:LEU:HB2	1.84	0.58
2:B:4751:PHE:O	2:B:4755:ARG:NH1	2.36	0.58
2:D:758:CYS:SG	2:D:759:LEU:N	2.77	0.58
2:F:4866:LEU:HD12	2:H:4871:PHE:HE2	1.69	0.58
2:B:248:PRO:O	2:B:257:ARG:NH2	2.37	0.58
2:H:693:LEU:HD21	2:H:798:ILE:HG21	1.86	0.58
2:F:802:PHE:HB2	2:F:1617:TRP:HB2	1.85	0.58
2:F:2142:LEU:HD23	2:F:2145:ARG:HD2	1.86	0.58
2:H:2142:LEU:HD23	2:H:2145:ARG:HD2	1.86	0.58
2:B:476:GLN:NE2	2:B:3679:GLU:OE1	2.37	0.58
2:B:2718:LEU:HD13	2:B:2780:LEU:HB3	1.86	0.58
2:B:4866:LEU:HD12	2:D:4871:PHE:HE2	1.69	0.58
2:D:2535:LEU:HD12	2:D:2537:ALA:H	1.69	0.58
2:F:2535:LEU:HD12	2:F:2537:ALA:H	1.69	0.58
2:B:4819:TYR:CD1	2:H:4845:ILE:HG23	2.39	0.57
2:D:248:PRO:O	2:D:257:ARG:NH2	2.37	0.57
2:D:756:SER:HB3	2:D:769:ARG:HB2	1.84	0.57
2:F:758:CYS:SG	2:F:759:LEU:N	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1589:GLN:NE2	2:D:1634:GLU:OE1	2.37	0.57
2:B:636:LEU:HD21	2:B:643:LEU:HD21	1.85	0.57
2:H:4640:SER:O	2:H:4643:ASN:ND2	2.38	0.57
2:B:758:CYS:SG	2:B:759:LEU:N	2.77	0.57
2:B:1089:ARG:HH21	2:B:1600:PRO:HG3	1.70	0.57
2:D:476:GLN:NE2	2:D:3679:GLU:OE1	2.37	0.57
2:D:2142:LEU:HD23	2:D:2145:ARG:HD2	1.86	0.57
2:D:2718:LEU:HD13	2:D:2780:LEU:HB3	1.86	0.57
2:D:4640:SER:O	2:D:4643:ASN:ND2	2.38	0.57
2:F:4865:GLY:HA2	2:H:4868:ILE:CD1	2.34	0.57
2:H:1089:ARG:HH21	2:H:1600:PRO:HG3	1.70	0.57
2:H:2718:LEU:HD13	2:H:2780:LEU:HB3	1.86	0.57
2:B:756:SER:HB3	2:B:769:ARG:HB2	1.84	0.57
2:B:1589:GLN:NE2	2:B:1634:GLU:OE1	2.37	0.57
2:D:693:LEU:HD21	2:D:798:ILE:HG21	1.86	0.57
2:H:758:CYS:SG	2:H:759:LEU:N	2.77	0.57
2:B:1631:HIS:HA	2:B:1638:SER:HA	1.87	0.57
2:B:2060:GLN:NE2	2:B:2092:GLN:O	2.38	0.57
2:B:2535:LEU:HD12	2:B:2537:ALA:H	1.69	0.57
2:F:4838:ASP:HB3	2:F:4841:GLU:HB2	1.87	0.57
2:H:476:GLN:NE2	2:H:3679:GLU:OE1	2.37	0.57
2:H:1121:GLY:O	2:H:1133:ARG:NH1	2.36	0.57
2:H:3808:ALA:HA	2:H:3811:ARG:HD3	1.87	0.57
2:B:3808:ALA:HA	2:B:3811:ARG:HD3	1.87	0.57
2:D:1631:HIS:HA	2:D:1638:SER:HA	1.87	0.57
2:D:1761:MET:N	2:D:1761:MET:SD	2.73	0.57
2:F:1089:ARG:HH21	2:F:1600:PRO:HG3	1.70	0.57
2:H:1043:LYS:HD3	2:H:1047:LYS:HE3	1.87	0.57
2:B:1121:GLY:O	2:B:1133:ARG:NH1	2.36	0.57
2:D:207:PHE:CE2	2:F:2326:ILE:CD1	2.88	0.57
2:F:248:PRO:O	2:F:257:ARG:NH2	2.37	0.57
2:F:476:GLN:NE2	2:F:3679:GLU:OE1	2.37	0.57
2:B:4814:TYR:HE2	2:B:4815:MET:HE1	1.70	0.57
2:B:4838:ASP:HB3	2:B:4841:GLU:HB2	1.87	0.57
2:B:2142:LEU:HD23	2:B:2145:ARG:HD2	1.86	0.57
2:D:1089:ARG:HH21	2:D:1600:PRO:HG3	1.70	0.57
2:D:4517:ILE:O	2:D:4519:LEU:N	2.32	0.57
1:E:87:HIS:NE2	2:F:1774:GLU:OE2	2.38	0.57
2:F:693:LEU:HD21	2:F:798:ILE:HG21	1.86	0.57
2:F:2060:GLN:NE2	2:F:2092:GLN:O	2.38	0.57
2:F:4857:VAL:CG1	2:H:4863:ILE:HG22	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:HIS:NE2	2:H:1774:GLU:OE2	2.38	0.57
2:H:150:GLN:NE2	2:H:158:CYS:SG	2.76	0.57
2:H:4814:TYR:HE2	2:H:4815:MET:HE1	1.70	0.57
2:H:4838:ASP:HB3	2:H:4841:GLU:HB2	1.87	0.57
2:B:657:PRO:HB3	2:B:834:VAL:HG22	1.87	0.56
2:B:4640:SER:O	2:B:4643:ASN:ND2	2.38	0.56
2:D:655:MET:HG2	2:D:836:HIS:HA	1.87	0.56
2:D:657:PRO:HB3	2:D:834:VAL:HG22	1.87	0.56
2:F:4138:GLU:OE2	2:F:4148:ARG:NH1	2.38	0.56
2:H:2535:LEU:HD12	2:H:2537:ALA:H	1.69	0.56
2:B:4138:GLU:OE2	2:B:4148:ARG:NH1	2.38	0.56
2:D:802:PHE:HB2	2:D:1617:TRP:HB2	1.85	0.56
2:F:2296:GLY:HA2	2:F:2299:TYR:HD2	1.70	0.56
2:H:802:PHE:HB2	2:H:1617:TRP:HB2	1.85	0.56
2:H:1631:HIS:HA	2:H:1638:SER:HA	1.87	0.56
1:A:87:HIS:NE2	2:B:1774:GLU:OE2	2.38	0.56
2:B:797:GLY:HA2	2:B:1622:LEU:HA	1.87	0.56
2:B:4871:PHE:HE2	2:H:4866:LEU:HD12	1.70	0.56
2:B:4888:LYS:HB3	2:B:4893:GLY:HA2	1.86	0.56
2:D:1043:LYS:HD3	2:D:1047:LYS:HE3	1.87	0.56
2:D:2060:GLN:NE2	2:D:2092:GLN:O	2.38	0.56
2:F:76:ARG:CB	2:H:3891:TRP:CG	2.88	0.56
2:F:1631:HIS:HA	2:F:1638:SER:HA	1.87	0.56
2:F:2421:ARG:NH2	2:F:2476:VAL:O	2.39	0.56
2:F:4520:PHE:HD1	2:F:4562:LEU:HD21	0.84	0.56
2:H:797:GLY:HA2	2:H:1622:LEU:HA	1.87	0.56
2:H:2060:GLN:NE2	2:H:2092:GLN:O	2.38	0.56
2:H:4138:GLU:OE2	2:H:4148:ARG:NH1	2.39	0.56
2:B:207:PHE:CD1	2:D:2326:ILE:HG23	2.33	0.56
2:B:802:PHE:HB2	2:B:1617:TRP:HB2	1.85	0.56
2:B:4845:ILE:HG23	2:D:4819:TYR:CD1	2.39	0.56
2:D:3808:ALA:HA	2:D:3811:ARG:HD3	1.87	0.56
2:D:4888:LYS:HB3	2:D:4893:GLY:HA2	1.86	0.56
2:F:2718:LEU:HD13	2:F:2780:LEU:HB3	1.86	0.56
2:H:655:MET:HG2	2:H:836:HIS:HA	1.87	0.56
2:H:4722:TYR:OH	2:H:4745:LEU:O	2.24	0.56
2:H:4888:LYS:HB3	2:H:4893:GLY:HA2	1.86	0.56
2:B:1043:LYS:HD3	2:B:1047:LYS:HE3	1.87	0.56
2:B:4520:PHE:HD1	2:B:4562:LEU:HD21	0.84	0.56
2:D:2296:GLY:HA2	2:D:2299:TYR:HD2	1.70	0.56
2:D:2421:ARG:NH2	2:D:2476:VAL:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4865:GLY:HA2	2:F:4868:ILE:CD1	2.35	0.56
2:F:150:GLN:NE2	2:F:158:CYS:SG	2.76	0.56
2:F:655:MET:HG2	2:F:836:HIS:HA	1.87	0.56
2:F:4888:LYS:HB3	2:F:4893:GLY:HA2	1.86	0.56
2:H:4136:ARG:NH2	2:H:4150:TYR:OH	2.38	0.56
2:D:15:ARG:HB3	2:D:110:HIS:HB3	1.88	0.56
2:F:15:ARG:HB3	2:F:110:HIS:HB3	1.88	0.56
2:F:1043:LYS:HD3	2:F:1047:LYS:HE3	1.87	0.56
2:F:4640:SER:O	2:F:4643:ASN:ND2	2.38	0.56
2:F:4722:TYR:OH	2:F:4745:LEU:O	2.24	0.56
2:D:4138:GLU:OE2	2:D:4148:ARG:NH1	2.38	0.56
2:H:15:ARG:HB3	2:H:110:HIS:HB3	1.88	0.56
2:B:4865:GLY:HA2	2:D:4868:ILE:CD1	2.36	0.56
2:D:4838:ASP:HB3	2:D:4841:GLU:HB2	1.87	0.56
2:B:15:ARG:HB3	2:B:110:HIS:HB3	1.88	0.56
2:B:2421:ARG:NH2	2:B:2476:VAL:O	2.39	0.56
2:D:4056:HIS:O	2:D:4058:HIS:ND1	2.39	0.56
2:F:3808:ALA:HA	2:F:3811:ARG:HD3	1.87	0.56
1:C:87:HIS:NE2	2:D:1774:GLU:OE2	2.38	0.56
2:D:2157:TYR:HH	2:D:2203:TYR:HH	1.54	0.56
2:F:2728:HIS:NE2	2:F:2829:MET:SD	2.79	0.56
2:H:2421:ARG:NH2	2:H:2476:VAL:O	2.39	0.56
2:B:2296:GLY:HA2	2:B:2299:TYR:HD2	1.70	0.55
2:B:4622:PRO:O	2:B:4630:GLN:NE2	2.39	0.55
2:F:657:PRO:HB3	2:F:834:VAL:HG22	1.87	0.55
2:B:4912:GLN:O	2:B:4915:ASN:ND2	2.40	0.55
2:D:517:VAL:HG23	2:D:520:ARG:HE	1.71	0.55
2:H:2296:GLY:HA2	2:H:2299:TYR:HD2	1.70	0.55
2:H:2728:HIS:NE2	2:H:2829:MET:SD	2.79	0.55
2:B:243:GLU:HA	2:B:264:GLY:HA2	1.88	0.55
2:F:207:PHE:CE2	2:H:2326:ILE:CD1	2.89	0.55
2:H:4056:HIS:O	2:H:4058:HIS:ND1	2.39	0.55
2:B:1128:LEU:HD13	2:B:1206:SER:HB2	1.89	0.55
2:B:1304:LEU:HG	2:B:1591:LEU:H	1.72	0.55
2:B:4056:HIS:O	2:B:4058:HIS:ND1	2.39	0.55
2:B:4868:ILE:CD1	2:H:4865:GLY:HA2	2.37	0.55
2:D:150:GLN:NE2	2:D:158:CYS:SG	2.76	0.55
2:H:243:GLU:HA	2:H:264:GLY:HA2	1.88	0.55
2:H:1827:THR:HA	2:H:1830:ILE:HD12	1.89	0.55
2:H:4912:GLN:O	2:H:4915:ASN:ND2	2.40	0.55
2:B:655:MET:HG2	2:B:836:HIS:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ARG:CB	2:F:3891:TRP:CG	2.89	0.55
2:D:1827:THR:HA	2:D:1830:ILE:HD12	1.89	0.55
2:D:2718:LEU:HB3	2:D:2780:LEU:HD13	1.89	0.55
2:F:1304:LEU:HG	2:F:1591:LEU:H	1.72	0.55
2:F:4622:PRO:O	2:F:4630:GLN:NE2	2.39	0.55
2:H:4622:PRO:O	2:H:4630:GLN:NE2	2.39	0.55
2:B:1827:THR:HA	2:B:1830:ILE:HD12	1.89	0.55
2:F:1827:THR:HA	2:F:1830:ILE:HD12	1.89	0.55
2:F:2718:LEU:HB3	2:F:2780:LEU:HD13	1.89	0.55
2:B:517:VAL:HG23	2:B:520:ARG:HE	1.71	0.55
2:D:1128:LEU:HD13	2:D:1206:SER:HB2	1.89	0.55
2:D:4845:ILE:HG23	2:F:4819:TYR:CD1	2.41	0.55
2:F:4056:HIS:O	2:F:4058:HIS:ND1	2.39	0.55
2:H:1257:GLN:O	2:H:1596:TRP:N	2.40	0.55
2:B:4722:TYR:OH	2:B:4745:LEU:O	2.24	0.55
2:D:797:GLY:HA2	2:D:1622:LEU:HA	1.87	0.55
2:D:1121:GLY:O	2:D:1133:ARG:NH1	2.36	0.55
2:D:1304:LEU:HG	2:D:1591:LEU:H	1.72	0.55
2:D:3917:VAL:O	2:D:3920:THR:OG1	2.24	0.55
2:D:4857:VAL:CG1	2:F:4863:ILE:HG22	2.36	0.55
2:F:4912:GLN:O	2:F:4915:ASN:ND2	2.40	0.55
2:H:299:HIS:HD2	2:H:302:THR:H	1.55	0.55
2:B:4002:ASP:OD1	2:B:4115:ARG:NH1	2.40	0.55
2:B:4857:VAL:CG1	2:D:4863:ILE:HG22	2.37	0.55
2:D:1014:GLN:HB3	2:D:1032:LEU:HD21	1.89	0.55
2:D:2072:GLN:NE2	2:D:3647:LYS:O	2.40	0.55
2:D:3771:ASN:ND2	2:D:3773:THR:OG1	2.40	0.55
2:D:4622:PRO:O	2:D:4630:GLN:NE2	2.39	0.55
2:D:4627:ILE:O	2:D:4631:TRP:CB	2.55	0.55
2:D:4722:TYR:OH	2:D:4745:LEU:O	2.23	0.55
2:F:797:GLY:HA2	2:F:1622:LEU:HA	1.87	0.55
2:H:657:PRO:HB3	2:H:834:VAL:HG22	1.87	0.55
2:H:1304:LEU:HG	2:H:1591:LEU:H	1.72	0.55
2:H:4002:ASP:OD1	2:H:4115:ARG:NH1	2.40	0.55
2:B:2072:GLN:NE2	2:B:3647:LYS:O	2.40	0.54
2:D:1160:ASP:OD1	2:D:1178:ASN:ND2	2.40	0.54
2:D:1257:GLN:O	2:D:1596:TRP:N	2.40	0.54
2:D:4912:GLN:O	2:D:4915:ASN:ND2	2.40	0.54
2:F:299:HIS:HD2	2:F:302:THR:H	1.55	0.54
2:F:687:THR:HG22	2:F:689:GLU:H	1.72	0.54
2:F:3771:ASN:ND2	2:F:3773:THR:OG1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4524:SER:HG	2:F:4558:VAL:N	2.05	0.54
2:H:2024:LEU:HD23	2:H:2026:ILE:H	1.73	0.54
2:H:2718:LEU:HB3	2:H:2780:LEU:HD13	1.89	0.54
2:B:2157:TYR:HH	2:B:2203:TYR:HH	1.50	0.54
2:D:556:ASP:HA	2:D:559:ILE:HD12	1.90	0.54
2:D:4002:ASP:OD1	2:D:4115:ARG:NH1	2.40	0.54
2:F:28:ILE:HD12	2:F:33:GLN:HG2	1.90	0.54
2:F:444:THR:OG1	2:F:445:VAL:N	2.40	0.54
2:F:4655:MET:HA	2:F:4667:ILE:HD12	1.90	0.54
2:F:1128:LEU:HD13	2:F:1206:SER:HB2	1.89	0.54
2:F:1154:ARG:NH2	2:F:1180:GLU:OE1	2.41	0.54
2:H:2072:GLN:NE2	2:H:3647:LYS:O	2.40	0.54
2:H:4520:PHE:HD1	2:H:4562:LEU:HD21	0.84	0.54
2:H:4524:SER:HG	2:H:4558:VAL:N	2.05	0.54
2:B:2718:LEU:HB3	2:B:2780:LEU:HD13	1.89	0.54
2:F:1160:ASP:OD1	2:F:1178:ASN:ND2	2.40	0.54
2:H:115:TYR:OH	2:H:179:ASP:OD2	2.26	0.54
2:H:3771:ASN:ND2	2:H:3773:THR:OG1	2.40	0.54
2:B:115:TYR:OH	2:B:179:ASP:OD2	2.26	0.54
2:B:3891:TRP:CG	2:H:76:ARG:CB	2.91	0.54
2:D:115:TYR:OH	2:D:179:ASP:OD2	2.26	0.54
2:H:1014:GLN:HB3	2:H:1032:LEU:HD21	1.89	0.54
2:H:1907:MET:HA	2:H:1910:LEU:HD23	1.90	0.54
2:H:4655:MET:HA	2:H:4667:ILE:HD12	1.90	0.54
2:B:1014:GLN:HB3	2:B:1032:LEU:HD21	1.89	0.54
2:B:1160:ASP:OD1	2:B:1178:ASN:ND2	2.40	0.54
2:B:2024:LEU:HD23	2:B:2026:ILE:H	1.72	0.54
1:C:7:ILE:H	1:C:72:ALA:HA	1.73	0.54
2:D:2024:LEU:HD23	2:D:2026:ILE:H	1.72	0.54
2:F:115:TYR:OH	2:F:179:ASP:OD2	2.26	0.54
2:F:681:HIS:HB2	2:F:799:LYS:HG2	1.90	0.54
2:F:3767:LEU:HD21	2:F:3774:VAL:HB	1.90	0.54
2:H:1086:ARG:HH22	2:H:1254:ARG:HD3	1.73	0.54
2:H:3767:LEU:HD21	2:H:3774:VAL:HB	1.90	0.54
2:B:1272:ARG:NH2	2:B:1590:PHE:O	2.41	0.54
2:D:444:THR:OG1	2:D:445:VAL:N	2.40	0.54
2:D:1154:ARG:NH2	2:D:1180:GLU:OE1	2.41	0.54
2:F:517:VAL:HG23	2:F:520:ARG:HE	1.71	0.54
2:F:1602:GLN:HE22	2:F:1642:LEU:HB3	1.73	0.54
2:H:28:ILE:HD12	2:H:33:GLN:HG2	1.90	0.54
2:H:517:VAL:HG23	2:H:520:ARG:HE	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1160:ASP:OD1	2:H:1178:ASN:ND2	2.40	0.54
2:H:1272:ARG:NH2	2:H:1590:PHE:O	2.41	0.54
2:H:1922:ARG:NH1	2:H:2038:THR:O	2.39	0.54
1:A:7:ILE:H	1:A:72:ALA:HA	1.73	0.54
2:B:1257:GLN:O	2:B:1596:TRP:N	2.40	0.54
2:B:1907:MET:HA	2:B:1910:LEU:HD23	1.90	0.54
2:B:3771:ASN:ND2	2:B:3773:THR:OG1	2.40	0.54
2:D:28:ILE:HD12	2:D:33:GLN:HG2	1.90	0.54
2:D:243:GLU:HA	2:D:264:GLY:HA2	1.88	0.54
2:D:687:THR:HG22	2:D:689:GLU:H	1.72	0.54
2:F:243:GLU:HA	2:F:264:GLY:HA2	1.88	0.54
2:F:371:TRP:N	2:F:394:HIS:O	2.38	0.54
2:F:1257:GLN:O	2:F:1596:TRP:N	2.40	0.54
2:F:2072:GLN:NE2	2:F:3647:LYS:O	2.40	0.54
2:F:4002:ASP:OD1	2:F:4115:ARG:NH1	2.40	0.54
2:F:4627:ILE:O	2:F:4631:TRP:CB	2.55	0.54
2:H:444:THR:OG1	2:H:445:VAL:N	2.40	0.54
2:B:1154:ARG:NH2	2:B:1180:GLU:OE1	2.41	0.54
2:B:4627:ILE:O	2:B:4631:TRP:CB	2.55	0.54
2:D:371:TRP:N	2:D:394:HIS:O	2.38	0.54
2:F:1014:GLN:HB3	2:F:1032:LEU:HD21	1.89	0.54
2:H:1128:LEU:HD13	2:H:1206:SER:HB2	1.89	0.54
2:B:444:THR:OG1	2:B:445:VAL:N	2.40	0.54
2:B:4863:ILE:HG22	2:H:4857:VAL:CG1	2.38	0.54
2:D:480:ARG:NH2	2:D:3679:GLU:OE2	2.41	0.54
2:D:4655:MET:HA	2:D:4667:ILE:HD12	1.90	0.54
2:H:235:ARG:NH2	2:H:268:SER:O	2.41	0.54
2:H:506:HIS:NE2	2:H:534:TYR:OH	2.40	0.54
2:H:4627:ILE:O	2:H:4631:TRP:CB	2.55	0.54
2:B:25:THR:HG22	2:B:34:LYS:HG2	1.90	0.53
2:B:371:TRP:N	2:B:394:HIS:O	2.38	0.53
2:B:375:GLN:N	2:B:390:LYS:O	2.41	0.53
2:B:687:THR:HG22	2:B:689:GLU:H	1.72	0.53
2:D:1224:LEU:HD13	2:D:1227:PHE:HD2	1.74	0.53
2:D:1907:MET:HA	2:D:1910:LEU:HD23	1.90	0.53
2:D:4814:TYR:HE2	2:D:4815:MET:CE	2.21	0.53
2:F:2840:ALA:HB3	2:F:2906:ARG:HD3	1.91	0.53
2:H:646:THR:HA	2:H:1630:LEU:HA	1.91	0.53
2:B:4136:ARG:NH2	2:B:4150:TYR:OH	2.38	0.53
2:D:246:THR:OG1	2:D:272:ARG:NH1	2.42	0.53
2:D:1029:ASN:HB3	2:D:1032:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1922:ARG:NH1	2:D:2038:THR:O	2.39	0.53
2:D:2728:HIS:NE2	2:D:2829:MET:SD	2.79	0.53
2:D:4037:ASP:OD2	2:D:4042:GLY:N	2.41	0.53
2:F:15:ARG:N	2:F:18:ASP:OD2	2.40	0.53
2:F:1907:MET:HA	2:F:1910:LEU:HD23	1.90	0.53
2:F:2024:LEU:HD23	2:F:2026:ILE:H	1.72	0.53
2:H:681:HIS:HB2	2:H:799:LYS:HG2	1.90	0.53
2:B:207:PHE:CE2	2:D:2326:ILE:CD1	2.91	0.53
2:B:1245:ARG:NH2	2:B:1797:GLU:OE2	2.42	0.53
2:B:2326:ILE:CD1	2:H:207:PHE:CE2	2.90	0.53
2:D:235:ARG:NH2	2:D:268:SER:O	2.41	0.53
2:D:1245:ARG:NH2	2:D:1797:GLU:OE2	2.42	0.53
2:D:1272:ARG:NH2	2:D:1590:PHE:O	2.41	0.53
2:D:3805:ASP:OD2	2:D:3808:ALA:N	2.41	0.53
2:D:4136:ARG:NH2	2:D:4150:TYR:OH	2.38	0.53
2:F:506:HIS:NE2	2:F:534:TYR:OH	2.40	0.53
2:F:646:THR:HA	2:F:1630:LEU:HA	1.90	0.53
2:F:1224:LEU:HD13	2:F:1227:PHE:HD2	1.74	0.53
2:B:246:THR:OG1	2:B:272:ARG:NH1	2.42	0.53
2:B:1086:ARG:HH22	2:B:1254:ARG:HD3	1.73	0.53
2:D:207:PHE:CD1	2:F:2326:ILE:HG22	2.42	0.53
2:D:646:THR:HA	2:D:1630:LEU:HA	1.90	0.53
2:D:1602:GLN:HE22	2:D:1642:LEU:HB3	1.72	0.53
2:D:2760:PRO:HD2	2:D:2763:LEU:HD12	1.91	0.53
2:D:2840:ALA:HB3	2:D:2906:ARG:HD3	1.91	0.53
2:D:4524:SER:HG	2:D:4558:VAL:N	2.05	0.53
2:F:1272:ARG:NH2	2:F:1590:PHE:O	2.41	0.53
2:F:4037:ASP:OD2	2:F:4042:GLY:N	2.41	0.53
2:H:1245:ARG:NH2	2:H:1797:GLU:OE2	2.42	0.53
2:H:3805:ASP:OD2	2:H:3808:ALA:N	2.40	0.53
2:H:4782:TYR:OH	2:H:4847:PHE:O	2.27	0.53
2:B:28:ILE:HD12	2:B:33:GLN:HG2	1.90	0.53
2:B:299:HIS:HD2	2:B:302:THR:H	1.55	0.53
2:B:556:ASP:HA	2:B:559:ILE:HD12	1.90	0.53
2:D:299:HIS:HD2	2:D:302:THR:H	1.55	0.53
2:D:565:LEU:HD11	2:D:603:LYS:HG2	1.91	0.53
2:D:1938:GLN:OE1	2:D:1942:ARG:NH1	2.42	0.53
2:F:556:ASP:HA	2:F:559:ILE:HD12	1.90	0.53
2:F:1938:GLN:OE1	2:F:1942:ARG:NH1	2.42	0.53
2:F:3919:ASN:O	2:F:3922:THR:OG1	2.27	0.53
2:H:480:ARG:NH2	2:H:3679:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1154:ARG:NH2	2:H:1180:GLU:OE1	2.41	0.53
2:H:1308:ILE:HD12	2:H:1539:LEU:HB2	1.90	0.53
2:H:1912:GLN:OE1	2:H:2091:ARG:NH1	2.42	0.53
2:B:196:TYR:O	2:B:201:LEU:N	2.42	0.53
2:B:1602:GLN:HE22	2:B:1642:LEU:HB3	1.73	0.53
2:B:4655:MET:HA	2:B:4667:ILE:HD12	1.90	0.53
2:D:25:THR:HG22	2:D:34:LYS:HG2	1.90	0.53
2:D:1912:GLN:OE1	2:D:2091:ARG:NH1	2.42	0.53
2:D:3904:GLN:NE2	2:D:3965:GLN:OE1	2.41	0.53
2:F:4782:TYR:OH	2:F:4847:PHE:O	2.27	0.53
1:G:7:ILE:H	1:G:72:ALA:HA	1.73	0.53
2:H:3904:GLN:NE2	2:H:3965:GLN:OE1	2.41	0.53
2:B:235:ARG:NH2	2:B:268:SER:O	2.41	0.53
2:B:4524:SER:HG	2:B:4558:VAL:N	2.05	0.53
2:D:681:HIS:HB2	2:D:799:LYS:HG2	1.90	0.53
2:D:3767:LEU:HD21	2:D:3774:VAL:HB	1.90	0.53
2:D:4866:LEU:HD12	2:F:4871:PHE:CE2	2.44	0.53
2:F:196:TYR:O	2:F:201:LEU:N	2.42	0.53
2:F:1086:ARG:HH22	2:F:1254:ARG:HD3	1.73	0.53
2:F:1640:ASP:OD1	2:F:1640:ASP:N	2.41	0.53
2:F:1908:CYS:HB2	2:F:2088:LEU:HD11	1.91	0.53
2:F:2157:TYR:HH	2:F:2203:TYR:HH	1.55	0.53
2:H:196:TYR:O	2:H:201:LEU:N	2.42	0.53
2:B:678:MET:HG3	2:B:754:VAL:HG22	1.91	0.53
2:B:1092:LYS:H	2:B:1250:TRP:HZ3	1.56	0.53
2:B:2728:HIS:NE2	2:B:2829:MET:SD	2.79	0.53
2:B:2760:PRO:HD2	2:B:2763:LEU:HD12	1.91	0.53
2:B:3919:ASN:O	2:B:3922:THR:OG1	2.27	0.53
2:D:1092:LYS:H	2:D:1250:TRP:HZ3	1.56	0.53
2:F:246:THR:OG1	2:F:272:ARG:NH1	2.42	0.53
2:H:556:ASP:HA	2:H:559:ILE:HD12	1.90	0.53
2:H:678:MET:HG3	2:H:754:VAL:HG22	1.91	0.53
2:H:1640:ASP:N	2:H:1640:ASP:OD1	2.41	0.53
2:B:480:ARG:NH2	2:B:3679:GLU:OE2	2.41	0.53
2:B:601:LEU:HB3	2:B:642:LEU:HD21	1.91	0.53
2:B:1029:ASN:HB3	2:B:1032:LEU:HG	1.91	0.53
2:B:4782:TYR:OH	2:B:4847:PHE:O	2.27	0.53
2:B:4814:TYR:HE2	2:B:4815:MET:CE	2.21	0.53
2:D:15:ARG:N	2:D:18:ASP:OD2	2.40	0.53
2:D:196:TYR:O	2:D:201:LEU:N	2.42	0.53
2:D:4640:SER:HB3	2:D:4643:ASN:HD21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:PHE:CE1	2:H:2326:ILE:HG21	2.40	0.53
2:F:480:ARG:NH2	2:F:3679:GLU:OE2	2.41	0.53
2:F:601:LEU:HB3	2:F:642:LEU:HD21	1.91	0.53
2:F:3805:ASP:OD2	2:F:3808:ALA:N	2.40	0.53
2:H:1173:MET:HB3	2:H:1192:PHE:HB2	1.91	0.53
2:H:2840:ALA:HB3	2:H:2906:ARG:HD3	1.91	0.53
2:B:76:ARG:CB	2:D:3891:TRP:CG	2.91	0.53
2:B:3805:ASP:OD2	2:B:3808:ALA:N	2.40	0.53
2:B:3904:GLN:NE2	2:B:3965:GLN:OE1	2.41	0.53
2:B:3983:LEU:O	2:B:3987:LEU:HB2	2.10	0.53
2:D:601:LEU:HB3	2:D:642:LEU:HD21	1.91	0.53
2:F:1308:ILE:HD12	2:F:1539:LEU:HB2	1.90	0.53
2:F:1761:MET:SD	2:F:1761:MET:N	2.73	0.53
2:F:3904:GLN:NE2	2:F:3965:GLN:OE1	2.41	0.53
2:F:4640:SER:HB3	2:F:4643:ASN:HD21	1.74	0.53
2:H:687:THR:HG22	2:H:689:GLU:H	1.72	0.53
2:H:4037:ASP:OD2	2:H:4042:GLY:N	2.41	0.53
2:B:1938:GLN:OE1	2:B:1942:ARG:NH1	2.42	0.52
2:B:2840:ALA:HB3	2:B:2906:ARG:HD3	1.91	0.52
2:B:4640:SER:HB3	2:B:4643:ASN:HD21	1.74	0.52
2:D:1086:ARG:HH22	2:D:1254:ARG:HD3	1.73	0.52
2:D:2204:PHE:O	2:D:2211:ASN:ND2	2.42	0.52
2:F:207:PHE:CD1	2:H:2326:ILE:HG22	2.43	0.52
2:F:235:ARG:NH2	2:F:268:SER:O	2.41	0.52
2:F:1029:ASN:HB3	2:F:1032:LEU:HG	1.91	0.52
2:F:2204:PHE:O	2:F:2211:ASN:ND2	2.42	0.52
2:F:2760:PRO:HD2	2:F:2763:LEU:HD12	1.91	0.52
2:F:3960:SER:HG	2:F:4070:CYS:HG	1.56	0.52
2:H:4640:SER:HB3	2:H:4643:ASN:HD21	1.74	0.52
2:H:4655:MET:O	2:H:4664:ARG:NH2	2.39	0.52
2:H:4814:TYR:HE2	2:H:4815:MET:CE	2.21	0.52
2:B:679:VAL:HA	2:B:800:VAL:HG12	1.92	0.52
2:B:681:HIS:HB2	2:B:799:LYS:HG2	1.90	0.52
2:B:1224:LEU:HD13	2:B:1227:PHE:HD2	1.74	0.52
2:B:1912:GLN:OE1	2:B:2091:ARG:NH1	2.42	0.52
2:B:3767:LEU:HD21	2:B:3774:VAL:HB	1.90	0.52
2:D:375:GLN:N	2:D:390:LYS:O	2.41	0.52
2:F:25:THR:HG22	2:F:34:LYS:HG2	1.90	0.52
2:F:565:LEU:HD11	2:F:603:LYS:HG2	1.91	0.52
2:F:4028:THR:HA	2:F:4033:PHE:HD2	1.75	0.52
2:F:4148:ARG:HH11	2:F:4959:PHE:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4655:MET:O	2:F:4664:ARG:NH2	2.39	0.52
2:H:601:LEU:HB3	2:H:642:LEU:HD21	1.91	0.52
2:H:1938:GLN:OE1	2:H:1942:ARG:NH1	2.42	0.52
2:H:3983:LEU:O	2:H:3987:LEU:HB2	2.10	0.52
2:H:4597:PRO:HA	2:H:4600:ILE:HG22	1.91	0.52
2:B:1308:ILE:HD12	2:B:1539:LEU:HB2	1.90	0.52
2:B:1996:GLN:HA	2:B:1997:LEU:HD23	1.92	0.52
2:D:678:MET:HG3	2:D:754:VAL:HG22	1.91	0.52
2:D:1640:ASP:OD1	2:D:1640:ASP:N	2.41	0.52
1:E:7:ILE:H	1:E:72:ALA:HA	1.73	0.52
2:F:1132:GLU:HB3	2:F:1147:GLN:HE21	1.74	0.52
2:F:1245:ARG:NH2	2:F:1797:GLU:OE2	2.42	0.52
2:H:371:TRP:N	2:H:394:HIS:O	2.38	0.52
2:H:1132:GLU:HB3	2:H:1147:GLN:HE21	1.74	0.52
2:H:1908:CYS:HB2	2:H:2088:LEU:HD11	1.91	0.52
2:H:4028:THR:HA	2:H:4033:PHE:HD2	1.75	0.52
2:B:646:THR:HA	2:B:1630:LEU:HA	1.90	0.52
2:B:1119:ARG:NH2	2:B:1196:ASP:O	2.39	0.52
2:B:2204:PHE:O	2:B:2211:ASN:ND2	2.42	0.52
2:D:4655:MET:O	2:D:4664:ARG:NH2	2.39	0.52
2:F:246:THR:N	2:F:261:HIS:O	2.42	0.52
2:F:1092:LYS:H	2:F:1250:TRP:HZ3	1.56	0.52
2:B:1640:ASP:N	2:B:1640:ASP:OD1	2.41	0.52
2:B:2326:ILE:HG22	2:H:207:PHE:CD1	2.44	0.52
2:B:4037:ASP:OD2	2:B:4042:GLY:N	2.41	0.52
2:D:1301:PHE:HE2	2:D:1453:TYR:HA	1.75	0.52
2:F:805:GLY:O	2:F:810:GLU:N	2.43	0.52
2:F:1173:MET:HB3	2:F:1192:PHE:HB2	1.91	0.52
2:F:1301:PHE:HE2	2:F:1453:TYR:HA	1.75	0.52
2:F:2857:LYS:HE3	2:F:2861:LEU:HD11	1.92	0.52
2:F:3983:LEU:O	2:F:3987:LEU:HB2	2.10	0.52
2:F:4136:ARG:NH2	2:F:4150:TYR:OH	2.38	0.52
2:F:4722:TYR:HD2	2:F:4723:LEU:HD12	1.75	0.52
2:F:4848:ASP:HB3	2:H:4819:TYR:CE1	2.39	0.52
2:H:679:VAL:HA	2:H:800:VAL:HG12	1.92	0.52
2:B:15:ARG:N	2:B:18:ASP:OD2	2.40	0.52
2:B:233:VAL:HG13	2:B:300:VAL:HG21	1.92	0.52
2:B:1922:ARG:NH1	2:B:2038:THR:O	2.39	0.52
2:B:3683:LEU:HD22	2:B:3748:SER:HB3	1.92	0.52
2:D:1173:MET:HB3	2:D:1192:PHE:HB2	1.91	0.52
2:D:4148:ARG:HH11	2:D:4959:PHE:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:375:GLN:N	2:F:390:LYS:O	2.41	0.52
2:F:1094:TYR:OH	2:F:1808:ASP:OD1	2.27	0.52
2:F:4597:PRO:HA	2:F:4600:ILE:HG22	1.91	0.52
2:H:15:ARG:N	2:H:18:ASP:OD2	2.40	0.52
2:H:25:THR:HG22	2:H:34:LYS:HG2	1.90	0.52
2:H:246:THR:N	2:H:261:HIS:O	2.42	0.52
2:H:1092:LYS:H	2:H:1250:TRP:HZ3	1.56	0.52
2:H:1301:PHE:HE2	2:H:1453:TYR:HA	1.75	0.52
2:H:2760:PRO:HD2	2:H:2763:LEU:HD12	1.91	0.52
2:D:805:GLY:O	2:D:810:GLU:N	2.43	0.52
2:D:1251:LEU:O	2:D:1601:ASN:N	2.43	0.52
2:D:1996:GLN:HA	2:D:1997:LEU:HD23	1.92	0.52
2:D:4782:TYR:OH	2:D:4847:PHE:O	2.27	0.52
2:F:748:LEU:HB2	2:F:750:ARG:HG3	1.92	0.52
2:F:1922:ARG:NH1	2:F:2038:THR:O	2.39	0.52
2:F:3683:LEU:HD22	2:F:3748:SER:HB3	1.92	0.52
2:F:3803:VAL:HG21	2:F:3881:ARG:HD2	1.92	0.52
2:H:246:THR:OG1	2:H:272:ARG:NH1	2.42	0.52
2:H:565:LEU:HD11	2:H:603:LYS:HG2	1.91	0.52
1:A:16:PRO:HD2	1:A:64:ALA:HA	1.92	0.52
2:B:207:PHE:CD1	2:D:2326:ILE:HG22	2.45	0.52
2:B:1301:PHE:HE2	2:B:1453:TYR:HA	1.75	0.52
2:B:3803:VAL:HG21	2:B:3881:ARG:HD2	1.92	0.52
2:B:4028:THR:HA	2:B:4033:PHE:HD2	1.75	0.52
2:B:4082:GLU:HA	2:B:4086:LYS:HD2	1.92	0.52
2:B:4617:TYR:OH	2:B:4629:GLY:O	2.28	0.52
2:D:1908:CYS:HB2	2:D:2088:LEU:HD11	1.91	0.52
2:D:2116:ASP:OD1	2:D:2153:ASN:ND2	2.43	0.52
2:D:3983:LEU:O	2:D:3987:LEU:HB2	2.10	0.52
2:D:4722:TYR:HD2	2:D:4723:LEU:HD12	1.75	0.52
2:F:2116:ASP:OD1	2:F:2153:ASN:ND2	2.43	0.52
2:F:4617:TYR:OH	2:F:4629:GLY:O	2.28	0.52
2:H:1224:LEU:HD13	2:H:1227:PHE:HD2	1.74	0.52
2:H:3683:LEU:HD22	2:H:3748:SER:HB3	1.92	0.52
2:B:1094:TYR:OH	2:B:1808:ASP:OD1	2.27	0.52
2:B:4597:PRO:HA	2:B:4600:ILE:HG22	1.91	0.52
2:D:486:GLN:NE2	2:D:539:ALA:O	2.43	0.52
2:D:1132:GLU:HB3	2:D:1147:GLN:HE21	1.74	0.52
2:D:3683:LEU:HD22	2:D:3748:SER:HB3	1.92	0.52
2:D:4597:PRO:HA	2:D:4600:ILE:HG22	1.91	0.52
1:E:16:PRO:HD2	1:E:64:ALA:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:679:VAL:HA	2:F:800:VAL:HG12	1.92	0.52
2:F:4866:LEU:HD12	2:H:4871:PHE:CE2	2.45	0.52
2:H:375:GLN:N	2:H:390:LYS:O	2.41	0.52
2:H:1602:GLN:HE22	2:H:1642:LEU:HB3	1.73	0.52
2:B:565:LEU:HD11	2:B:603:LYS:HG2	1.91	0.52
2:B:909:ASP:HB2	2:B:914:GLN:HB2	1.91	0.52
2:B:1098:ALA:O	2:B:1101:TRP:NE1	2.42	0.52
2:B:4568:TYR:O	2:B:4572:THR:OG1	2.22	0.52
1:C:16:PRO:HD2	1:C:64:ALA:HA	1.92	0.52
2:D:748:LEU:HB2	2:D:750:ARG:HG3	1.92	0.52
2:D:4518:LEU:N	2:D:4518:LEU:CD2	2.73	0.52
2:F:909:ASP:HB2	2:F:914:GLN:HB2	1.91	0.52
2:F:1912:GLN:OE1	2:F:2091:ARG:NH1	2.42	0.52
2:H:486:GLN:NE2	2:H:539:ALA:O	2.43	0.52
2:H:725:TYR:HA	2:H:732:LEU:HA	1.92	0.52
2:H:4617:TYR:OH	2:H:4629:GLY:O	2.28	0.52
2:B:1132:GLU:HB3	2:B:1147:GLN:HE21	1.74	0.51
2:B:2160:PRO:HB3	2:B:2207:ILE:HD12	1.91	0.51
2:B:2857:LYS:HE3	2:B:2861:LEU:HD11	1.92	0.51
2:B:4572:THR:O	2:B:4576:LEU:HB2	2.10	0.51
2:D:3803:VAL:HG21	2:D:3881:ARG:HD2	1.92	0.51
2:F:657:PRO:HA	2:F:834:VAL:HA	1.92	0.51
2:F:678:MET:HG3	2:F:754:VAL:HG22	1.91	0.51
2:F:3848:CYS:HB3	2:F:3856:GLN:HE21	1.76	0.51
2:H:162:ILE:HG23	2:H:181:LEU:HD13	1.92	0.51
2:H:657:PRO:HA	2:H:834:VAL:HA	1.92	0.51
2:H:805:GLY:O	2:H:810:GLU:N	2.43	0.51
2:H:1098:ALA:O	2:H:1101:TRP:NE1	2.42	0.51
2:B:748:LEU:HB2	2:B:750:ARG:HG3	1.92	0.51
2:B:2221:TYR:O	2:B:2225:ASN:ND2	2.44	0.51
2:B:4148:ARG:HH11	2:B:4959:PHE:HB3	1.75	0.51
2:B:4655:MET:O	2:B:4664:ARG:NH2	2.39	0.51
2:D:1308:ILE:HD12	2:D:1539:LEU:HB2	1.90	0.51
2:D:4572:THR:O	2:D:4576:LEU:HB2	2.10	0.51
2:D:4617:TYR:OH	2:D:4629:GLY:O	2.28	0.51
1:G:16:PRO:HD2	1:G:64:ALA:HA	1.92	0.51
2:H:233:VAL:HG13	2:H:300:VAL:HG21	1.92	0.51
2:H:1029:ASN:HB3	2:H:1032:LEU:HG	1.91	0.51
2:H:2160:PRO:HB3	2:H:2207:ILE:HD12	1.91	0.51
2:D:909:ASP:HB2	2:D:914:GLN:HB2	1.91	0.51
2:D:1094:TYR:OH	2:D:1808:ASP:OD1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2096:ILE:O	2:D:2100:VAL:N	2.43	0.51
2:D:2221:TYR:O	2:D:2225:ASN:ND2	2.44	0.51
2:D:3848:CYS:HB3	2:D:3856:GLN:HE21	1.76	0.51
2:F:162:ILE:HG23	2:F:181:LEU:HD13	1.93	0.51
2:F:725:TYR:HA	2:F:732:LEU:HA	1.92	0.51
2:F:2157:TYR:OH	2:F:2203:TYR:OH	2.26	0.51
2:H:483:LYS:O	2:H:544:ASN:ND2	2.38	0.51
2:H:3803:VAL:HG21	2:H:3881:ARG:HD2	1.92	0.51
2:B:506:HIS:NE2	2:B:534:TYR:OH	2.40	0.51
2:B:1251:LEU:O	2:B:1601:ASN:N	2.43	0.51
2:B:1908:CYS:HB2	2:B:2088:LEU:HD11	1.91	0.51
2:B:3848:CYS:HB3	2:B:3856:GLN:HE21	1.76	0.51
2:B:3917:VAL:O	2:B:3920:THR:OG1	2.24	0.51
2:B:4518:LEU:CD2	2:B:4518:LEU:N	2.73	0.51
2:B:4866:LEU:HD12	2:D:4871:PHE:CE2	2.44	0.51
2:D:1098:ALA:O	2:D:1101:TRP:NE1	2.42	0.51
2:D:4891:ILE:HD13	2:D:4914:HIS:HB3	1.92	0.51
2:H:2221:TYR:O	2:H:2225:ASN:ND2	2.44	0.51
2:H:2857:LYS:HE3	2:H:2861:LEU:HD11	1.92	0.51
2:B:1570:LEU:O	2:B:1573:SER:OG	2.27	0.51
2:B:1799:VAL:HG22	2:B:1894:LEU:HD13	1.93	0.51
1:C:42:ARG:NH2	2:D:1766:PRO:O	2.44	0.51
2:D:679:VAL:HA	2:D:800:VAL:HG12	1.92	0.51
2:D:1799:VAL:HG22	2:D:1894:LEU:HD13	1.93	0.51
1:E:28:GLY:N	1:E:37:ASP:O	2.37	0.51
2:F:1666:ALA:N	2:F:1669:ASN:OD1	2.41	0.51
2:F:4798:GLU:O	2:F:4802:THR:OG1	2.27	0.51
2:H:1996:GLN:HA	2:H:1997:LEU:HD23	1.92	0.51
2:H:3848:CYS:HB3	2:H:3856:GLN:HE21	1.76	0.51
2:H:4148:ARG:HH11	2:H:4959:PHE:HB3	1.75	0.51
2:B:486:GLN:NE2	2:B:539:ALA:O	2.43	0.51
2:B:776:GLN:HB3	2:B:1470:GLY:HA3	1.93	0.51
2:D:40:GLU:HB2	2:D:48:PHE:HE1	1.76	0.51
2:D:233:VAL:HG13	2:D:300:VAL:HG21	1.92	0.51
2:D:646:THR:OG1	2:D:1684:GLN:NE2	2.44	0.51
2:D:4118:THR:O	2:D:4122:LEU:HB2	2.11	0.51
2:F:1119:ARG:NH2	2:F:1196:ASP:O	2.39	0.51
2:F:1799:VAL:HG22	2:F:1894:LEU:HD13	1.93	0.51
2:F:4082:GLU:HA	2:F:4086:LYS:HD2	1.92	0.51
2:F:4118:THR:O	2:F:4122:LEU:HB2	2.11	0.51
2:F:4891:ILE:HD13	2:F:4914:HIS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:GLU:HB2	2:H:48:PHE:HE1	1.76	0.51
2:H:2116:ASP:OD1	2:H:2153:ASN:ND2	2.43	0.51
2:B:805:GLY:O	2:B:810:GLU:N	2.43	0.51
2:D:4082:GLU:HA	2:D:4086:LYS:HD2	1.92	0.51
2:F:486:GLN:NE2	2:F:539:ALA:O	2.43	0.51
2:F:1300:MET:HB2	2:F:1545:ALA:HB3	1.93	0.51
2:F:4572:THR:O	2:F:4576:LEU:HB2	2.10	0.51
2:H:1300:MET:HB2	2:H:1545:ALA:HB3	1.93	0.51
2:H:2083:ARG:NH2	2:H:3686:ASP:OD1	2.43	0.51
2:H:4572:THR:O	2:H:4576:LEU:HB2	2.10	0.51
2:H:4794:TYR:HB2	2:H:4806:LYS:HD2	1.93	0.51
2:B:300:VAL:HG12	2:B:420:ARG:HH22	1.76	0.51
2:B:1173:MET:HB3	2:B:1192:PHE:HB2	1.91	0.51
2:B:2222:LEU:O	2:B:2226:SER:N	2.35	0.51
2:B:4085:VAL:O	2:B:4089:HIS:N	2.44	0.51
2:B:4871:PHE:CE2	2:H:4866:LEU:HD12	2.46	0.51
2:B:4891:ILE:HD13	2:B:4914:HIS:HB3	1.92	0.51
2:D:510:SER:O	2:D:520:ARG:NH2	2.44	0.51
2:D:2160:PRO:HB3	2:D:2207:ILE:HD12	1.91	0.51
2:F:290:ARG:HG2	2:F:353:GLU:HB2	1.93	0.51
2:F:510:SER:O	2:F:520:ARG:NH2	2.44	0.51
2:F:4124:GLU:HG3	2:F:4128:ASN:HD21	1.76	0.51
2:H:165:ALA:HB2	2:H:182:ILE:HG12	1.93	0.51
2:H:2558:LYS:O	2:H:2562:LEU:N	2.44	0.51
2:H:4085:VAL:O	2:H:4089:HIS:N	2.44	0.51
2:H:4722:TYR:HD2	2:H:4723:LEU:HD12	1.75	0.51
2:B:246:THR:N	2:B:261:HIS:O	2.42	0.51
2:B:646:THR:OG1	2:B:1684:GLN:NE2	2.44	0.51
2:D:2083:ARG:NH2	2:D:3686:ASP:OD1	2.43	0.51
2:D:4028:THR:HA	2:D:4033:PHE:HD2	1.75	0.51
2:F:1098:ALA:O	2:F:1101:TRP:NE1	2.42	0.51
2:F:1996:GLN:HA	2:F:1997:LEU:HD23	1.92	0.51
1:G:42:ARG:NH2	2:H:1766:PRO:O	2.44	0.51
2:H:646:THR:OG1	2:H:1684:GLN:NE2	2.44	0.51
2:H:776:GLN:HB3	2:H:1470:GLY:HA3	1.93	0.51
2:H:909:ASP:HB2	2:H:914:GLN:HB2	1.91	0.51
2:H:3919:ASN:O	2:H:3922:THR:OG1	2.27	0.51
2:H:4518:LEU:CD2	2:H:4518:LEU:N	2.73	0.51
2:D:1252:SER:HB2	2:D:1598:ARG:HB2	1.93	0.51
1:E:42:ARG:NH2	2:F:1766:PRO:O	2.44	0.51
2:F:40:GLU:HB2	2:F:48:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2096:ILE:O	2:F:2100:VAL:N	2.43	0.51
2:F:2193:MET:HA	2:F:2196:ASN:HD22	1.76	0.51
2:H:694:ARG:O	2:H:793:SER:N	2.42	0.51
2:H:2204:PHE:O	2:H:2211:ASN:ND2	2.42	0.51
2:H:3806:LEU:O	2:H:3810:GLU:N	2.43	0.51
2:B:40:GLU:HB2	2:B:48:PHE:HE1	1.76	0.50
2:B:694:ARG:O	2:B:793:SER:N	2.42	0.50
2:B:2773:ARG:HA	2:B:2776:ILE:HD12	1.93	0.50
2:B:4124:GLU:HG3	2:B:4128:ASN:HD21	1.76	0.50
2:B:4722:TYR:HD2	2:B:4723:LEU:HD12	1.75	0.50
2:D:1119:ARG:NH2	2:D:1196:ASP:O	2.39	0.50
2:D:1171:HIS:O	2:D:1194:ASP:N	2.44	0.50
2:D:4848:ASP:HB3	2:F:4819:TYR:CE1	2.41	0.50
2:F:233:VAL:HG13	2:F:300:VAL:HG21	1.92	0.50
2:F:2221:TYR:O	2:F:2225:ASN:ND2	2.44	0.50
2:F:4018:PHE:O	2:F:4022:LEU:HB2	2.11	0.50
2:F:4794:TYR:HB2	2:F:4806:LYS:HD2	1.93	0.50
2:H:4568:TYR:O	2:H:4572:THR:OG1	2.22	0.50
2:H:4651:LYS:NZ	2:H:4670:LEU:O	2.45	0.50
1:A:42:ARG:NH2	2:B:1766:PRO:O	2.44	0.50
2:B:207:PHE:CE1	2:D:2326:ILE:HG21	2.42	0.50
2:B:2083:ARG:NH2	2:B:3686:ASP:OD1	2.43	0.50
2:B:4591:TYR:OH	2:B:4717:ASP:OD2	2.29	0.50
2:B:4798:GLU:O	2:B:4802:THR:OG1	2.27	0.50
2:D:2193:MET:HA	2:D:2196:ASN:HD22	1.76	0.50
2:D:4590:GLY:O	2:D:4594:LEU:N	2.44	0.50
2:D:4794:TYR:HB2	2:D:4806:LYS:HD2	1.93	0.50
2:F:1171:HIS:O	2:F:1194:ASP:N	2.44	0.50
2:F:2160:PRO:HB3	2:F:2207:ILE:HD12	1.91	0.50
2:F:3810:GLU:O	2:F:3814:LYS:HB2	2.12	0.50
2:F:4518:LEU:N	2:F:4518:LEU:CD2	2.74	0.50
2:H:748:LEU:HB2	2:H:750:ARG:HG3	1.92	0.50
2:H:1094:TYR:OH	2:H:1808:ASP:OD1	2.27	0.50
2:H:1666:ALA:N	2:H:1669:ASN:OD1	2.41	0.50
2:B:2116:ASP:OD1	2:B:2153:ASN:ND2	2.43	0.50
2:D:2773:ARG:HA	2:D:2776:ILE:HD12	1.93	0.50
2:F:165:ALA:HB2	2:F:182:ILE:HG12	1.93	0.50
2:F:2083:ARG:NH2	2:F:3686:ASP:OD1	2.44	0.50
2:F:4085:VAL:O	2:F:4089:HIS:N	2.44	0.50
2:F:4651:LYS:NZ	2:F:4670:LEU:O	2.45	0.50
2:H:300:VAL:HG12	2:H:420:ARG:HH22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:PRO:HA	2:B:834:VAL:HA	1.92	0.50
2:B:1799:VAL:O	2:B:1803:SER:CB	2.60	0.50
2:D:162:ILE:HG23	2:D:181:LEU:HD13	1.93	0.50
2:D:657:PRO:HA	2:D:834:VAL:HA	1.92	0.50
2:D:4085:VAL:O	2:D:4089:HIS:N	2.44	0.50
2:D:4520:PHE:HD1	2:D:4562:LEU:HD21	0.84	0.50
1:E:89:GLY:HA3	2:F:1671:ARG:HH12	1.76	0.50
2:F:646:THR:OG1	2:F:1684:GLN:NE2	2.44	0.50
2:H:290:ARG:HG2	2:H:353:GLU:HB2	1.93	0.50
2:H:904:TYR:HB2	2:H:918:LEU:HB2	1.93	0.50
2:H:2193:MET:HA	2:H:2196:ASN:HD22	1.76	0.50
2:H:4082:GLU:HA	2:H:4086:LYS:HD2	1.92	0.50
2:H:4891:ILE:HD13	2:H:4914:HIS:HB3	1.92	0.50
2:B:165:ALA:HB2	2:B:182:ILE:HG12	1.93	0.50
2:B:1611:ILE:HB	2:B:1620:GLN:HB3	1.94	0.50
2:B:2193:MET:HA	2:B:2196:ASN:HD22	1.76	0.50
2:B:4118:THR:O	2:B:4122:LEU:HB2	2.11	0.50
2:D:776:GLN:HB3	2:D:1470:GLY:HA3	1.93	0.50
2:F:300:VAL:HG12	2:F:420:ARG:HH22	1.76	0.50
2:F:802:PHE:N	2:F:1616:GLY:O	2.45	0.50
2:H:802:PHE:N	2:H:1616:GLY:O	2.45	0.50
1:A:89:GLY:HA3	2:B:1671:ARG:HH12	1.76	0.50
2:B:620:CYS:N	2:B:623:VAL:O	2.39	0.50
2:D:207:PHE:CD2	2:F:2326:ILE:O	2.65	0.50
2:D:290:ARG:HG2	2:D:353:GLU:HB2	1.93	0.50
2:H:4118:THR:O	2:H:4122:LEU:HB2	2.11	0.50
2:B:1666:ALA:N	2:B:1669:ASN:OD1	2.41	0.50
2:B:4794:TYR:HB2	2:B:4806:LYS:HD2	1.93	0.50
2:D:300:VAL:HG12	2:D:420:ARG:HH22	1.76	0.50
2:F:1184:ASP:OD2	2:F:1188:SER:OG	2.30	0.50
2:F:1252:SER:HB2	2:F:1598:ARG:HB2	1.93	0.50
2:F:2773:ARG:HA	2:F:2776:ILE:HD12	1.93	0.50
2:F:4568:TYR:O	2:F:4572:THR:OG1	2.22	0.50
2:H:559:ILE:HD13	2:H:593:HIS:HB3	1.94	0.50
2:H:1611:ILE:HB	2:H:1620:GLN:HB3	1.94	0.50
2:B:289:ILE:HA	2:B:293:GLN:HE22	1.77	0.50
2:B:652:VAL:HA	2:B:795:SER:HB2	1.94	0.50
2:B:694:ARG:HB2	2:B:793:SER:HB2	1.94	0.50
2:B:725:TYR:HA	2:B:732:LEU:HA	1.92	0.50
2:B:3810:GLU:O	2:B:3814:LYS:HB2	2.12	0.50
2:D:289:ILE:HA	2:D:293:GLN:HE22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2857:LYS:HE3	2:D:2861:LEU:HD11	1.92	0.50
2:D:4651:LYS:NZ	2:D:4670:LEU:O	2.45	0.50
1:E:75:THR:HG23	1:E:98:ILE:HG12	1.94	0.50
2:H:1682:GLU:HA	2:H:1685:LEU:HD13	1.93	0.50
2:H:3810:GLU:O	2:H:3814:LYS:HB2	2.12	0.50
2:B:510:SER:O	2:B:520:ARG:NH2	2.44	0.50
2:B:559:ILE:HD13	2:B:593:HIS:HB3	1.94	0.50
2:B:2071:ALA:HA	2:B:2076:ILE:HD11	1.94	0.50
2:B:4651:LYS:NZ	2:B:4670:LEU:O	2.45	0.50
2:B:4814:TYR:CE2	2:B:4815:MET:CE	2.95	0.50
1:C:75:THR:HG23	1:C:98:ILE:HG12	1.94	0.50
2:D:904:TYR:HB2	2:D:918:LEU:HB2	1.93	0.50
2:D:3810:GLU:O	2:D:3814:LYS:HB2	2.12	0.50
2:D:4931:GLU:OE2	2:D:4942:TRP:NE1	2.45	0.50
2:H:510:SER:O	2:H:520:ARG:NH2	2.44	0.50
2:H:1799:VAL:O	2:H:1803:SER:CB	2.60	0.50
2:H:4018:PHE:O	2:H:4022:LEU:HB2	2.11	0.50
2:B:802:PHE:N	2:B:1616:GLY:O	2.45	0.49
2:B:1682:GLU:HA	2:B:1685:LEU:HD13	1.94	0.49
2:B:4515:ASN:HA	2:H:4780:TYR:OH	2.12	0.49
2:B:4931:GLU:OE2	2:B:4942:TRP:NE1	2.45	0.49
2:D:694:ARG:O	2:D:793:SER:N	2.42	0.49
2:D:725:TYR:HA	2:D:732:LEU:HA	1.92	0.49
2:D:1611:ILE:HB	2:D:1620:GLN:HB3	1.94	0.49
2:D:4018:PHE:O	2:D:4022:LEU:HB2	2.11	0.49
2:F:776:GLN:HB3	2:F:1470:GLY:HA3	1.93	0.49
2:F:4931:GLU:OE2	2:F:4942:TRP:NE1	2.45	0.49
2:H:652:VAL:HA	2:H:795:SER:HB2	1.94	0.49
2:H:1171:HIS:O	2:H:1194:ASP:N	2.44	0.49
2:H:1799:VAL:HG22	2:H:1894:LEU:HD13	1.93	0.49
2:H:4931:GLU:OE2	2:H:4942:TRP:NE1	2.45	0.49
2:B:162:ILE:HG23	2:B:181:LEU:HD13	1.92	0.49
2:B:1252:SER:HB2	2:B:1598:ARG:HB2	1.93	0.49
2:D:375:GLN:HE21	2:D:392:ILE:HD13	1.77	0.49
2:D:3810:GLU:O	2:D:3814:LYS:CB	2.60	0.49
1:E:54:GLU:OE1	2:F:1772:ASN:ND2	2.45	0.49
2:F:904:TYR:HB2	2:F:918:LEU:HB2	1.93	0.49
2:F:1251:LEU:O	2:F:1601:ASN:N	2.43	0.49
2:F:4814:TYR:HE2	2:F:4815:MET:CE	2.21	0.49
2:H:3763:GLY:HA2	2:H:3766:ILE:HD12	1.94	0.49
2:H:4590:GLY:O	2:H:4594:LEU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4814:TYR:CE2	2:H:4815:MET:CE	2.95	0.49
2:B:3856:GLN:NE2	2:B:3923:GLU:O	2.45	0.49
2:D:1682:GLU:HA	2:D:1685:LEU:HD13	1.93	0.49
2:D:2026:ILE:HG23	2:D:2030:LEU:HD12	1.94	0.49
2:D:2301:ASP:OD1	2:D:2304:ARG:NH2	2.46	0.49
2:D:3806:LEU:O	2:D:3810:GLU:N	2.43	0.49
2:D:4124:GLU:HG3	2:D:4128:ASN:HD21	1.76	0.49
2:F:2558:LYS:O	2:F:2562:LEU:N	2.44	0.49
2:F:3810:GLU:O	2:F:3814:LYS:CB	2.60	0.49
2:H:707:PRO:HD3	2:H:840:TYR:HE1	1.78	0.49
2:H:1443:VAL:O	2:H:1489:CYS:N	2.43	0.49
2:H:2773:ARG:HA	2:H:2776:ILE:HD12	1.93	0.49
2:H:4124:GLU:HG3	2:H:4128:ASN:HD21	1.76	0.49
2:B:1041:ARG:HA	2:B:1044:LYS:HG3	1.94	0.49
2:B:3763:GLY:HA2	2:B:3766:ILE:HD12	1.94	0.49
2:B:3810:GLU:O	2:B:3814:LYS:CB	2.60	0.49
2:B:4523:VAL:HG22	2:B:4559:HIS:HE1	1.78	0.49
1:C:89:GLY:HA3	2:D:1671:ARG:HH12	1.76	0.49
2:D:165:ALA:HB2	2:D:182:ILE:HG12	1.93	0.49
2:D:1300:MET:HB2	2:D:1545:ALA:HB3	1.93	0.49
2:D:4523:VAL:HG22	2:D:4559:HIS:HE1	1.78	0.49
2:F:375:GLN:HE21	2:F:392:ILE:HD13	1.77	0.49
2:F:559:ILE:HD13	2:F:593:HIS:HB3	1.94	0.49
2:F:1041:ARG:HA	2:F:1044:LYS:HG3	1.94	0.49
2:F:3806:LEU:O	2:F:3810:GLU:N	2.43	0.49
1:G:75:THR:HG23	1:G:98:ILE:HG12	1.94	0.49
1:G:89:GLY:HA3	2:H:1671:ARG:HH12	1.76	0.49
2:H:4176:ASP:HA	2:H:4180:GLU:HB3	1.95	0.49
1:A:54:GLU:OE1	2:B:1772:ASN:ND2	2.45	0.49
1:A:75:THR:HG23	1:A:98:ILE:HG12	1.94	0.49
2:B:904:TYR:HB2	2:B:918:LEU:HB2	1.93	0.49
2:B:2026:ILE:HG23	2:B:2030:LEU:HD12	1.94	0.49
2:B:2301:ASP:OD1	2:B:2304:ARG:NH2	2.46	0.49
1:C:54:GLU:OE1	2:D:1772:ASN:ND2	2.46	0.49
2:D:1666:ALA:N	2:D:1669:ASN:OD1	2.41	0.49
2:D:4796:LYS:HD2	2:D:4805:MET:HB3	1.95	0.49
2:H:1252:SER:HB2	2:H:1598:ARG:HB2	1.93	0.49
2:B:290:ARG:HG2	2:B:353:GLU:HB2	1.93	0.49
2:B:542:ARG:NE	2:B:577:CYS:SG	2.85	0.49
2:B:4176:ASP:HA	2:B:4180:GLU:HB3	1.95	0.49
2:D:4176:ASP:HA	2:D:4180:GLU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1682:GLU:HA	2:F:1685:LEU:HD13	1.94	0.49
2:F:1799:VAL:O	2:F:1803:SER:CB	2.60	0.49
2:F:3763:GLY:HA2	2:F:3766:ILE:HD12	1.94	0.49
2:F:4523:VAL:HG22	2:F:4559:HIS:HE1	1.78	0.49
2:F:4713:VAL:O	2:F:4716:THR:OG1	2.27	0.49
2:H:289:ILE:HA	2:H:293:GLN:HE22	1.77	0.49
2:B:207:PHE:CD2	2:D:2326:ILE:O	2.66	0.49
2:B:4018:PHE:O	2:B:4022:LEU:HB2	2.12	0.49
2:D:207:PHE:CE1	2:F:2326:ILE:HG21	2.39	0.49
2:D:4520:PHE:CB	2:D:4562:LEU:HD21	2.43	0.49
2:F:1611:ILE:HB	2:F:1620:GLN:HB3	1.94	0.49
2:F:4759:SER:HA	2:F:4762:THR:HG22	1.95	0.49
2:H:620:CYS:N	2:H:623:VAL:O	2.39	0.49
2:H:2096:ILE:O	2:H:2100:VAL:N	2.43	0.49
2:H:2301:ASP:OD1	2:H:2304:ARG:NH2	2.46	0.49
2:H:3921:LEU:HD23	2:H:3924:TYR:HD2	1.78	0.49
2:H:4798:GLU:O	2:H:4802:THR:OG1	2.27	0.49
2:B:2096:ILE:O	2:B:2100:VAL:N	2.43	0.49
2:B:2326:ILE:O	2:H:207:PHE:CD2	2.66	0.49
2:B:3806:LEU:O	2:B:3810:GLU:N	2.43	0.49
1:C:28:GLY:N	1:C:37:ASP:O	2.37	0.49
2:D:506:HIS:NE2	2:D:534:TYR:OH	2.40	0.49
2:D:559:ILE:HD13	2:D:593:HIS:HB3	1.94	0.49
2:D:802:PHE:N	2:D:1616:GLY:O	2.45	0.49
2:D:1799:VAL:O	2:D:1803:SER:CB	2.60	0.49
2:D:3763:GLY:HA2	2:D:3766:ILE:HD12	1.94	0.49
2:D:4798:GLU:O	2:D:4802:THR:OG1	2.27	0.49
2:D:4857:VAL:HG13	2:F:4863:ILE:HG21	1.93	0.49
2:F:207:PHE:CD2	2:H:2326:ILE:O	2.65	0.49
2:F:289:ILE:HA	2:F:293:GLN:HE22	1.77	0.49
2:F:694:ARG:HB2	2:F:793:SER:HB2	1.94	0.49
2:F:4590:GLY:O	2:F:4594:LEU:N	2.44	0.49
2:F:4796:LYS:HD2	2:F:4805:MET:HB3	1.95	0.49
2:B:694:ARG:HB3	2:B:716:ASN:HB3	1.94	0.49
2:B:4193:PHE:O	2:B:4197:THR:OG1	2.25	0.49
2:B:4796:LYS:HD2	2:B:4805:MET:HB3	1.95	0.49
2:B:4819:TYR:CE1	2:H:4848:ASP:HB3	2.42	0.49
2:B:4848:ASP:HB3	2:D:4819:TYR:CE1	2.42	0.49
2:D:694:ARG:HB2	2:D:793:SER:HB2	1.94	0.49
2:D:1041:ARG:HA	2:D:1044:LYS:HG3	1.94	0.49
2:F:2738:LEU:HD13	2:F:2819:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2835:SER:H	2:F:2838:LEU:HB2	1.78	0.49
1:G:54:GLU:OE1	2:H:1772:ASN:ND2	2.45	0.49
2:H:375:GLN:HE21	2:H:392:ILE:HD13	1.77	0.49
2:H:750:ARG:N	2:H:753:ASP:OD2	2.46	0.49
2:H:1926:ILE:HD11	2:H:2034:VAL:HG22	1.95	0.49
2:B:1300:MET:HB2	2:B:1545:ALA:HB3	1.93	0.49
2:B:2326:ILE:HG21	2:H:207:PHE:CE1	2.41	0.49
2:B:2835:SER:H	2:B:2838:LEU:HB2	1.78	0.49
2:D:4814:TYR:CE2	2:D:4815:MET:CE	2.95	0.49
2:F:228:LEU:HB3	2:F:289:ILE:HB	1.95	0.49
2:F:1926:ILE:HD11	2:F:2034:VAL:HG22	1.95	0.49
2:F:2071:ALA:HA	2:F:2076:ILE:HD11	1.94	0.49
2:F:3856:GLN:NE2	2:F:3923:GLU:O	2.45	0.49
2:F:4569:MET:O	2:F:4573:LEU:HB2	2.13	0.49
2:F:4591:TYR:OH	2:F:4717:ASP:OD2	2.29	0.49
2:H:1041:ARG:HA	2:H:1044:LYS:HG3	1.94	0.49
2:H:2738:LEU:HD13	2:H:2819:ALA:HB3	1.95	0.49
2:B:483:LYS:O	2:B:544:ASN:ND2	2.38	0.48
2:B:2558:LYS:O	2:B:2562:LEU:N	2.44	0.48
2:B:4780:TYR:OH	2:D:4515:ASN:HA	2.12	0.48
2:D:207:PHE:HB3	2:F:2326:ILE:O	2.13	0.48
2:D:246:THR:N	2:D:261:HIS:O	2.42	0.48
2:D:483:LYS:O	2:D:544:ASN:ND2	2.38	0.48
2:D:707:PRO:HD3	2:D:840:TYR:HE1	1.78	0.48
2:D:2835:SER:H	2:D:2838:LEU:HB2	1.78	0.48
2:D:3856:GLN:NE2	2:D:3923:GLU:O	2.45	0.48
2:F:556:ASP:OD1	2:F:556:ASP:N	2.46	0.48
2:F:1570:LEU:O	2:F:1573:SER:OG	2.27	0.48
2:F:4176:ASP:HA	2:F:4180:GLU:HB3	1.95	0.48
2:H:556:ASP:OD1	2:H:556:ASP:N	2.46	0.48
2:H:1184:ASP:OD2	2:H:1188:SER:OG	2.30	0.48
2:H:2835:SER:H	2:H:2838:LEU:HB2	1.78	0.48
2:H:4759:SER:HA	2:H:4762:THR:HG22	1.95	0.48
2:B:707:PRO:HD3	2:B:840:TYR:HE1	1.78	0.48
2:B:803:LEU:HD13	2:B:813:PHE:H	1.78	0.48
2:B:4520:PHE:CB	2:B:4562:LEU:HD21	2.43	0.48
2:D:228:LEU:HB3	2:D:289:ILE:HB	1.95	0.48
2:F:542:ARG:NE	2:F:577:CYS:SG	2.85	0.48
2:F:3921:LEU:HD23	2:F:3924:TYR:HD2	1.78	0.48
2:F:4899:PHE:HB2	2:F:4906:PHE:HD1	1.78	0.48
2:H:3810:GLU:O	2:H:3814:LYS:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3917:VAL:O	2:H:3920:THR:OG1	2.24	0.48
2:B:375:GLN:HE21	2:B:392:ILE:HD13	1.77	0.48
2:B:556:ASP:N	2:B:556:ASP:OD1	2.46	0.48
2:D:652:VAL:HA	2:D:795:SER:HB2	1.94	0.48
2:D:694:ARG:HB3	2:D:716:ASN:HB3	1.94	0.48
2:D:2837:ASP:OD1	2:D:2906:ARG:NE	2.42	0.48
2:F:707:PRO:HD3	2:F:840:TYR:HE1	1.78	0.48
1:A:42:ARG:HG3	1:A:44:LYS:HB3	1.95	0.48
2:B:750:ARG:N	2:B:753:ASP:OD2	2.46	0.48
2:B:2425:ARG:HG3	2:B:2477:TYR:CE1	2.48	0.48
2:B:2738:LEU:HD13	2:B:2819:ALA:HB3	1.95	0.48
2:B:4759:SER:HA	2:B:4762:THR:HG22	1.95	0.48
2:B:4899:PHE:HB2	2:B:4906:PHE:HD1	1.78	0.48
2:D:803:LEU:HD13	2:D:813:PHE:H	1.78	0.48
2:D:4569:MET:O	2:D:4573:LEU:HB2	2.13	0.48
2:F:652:VAL:HA	2:F:795:SER:HB2	1.94	0.48
2:H:457:GLN:HA	2:H:460:ILE:HD12	1.95	0.48
2:H:694:ARG:HB3	2:H:716:ASN:HB3	1.94	0.48
2:H:4523:VAL:HG22	2:H:4559:HIS:HE1	1.78	0.48
2:B:122:ARG:HE	2:B:127:GLY:HA2	1.79	0.48
2:B:434:ASP:O	2:B:438:LYS:NZ	2.43	0.48
2:B:457:GLN:HA	2:B:460:ILE:HD12	1.95	0.48
2:D:207:PHE:HZ	2:F:2326:ILE:HD12	1.70	0.48
2:D:556:ASP:N	2:D:556:ASP:OD1	2.46	0.48
2:F:434:ASP:O	2:F:438:LYS:NZ	2.43	0.48
2:F:1443:VAL:O	2:F:1489:CYS:N	2.43	0.48
2:F:4520:PHE:CB	2:F:4562:LEU:HD21	2.43	0.48
1:G:74:LEU:HB2	1:G:99:PHE:HB2	1.95	0.48
2:H:542:ARG:NE	2:H:577:CYS:SG	2.85	0.48
2:H:694:ARG:HB2	2:H:793:SER:HB2	1.94	0.48
2:H:2026:ILE:HG23	2:H:2030:LEU:HD12	1.94	0.48
2:H:2071:ALA:HA	2:H:2076:ILE:HD11	1.94	0.48
2:H:2731:ASP:OD1	2:H:2822:TYR:OH	2.30	0.48
2:H:4569:MET:O	2:H:4573:LEU:HB2	2.13	0.48
2:H:4649:PHE:HB3	2:H:4653:LYS:HE3	1.96	0.48
2:H:4796:LYS:HD2	2:H:4805:MET:HB3	1.95	0.48
1:C:23:VAL:HB	1:C:105:ASN:H	1.79	0.48
2:D:2071:ALA:HA	2:D:2076:ILE:HD11	1.94	0.48
2:D:2222:LEU:O	2:D:2226:SER:N	2.35	0.48
2:D:4568:TYR:O	2:D:4572:THR:OG1	2.22	0.48
2:D:4649:PHE:HB3	2:D:4653:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:ARG:HE	2:F:127:GLY:HA2	1.79	0.48
2:F:750:ARG:N	2:F:753:ASP:OD2	2.46	0.48
2:F:2026:ILE:HG23	2:F:2030:LEU:HD12	1.94	0.48
2:F:2301:ASP:OD1	2:F:2304:ARG:NH2	2.46	0.48
2:F:4814:TYR:CE2	2:F:4815:MET:CE	2.95	0.48
2:H:122:ARG:HE	2:H:127:GLY:HA2	1.79	0.48
2:H:1119:ARG:NH2	2:H:1196:ASP:O	2.39	0.48
2:B:4089:HIS:O	2:B:4093:LYS:N	2.44	0.48
2:D:4759:SER:HA	2:D:4762:THR:HG22	1.95	0.48
2:H:3856:GLN:NE2	2:H:3923:GLU:O	2.45	0.48
2:B:4569:MET:O	2:B:4573:LEU:HB2	2.13	0.48
2:D:2738:LEU:HD13	2:D:2819:ALA:HB3	1.95	0.48
2:F:803:LEU:HD13	2:F:813:PHE:H	1.78	0.48
2:H:4089:HIS:O	2:H:4093:LYS:N	2.44	0.48
2:B:4668:SER:HA	2:B:4671:LEU:HD12	1.96	0.48
2:D:185:SER:OG	2:D:186:VAL:N	2.47	0.48
2:D:1197:VAL:HA	2:D:1201:PHE:HE2	1.79	0.48
2:D:1209:VAL:N	2:D:1211:GLN:OE1	2.47	0.48
1:E:42:ARG:HG3	1:E:44:LYS:HB3	1.95	0.48
2:F:694:ARG:O	2:F:793:SER:N	2.42	0.48
2:F:1209:VAL:N	2:F:1211:GLN:OE1	2.47	0.48
2:H:803:LEU:HD13	2:H:813:PHE:H	1.78	0.48
1:C:74:LEU:HB2	1:C:99:PHE:HB2	1.95	0.48
2:D:122:ARG:HE	2:D:127:GLY:HA2	1.79	0.48
2:D:1310:CYS:HB2	2:D:1536:SER:HA	1.95	0.48
2:D:1799:VAL:O	2:D:1803:SER:OG	2.30	0.48
2:D:2558:LYS:O	2:D:2562:LEU:N	2.44	0.48
2:D:3748:SER:O	2:D:3793:SER:OG	2.30	0.48
2:F:185:SER:OG	2:F:186:VAL:N	2.47	0.48
2:F:1197:VAL:HA	2:F:1201:PHE:HE2	1.79	0.48
2:H:434:ASP:O	2:H:438:LYS:NZ	2.43	0.48
2:H:656:ARG:HH12	2:H:700:THR:HG22	1.79	0.48
2:H:1799:VAL:O	2:H:1803:SER:OG	2.30	0.48
2:H:2135:MET:HA	2:H:2136:GLY:HA3	1.68	0.48
2:H:4520:PHE:CB	2:H:4562:LEU:HD21	2.43	0.48
2:B:1184:ASP:OD2	2:B:1188:SER:OG	2.30	0.47
2:B:1926:ILE:HD11	2:B:2034:VAL:HG22	1.95	0.47
2:D:750:ARG:N	2:D:753:ASP:OD2	2.46	0.47
2:D:1443:VAL:O	2:D:1489:CYS:N	2.43	0.47
2:D:1926:ILE:HD11	2:D:2034:VAL:HG22	1.95	0.47
2:D:4642:PRO:HG2	2:D:4648:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:LEU:HB3	2:F:289:ILE:HD12	1.96	0.47
2:F:457:GLN:HA	2:F:460:ILE:HD12	1.95	0.47
2:F:694:ARG:HB3	2:F:716:ASN:HB3	1.94	0.47
2:F:2835:SER:O	2:F:2839:HIS:N	2.38	0.47
2:F:4594:LEU:O	2:F:4596:VAL:N	2.47	0.47
2:B:656:ARG:HH12	2:B:700:THR:HG22	1.79	0.47
2:B:4594:LEU:O	2:B:4596:VAL:N	2.47	0.47
2:D:457:GLN:HA	2:D:460:ILE:HD12	1.95	0.47
2:D:1302:TYR:HB2	2:D:1543:VAL:HB	1.96	0.47
2:D:4193:PHE:O	2:D:4197:THR:OG1	2.25	0.47
2:D:4627:ILE:HA	2:D:4630:GLN:HB2	1.96	0.47
1:E:74:LEU:HB2	1:E:99:PHE:HB2	1.95	0.47
2:F:4857:VAL:HG13	2:H:4863:ILE:HG21	1.93	0.47
2:B:443:SER:HA	2:B:444:THR:HA	1.64	0.47
2:B:1171:HIS:O	2:B:1194:ASP:N	2.44	0.47
2:B:1310:CYS:HB2	2:B:1536:SER:HA	1.96	0.47
2:B:1648:GLU:HA	2:B:1651:LEU:HB3	1.97	0.47
2:D:2038:THR:OG1	2:D:2039:TYR:N	2.47	0.47
1:E:23:VAL:HB	1:E:105:ASN:H	1.79	0.47
2:F:443:SER:HA	2:F:444:THR:HA	1.64	0.47
2:H:228:LEU:HB3	2:H:289:ILE:HB	1.95	0.47
2:H:443:SER:HA	2:H:444:THR:HA	1.64	0.47
2:H:4804:ASP:N	2:H:4804:ASP:OD1	2.47	0.47
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.95	0.47
2:B:228:LEU:HB3	2:B:289:ILE:HB	1.95	0.47
2:B:420:ARG:HE	2:B:420:ARG:H	1.63	0.47
2:B:2038:THR:OG1	2:B:2039:TYR:N	2.47	0.47
2:B:3921:LEU:HD23	2:B:3924:TYR:HD2	1.78	0.47
2:D:542:ARG:NE	2:D:577:CYS:SG	2.85	0.47
2:D:2256:LEU:HD11	2:D:3815:ALA:HB3	1.97	0.47
2:D:3919:ASN:O	2:D:3922:THR:OG1	2.27	0.47
2:D:4899:PHE:HB2	2:D:4906:PHE:HD1	1.78	0.47
2:F:1043:LYS:HA	2:F:1046:ASN:HB2	1.97	0.47
2:F:4804:ASP:OD1	2:F:4804:ASP:N	2.47	0.47
2:H:125:TYR:CZ	2:H:417:ARG:HB3	2.50	0.47
2:B:2256:LEU:HD11	2:B:3815:ALA:HB3	1.97	0.47
2:B:4627:ILE:HA	2:B:4630:GLN:HB2	1.96	0.47
2:D:1689:ILE:HG12	2:D:1703:TYR:HE1	1.80	0.47
2:D:4594:LEU:O	2:D:4596:VAL:N	2.47	0.47
2:F:218:SER:HB3	2:F:286:GLY:HA3	1.96	0.47
2:H:185:SER:OG	2:H:186:VAL:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1043:LYS:HA	2:H:1046:ASN:HB2	1.97	0.47
2:H:1209:VAL:N	2:H:1211:GLN:OE1	2.47	0.47
2:H:1251:LEU:O	2:H:1601:ASN:N	2.43	0.47
2:H:4899:PHE:HB2	2:H:4906:PHE:HD1	1.78	0.47
2:B:228:LEU:HB3	2:B:289:ILE:HD12	1.96	0.47
2:B:1197:VAL:HA	2:B:1201:PHE:HE2	1.79	0.47
2:B:1209:VAL:N	2:B:1211:GLN:OE1	2.47	0.47
2:B:1302:TYR:HB2	2:B:1543:VAL:HB	1.96	0.47
2:B:1689:ILE:HG12	2:B:1703:TYR:HE1	1.80	0.47
2:B:2425:ARG:HG3	2:B:2477:TYR:HE1	1.79	0.47
2:D:228:LEU:HB3	2:D:289:ILE:HD12	1.96	0.47
2:D:656:ARG:HH12	2:D:700:THR:HG22	1.79	0.47
2:D:3956:GLN:HE21	2:D:3976:GLN:HE22	1.63	0.47
2:D:4780:TYR:OH	2:F:4515:ASN:HA	2.15	0.47
2:F:2256:LEU:HD11	2:F:3815:ALA:HB3	1.97	0.47
2:F:2858:LYS:HG2	2:F:2872:LEU:HD22	1.97	0.47
1:G:28:GLY:N	1:G:37:ASP:O	2.37	0.47
2:H:1310:CYS:HB2	2:H:1536:SER:HA	1.96	0.47
2:H:2488:LEU:O	2:H:2492:GLY:N	2.48	0.47
2:H:4642:PRO:HG2	2:H:4648:LYS:HD2	1.96	0.47
1:A:68:LEU:HA	1:A:103:LEU:HD23	1.97	0.47
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.96	0.47
2:B:1043:LYS:HA	2:B:1046:ASN:HB2	1.97	0.47
1:C:42:ARG:HG3	1:C:44:LYS:HB3	1.95	0.47
2:D:1748:LEU:HD22	2:D:1749:PRO:HD2	1.95	0.47
2:D:4591:TYR:OH	2:D:4717:ASP:OD2	2.29	0.47
2:D:4668:SER:HA	2:D:4671:LEU:HD12	1.96	0.47
2:F:125:TYR:CZ	2:F:417:ARG:HB3	2.50	0.47
2:F:656:ARG:HH12	2:F:700:THR:HG22	1.79	0.47
2:F:672:LYS:HA	2:F:760:ASP:HA	1.97	0.47
2:F:1302:TYR:HB2	2:F:1543:VAL:HB	1.96	0.47
2:F:4089:HIS:O	2:F:4093:LYS:N	2.44	0.47
2:F:4857:VAL:CG1	2:H:4863:ILE:HG21	2.43	0.47
1:G:42:ARG:HG3	1:G:44:LYS:HB3	1.95	0.47
2:H:64:ILE:HA	2:H:123:HIS:HE1	1.80	0.47
2:H:218:SER:HB3	2:H:286:GLY:HA3	1.96	0.47
2:H:228:LEU:HB3	2:H:289:ILE:HD12	1.96	0.47
2:H:420:ARG:H	2:H:420:ARG:HE	1.63	0.47
2:H:1115:VAL:O	2:H:1137:PHE:N	2.48	0.47
2:H:1648:GLU:HA	2:H:1651:LEU:HB3	1.96	0.47
2:H:1748:LEU:HD22	2:H:1749:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2256:LEU:HD11	2:H:3815:ALA:HB3	1.96	0.47
2:H:3960:SER:HG	2:H:4070:CYS:HG	1.62	0.47
2:B:185:SER:OG	2:B:186:VAL:N	2.47	0.47
2:B:673:TRP:HB2	2:B:759:LEU:HB3	1.97	0.47
2:B:4648:LYS:O	2:B:4652:ARG:NE	2.48	0.47
2:D:653:SER:OG	2:D:794:PHE:O	2.31	0.47
2:D:673:TRP:HB2	2:D:759:LEU:HB3	1.96	0.47
1:E:40:ARG:HB3	2:F:688:ALA:HB1	1.97	0.47
2:F:64:ILE:HA	2:F:123:HIS:HE1	1.79	0.47
2:F:420:ARG:H	2:F:420:ARG:HE	1.63	0.47
2:F:483:LYS:O	2:F:544:ASN:ND2	2.38	0.47
2:F:1310:CYS:HB2	2:F:1536:SER:HA	1.96	0.47
2:F:2135:MET:HA	2:F:2136:GLY:HA3	1.68	0.47
2:F:2837:ASP:OD1	2:F:2906:ARG:NE	2.42	0.47
2:F:4648:LYS:O	2:F:4652:ARG:NE	2.48	0.47
2:H:4100:ALA:O	2:H:4104:THR:OG1	2.30	0.47
2:B:3956:GLN:HE21	2:B:3976:GLN:HE22	1.63	0.47
2:B:4052:ALA:O	2:B:4056:HIS:ND1	2.47	0.47
2:D:218:SER:HB3	2:D:286:GLY:HA3	1.96	0.47
2:D:420:ARG:HE	2:D:420:ARG:H	1.63	0.47
2:D:4857:VAL:CG1	2:F:4863:ILE:HG21	2.45	0.47
2:F:1934:VAL:HG21	2:F:3618:VAL:HA	1.97	0.47
2:F:2102:ALA:O	2:F:2106:THR:N	2.46	0.47
2:F:4717:ASP:HB3	2:F:4720:PHE:HB3	1.97	0.47
2:H:394:HIS:NE2	2:H:396:GLU:OE1	2.48	0.47
2:H:2148:GLY:O	2:H:2152:ASN:ND2	2.48	0.47
2:H:4594:LEU:O	2:H:4596:VAL:N	2.47	0.47
2:H:4668:SER:HA	2:H:4671:LEU:HD12	1.96	0.47
1:A:40:ARG:HB3	2:B:688:ALA:HB1	1.97	0.47
2:B:64:ILE:HA	2:B:123:HIS:HE1	1.79	0.47
2:B:394:HIS:NE2	2:B:396:GLU:OE1	2.48	0.47
2:B:653:SER:OG	2:B:794:PHE:O	2.31	0.47
2:B:2148:GLY:O	2:B:2152:ASN:ND2	2.48	0.47
2:B:4642:PRO:HG2	2:B:4648:LYS:HD2	1.96	0.47
2:B:4804:ASP:N	2:B:4804:ASP:OD1	2.47	0.47
1:C:68:LEU:HA	1:C:103:LEU:HD23	1.97	0.47
2:D:1115:VAL:O	2:D:1137:PHE:N	2.48	0.47
2:D:2858:LYS:HG2	2:D:2872:LEU:HD22	1.97	0.47
2:D:4804:ASP:OD1	2:D:4804:ASP:N	2.47	0.47
2:F:1306:MET:HB3	2:F:1575:HIS:CE1	2.50	0.47
2:F:1748:LEU:HD22	2:F:1749:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4649:PHE:HB3	2:F:4653:LYS:HE3	1.96	0.47
2:F:4668:SER:HA	2:F:4671:LEU:HD12	1.96	0.47
1:G:23:VAL:HB	1:G:105:ASN:H	1.79	0.47
2:H:190:ARG:HG2	2:H:207:PHE:HE1	1.80	0.47
2:H:1306:MET:HB3	2:H:1575:HIS:CE1	2.49	0.47
2:B:681:HIS:HD2	2:B:799:LYS:HD3	1.80	0.46
2:B:848:ARG:NH1	2:B:1605:LYS:O	2.48	0.46
2:B:1115:VAL:O	2:B:1137:PHE:N	2.48	0.46
2:B:1748:LEU:HD22	2:B:1749:PRO:HD2	1.96	0.46
2:B:1929:PHE:HZ	2:B:2030:LEU:HB3	1.80	0.46
2:B:3925:ILE:HD11	2:B:3936:LEU:HD13	1.97	0.46
2:B:4100:ALA:O	2:B:4104:THR:OG1	2.30	0.46
1:C:49:ARG:HB3	1:C:52:LYS:HE2	1.97	0.46
2:D:1306:MET:HB3	2:D:1575:HIS:CE1	2.49	0.46
2:D:1570:LEU:O	2:D:1573:SER:OG	2.27	0.46
2:D:1648:GLU:HA	2:D:1651:LEU:HB3	1.97	0.46
2:D:1929:PHE:HZ	2:D:2030:LEU:HB3	1.80	0.46
2:D:3925:ILE:HD11	2:D:3936:LEU:HD13	1.97	0.46
2:F:4518:LEU:HD13	2:F:4521:TYR:HE2	1.80	0.46
2:F:4780:TYR:OH	2:H:4515:ASN:HA	2.15	0.46
2:H:1197:VAL:HA	2:H:1201:PHE:HE2	1.79	0.46
2:H:1302:TYR:HB2	2:H:1543:VAL:HB	1.96	0.46
2:H:4627:ILE:HA	2:H:4630:GLN:HB2	1.96	0.46
2:B:190:ARG:HG2	2:B:207:PHE:HE1	1.80	0.46
2:B:2326:ILE:O	2:H:207:PHE:HB3	2.15	0.46
2:D:64:ILE:HA	2:D:123:HIS:HE1	1.80	0.46
2:D:2102:ALA:O	2:D:2106:THR:N	2.46	0.46
2:D:2488:LEU:O	2:D:2492:GLY:N	2.48	0.46
2:D:3921:LEU:HD23	2:D:3924:TYR:HD2	1.78	0.46
2:D:4648:LYS:O	2:D:4652:ARG:NE	2.48	0.46
2:F:207:PHE:HB3	2:H:2326:ILE:O	2.15	0.46
2:F:673:TRP:HB2	2:F:759:LEU:HB3	1.97	0.46
2:F:1699:ARG:HH22	2:F:1821:LEU:HD11	1.80	0.46
2:F:1738:LEU:HD22	2:F:1739:PHE:H	1.79	0.46
2:F:3925:ILE:HD11	2:F:3936:LEU:HD13	1.97	0.46
2:F:4627:ILE:HA	2:F:4630:GLN:HB2	1.96	0.46
2:F:4642:PRO:HG2	2:F:4648:LYS:HD2	1.96	0.46
2:F:4733:GLY:HA3	2:F:4740:PHE:HD1	1.80	0.46
2:H:506:HIS:HE2	2:H:534:TYR:HH	1.61	0.46
2:H:673:TRP:HB2	2:H:759:LEU:HB3	1.97	0.46
2:H:1934:VAL:HG21	2:H:3618:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3925:ILE:HD11	2:H:3936:LEU:HD13	1.97	0.46
2:B:672:LYS:HA	2:B:760:ASP:HA	1.97	0.46
2:B:1699:ARG:HH22	2:B:1821:LEU:HD11	1.80	0.46
2:B:1738:LEU:HD22	2:B:1739:PHE:H	1.80	0.46
2:B:4013:MET:N	2:B:4013:MET:SD	2.89	0.46
2:B:4649:PHE:HB3	2:B:4653:LYS:HE3	1.96	0.46
2:D:190:ARG:HG2	2:D:207:PHE:HE1	1.80	0.46
2:F:137:ARG:N	2:F:146:ASP:OD2	2.49	0.46
2:F:4052:ALA:O	2:F:4056:HIS:ND1	2.47	0.46
2:H:1484:ASN:H	2:H:1486:TYR:HA	1.80	0.46
2:H:4591:TYR:OH	2:H:4717:ASP:OD2	2.29	0.46
2:H:4623:SER:O	2:H:4630:GLN:NE2	2.48	0.46
2:B:3860:ARG:HH21	2:B:3932:ASN:HB2	1.80	0.46
2:D:707:PRO:HD2	2:D:1604:LEU:HD22	1.98	0.46
2:D:848:ARG:NH1	2:D:1605:LYS:O	2.48	0.46
2:D:4138:GLU:HG2	2:D:4148:ARG:HB3	1.98	0.46
2:D:4733:GLY:HA3	2:D:4740:PHE:HD1	1.80	0.46
1:E:68:LEU:HA	1:E:103:LEU:HD23	1.97	0.46
2:F:2488:LEU:O	2:F:2492:GLY:N	2.48	0.46
2:F:4046:LYS:N	2:F:4077:GLU:OE1	2.49	0.46
2:H:137:ARG:N	2:H:146:ASP:OD2	2.49	0.46
2:H:419:ILE:HG12	2:H:489:PHE:HE1	1.81	0.46
2:H:506:HIS:HB3	2:H:564:ARG:HH22	1.81	0.46
2:H:848:ARG:NH1	2:H:1605:LYS:O	2.48	0.46
2:H:4113:ASP:O	2:H:4117:GLN:N	2.46	0.46
2:H:4648:LYS:O	2:H:4652:ARG:NE	2.48	0.46
1:A:23:VAL:HB	1:A:105:ASN:H	1.79	0.46
2:B:707:PRO:HD2	2:B:1604:LEU:HD22	1.98	0.46
2:B:1306:MET:HB3	2:B:1575:HIS:CE1	2.49	0.46
2:B:4713:VAL:O	2:B:4716:THR:OG1	2.27	0.46
2:B:4733:GLY:HA3	2:B:4740:PHE:HD1	1.80	0.46
2:D:394:HIS:NE2	2:D:396:GLU:OE1	2.48	0.46
2:D:4013:MET:N	2:D:4013:MET:SD	2.89	0.46
2:F:190:ARG:HG2	2:F:207:PHE:HE1	1.80	0.46
2:F:3860:ARG:HH21	2:F:3932:ASN:HB2	1.80	0.46
2:F:4138:GLU:HG2	2:F:4148:ARG:HB3	1.98	0.46
2:H:1570:LEU:O	2:H:1573:SER:OG	2.27	0.46
2:H:1689:ILE:HG12	2:H:1703:TYR:HE1	1.80	0.46
2:B:1716:THR:HA	2:B:1719:LEU:HD12	1.98	0.46
2:B:4138:GLU:HG2	2:B:4148:ARG:HB3	1.98	0.46
1:C:40:ARG:HB3	2:D:688:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1184:ASP:OD2	2:D:1188:SER:OG	2.30	0.46
2:D:3924:TYR:O	2:D:3932:ASN:ND2	2.48	0.46
2:D:4717:ASP:HB3	2:D:4720:PHE:HB3	1.97	0.46
2:F:228:LEU:HD23	2:F:228:LEU:HA	1.82	0.46
2:F:394:HIS:NE2	2:F:396:GLU:OE1	2.48	0.46
2:F:1686:LEU:HA	2:F:1689:ILE:HD12	1.98	0.46
2:F:1689:ILE:HG12	2:F:1703:TYR:HE1	1.80	0.46
2:F:3917:VAL:O	2:F:3920:THR:OG1	2.24	0.46
2:F:3956:GLN:HE21	2:F:3976:GLN:HE22	1.63	0.46
2:H:1716:THR:HA	2:H:1719:LEU:HD12	1.98	0.46
2:H:1738:LEU:HD22	2:H:1739:PHE:H	1.79	0.46
2:H:2858:LYS:HG2	2:H:2872:LEU:HD22	1.97	0.46
2:H:3859:LEU:HD22	2:H:3871:ILE:HG21	1.98	0.46
2:H:4046:LYS:N	2:H:4077:GLU:OE1	2.49	0.46
2:B:207:PHE:HB3	2:D:2326:ILE:O	2.16	0.46
2:B:1611:ILE:N	2:B:1620:GLN:O	2.44	0.46
2:B:4523:VAL:CG2	2:H:4808:ASP:CG	2.62	0.46
2:D:1043:LYS:HA	2:D:1046:ASN:HB2	1.97	0.46
2:D:4623:SER:O	2:D:4630:GLN:NE2	2.49	0.46
2:F:419:ILE:HG12	2:F:489:PHE:HE1	1.81	0.46
2:F:848:ARG:NH1	2:F:1605:LYS:O	2.48	0.46
2:F:1648:GLU:HA	2:F:1651:LEU:HB3	1.97	0.46
2:F:2148:GLY:O	2:F:2152:ASN:ND2	2.48	0.46
1:G:68:LEU:HA	1:G:103:LEU:HD23	1.97	0.46
2:H:681:HIS:HD2	2:H:799:LYS:HD3	1.80	0.46
2:H:1686:LEU:HA	2:H:1689:ILE:HD12	1.98	0.46
2:H:3956:GLN:HE21	2:H:3976:GLN:HE22	1.63	0.46
2:H:4138:GLU:HG2	2:H:4148:ARG:HB3	1.98	0.46
2:B:137:ARG:N	2:B:146:ASP:OD2	2.49	0.46
2:B:1686:LEU:HA	2:B:1689:ILE:HD12	1.98	0.46
2:B:2791:GLU:H	2:B:2903:ALA:HB3	1.81	0.46
2:B:4113:ASP:O	2:B:4117:GLN:N	2.46	0.46
2:D:137:ARG:N	2:D:146:ASP:OD2	2.49	0.46
2:D:681:HIS:HD2	2:D:799:LYS:HD3	1.80	0.46
2:D:1738:LEU:HD22	2:D:1739:PHE:H	1.79	0.46
2:D:1934:VAL:HG21	2:D:3618:VAL:HA	1.97	0.46
2:D:2116:ASP:OD2	2:D:2154:LYS:N	2.49	0.46
2:D:4046:LYS:N	2:D:4077:GLU:OE1	2.49	0.46
2:F:1736:ILE:HG12	2:F:1753:LEU:HD12	1.98	0.46
2:F:3924:TYR:O	2:F:3932:ASN:ND2	2.49	0.46
1:G:40:ARG:HB3	2:H:688:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:672:LYS:HA	2:H:760:ASP:HA	1.97	0.46
2:H:4002:ASP:HA	2:H:4115:ARG:HH22	1.81	0.46
2:B:506:HIS:HB3	2:B:564:ARG:HH22	1.81	0.46
2:B:2488:LEU:O	2:B:2492:GLY:N	2.48	0.46
2:B:4160:GLN:HG3	2:B:4205:ALA:HB2	1.98	0.46
2:B:4857:VAL:HG13	2:D:4863:ILE:HG21	1.96	0.46
2:D:125:TYR:CZ	2:D:417:ARG:HB3	2.50	0.46
2:D:2040:LEU:HD11	2:D:3634:GLU:HG2	1.98	0.46
2:D:2148:GLY:O	2:D:2152:ASN:ND2	2.48	0.46
2:D:3860:ARG:HH21	2:D:3932:ASN:HB2	1.80	0.46
2:F:21:VAL:HG13	2:F:217:ILE:HG13	1.98	0.46
2:F:3859:LEU:HD22	2:F:3871:ILE:HG21	1.98	0.46
2:F:4013:MET:N	2:F:4013:MET:SD	2.89	0.46
2:H:115:TYR:HB2	2:H:171:GLU:HA	1.98	0.46
2:H:3924:TYR:O	2:H:3932:ASN:ND2	2.49	0.46
1:A:28:GLY:N	1:A:37:ASP:O	2.37	0.46
2:B:21:VAL:HG13	2:B:217:ILE:HG13	1.98	0.46
2:B:125:TYR:CZ	2:B:417:ARG:HB3	2.50	0.46
2:B:2835:SER:O	2:B:2839:HIS:N	2.38	0.46
2:D:699:SER:OG	2:D:701:GLU:O	2.31	0.46
2:D:1143:GLN:HA	2:D:1151:HIS:HA	1.98	0.46
2:D:1716:THR:HA	2:D:1719:LEU:HD12	1.98	0.46
2:F:506:HIS:HB3	2:F:564:ARG:HH22	1.81	0.46
2:F:2040:LEU:HD11	2:F:3634:GLU:HG2	1.98	0.46
2:F:4160:GLN:HG3	2:F:4205:ALA:HB2	1.98	0.46
2:H:565:LEU:HG	2:H:604:HIS:CE1	2.51	0.46
2:H:4013:MET:SD	2:H:4013:MET:N	2.89	0.46
2:H:4160:GLN:HG3	2:H:4205:ALA:HB2	1.98	0.46
2:B:1443:VAL:O	2:B:1489:CYS:N	2.43	0.45
2:B:3924:TYR:O	2:B:3932:ASN:ND2	2.49	0.45
2:B:4857:VAL:CG1	2:D:4863:ILE:HG21	2.46	0.45
2:D:20:VAL:HG12	2:D:216:PRO:HA	1.99	0.45
2:D:506:HIS:HB3	2:D:564:ARG:HH22	1.81	0.45
2:D:1699:ARG:HH22	2:D:1821:LEU:HD11	1.80	0.45
2:D:3845:GLN:HB2	2:D:3920:THR:HG22	1.98	0.45
1:E:49:ARG:HB3	1:E:52:LYS:HE2	1.97	0.45
2:F:1210:ALA:N	2:F:1211:GLN:OE1	2.50	0.45
2:F:1484:ASN:H	2:F:1486:TYR:HA	1.80	0.45
2:F:3845:GLN:HB2	2:F:3920:THR:HG22	1.98	0.45
2:H:699:SER:OG	2:H:701:GLU:O	2.31	0.45
2:H:2837:ASP:OD1	2:H:2906:ARG:NE	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TYR:HB2	2:B:171:GLU:HA	1.98	0.45
2:B:2102:ALA:O	2:B:2106:THR:N	2.46	0.45
2:B:4519:LEU:HA	2:H:4810:MET:HB3	1.97	0.45
2:D:101:MET:HE2	2:D:104:THR:HG22	1.98	0.45
2:D:115:TYR:HB2	2:D:171:GLU:HA	1.98	0.45
2:D:207:PHE:CG	2:F:2326:ILE:HG23	2.51	0.45
2:D:456:LEU:HD12	2:D:536:LEU:HD13	1.99	0.45
2:D:1736:ILE:HG12	2:D:1753:LEU:HD12	1.98	0.45
2:D:3779:LEU:HD13	2:D:3855:PHE:HD1	1.81	0.45
2:F:565:LEU:HG	2:F:604:HIS:CE1	2.51	0.45
2:H:195:SER:OG	2:H:196:TYR:N	2.49	0.45
2:H:731:HIS:ND1	2:H:739:ARG:O	2.50	0.45
2:H:1210:ALA:N	2:H:1211:GLN:OE1	2.50	0.45
2:H:1699:ARG:HH22	2:H:1821:LEU:HD11	1.80	0.45
2:H:2038:THR:OG1	2:H:2039:TYR:N	2.47	0.45
2:H:3682:LYS:HZ3	2:H:3684:GLU:HG2	1.81	0.45
1:A:14:THR:HB	1:A:68:LEU:HB2	1.99	0.45
1:A:49:ARG:HB3	1:A:52:LYS:HE2	1.97	0.45
2:B:456:LEU:HD12	2:B:536:LEU:HD13	1.99	0.45
2:B:2040:LEU:HD11	2:B:3634:GLU:HG2	1.98	0.45
2:B:2116:ASP:OD2	2:B:2154:LYS:N	2.49	0.45
2:B:2858:LYS:HG2	2:B:2872:LEU:HD22	1.97	0.45
2:D:1686:LEU:HA	2:D:1689:ILE:HD12	1.98	0.45
2:D:2791:GLU:H	2:D:2903:ALA:HB3	1.81	0.45
2:D:4160:GLN:HG3	2:D:4205:ALA:HB2	1.98	0.45
2:F:1143:GLN:HA	2:F:1151:HIS:HA	1.98	0.45
2:F:1929:PHE:HZ	2:F:2030:LEU:HB3	1.80	0.45
2:F:3897:ASP:OD1	2:F:3958:LYS:NZ	2.40	0.45
2:F:4623:SER:O	2:F:4630:GLN:NE2	2.49	0.45
2:H:935:MET:O	2:H:939:THR:OG1	2.34	0.45
2:H:1736:ILE:HG12	2:H:1753:LEU:HD12	1.98	0.45
2:H:2116:ASP:OD2	2:H:2154:LYS:N	2.49	0.45
2:H:3860:ARG:HH21	2:H:3932:ASN:HB2	1.81	0.45
2:B:1934:VAL:HG21	2:B:3618:VAL:HA	1.97	0.45
2:B:3831:LEU:HA	2:B:3832:GLN:HA	1.57	0.45
2:D:21:VAL:HG13	2:D:217:ILE:HG13	1.98	0.45
2:D:626:ARG:NH2	2:D:1668:GLY:O	2.36	0.45
2:D:672:LYS:HA	2:D:760:ASP:HA	1.97	0.45
2:D:1210:ALA:N	2:D:1211:GLN:OE1	2.50	0.45
2:H:4518:LEU:HD13	2:H:4521:TYR:HE2	1.79	0.45
2:B:1210:ALA:N	2:B:1211:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3779:LEU:HD13	2:B:3855:PHE:HD1	1.82	0.45
2:B:4590:GLY:O	2:B:4594:LEU:N	2.44	0.45
2:B:4717:ASP:HB3	2:B:4720:PHE:HB3	1.97	0.45
2:D:565:LEU:HG	2:D:604:HIS:CE1	2.51	0.45
2:D:2135:MET:HA	2:D:2136:GLY:HA3	1.68	0.45
2:D:4002:ASP:HA	2:D:4115:ARG:HH22	1.81	0.45
2:F:835:GLU:HG3	2:F:837:SER:H	1.82	0.45
2:F:2116:ASP:OD2	2:F:2154:LYS:N	2.49	0.45
1:G:14:THR:HB	1:G:68:LEU:HB2	1.99	0.45
2:H:713:TRP:CZ3	2:H:1627:PHE:HB2	2.52	0.45
2:H:1143:GLN:HA	2:H:1151:HIS:HA	1.98	0.45
2:H:1929:PHE:HZ	2:H:2030:LEU:HB3	1.80	0.45
2:H:4052:ALA:O	2:H:4056:HIS:ND1	2.47	0.45
2:B:20:VAL:HG12	2:B:216:PRO:HA	1.99	0.45
2:B:4623:SER:O	2:B:4630:GLN:NE2	2.48	0.45
2:D:713:TRP:CZ3	2:D:1627:PHE:HB2	2.52	0.45
2:D:731:HIS:ND1	2:D:739:ARG:O	2.50	0.45
2:D:1846:ILE:HG12	2:D:1894:LEU:HB3	1.99	0.45
2:F:681:HIS:HD2	2:F:799:LYS:HD3	1.80	0.45
2:F:707:PRO:HD2	2:F:1604:LEU:HD22	1.98	0.45
2:H:835:GLU:HG3	2:H:837:SER:H	1.82	0.45
1:A:67:SER:H	1:A:70:GLN:HB3	1.82	0.45
2:B:180:ASP:HB3	2:B:211:LEU:HD22	1.99	0.45
2:B:4518:LEU:HD13	2:B:4521:TYR:HE2	1.80	0.45
2:D:3859:LEU:HD22	2:D:3871:ILE:HG21	1.98	0.45
2:F:2791:GLU:H	2:F:2903:ALA:HB3	1.81	0.45
2:F:3907:PHE:HD2	2:F:3968:LEU:HD11	1.82	0.45
1:G:49:ARG:HB3	1:G:52:LYS:HE2	1.97	0.45
2:H:614:LEU:HD23	2:H:617:LEU:HD12	1.99	0.45
2:H:1846:ILE:HG12	2:H:1894:LEU:HB3	1.99	0.45
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.99	0.45
2:B:419:ILE:HG12	2:B:489:PHE:HE1	1.81	0.45
2:B:680:ASP:HB2	2:B:799:LYS:HG3	1.98	0.45
2:B:4002:ASP:HA	2:B:4115:ARG:HH22	1.81	0.45
2:B:4046:LYS:N	2:B:4077:GLU:OE1	2.49	0.45
2:B:4131:GLN:HA	2:B:4134:LEU:HD23	1.99	0.45
2:B:4138:GLU:HA	2:B:4148:ARG:HA	1.99	0.45
2:D:835:GLU:HG3	2:D:837:SER:H	1.82	0.45
2:D:1433:PHE:HB2	2:D:1552:VAL:HA	1.99	0.45
2:D:1484:ASN:H	2:D:1486:TYR:HA	1.80	0.45
2:D:1620:GLN:HE21	2:D:1622:LEU:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3907:PHE:HD2	2:D:3968:LEU:HD11	1.82	0.45
2:D:4869:ASP:OD1	2:F:4875:ARG:HD3	2.17	0.45
2:F:180:ASP:HB3	2:F:211:LEU:HD22	1.99	0.45
2:F:195:SER:OG	2:F:196:TYR:N	2.49	0.45
2:F:207:PHE:CG	2:H:2326:ILE:HG23	2.52	0.45
2:F:1620:GLN:HE21	2:F:1622:LEU:HD21	1.81	0.45
2:F:1846:ILE:HG12	2:F:1894:LEU:HB3	1.99	0.45
2:F:2196:ASN:OD1	2:F:2199:ARG:NH1	2.50	0.45
2:F:4002:ASP:HA	2:F:4115:ARG:HH22	1.81	0.45
1:G:67:SER:H	1:G:70:GLN:HB3	1.82	0.45
2:H:180:ASP:HB3	2:H:211:LEU:HD22	1.99	0.45
2:H:2040:LEU:HD11	2:H:3634:GLU:HG2	1.98	0.45
2:H:2988:SER:O	2:H:2992:CYS:N	2.47	0.45
2:H:4138:GLU:HA	2:H:4148:ARG:HA	1.99	0.45
2:H:4717:ASP:HB3	2:H:4720:PHE:HB3	1.97	0.45
2:B:993:GLU:HG2	2:B:1051:ARG:HG2	1.99	0.45
2:B:1040:ASP:HA	2:B:1043:LYS:HB2	1.99	0.45
2:B:1484:ASN:H	2:B:1486:TYR:HA	1.80	0.45
2:B:2837:ASP:OD1	2:B:2906:ARG:NE	2.42	0.45
2:B:3892:TYR:O	2:B:3896:LYS:NZ	2.50	0.45
2:B:3907:PHE:HD2	2:B:3968:LEU:HD11	1.82	0.45
2:D:18:ASP:HB2	2:D:69:LEU:HD12	1.99	0.45
2:D:180:ASP:HB3	2:D:211:LEU:HD22	1.99	0.45
2:D:238:HIS:HB3	2:D:243:GLU:HB3	1.99	0.45
2:D:419:ILE:HG12	2:D:489:PHE:HE1	1.81	0.45
2:D:614:LEU:HD23	2:D:617:LEU:HD12	1.99	0.45
2:D:2464:ASP:OD1	2:D:2464:ASP:N	2.50	0.45
2:D:4131:GLN:HA	2:D:4134:LEU:HD23	1.99	0.45
2:F:49:LEU:HD12	2:F:201:LEU:HB3	1.99	0.45
2:F:935:MET:O	2:F:939:THR:OG1	2.34	0.45
2:F:1716:THR:HA	2:F:1719:LEU:HD12	1.98	0.45
2:F:4083:GLU:HA	2:F:4087:ARG:HD2	1.98	0.45
2:H:49:LEU:HD12	2:H:201:LEU:HB3	1.99	0.45
2:H:707:PRO:HD2	2:H:1604:LEU:HD22	1.98	0.45
2:B:565:LEU:HG	2:B:604:HIS:CE1	2.51	0.45
2:B:674:TYR:OH	2:B:676:GLU:OE2	2.24	0.45
2:B:731:HIS:ND1	2:B:739:ARG:O	2.50	0.45
2:B:1736:ILE:HG12	2:B:1753:LEU:HD12	1.98	0.45
2:B:1846:ILE:HG12	2:B:1894:LEU:HB3	1.99	0.45
2:B:3859:LEU:HD22	2:B:3871:ILE:HG21	1.98	0.45
1:C:67:SER:H	1:C:70:GLN:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1221:VAL:HG13	2:D:1224:LEU:HD12	1.99	0.45
2:D:2835:SER:O	2:D:2839:HIS:N	2.38	0.45
2:F:680:ASP:HB2	2:F:799:LYS:HG3	1.98	0.45
2:F:713:TRP:CZ3	2:F:1627:PHE:HB2	2.52	0.45
2:F:745:ASN:HB3	2:F:747:HIS:HB2	1.99	0.45
2:F:1799:VAL:O	2:F:1803:SER:HB3	2.17	0.45
2:H:1261:VAL:HA	2:H:1596:TRP:HH2	1.82	0.45
2:H:3779:LEU:HD13	2:H:3855:PHE:HD1	1.82	0.45
2:H:3845:GLN:HB2	2:H:3920:THR:HG22	1.98	0.45
2:B:195:SER:OG	2:B:196:TYR:N	2.50	0.44
2:B:835:GLU:HG3	2:B:837:SER:H	1.82	0.44
2:B:1799:VAL:O	2:B:1803:SER:HB3	2.17	0.44
2:B:3845:GLN:HB2	2:B:3920:THR:HG22	1.98	0.44
2:B:4875:ARG:HD3	2:H:4869:ASP:OD1	2.18	0.44
1:C:14:THR:HB	1:C:68:LEU:HB2	1.99	0.44
2:D:195:SER:OG	2:D:196:TYR:N	2.49	0.44
2:D:207:PHE:CG	2:F:2326:ILE:CG2	3.00	0.44
2:D:4089:HIS:O	2:D:4093:LYS:N	2.44	0.44
2:F:456:LEU:HD12	2:F:536:LEU:HD13	1.99	0.44
2:F:1115:VAL:O	2:F:1137:PHE:N	2.48	0.44
2:F:1170:GLU:O	2:F:1172:THR:N	2.49	0.44
2:F:1261:VAL:HA	2:F:1596:TRP:HH2	1.82	0.44
2:F:1433:PHE:HB2	2:F:1552:VAL:HA	1.99	0.44
2:H:456:LEU:HD12	2:H:536:LEU:HD13	1.99	0.44
2:H:680:ASP:HB2	2:H:799:LYS:HG3	1.98	0.44
2:H:993:GLU:HG2	2:H:1051:ARG:HG2	1.99	0.44
2:H:2157:TYR:HH	2:H:2203:TYR:HH	1.54	0.44
2:H:4733:GLY:HA3	2:H:4740:PHE:HD1	1.80	0.44
2:B:2212:GLN:HE22	2:B:2250:ASP:H	1.65	0.44
1:C:75:THR:HA	1:C:98:ILE:HA	1.99	0.44
2:D:4767:GLN:O	2:D:4771:THR:OG1	2.28	0.44
2:D:4832:ILE:HD11	2:D:4844:ARG:HG3	2.00	0.44
1:E:14:THR:HB	1:E:68:LEU:HB2	1.99	0.44
2:F:115:TYR:HB2	2:F:171:GLU:HA	1.98	0.44
2:F:731:HIS:ND1	2:F:739:ARG:O	2.50	0.44
2:H:1926:ILE:HD12	2:H:1926:ILE:HA	1.89	0.44
2:H:2127:ILE:HD12	2:H:2127:ILE:HA	1.89	0.44
2:H:2791:GLU:H	2:H:2903:ALA:HB3	1.81	0.44
2:H:3892:TYR:O	2:H:3896:LYS:NZ	2.50	0.44
2:B:713:TRP:CZ3	2:B:1627:PHE:HB2	2.52	0.44
2:D:49:LEU:HD12	2:D:201:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:680:ASP:HB2	2:D:799:LYS:HG3	1.98	0.44
2:D:1799:VAL:O	2:D:1803:SER:HB3	2.17	0.44
2:D:3831:LEU:HA	2:D:3832:GLN:HA	1.57	0.44
2:F:644:LEU:HD22	2:F:1632:ILE:HG22	1.99	0.44
2:F:1221:VAL:HG13	2:F:1224:LEU:HD12	1.99	0.44
2:F:3831:LEU:HA	2:F:3832:GLN:HA	1.57	0.44
2:H:21:VAL:HG13	2:H:217:ILE:HG13	1.98	0.44
2:H:644:LEU:HD22	2:H:1632:ILE:HG22	1.99	0.44
2:H:1602:GLN:HB3	2:H:1604:LEU:HD12	2.00	0.44
2:H:2196:ASN:OD1	2:H:2199:ARG:NH1	2.50	0.44
2:B:207:PHE:HZ	2:D:2326:ILE:HD12	1.72	0.44
2:B:1143:GLN:HA	2:B:1151:HIS:HA	1.98	0.44
2:B:1253:LYS:HE2	2:B:1257:GLN:HE21	1.82	0.44
2:B:2103:LEU:HA	2:B:2106:THR:HG22	2.00	0.44
2:D:434:ASP:O	2:D:438:LYS:NZ	2.43	0.44
2:D:745:ASN:HB3	2:D:747:HIS:HB2	1.99	0.44
2:D:935:MET:O	2:D:939:THR:OG1	2.34	0.44
2:D:1040:ASP:HA	2:D:1043:LYS:HB2	1.99	0.44
2:D:3682:LYS:HZ3	2:D:3684:GLU:HG2	1.82	0.44
2:D:4093:LYS:HE2	2:D:4093:LYS:HB3	1.84	0.44
2:F:20:VAL:HG12	2:F:216:PRO:HA	1.99	0.44
2:F:77:ALA:HA	2:H:3891:TRP:CZ3	2.53	0.44
2:F:1253:LYS:HE2	2:F:1257:GLN:HE21	1.82	0.44
2:F:1926:ILE:HD12	2:F:1926:ILE:HA	1.89	0.44
2:F:2464:ASP:N	2:F:2464:ASP:OD1	2.50	0.44
2:F:3779:LEU:HD13	2:F:3855:PHE:HD1	1.82	0.44
2:H:1245:ARG:HE	2:H:1692:LYS:HD2	1.83	0.44
2:B:49:LEU:HD12	2:B:201:LEU:HB3	1.99	0.44
2:B:1620:GLN:HE21	2:B:1622:LEU:HD21	1.81	0.44
2:B:1699:ARG:NH1	2:B:1816:PHE:O	2.51	0.44
2:B:1799:VAL:O	2:B:1803:SER:OG	2.30	0.44
2:B:2135:MET:HA	2:B:2136:GLY:HA3	1.68	0.44
2:B:4863:ILE:HG21	2:H:4857:VAL:CG1	2.47	0.44
2:B:4869:ASP:OD1	2:D:4875:ARG:HD3	2.16	0.44
2:D:234:LEU:HD21	2:D:277:LEU:HD12	2.00	0.44
2:D:434:ASP:OD1	2:D:504:ARG:NE	2.41	0.44
2:D:4138:GLU:HA	2:D:4148:ARG:HA	1.99	0.44
2:F:238:HIS:HB3	2:F:243:GLU:HB3	2.00	0.44
2:F:1245:ARG:HE	2:F:1692:LYS:HD2	1.83	0.44
2:H:20:VAL:HG12	2:H:216:PRO:HA	1.99	0.44
2:H:1253:LYS:HE2	2:H:1257:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1699:ARG:NH1	2:H:1816:PHE:O	2.51	0.44
2:H:2103:LEU:HA	2:H:2106:THR:HG22	2.00	0.44
2:H:4173:PHE:HZ	2:H:4190:PHE:HA	1.83	0.44
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.50	0.44
2:B:4810:MET:HB3	2:D:4519:LEU:HA	1.98	0.44
2:D:993:GLU:HG2	2:D:1051:ARG:HG2	1.99	0.44
2:D:1114:ARG:HH12	2:D:1127:GLU:HB3	1.82	0.44
2:D:1245:ARG:HE	2:D:1692:LYS:HD2	1.83	0.44
2:D:3983:LEU:HD12	2:D:3983:LEU:HA	1.87	0.44
2:D:4083:GLU:HA	2:D:4087:ARG:HD2	1.98	0.44
1:E:67:SER:H	1:E:70:GLN:HB3	1.82	0.44
2:F:234:LEU:HD21	2:F:277:LEU:HD12	2.00	0.44
2:F:614:LEU:HD23	2:F:617:LEU:HD12	1.99	0.44
1:G:75:THR:HA	1:G:98:ILE:HA	1.99	0.44
2:H:238:HIS:HB3	2:H:243:GLU:HB3	1.99	0.44
2:H:1620:GLN:HE21	2:H:1622:LEU:HD21	1.81	0.44
2:H:2212:GLN:HE22	2:H:2250:ASP:H	1.65	0.44
2:B:844:ARG:NH1	2:B:849:ASP:OD2	2.51	0.44
2:B:1114:ARG:HH12	2:B:1127:GLU:HB3	1.82	0.44
2:B:4173:PHE:HZ	2:B:4190:PHE:HA	1.83	0.44
2:D:77:ALA:HA	2:F:3891:TRP:CZ3	2.52	0.44
2:D:4173:PHE:HZ	2:D:4190:PHE:HA	1.83	0.44
1:E:75:THR:HA	1:E:98:ILE:HA	1.99	0.44
2:F:993:GLU:HG2	2:F:1051:ARG:HG2	2.00	0.44
2:F:4832:ILE:HD11	2:F:4844:ARG:HG3	2.00	0.44
2:F:4869:ASP:OD1	2:H:4875:ARG:HD3	2.17	0.44
2:H:4131:GLN:HA	2:H:4134:LEU:HD23	1.99	0.44
2:H:4832:ILE:HD11	2:H:4844:ARG:HG3	2.00	0.44
2:B:238:HIS:HB3	2:B:243:GLU:HB3	2.00	0.44
2:B:644:LEU:HD22	2:B:1632:ILE:HG22	1.99	0.44
2:B:745:ASN:HB3	2:B:747:HIS:HB2	1.99	0.44
2:B:1245:ARG:HE	2:B:1692:LYS:HD2	1.83	0.44
2:B:1602:GLN:HB3	2:B:1604:LEU:HD12	2.00	0.44
2:D:412:GLU:O	2:D:415:THR:OG1	2.33	0.44
2:D:644:LEU:HD22	2:D:1632:ILE:HG22	1.99	0.44
2:D:2212:GLN:HE22	2:D:2250:ASP:H	1.65	0.44
2:D:4750:GLY:H	2:D:4755:ARG:NE	2.16	0.44
2:F:1228:THR:HA	2:F:1232:LEU:HD12	1.99	0.44
2:F:4857:VAL:HG11	2:H:4863:ILE:HG22	1.98	0.44
2:H:1086:ARG:N	2:H:1207:LEU:O	2.48	0.44
2:H:3800:SER:OG	2:H:3801:CYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4083:GLU:HA	2:H:4087:ARG:HD2	1.99	0.44
2:B:614:LEU:HD23	2:B:617:LEU:HD12	1.99	0.44
2:B:1221:VAL:HG13	2:B:1224:LEU:HD12	1.99	0.44
2:B:1433:PHE:HB2	2:B:1552:VAL:HA	1.99	0.44
2:B:2123:SER:O	2:B:2126:GLN:NE2	2.51	0.44
2:B:2793:THR:OG1	2:B:2901:GLY:O	2.30	0.44
2:D:2123:SER:O	2:D:2126:GLN:NE2	2.51	0.44
2:D:2196:ASN:OD1	2:D:2199:ARG:NH1	2.50	0.44
2:D:2832:VAL:O	2:D:2895:LYS:NZ	2.44	0.44
2:D:4113:ASP:O	2:D:4117:GLN:N	2.46	0.44
2:F:1570:LEU:HD23	2:F:1570:LEU:HA	1.84	0.44
2:F:2127:ILE:HD12	2:F:2127:ILE:HA	1.89	0.44
2:F:4657:LYS:HD2	2:F:4658:TYR:CZ	2.53	0.44
2:H:18:ASP:HB2	2:H:69:LEU:HD12	1.99	0.44
2:H:1104:GLU:HG2	2:H:1216:ASN:HB2	2.00	0.44
2:H:1272:ARG:NH1	2:H:1587:HIS:O	2.51	0.44
2:B:1104:GLU:HG2	2:B:1216:ASN:HB2	2.00	0.43
2:B:1228:THR:HA	2:B:1232:LEU:HD12	1.99	0.43
2:B:1261:VAL:HA	2:B:1596:TRP:HH2	1.82	0.43
2:D:459:LEU:HD23	2:D:459:LEU:HA	1.86	0.43
2:D:1445:TRP:HB3	2:D:1539:LEU:HD13	2.00	0.43
2:D:3892:TYR:O	2:D:3896:LYS:NZ	2.50	0.43
2:D:4052:ALA:O	2:D:4056:HIS:ND1	2.47	0.43
2:F:18:ASP:HB2	2:F:69:LEU:HD12	1.99	0.43
2:F:766:ILE:HB	2:F:779:PHE:HB2	2.00	0.43
2:F:1434:PRO:HD2	2:F:1552:VAL:HG23	2.00	0.43
2:F:1445:TRP:HB3	2:F:1539:LEU:HD13	2.00	0.43
2:F:1699:ARG:NH1	2:F:1816:PHE:O	2.51	0.43
2:F:3892:TYR:O	2:F:3896:LYS:NZ	2.50	0.43
1:G:21:THR:OG1	1:G:49:ARG:NE	2.50	0.43
2:H:1221:VAL:HG13	2:H:1224:LEU:HD12	1.99	0.43
2:H:1799:VAL:O	2:H:1803:SER:HB3	2.17	0.43
2:B:3767:LEU:HA	2:B:3767:LEU:HD23	1.84	0.43
2:D:1261:VAL:HA	2:D:1596:TRP:HH2	1.82	0.43
2:D:4576:LEU:HD13	2:D:4579:LEU:HD22	2.01	0.43
2:F:4138:GLU:HA	2:F:4148:ARG:HA	1.99	0.43
2:F:4750:GLY:H	2:F:4755:ARG:NE	2.16	0.43
2:H:745:ASN:HB3	2:H:747:HIS:HB2	1.99	0.43
2:H:766:ILE:HB	2:H:779:PHE:HB2	2.00	0.43
2:H:1433:PHE:HB2	2:H:1552:VAL:HA	1.99	0.43
2:B:234:LEU:HD21	2:B:277:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2473:LEU:HD12	2:B:2477:TYR:HD2	1.83	0.43
2:B:4832:ILE:HD11	2:B:4844:ARG:HG3	2.00	0.43
2:B:4857:VAL:HG11	2:D:4863:ILE:HG22	2.01	0.43
2:D:1253:LYS:HE2	2:D:1257:GLN:HE21	1.82	0.43
2:D:1272:ARG:NH1	2:D:1587:HIS:O	2.51	0.43
2:D:4657:LYS:HD2	2:D:4658:TYR:CZ	2.53	0.43
2:F:1272:ARG:NH1	2:F:1587:HIS:O	2.51	0.43
2:F:4131:GLN:HA	2:F:4134:LEU:HD23	1.99	0.43
2:H:234:LEU:HD21	2:H:277:LEU:HD12	2.00	0.43
2:H:2835:SER:O	2:H:2839:HIS:N	2.38	0.43
2:H:4766:LYS:HE3	2:H:4770:LEU:HD11	2.00	0.43
2:B:1272:ARG:NH1	2:B:1587:HIS:O	2.51	0.43
2:B:4657:LYS:HD2	2:B:4658:TYR:CZ	2.53	0.43
1:C:44:LYS:HA	1:C:45:PRO:HD3	1.90	0.43
2:D:2473:LEU:HD12	2:D:2477:TYR:HD2	1.83	0.43
2:D:4750:GLY:H	2:D:4755:ARG:HE	1.66	0.43
2:F:439:LYS:HD3	2:F:441:LYS:HB2	2.01	0.43
2:F:699:SER:OG	2:F:701:GLU:O	2.31	0.43
2:F:1086:ARG:N	2:F:1207:LEU:O	2.48	0.43
2:F:1602:GLN:HB3	2:F:1604:LEU:HD12	2.00	0.43
2:F:1696:GLY:HA2	2:F:1699:ARG:HB3	2.00	0.43
2:F:2222:LEU:O	2:F:2226:SER:N	2.35	0.43
2:F:2793:THR:OG1	2:F:2901:GLY:O	2.30	0.43
2:F:4173:PHE:HZ	2:F:4190:PHE:HA	1.83	0.43
2:H:844:ARG:NH1	2:H:849:ASP:OD2	2.51	0.43
2:H:4657:LYS:HD2	2:H:4658:TYR:CZ	2.53	0.43
2:B:935:MET:O	2:B:939:THR:OG1	2.34	0.43
2:B:4083:GLU:HA	2:B:4087:ARG:HD2	1.99	0.43
2:B:4750:GLY:H	2:B:4755:ARG:NE	2.16	0.43
2:D:620:CYS:N	2:D:623:VAL:O	2.39	0.43
2:D:836:HIS:CE1	2:D:1610:ARG:HB2	2.54	0.43
2:D:1699:ARG:NH1	2:D:1816:PHE:O	2.51	0.43
2:D:4857:VAL:HG11	2:F:4863:ILE:HG22	2.00	0.43
2:F:306:LEU:HG	2:F:314:LEU:HD11	2.00	0.43
2:F:1040:ASP:HA	2:F:1043:LYS:HB2	1.99	0.43
2:F:1114:ARG:HH12	2:F:1127:GLU:HB3	1.82	0.43
2:H:306:LEU:HG	2:H:314:LEU:HD11	2.00	0.43
2:H:1040:ASP:HA	2:H:1043:LYS:HB2	2.00	0.43
2:B:861:ALA:HB3	2:B:863:THR:HG23	2.01	0.43
2:B:1505:LEU:O	2:B:1523:ASN:N	2.52	0.43
1:C:29:MET:HB3	1:C:35:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:796:ALA:HB3	2:D:798:ILE:HG13	2.00	0.43
2:D:4611:LEU:HD21	2:D:4617:TYR:HD2	1.84	0.43
2:F:836:HIS:CE1	2:F:1610:ARG:HB2	2.54	0.43
2:F:2103:LEU:HA	2:F:2106:THR:HG22	2.00	0.43
2:F:2123:SER:O	2:F:2126:GLN:NE2	2.51	0.43
2:F:2212:GLN:HE22	2:F:2250:ASP:H	1.65	0.43
2:F:4750:GLY:H	2:F:4755:ARG:HE	1.67	0.43
2:H:1466:THR:HG22	2:H:1482:ARG:HA	2.01	0.43
2:H:2102:ALA:O	2:H:2106:THR:N	2.46	0.43
2:H:2123:SER:O	2:H:2126:GLN:NE2	2.51	0.43
2:B:3797:LEU:HD23	2:B:3797:LEU:HA	1.88	0.43
2:B:4766:LYS:HE3	2:B:4770:LEU:HD11	2.00	0.43
2:D:1104:GLU:HG2	2:D:1216:ASN:HB2	2.00	0.43
2:D:1449:ASP:OD1	2:D:1449:ASP:N	2.52	0.43
2:D:1696:GLY:HA2	2:D:1699:ARG:HB3	2.00	0.43
2:D:2198:CYS:HA	2:D:2201:LEU:HD12	2.01	0.43
2:D:3997:GLY:HA2	2:D:4000:MET:SD	2.59	0.43
2:D:4023:LYS:HA	2:D:4026:ASP:HB2	2.01	0.43
2:D:4713:VAL:O	2:D:4716:THR:OG1	2.27	0.43
2:F:1176:THR:HG22	2:F:1181:ILE:HG12	2.01	0.43
2:F:2038:THR:OG1	2:F:2039:TYR:N	2.47	0.43
2:H:1114:ARG:HH12	2:H:1127:GLU:HB3	1.82	0.43
2:H:1190:LEU:HD12	2:H:1193:LYS:HE2	2.00	0.43
2:H:1228:THR:HA	2:H:1232:LEU:HD12	1.99	0.43
2:H:1445:TRP:HB3	2:H:1539:LEU:HD13	2.00	0.43
2:H:1675:ALA:O	2:H:1679:HIS:ND1	2.48	0.43
2:H:3907:PHE:HD2	2:H:3968:LEU:HD11	1.82	0.43
1:A:75:THR:HA	1:A:98:ILE:HA	1.99	0.43
2:B:256:GLN:O	2:B:304:LYS:NZ	2.48	0.43
2:B:452:VAL:O	2:B:456:LEU:HB2	2.19	0.43
2:B:1466:THR:HG22	2:B:1482:ARG:HA	2.01	0.43
2:B:3800:SER:OG	2:B:3801:CYS:N	2.51	0.43
2:B:4521:TYR:H	2:H:4810:MET:CG	2.32	0.43
2:D:861:ALA:HB3	2:D:863:THR:HG23	2.01	0.43
2:D:1434:PRO:HD2	2:D:1552:VAL:HG23	2.00	0.43
2:F:35:LEU:HA	2:F:51:SER:HA	2.01	0.43
2:F:207:PHE:CG	2:H:2326:ILE:CG2	3.01	0.43
2:F:1449:ASP:OD1	2:F:1449:ASP:N	2.52	0.43
2:F:1466:THR:HG22	2:F:1482:ARG:HA	2.01	0.43
2:F:4632:ASP:OD1	2:F:4709:TRP:NE1	2.48	0.43
2:H:233:VAL:HG22	2:H:276:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:297:LEU:HD23	2:H:297:LEU:HA	1.87	0.43
2:H:836:HIS:CE1	2:H:1610:ARG:HB2	2.54	0.43
2:H:2731:ASP:HB3	2:H:2826:ALA:HB2	2.00	0.43
2:H:4778:VAL:O	2:H:4782:TYR:HB2	2.19	0.43
2:B:644:LEU:HB2	2:B:1654:HIS:HD2	1.84	0.43
2:B:796:ALA:HB3	2:B:798:ILE:HG13	2.00	0.43
2:D:1228:THR:HA	2:D:1232:LEU:HD12	1.99	0.43
2:D:2103:LEU:HA	2:D:2106:THR:HG22	2.00	0.43
1:E:29:MET:HB3	1:E:35:LYS:HG2	2.01	0.43
2:F:434:ASP:OD1	2:F:504:ARG:NE	2.40	0.43
2:F:452:VAL:O	2:F:456:LEU:HB2	2.19	0.43
2:F:626:ARG:NH2	2:F:1668:GLY:O	2.36	0.43
2:F:2731:ASP:HB3	2:F:2826:ALA:HB2	2.00	0.43
2:F:3997:GLY:HA2	2:F:4000:MET:SD	2.59	0.43
2:F:4737:ASN:HA	2:F:4740:PHE:HB2	2.01	0.43
2:H:794:PHE:HE2	2:H:1621:CYS:HB2	1.83	0.43
2:H:796:ALA:HB3	2:H:798:ILE:HG13	2.00	0.43
2:H:2198:CYS:HA	2:H:2201:LEU:HD12	2.01	0.43
2:H:2473:LEU:HD12	2:H:2477:TYR:HD2	1.83	0.43
2:H:3831:LEU:HA	2:H:3832:GLN:HA	1.57	0.43
2:H:4737:ASN:HA	2:H:4740:PHE:HB2	2.01	0.43
2:B:647:ARG:HA	2:B:647:ARG:HD2	1.84	0.43
2:B:1170:GLU:O	2:B:1172:THR:N	2.49	0.43
2:B:1190:LEU:HD12	2:B:1193:LYS:HE2	2.00	0.43
2:B:2326:ILE:HG23	2:H:207:PHE:CG	2.53	0.43
2:D:256:GLN:O	2:D:304:LYS:NZ	2.48	0.43
2:F:305:TYR:HE2	2:F:319:LYS:HG2	1.83	0.43
2:F:844:ARG:NH1	2:F:849:ASP:OD2	2.51	0.43
2:F:1190:LEU:HD12	2:F:1193:LYS:HE2	2.00	0.43
2:F:2834:LEU:HB2	2:F:2839:HIS:CE1	2.54	0.43
2:F:4652:ARG:HA	2:F:4655:MET:HB2	2.01	0.43
1:G:29:MET:HB3	1:G:35:LYS:HG2	2.01	0.43
2:H:439:LYS:HD3	2:H:441:LYS:HB2	2.01	0.43
2:H:551:PHE:HD1	2:H:551:PHE:HA	1.70	0.43
2:B:101:MET:HE2	2:B:104:THR:HG22	2.01	0.42
2:B:794:PHE:HE2	2:B:1621:CYS:HB2	1.83	0.42
2:B:836:HIS:CE1	2:B:1610:ARG:HB2	2.54	0.42
2:B:1033:VAL:HG23	2:B:1038:LEU:HB3	2.01	0.42
2:B:1250:TRP:HB3	2:B:1600:PRO:HB2	2.01	0.42
2:B:1809:PRO:HA	2:B:1817:LEU:HD13	2.01	0.42
2:B:4046:LYS:HA	2:B:4049:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4576:LEU:HD13	2:B:4579:LEU:HD22	2.01	0.42
2:D:644:LEU:HB2	2:D:1654:HIS:HD2	1.84	0.42
2:D:1789:ALA:HA	2:D:1792:ILE:HD12	2.01	0.42
2:D:4834:ASP:OD1	2:D:4834:ASP:N	2.52	0.42
2:F:763:ALA:O	2:F:765:SER:N	2.51	0.42
2:F:1104:GLU:HG2	2:F:1216:ASN:HB2	2.00	0.42
2:F:4576:LEU:HD13	2:F:4579:LEU:HD22	2.01	0.42
2:H:452:VAL:O	2:H:456:LEU:HB2	2.19	0.42
2:H:644:LEU:HB2	2:H:1654:HIS:HD2	1.84	0.42
2:H:1250:TRP:HB3	2:H:1600:PRO:HB2	2.01	0.42
2:H:1676:LEU:HD23	2:H:1676:LEU:HA	1.87	0.42
2:H:2832:VAL:O	2:H:2895:LYS:NZ	2.44	0.42
2:H:4046:LYS:HA	2:H:4049:PHE:HB3	2.01	0.42
2:H:4652:ARG:HA	2:H:4655:MET:HB2	2.01	0.42
2:H:4750:GLY:H	2:H:4755:ARG:HE	1.66	0.42
1:A:29:MET:HB3	1:A:35:LYS:HG2	2.01	0.42
2:B:3730:ALA:HA	2:B:3733:HIS:CE1	2.54	0.42
2:B:4778:VAL:O	2:B:4782:TYR:HB2	2.19	0.42
2:B:4863:ILE:HG21	2:H:4857:VAL:HG13	1.96	0.42
2:D:233:VAL:HG22	2:D:276:ARG:HB2	2.01	0.42
2:D:1170:GLU:O	2:D:1172:THR:N	2.49	0.42
2:D:1602:GLN:HB3	2:D:1604:LEU:HD12	2.00	0.42
2:D:1611:ILE:N	2:D:1620:GLN:O	2.44	0.42
2:F:1676:LEU:HD23	2:F:1676:LEU:HA	1.87	0.42
2:F:2473:LEU:HD12	2:F:2477:TYR:HD2	1.83	0.42
2:F:4023:LYS:HA	2:F:4026:ASP:HB2	2.01	0.42
2:H:861:ALA:HB3	2:H:863:THR:HG23	2.01	0.42
2:H:1434:PRO:HD2	2:H:1552:VAL:HG23	2.00	0.42
2:H:1757:LEU:HD13	2:H:1757:LEU:HA	1.83	0.42
2:H:1809:PRO:HA	2:H:1817:LEU:HD13	2.01	0.42
2:H:4750:GLY:H	2:H:4755:ARG:NE	2.16	0.42
2:B:1090:ALA:HA	2:B:1249:MET:HG2	2.02	0.42
2:B:1434:PRO:HD2	2:B:1552:VAL:HG23	2.00	0.42
2:B:1789:ALA:HA	2:B:1792:ILE:HD12	2.01	0.42
2:B:3997:GLY:HA2	2:B:4000:MET:SD	2.59	0.42
2:D:77:ALA:HB2	2:F:3891:TRP:CH2	2.54	0.42
2:D:439:LYS:HD3	2:D:441:LYS:HB2	2.01	0.42
2:D:794:PHE:HE2	2:D:1621:CYS:HB2	1.83	0.42
2:D:1086:ARG:N	2:D:1207:LEU:O	2.48	0.42
2:D:1190:LEU:HD12	2:D:1193:LYS:HE2	2.00	0.42
2:D:1809:PRO:HA	2:D:1817:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4652:ARG:HA	2:D:4655:MET:HB2	2.01	0.42
2:F:794:PHE:HE2	2:F:1621:CYS:HB2	1.83	0.42
2:F:1033:VAL:HG23	2:F:1038:LEU:HB3	2.01	0.42
2:F:1505:LEU:O	2:F:1523:ASN:N	2.52	0.42
2:F:3730:ALA:HA	2:F:3733:HIS:CE1	2.54	0.42
2:F:4202:GLN:O	2:F:4206:GLN:HB3	2.20	0.42
2:H:256:GLN:O	2:H:304:LYS:NZ	2.47	0.42
2:H:1153:GLY:N	2:H:1183:LEU:O	2.53	0.42
2:H:4061:GLN:O	2:H:4064:THR:OG1	2.27	0.42
2:B:35:LEU:HA	2:B:51:SER:HA	2.01	0.42
2:B:1696:GLY:HA2	2:B:1699:ARG:HB3	2.00	0.42
2:B:2422:SER:O	2:B:2426:SER:N	2.48	0.42
2:B:4652:ARG:HA	2:B:4655:MET:HB2	2.01	0.42
2:B:4792:LYS:HE3	2:B:4792:LYS:HB3	1.92	0.42
2:D:766:ILE:HB	2:D:779:PHE:HB2	2.00	0.42
2:D:844:ARG:NH1	2:D:849:ASP:OD2	2.51	0.42
2:D:1466:THR:HG22	2:D:1482:ARG:HA	2.01	0.42
2:D:1926:ILE:HD12	2:D:1926:ILE:HA	1.89	0.42
1:E:44:LYS:HA	1:E:45:PRO:HD3	1.90	0.42
2:F:875:PRO:HG2	2:F:878:LEU:HD12	2.02	0.42
2:F:3800:SER:OG	2:F:3801:CYS:N	2.51	0.42
2:F:4766:LYS:HE3	2:F:4770:LEU:HD11	2.00	0.42
2:F:4778:VAL:O	2:F:4782:TYR:HB2	2.19	0.42
2:H:1090:ALA:HA	2:H:1249:MET:HG2	2.02	0.42
2:H:1764:SER:N	2:H:1779:SER:O	2.53	0.42
2:B:207:PHE:CG	2:D:2326:ILE:HG23	2.55	0.42
2:B:306:LEU:HG	2:B:314:LEU:HD11	2.00	0.42
2:B:766:ILE:HB	2:B:779:PHE:HB2	2.00	0.42
2:B:875:PRO:HG2	2:B:878:LEU:HD12	2.02	0.42
2:B:897:LYS:HE2	2:B:915:HIS:CG	2.55	0.42
2:B:4811:LEU:O	2:B:4814:TYR:HB3	2.19	0.42
2:D:2894:LEU:HA	2:D:2897:LEU:HD12	2.02	0.42
2:D:4202:GLN:O	2:D:4206:GLN:HB3	2.20	0.42
2:F:796:ALA:HB3	2:F:798:ILE:HG13	2.00	0.42
2:F:897:LYS:HE2	2:F:915:HIS:CG	2.55	0.42
2:F:1628:MET:HB2	2:F:1687:TYR:HE2	1.84	0.42
2:F:3797:LEU:HD23	2:F:3797:LEU:HA	1.88	0.42
2:F:4611:LEU:HD21	2:F:4617:TYR:HD2	1.84	0.42
2:H:682:THR:H	2:H:751:THR:HG22	1.85	0.42
2:H:763:ALA:O	2:H:765:SER:N	2.52	0.42
2:H:1628:MET:HB2	2:H:1687:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1696:GLY:HA2	2:H:1699:ARG:HB3	2.00	0.42
2:H:3997:GLY:HA2	2:H:4000:MET:SD	2.59	0.42
2:H:4811:LEU:O	2:H:4814:TYR:HB3	2.20	0.42
2:B:233:VAL:HG22	2:B:276:ARG:HB2	2.01	0.42
2:B:394:HIS:CD2	2:B:396:GLU:H	2.38	0.42
2:B:1176:THR:HG22	2:B:1181:ILE:HG12	2.01	0.42
2:B:1628:MET:HB2	2:B:1687:TYR:HE2	1.84	0.42
2:B:1764:SER:N	2:B:1779:SER:O	2.53	0.42
2:B:3834:ASP:OD1	2:B:3834:ASP:N	2.53	0.42
2:B:4037:ASP:OD2	2:B:4041:LYS:N	2.53	0.42
2:D:416:ALA:HA	2:D:419:ILE:HD12	2.01	0.42
2:D:661:LEU:O	2:D:788:PHE:N	2.53	0.42
2:D:763:ALA:O	2:D:765:SER:N	2.51	0.42
2:D:1176:THR:HG22	2:D:1181:ILE:HG12	2.01	0.42
2:D:3762:LEU:HD12	2:D:3762:LEU:HA	1.86	0.42
2:D:3800:SER:OG	2:D:3801:CYS:N	2.51	0.42
2:F:233:VAL:HG22	2:F:276:ARG:HB2	2.00	0.42
2:F:420:ARG:HA	2:F:423:VAL:HB	2.02	0.42
2:F:644:LEU:HB2	2:F:1654:HIS:HD2	1.84	0.42
2:F:1611:ILE:N	2:F:1620:GLN:O	2.43	0.42
2:F:2894:LEU:HA	2:F:2897:LEU:HD12	2.02	0.42
2:H:394:HIS:CD2	2:H:396:GLU:H	2.38	0.42
2:H:897:LYS:HE2	2:H:915:HIS:CG	2.55	0.42
2:H:1505:LEU:O	2:H:1523:ASN:N	2.52	0.42
2:H:2222:LEU:O	2:H:2226:SER:N	2.35	0.42
2:H:4202:GLN:O	2:H:4206:GLN:HB3	2.20	0.42
2:H:4611:LEU:HD21	2:H:4617:TYR:HD2	1.84	0.42
2:B:52:THR:HG22	2:B:60:PRO:HG3	2.02	0.42
2:B:682:THR:H	2:B:751:THR:HG22	1.85	0.42
2:B:2464:ASP:OD1	2:B:2464:ASP:N	2.50	0.42
2:B:4093:LYS:HE2	2:B:4093:LYS:HB3	1.84	0.42
2:B:4750:GLY:H	2:B:4755:ARG:HE	1.66	0.42
1:C:21:THR:OG1	1:C:49:ARG:NE	2.50	0.42
2:D:305:TYR:HE2	2:D:319:LYS:HG2	1.84	0.42
2:D:306:LEU:HG	2:D:314:LEU:HD11	2.00	0.42
2:D:678:MET:O	2:D:801:ARG:N	2.46	0.42
2:D:4518:LEU:HD13	2:D:4521:TYR:HE2	1.80	0.42
2:F:77:ALA:HB2	2:H:3891:TRP:CH2	2.54	0.42
2:F:121:LEU:HD23	2:F:121:LEU:HA	1.86	0.42
2:F:647:ARG:HD2	2:F:647:ARG:HA	1.84	0.42
2:F:861:ALA:HB3	2:F:863:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1153:GLY:N	2:F:1183:LEU:O	2.53	0.42
2:F:2198:CYS:HA	2:F:2201:LEU:HD12	2.01	0.42
2:H:35:LEU:HA	2:H:51:SER:HA	2.01	0.42
2:H:1170:GLU:O	2:H:1172:THR:N	2.49	0.42
1:A:82:TYR:OH	2:B:1768:PHE:O	2.28	0.42
2:B:305:TYR:HE2	2:B:319:LYS:HG2	1.84	0.42
2:B:439:LYS:HD3	2:B:441:LYS:HB2	2.01	0.42
2:B:1153:GLY:N	2:B:1183:LEU:O	2.53	0.42
2:B:1445:TRP:HB3	2:B:1539:LEU:HD13	2.00	0.42
2:B:2198:CYS:HA	2:B:2201:LEU:HD12	2.01	0.42
2:B:2731:ASP:HB3	2:B:2826:ALA:HB2	2.00	0.42
2:B:2988:SER:O	2:B:2992:CYS:N	2.47	0.42
2:D:52:THR:HG22	2:D:60:PRO:HG3	2.02	0.42
2:D:3834:ASP:N	2:D:3834:ASP:OD1	2.53	0.42
2:F:1250:TRP:HB3	2:F:1600:PRO:HB2	2.01	0.42
2:F:1572:LYS:HB3	2:F:1584:PRO:HA	2.01	0.42
2:F:1626:GLN:O	2:F:1687:TYR:OH	2.36	0.42
2:F:2843:GLU:OE2	2:F:2875:TYR:OH	2.34	0.42
2:F:2988:SER:O	2:F:2992:CYS:N	2.47	0.42
2:F:4635:VAL:O	2:F:4638:THR:OG1	2.31	0.42
2:H:52:THR:HG22	2:H:60:PRO:HG3	2.02	0.42
2:H:305:TYR:HE2	2:H:319:LYS:HG2	1.83	0.42
2:H:4036:TYR:HE2	2:H:4048:ASP:HB3	1.85	0.42
2:H:4093:LYS:HE2	2:H:4093:LYS:HB3	1.84	0.42
2:H:4576:LEU:HD13	2:H:4579:LEU:HD22	2.01	0.42
1:A:15:PHE:HA	1:A:67:SER:HA	2.01	0.42
2:B:661:LEU:O	2:B:788:PHE:N	2.53	0.42
2:B:3891:TRP:CZ3	2:H:77:ALA:HA	2.54	0.42
2:B:4737:ASN:HA	2:B:4740:PHE:HB2	2.01	0.42
2:D:1628:MET:HB2	2:D:1687:TYR:HE2	1.84	0.42
2:D:3730:ALA:HA	2:D:3733:HIS:CE1	2.54	0.42
2:D:4766:LYS:HE3	2:D:4770:LEU:HD11	2.00	0.42
1:E:15:PHE:HA	1:E:67:SER:HA	2.02	0.42
2:F:4808:ASP:CG	2:H:4523:VAL:CG2	2.66	0.42
2:B:554:SER:O	2:B:558:LEU:N	2.49	0.42
2:B:763:ALA:O	2:B:765:SER:N	2.51	0.42
2:B:2731:ASP:OD1	2:B:2822:TYR:OH	2.30	0.42
2:B:2834:LEU:HB2	2:B:2839:HIS:CE1	2.54	0.42
2:B:3897:ASP:OD1	2:B:3958:LYS:NZ	2.40	0.42
2:B:4808:ASP:OD2	2:D:4523:VAL:HG11	2.20	0.42
2:D:452:VAL:O	2:D:456:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1572:LYS:HB3	2:D:1584:PRO:HA	2.02	0.42
2:D:1607:ASP:HB3	2:D:1608:VAL:HG23	2.02	0.42
2:D:3854:ASP:OD1	2:D:3854:ASP:N	2.53	0.42
2:D:4036:TYR:HE2	2:D:4048:ASP:HB3	1.85	0.42
2:D:4037:ASP:OD2	2:D:4041:LYS:N	2.53	0.42
2:D:4737:ASN:HA	2:D:4740:PHE:HB2	2.01	0.42
2:D:4767:GLN:CG	2:F:4753:THR:OG1	2.67	0.42
2:D:4810:MET:HB3	2:F:4519:LEU:HA	2.01	0.42
2:F:119:ILE:HD13	2:F:162:ILE:HD11	2.02	0.42
2:F:195:SER:HB3	2:F:202:HIS:HB2	2.02	0.42
2:F:394:HIS:CD2	2:F:396:GLU:H	2.38	0.42
2:F:3696:MET:O	2:F:3699:SER:OG	2.28	0.42
2:H:1176:THR:HG22	2:H:1181:ILE:HG12	2.01	0.42
2:H:2834:LEU:HB2	2:H:2839:HIS:CE1	2.54	0.42
2:B:123:HIS:CD2	2:B:126:SER:H	2.38	0.41
2:B:626:ARG:NH2	2:B:1668:GLY:O	2.36	0.41
2:B:3677:LEU:HD23	2:B:3677:LEU:HA	1.91	0.41
2:B:4863:ILE:HG22	2:H:4857:VAL:HG13	1.98	0.41
2:D:394:HIS:CD2	2:D:396:GLU:H	2.38	0.41
2:D:682:THR:H	2:D:751:THR:HG22	1.85	0.41
2:D:897:LYS:HE2	2:D:915:HIS:CG	2.55	0.41
2:D:1090:ALA:HA	2:D:1249:MET:HG2	2.02	0.41
2:D:1250:TRP:HB3	2:D:1600:PRO:HB2	2.01	0.41
2:F:620:CYS:N	2:F:623:VAL:O	2.39	0.41
2:F:4036:TYR:HE2	2:F:4048:ASP:HB3	1.85	0.41
2:F:4046:LYS:HA	2:F:4049:PHE:HB3	2.01	0.41
2:F:4834:ASP:N	2:F:4834:ASP:OD1	2.52	0.41
2:H:1033:VAL:HG23	2:H:1038:LEU:HB3	2.01	0.41
2:H:2834:LEU:HD22	2:H:2838:LEU:HB3	2.02	0.41
2:H:4037:ASP:OD2	2:H:4041:LYS:N	2.53	0.41
2:B:1607:ASP:HB3	2:B:1608:VAL:HG23	2.02	0.41
2:B:2326:ILE:CG2	2:H:207:PHE:CG	3.02	0.41
2:B:2894:LEU:HA	2:B:2897:LEU:HD12	2.02	0.41
2:B:3983:LEU:HD12	2:B:3983:LEU:HA	1.88	0.41
2:D:35:LEU:HA	2:D:51:SER:HA	2.01	0.41
2:D:119:ILE:HD13	2:D:162:ILE:HD11	2.02	0.41
2:D:875:PRO:HG2	2:D:878:LEU:HD12	2.02	0.41
2:D:4808:ASP:OD2	2:F:4523:VAL:HG11	2.19	0.41
2:F:52:THR:HG22	2:F:60:PRO:HG3	2.02	0.41
2:F:290:ARG:HA	2:F:353:GLU:HG2	2.02	0.41
2:F:1809:PRO:HA	2:F:1817:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3993:ASN:HD22	2:F:4110:MET:HA	1.84	0.41
2:H:130:LEU:HA	2:H:149:LEU:HD23	2.03	0.41
2:H:195:SER:HB3	2:H:202:HIS:HB2	2.02	0.41
2:H:420:ARG:HA	2:H:423:VAL:HB	2.02	0.41
2:H:585:ALA:HA	2:H:588:ILE:HD12	2.02	0.41
2:H:647:ARG:HD2	2:H:647:ARG:HA	1.84	0.41
2:H:2730:HIS:CE1	2:H:2764:LEU:HD11	2.56	0.41
2:H:4023:LYS:HA	2:H:4026:ASP:HB2	2.01	0.41
2:B:551:PHE:HD1	2:B:551:PHE:HA	1.70	0.41
2:B:4810:MET:CG	2:D:4521:TYR:H	2.34	0.41
2:D:195:SER:HB3	2:D:202:HIS:HB2	2.02	0.41
2:D:2731:ASP:HB3	2:D:2826:ALA:HB2	2.00	0.41
2:D:3993:ASN:HD22	2:D:4110:MET:HA	1.84	0.41
2:D:4046:LYS:HA	2:D:4049:PHE:HB3	2.01	0.41
2:D:4778:VAL:O	2:D:4782:TYR:HB2	2.19	0.41
1:E:21:THR:OG1	1:E:49:ARG:NE	2.50	0.41
2:F:64:ILE:H	2:F:64:ILE:HG13	1.74	0.41
2:F:1090:ALA:HA	2:F:1249:MET:HG2	2.01	0.41
2:F:1607:ASP:HB3	2:F:1608:VAL:HG23	2.02	0.41
2:F:3760:LEU:HD23	2:F:3760:LEU:HA	1.89	0.41
2:F:3854:ASP:N	2:F:3854:ASP:OD1	2.53	0.41
2:F:4037:ASP:OD2	2:F:4041:LYS:N	2.53	0.41
2:F:4810:MET:HB3	2:H:4519:LEU:HA	2.01	0.41
2:H:412:GLU:O	2:H:415:THR:OG1	2.33	0.41
2:H:1253:LYS:HD2	2:H:1255:LEU:HB2	2.02	0.41
2:H:1607:ASP:HB3	2:H:1608:VAL:HG23	2.02	0.41
2:H:2464:ASP:N	2:H:2464:ASP:OD1	2.50	0.41
2:H:3730:ALA:HA	2:H:3733:HIS:CE1	2.54	0.41
2:B:77:ALA:HA	2:D:3891:TRP:CZ3	2.56	0.41
2:B:372:LEU:HD11	2:B:391:ALA:HB1	2.03	0.41
2:B:416:ALA:O	2:B:420:ARG:NH2	2.51	0.41
2:B:782:PHE:HZ	2:B:1467:VAL:HG22	1.86	0.41
2:B:2730:HIS:CE1	2:B:2764:LEU:HD11	2.56	0.41
2:D:1505:LEU:O	2:D:1523:ASN:N	2.52	0.41
2:D:2834:LEU:HB2	2:D:2839:HIS:CE1	2.54	0.41
2:D:4011:VAL:HA	2:D:4014:ILE:HG12	2.03	0.41
2:F:682:THR:H	2:F:751:THR:HG22	1.85	0.41
2:F:1843:LEU:O	2:F:1846:ILE:N	2.54	0.41
2:F:3682:LYS:HZ3	2:F:3684:GLU:HA	1.84	0.41
2:B:195:SER:HB3	2:B:202:HIS:HB2	2.02	0.41
2:B:416:ALA:HA	2:B:419:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2834:LEU:HD22	2:B:2838:LEU:HB3	2.02	0.41
2:B:3682:LYS:HZ3	2:B:3684:GLU:HG2	1.85	0.41
2:D:420:ARG:HA	2:D:423:VAL:HB	2.02	0.41
2:D:1843:LEU:O	2:D:1846:ILE:N	2.54	0.41
2:F:1764:SER:N	2:F:1779:SER:O	2.53	0.41
2:F:3983:LEU:HD12	2:F:3983:LEU:HA	1.87	0.41
2:F:4189:LEU:HA	2:F:4192:ASN:HD22	1.86	0.41
2:H:123:HIS:CD2	2:H:126:SER:H	2.38	0.41
2:H:1156:TRP:CZ3	2:H:1158:ALA:HA	2.56	0.41
2:H:1572:LYS:HB3	2:H:1584:PRO:HA	2.02	0.41
2:H:1738:LEU:HD21	2:H:2039:TYR:HE1	1.86	0.41
2:H:2843:GLU:OE2	2:H:2875:TYR:OH	2.34	0.41
2:H:3797:LEU:HA	2:H:3797:LEU:HD23	1.88	0.41
2:H:3834:ASP:OD1	2:H:3834:ASP:N	2.53	0.41
2:H:4189:LEU:HA	2:H:4192:ASN:HD22	1.86	0.41
2:B:585:ALA:HA	2:B:588:ILE:HD12	2.02	0.41
2:B:1169:THR:OG1	2:B:1170:GLU:N	2.54	0.41
2:B:1285:VAL:HG12	2:B:1286:THR:HG23	2.03	0.41
2:B:3854:ASP:OD1	2:B:3854:ASP:N	2.53	0.41
2:B:4863:ILE:HG22	2:H:4857:VAL:HG11	2.01	0.41
1:C:15:PHE:HA	1:C:67:SER:HA	2.02	0.41
2:D:554:SER:O	2:D:558:LEU:N	2.49	0.41
2:D:1033:VAL:HG23	2:D:1038:LEU:HB3	2.01	0.41
2:D:2063:ILE:O	2:D:2067:MET:HG2	2.21	0.41
2:D:3897:ASP:OD1	2:D:3958:LYS:NZ	2.40	0.41
2:D:4811:LEU:O	2:D:4814:TYR:HB3	2.19	0.41
2:F:1156:TRP:CZ3	2:F:1158:ALA:HA	2.56	0.41
2:F:1253:LYS:HD2	2:F:1255:LEU:HB2	2.02	0.41
2:F:1267:HIS:NE2	2:F:1293:GLN:OE1	2.53	0.41
2:F:1738:LEU:HD21	2:F:2039:TYR:HE1	1.86	0.41
2:F:2063:ILE:O	2:F:2067:MET:HG2	2.21	0.41
2:F:4811:LEU:O	2:F:4814:TYR:HB3	2.20	0.41
2:F:4889:CYS:HB2	2:F:4892:CYS:HB3	2.03	0.41
2:H:290:ARG:HA	2:H:353:GLU:HG2	2.02	0.41
2:H:875:PRO:HG2	2:H:878:LEU:HD12	2.02	0.41
2:H:1449:ASP:OD1	2:H:1449:ASP:N	2.52	0.41
2:B:290:ARG:HA	2:B:353:GLU:HG2	2.02	0.41
2:B:1156:TRP:CZ3	2:B:1158:ALA:HA	2.56	0.41
2:B:3993:ASN:HD22	2:B:4110:MET:HA	1.84	0.41
2:B:4189:LEU:HA	2:B:4192:ASN:HD22	1.86	0.41
2:D:123:HIS:CD2	2:D:126:SER:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:585:ALA:HA	2:D:588:ILE:HD12	2.02	0.41
2:D:782:PHE:HZ	2:D:1467:VAL:HG22	1.86	0.41
2:D:1153:GLY:N	2:D:1183:LEU:O	2.53	0.41
2:D:1156:TRP:CZ3	2:D:1158:ALA:HA	2.56	0.41
2:D:4810:MET:CG	2:F:4521:TYR:H	2.34	0.41
2:F:2730:HIS:CE1	2:F:2764:LEU:HD11	2.56	0.41
2:F:4865:GLY:HA2	2:H:4868:ILE:HD11	2.03	0.41
2:H:64:ILE:H	2:H:64:ILE:HG13	1.74	0.41
2:H:372:LEU:HD11	2:H:391:ALA:HB1	2.03	0.41
2:H:554:SER:O	2:H:558:LEU:N	2.49	0.41
2:H:1169:THR:OG1	2:H:1170:GLU:N	2.54	0.41
2:H:4834:ASP:OD1	2:H:4834:ASP:N	2.52	0.41
2:B:411:GLU:HA	2:B:414:ARG:HB2	2.03	0.41
2:B:1843:LEU:O	2:B:1846:ILE:N	2.54	0.41
2:B:2063:ILE:O	2:B:2067:MET:HG2	2.21	0.41
2:F:416:ALA:HA	2:F:419:ILE:HD12	2.02	0.41
2:F:1757:LEU:HA	2:F:1757:LEU:HD13	1.83	0.41
2:F:4125:SER:HA	2:F:4128:ASN:HD22	1.86	0.41
2:F:4857:VAL:HG13	2:H:4863:ILE:HG22	1.96	0.41
2:H:416:ALA:HA	2:H:419:ILE:HD12	2.02	0.41
2:H:1843:LEU:HD23	2:H:1843:LEU:HA	1.88	0.41
2:H:3993:ASN:HD22	2:H:4110:MET:HA	1.84	0.41
2:H:4011:VAL:HA	2:H:4014:ILE:HG12	2.03	0.41
2:H:4518:LEU:HD23	2:H:4518:LEU:H	1.86	0.41
1:A:21:THR:OG1	1:A:49:ARG:NE	2.50	0.41
2:B:26:ALA:O	2:B:33:GLN:N	2.49	0.41
2:B:130:LEU:HA	2:B:149:LEU:HD23	2.03	0.41
2:B:420:ARG:HA	2:B:423:VAL:HB	2.02	0.41
2:B:1676:LEU:HD23	2:B:1676:LEU:HA	1.87	0.41
2:B:1738:LEU:HD21	2:B:2039:TYR:HE1	1.86	0.41
2:B:3762:LEU:HD12	2:B:3762:LEU:HA	1.86	0.41
2:B:4202:GLN:O	2:B:4206:GLN:HB3	2.20	0.41
2:B:4611:LEU:HD21	2:B:4617:TYR:HD2	1.84	0.41
2:D:130:LEU:HA	2:D:149:LEU:HD23	2.03	0.41
2:D:150:GLN:NE2	2:D:152:ASP:O	2.54	0.41
2:D:486:GLN:OE1	2:D:547:ASN:ND2	2.54	0.41
2:D:3767:LEU:HD23	2:D:3767:LEU:HA	1.84	0.41
2:D:4780:TYR:OH	2:F:4518:LEU:HB2	2.21	0.41
2:D:4889:CYS:HB2	2:D:4892:CYS:HB3	2.03	0.41
2:F:123:HIS:CD2	2:F:126:SER:H	2.38	0.41
2:F:415:THR:O	2:F:419:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1440:ASN:HB2	2:F:1548:THR:HG21	2.03	0.41
2:F:1789:ALA:HA	2:F:1792:ILE:HD12	2.01	0.41
2:F:1999:ASP:O	2:F:2003:ASP:N	2.54	0.41
1:G:15:PHE:HA	1:G:67:SER:HA	2.02	0.41
2:H:121:LEU:HD23	2:H:121:LEU:HA	1.86	0.41
2:H:1157:GLN:N	2:H:1160:ASP:OD2	2.54	0.41
2:H:1177:LEU:N	2:H:1180:GLU:O	2.54	0.41
2:H:1285:VAL:HG12	2:H:1286:THR:HG23	2.03	0.41
2:H:1999:ASP:O	2:H:2003:ASP:N	2.54	0.41
2:H:2011:GLU:O	2:H:2027:ARG:NH2	2.54	0.41
2:H:2063:ILE:O	2:H:2067:MET:HG2	2.21	0.41
2:H:2894:LEU:HA	2:H:2897:LEU:HD12	2.02	0.41
2:H:3831:LEU:HA	2:H:3831:LEU:HD23	1.85	0.41
2:B:486:GLN:OE1	2:B:547:ASN:ND2	2.54	0.41
2:B:1136:ALA:HB3	2:B:1145:TRP:HB2	2.03	0.41
2:B:2326:ILE:HD12	2:H:207:PHE:HZ	1.72	0.41
2:B:4834:ASP:N	2:B:4834:ASP:OD1	2.52	0.41
2:D:1440:ASN:HB2	2:D:1548:THR:HG21	2.03	0.41
2:D:1753:LEU:HD11	2:D:1921:HIS:CD2	2.56	0.41
2:D:1764:SER:N	2:D:1779:SER:O	2.53	0.41
2:D:2549:LEU:O	2:D:2553:VAL:N	2.54	0.41
2:D:4189:LEU:HA	2:D:4192:ASN:HD22	1.86	0.41
2:F:123:HIS:NE2	2:F:125:TYR:HB3	2.36	0.41
2:F:130:LEU:HA	2:F:149:LEU:HD23	2.03	0.41
2:F:486:GLN:OE1	2:F:547:ASN:ND2	2.54	0.41
2:F:2088:LEU:O	2:F:2092:GLN:HG2	2.21	0.41
2:F:2177:VAL:HG22	2:F:2221:TYR:CZ	2.56	0.41
2:F:4113:ASP:O	2:F:4117:GLN:N	2.46	0.41
2:H:486:GLN:OE1	2:H:547:ASN:ND2	2.54	0.41
2:H:1255:LEU:HA	2:H:1256:PRO:HD3	1.88	0.41
2:H:1611:ILE:N	2:H:1620:GLN:O	2.44	0.41
2:H:1789:ALA:HA	2:H:1792:ILE:HD12	2.01	0.41
2:H:2298:ARG:HD3	2:H:2298:ARG:HA	1.90	0.41
2:H:3767:LEU:HA	2:H:3767:LEU:HD23	1.84	0.41
2:B:123:HIS:NE2	2:B:125:TYR:HB3	2.36	0.40
2:B:699:SER:OG	2:B:701:GLU:O	2.31	0.40
2:B:1572:LYS:HB3	2:B:1584:PRO:HA	2.02	0.40
2:B:1655:TYR:OH	2:B:1659:ARG:NH2	2.51	0.40
2:B:3871:ILE:O	2:B:3874:SER:OG	2.40	0.40
2:B:4113:ASP:HB2	2:B:4116:LEU:HB3	2.03	0.40
2:D:1177:LEU:N	2:D:1180:GLU:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4011:VAL:HA	2:F:4014:ILE:HG12	2.03	0.40
2:H:119:ILE:HD13	2:H:162:ILE:HD11	2.02	0.40
2:H:1136:ALA:HB3	2:H:1145:TRP:HB2	2.03	0.40
2:H:1843:LEU:O	2:H:1846:ILE:N	2.54	0.40
2:H:1940:ASN:O	2:H:1944:ARG:HG2	2.21	0.40
2:H:2177:VAL:HG22	2:H:2221:TYR:CZ	2.56	0.40
2:H:3663:ASP:HA	2:H:3664:PRO:HD3	1.95	0.40
2:B:1157:GLN:N	2:B:1160:ASP:OD2	2.54	0.40
2:B:1177:LEU:N	2:B:1180:GLU:O	2.54	0.40
2:B:1255:LEU:HA	2:B:1256:PRO:HD3	1.88	0.40
2:B:2177:VAL:HG22	2:B:2221:TYR:CZ	2.56	0.40
2:B:4011:VAL:HA	2:B:4014:ILE:HG12	2.03	0.40
2:B:4036:TYR:HE2	2:B:4048:ASP:HB3	1.85	0.40
2:B:4889:CYS:HB2	2:B:4892:CYS:HB3	2.03	0.40
2:D:411:GLU:HA	2:D:414:ARG:HB2	2.03	0.40
2:D:415:THR:O	2:D:419:ILE:HG13	2.21	0.40
2:D:1253:LYS:HD2	2:D:1255:LEU:HB2	2.02	0.40
2:D:1645:THR:H	2:D:1645:THR:HG23	1.68	0.40
2:D:4957:ASP:OD1	2:D:4957:ASP:N	2.54	0.40
2:F:191:TYR:N	2:F:206:ALA:O	2.54	0.40
2:H:411:GLU:HA	2:H:414:ARG:HB2	2.03	0.40
2:H:782:PHE:HZ	2:H:1467:VAL:HG22	1.86	0.40
2:H:2157:TYR:OH	2:H:2203:TYR:OH	2.26	0.40
2:H:3871:ILE:O	2:H:3874:SER:OG	2.40	0.40
2:H:3983:LEU:HD12	2:H:3983:LEU:HA	1.88	0.40
2:H:4713:VAL:O	2:H:4716:THR:OG1	2.27	0.40
2:B:119:ILE:HD13	2:B:162:ILE:HD11	2.02	0.40
2:B:717:GLY:H	2:B:722:LEU:HB3	1.86	0.40
2:B:1137:PHE:CE2	2:B:1139:GLY:HA2	2.57	0.40
2:B:1709:ILE:HD13	2:B:1709:ILE:HA	1.94	0.40
2:B:1753:LEU:HD11	2:B:1921:HIS:CD2	2.56	0.40
2:B:4023:LYS:HA	2:B:4026:ASP:HB2	2.01	0.40
2:B:4808:ASP:CG	2:D:4523:VAL:CG2	2.62	0.40
2:D:1157:GLN:N	2:D:1160:ASP:OD2	2.54	0.40
2:D:1999:ASP:O	2:D:2003:ASP:N	2.54	0.40
2:D:2157:TYR:OH	2:D:2203:TYR:OH	2.26	0.40
2:D:2834:LEU:HD22	2:D:2838:LEU:HB3	2.02	0.40
1:E:78:PRO:HA	1:E:81:ALA:HB3	2.04	0.40
2:F:297:LEU:HD23	2:F:297:LEU:HA	1.87	0.40
2:F:585:ALA:HA	2:F:588:ILE:HD12	2.02	0.40
2:F:653:SER:OG	2:F:794:PHE:O	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2011:GLU:O	2:F:2027:ARG:NH2	2.54	0.40
2:H:415:THR:O	2:H:419:ILE:HG13	2.21	0.40
2:H:517:VAL:HG23	2:H:520:ARG:NE	2.35	0.40
2:H:678:MET:O	2:H:801:ARG:N	2.46	0.40
2:H:3762:LEU:HA	2:H:3762:LEU:HD12	1.86	0.40
2:H:4113:ASP:HB2	2:H:4116:LEU:HB3	2.03	0.40
2:B:3893:TYR:CE2	2:B:3899:ILE:HG23	2.57	0.40
2:D:123:HIS:NE2	2:D:125:TYR:HB3	2.36	0.40
2:D:228:LEU:HD23	2:D:228:LEU:HA	1.82	0.40
2:D:976:TYR:CZ	2:D:978:PRO:HG3	2.57	0.40
2:D:1136:ALA:HB3	2:D:1145:TRP:HB2	2.03	0.40
2:D:1505:LEU:HD23	2:D:1505:LEU:HA	1.97	0.40
2:D:2088:LEU:O	2:D:2092:GLN:HG2	2.21	0.40
2:D:4518:LEU:H	2:D:4518:LEU:HD23	1.86	0.40
2:F:459:LEU:HD23	2:F:459:LEU:HA	1.86	0.40
2:F:973:THR:HG23	2:F:977:LYS:HB3	2.04	0.40
2:F:976:TYR:CZ	2:F:978:PRO:HG3	2.57	0.40
2:F:1177:LEU:N	2:F:1180:GLU:O	2.54	0.40
2:F:1305:SER:HB2	2:F:1593:HIS:CD2	2.57	0.40
2:F:1707:ILE:HG22	2:F:1712:SER:HB3	2.04	0.40
2:F:4518:LEU:HD23	2:F:4518:LEU:H	1.86	0.40
2:H:626:ARG:NH2	2:H:1668:GLY:O	2.36	0.40
2:H:1902:PRO:HA	2:H:1905:LEU:HB3	2.04	0.40
2:H:4125:SER:HA	2:H:4128:ASN:HD22	1.86	0.40
2:B:1253:LYS:HD2	2:B:1255:LEU:HB2	2.02	0.40
2:B:2088:LEU:O	2:B:2092:GLN:HG2	2.21	0.40
2:B:4518:LEU:H	2:B:4518:LEU:HD23	1.86	0.40
2:D:517:VAL:HG23	2:D:520:ARG:NE	2.35	0.40
2:D:647:ARG:HD2	2:D:647:ARG:HA	1.84	0.40
2:D:4113:ASP:HB2	2:D:4116:LEU:HB3	2.03	0.40
2:F:36:CYS:O	2:F:50:GLU:N	2.55	0.40
2:F:412:GLU:O	2:F:415:THR:OG1	2.33	0.40
2:H:36:CYS:O	2:H:50:GLU:N	2.55	0.40
2:H:1753:LEU:HD11	2:H:1921:HIS:CD2	2.56	0.40
2:H:1833:ILE:HG22	2:H:1834:PHE:H	1.87	0.40
2:H:1905:LEU:HB2	2:H:2081:LEU:HD12	2.04	0.40
2:H:3893:TYR:CE2	2:H:3899:ILE:HG23	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	C	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	E	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	G	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3365/4968 (68%)	2969 (88%)	382 (11%)	14 (0%)	34	72
2	D	3365/4968 (68%)	2969 (88%)	382 (11%)	14 (0%)	34	72
2	F	3365/4968 (68%)	2968 (88%)	383 (11%)	14 (0%)	34	72
2	H	3365/4968 (68%)	2968 (88%)	383 (11%)	14 (0%)	34	72
All	All	13880/20304 (68%)	12254 (88%)	1570 (11%)	56 (0%)	38	72

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	143	LEU
2	B	4595	LYS
2	D	143	LEU
2	D	4595	LYS
2	F	143	LEU
2	F	4595	LYS
2	H	143	LEU
2	H	4595	LYS
2	B	730	LEU
2	B	4518	LEU
2	D	730	LEU
2	D	4518	LEU
2	F	730	LEU
2	F	4518	LEU
2	H	730	LEU
2	H	4518	LEU
2	B	142	LYS

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Mol	Chain	Res	Type
2	B	1580	PRO
2	B	4071	ALA
2	D	142	LYS
2	D	1580	PRO
2	D	4071	ALA
2	F	142	LYS
2	F	1580	PRO
2	F	4071	ALA
2	H	142	LYS
2	H	1580	PRO
2	H	4071	ALA
2	B	4903	PRO
2	F	4903	PRO
2	H	4903	PRO
2	B	2233	PRO
2	D	2233	PRO
2	D	4903	PRO
2	F	2233	PRO
2	H	2233	PRO
2	B	1848	PRO
2	D	1848	PRO
2	F	1848	PRO
2	H	1848	PRO
2	B	3803	VAL
2	D	3803	VAL
2	F	3803	VAL
2	B	853	PRO
2	B	1535	PRO
2	D	853	PRO
2	F	853	PRO
2	H	853	PRO
2	H	1535	PRO
2	H	3803	VAL
2	B	828	PRO
2	D	828	PRO
2	D	1535	PRO
2	F	828	PRO
2	F	1535	PRO
2	H	828	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/89 (99%)	87 (99%)	1 (1%)	73 85
1	C	88/89 (99%)	87 (99%)	1 (1%)	73 85
1	E	88/89 (99%)	87 (99%)	1 (1%)	73 85
1	G	88/89 (99%)	87 (99%)	1 (1%)	73 85
2	B	2688/4355 (62%)	2655 (99%)	33 (1%)	71 84
2	D	2688/4355 (62%)	2655 (99%)	33 (1%)	71 84
2	F	2688/4355 (62%)	2655 (99%)	33 (1%)	71 84
2	H	2689/4355 (62%)	2655 (99%)	34 (1%)	69 82
All	All	11105/17776 (62%)	10968 (99%)	137 (1%)	72 84

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
2	B	44	ASN
2	B	84	ASN
2	B	298	ARG
2	B	420	ARG
2	B	531	ASN
2	B	628	ASN
2	B	658	ASN
2	B	841	LYS
2	B	854	THR
2	B	925	PRO
2	B	990	PRO
2	B	1054	VAL
2	B	1089	ARG
2	B	2027	ARG
2	B	2118	ILE
2	B	2206	ARG
2	B	2211	ASN
2	B	2328	ARG

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Mol	Chain	Res	Type
2	B	3813	ASN
2	B	3870	ASN
2	B	3906	ASN
2	B	4087	ARG
2	B	4136	ARG
2	B	4171	ARG
2	B	4179	ASN
2	B	4499	ASN
2	B	4518	LEU
2	B	4519	LEU
2	B	4652	ARG
2	B	4792	LYS
2	B	4809	ASP
2	B	4900	ASP
2	B	4902	VAL
1	C	13	ARG
2	D	44	ASN
2	D	84	ASN
2	D	298	ARG
2	D	420	ARG
2	D	531	ASN
2	D	628	ASN
2	D	658	ASN
2	D	841	LYS
2	D	854	THR
2	D	925	PRO
2	D	950	VAL
2	D	990	PRO
2	D	1089	ARG
2	D	2027	ARG
2	D	2118	ILE
2	D	2206	ARG
2	D	2211	ASN
2	D	2328	ARG
2	D	3813	ASN
2	D	3870	ASN
2	D	3906	ASN
2	D	4087	ARG
2	D	4136	ARG
2	D	4171	ARG
2	D	4179	ASN
2	D	4499	ASN

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Mol	Chain	Res	Type
2	D	4518	LEU
2	D	4519	LEU
2	D	4652	ARG
2	D	4792	LYS
2	D	4809	ASP
2	D	4900	ASP
2	D	4902	VAL
1	E	13	ARG
2	F	44	ASN
2	F	84	ASN
2	F	298	ARG
2	F	420	ARG
2	F	531	ASN
2	F	628	ASN
2	F	658	ASN
2	F	841	LYS
2	F	854	THR
2	F	925	PRO
2	F	950	VAL
2	F	990	PRO
2	F	1089	ARG
2	F	2027	ARG
2	F	2118	ILE
2	F	2206	ARG
2	F	2211	ASN
2	F	2328	ARG
2	F	3813	ASN
2	F	3870	ASN
2	F	3906	ASN
2	F	4087	ARG
2	F	4136	ARG
2	F	4171	ARG
2	F	4179	ASN
2	F	4499	ASN
2	F	4518	LEU
2	F	4519	LEU
2	F	4652	ARG
2	F	4792	LYS
2	F	4809	ASP
2	F	4900	ASP
2	F	4902	VAL
1	G	13	ARG

Continued on next page...

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Mol	Chain	Res	Type
2	H	44	ASN
2	H	84	ASN
2	H	298	ARG
2	H	420	ARG
2	H	531	ASN
2	H	628	ASN
2	H	658	ASN
2	H	841	LYS
2	H	854	THR
2	H	925	PRO
2	H	950	VAL
2	H	990	PRO
2	H	1054	VAL
2	H	1089	ARG
2	H	2027	ARG
2	H	2118	ILE
2	H	2206	ARG
2	H	2211	ASN
2	H	2328	ARG
2	H	3813	ASN
2	H	3870	ASN
2	H	3906	ASN
2	H	4087	ARG
2	H	4136	ARG
2	H	4171	ARG
2	H	4179	ASN
2	H	4499	ASN
2	H	4518	LEU
2	H	4519	LEU
2	H	4652	ARG
2	H	4792	LYS
2	H	4809	ASP
2	H	4900	ASP
2	H	4902	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	B	44	ASN
2	B	57	ASN
2	B	123	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	150	GLN
2	B	252	HIS
2	B	293	GLN
2	B	375	GLN
2	B	394	HIS
2	B	398	HIS
2	B	477	ASN
2	B	531	ASN
2	B	547	ASN
2	B	628	ASN
2	B	681	HIS
2	B	776	GLN
2	B	888	ASN
2	B	1147	GLN
2	B	1265	HIS
2	B	1620	GLN
2	B	1656	HIS
2	B	1691	ASN
2	B	1722	ASN
2	B	1772	ASN
2	B	1918	GLN
2	B	1940	ASN
2	B	2060	GLN
2	B	2152	ASN
2	B	2225	ASN
2	B	2317	ASN
2	B	2831	ASN
2	B	3813	ASN
2	B	3852	ASN
2	B	3856	GLN
2	B	3870	ASN
2	B	3904	GLN
2	B	3906	ASN
2	B	3919	ASN
2	B	3954	HIS
2	B	3956	GLN
2	B	3965	GLN
2	B	3993	ASN
2	B	3999	GLN
2	B	4128	ASN
2	B	4160	GLN
2	B	4499	ASN

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Mol	Chain	Res	Type
2	B	4643	ASN
2	B	4817	HIS
2	B	4878	GLN
2	B	4918	ASN
2	D	23	GLN
2	D	44	ASN
2	D	57	ASN
2	D	123	HIS
2	D	150	GLN
2	D	252	HIS
2	D	293	GLN
2	D	375	GLN
2	D	394	HIS
2	D	398	HIS
2	D	477	ASN
2	D	531	ASN
2	D	547	ASN
2	D	628	ASN
2	D	681	HIS
2	D	888	ASN
2	D	1147	GLN
2	D	1265	HIS
2	D	1620	GLN
2	D	1656	HIS
2	D	1691	ASN
2	D	1722	ASN
2	D	1772	ASN
2	D	1918	GLN
2	D	1921	HIS
2	D	1940	ASN
2	D	2060	GLN
2	D	2152	ASN
2	D	2225	ASN
2	D	2317	ASN
2	D	2831	ASN
2	D	3813	ASN
2	D	3852	ASN
2	D	3856	GLN
2	D	3870	ASN
2	D	3904	GLN
2	D	3906	ASN
2	D	3919	ASN

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Mol	Chain	Res	Type
2	D	3954	HIS
2	D	3956	GLN
2	D	3965	GLN
2	D	3993	ASN
2	D	3999	GLN
2	D	4128	ASN
2	D	4160	GLN
2	D	4179	ASN
2	D	4499	ASN
2	D	4643	ASN
2	D	4817	HIS
2	D	4878	GLN
2	D	4918	ASN
2	F	23	GLN
2	F	44	ASN
2	F	57	ASN
2	F	123	HIS
2	F	150	GLN
2	F	252	HIS
2	F	293	GLN
2	F	375	GLN
2	F	394	HIS
2	F	398	HIS
2	F	477	ASN
2	F	531	ASN
2	F	547	ASN
2	F	628	ASN
2	F	681	HIS
2	F	776	GLN
2	F	888	ASN
2	F	1147	GLN
2	F	1265	HIS
2	F	1620	GLN
2	F	1656	HIS
2	F	1691	ASN
2	F	1772	ASN
2	F	1918	GLN
2	F	1940	ASN
2	F	2152	ASN
2	F	2225	ASN
2	F	2317	ASN
2	F	2831	ASN

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Mol	Chain	Res	Type
2	F	3813	ASN
2	F	3852	ASN
2	F	3856	GLN
2	F	3870	ASN
2	F	3904	GLN
2	F	3906	ASN
2	F	3919	ASN
2	F	3954	HIS
2	F	3956	GLN
2	F	3965	GLN
2	F	3993	ASN
2	F	3999	GLN
2	F	4128	ASN
2	F	4160	GLN
2	F	4179	ASN
2	F	4499	ASN
2	F	4643	ASN
2	F	4817	HIS
2	F	4878	GLN
2	F	4918	ASN
2	H	23	GLN
2	H	44	ASN
2	H	57	ASN
2	H	123	HIS
2	H	150	GLN
2	H	252	HIS
2	H	293	GLN
2	H	375	GLN
2	H	394	HIS
2	H	398	HIS
2	H	477	ASN
2	H	531	ASN
2	H	547	ASN
2	H	628	ASN
2	H	681	HIS
2	H	888	ASN
2	H	1147	GLN
2	H	1265	HIS
2	H	1620	GLN
2	H	1656	HIS
2	H	1691	ASN
2	H	1772	ASN

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Mol	Chain	Res	Type
2	H	1918	GLN
2	H	1940	ASN
2	H	2152	ASN
2	H	2225	ASN
2	H	2317	ASN
2	H	2831	ASN
2	H	3813	ASN
2	H	3852	ASN
2	H	3856	GLN
2	H	3870	ASN
2	H	3904	GLN
2	H	3906	ASN
2	H	3919	ASN
2	H	3954	HIS
2	H	3956	GLN
2	H	3965	GLN
2	H	3993	ASN
2	H	3999	GLN
2	H	4128	ASN
2	H	4160	GLN
2	H	4179	ASN
2	H	4499	ASN
2	H	4643	ASN
2	H	4817	HIS
2	H	4878	GLN
2	H	4918	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

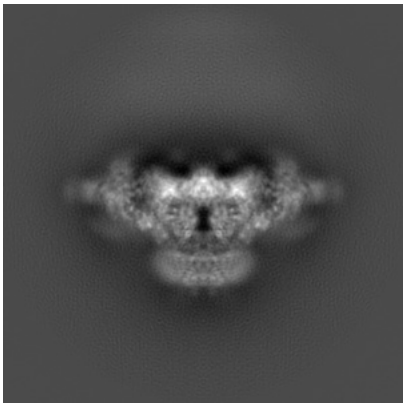
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9824. These allow visual inspection of the internal detail of the map and identification of artifacts.

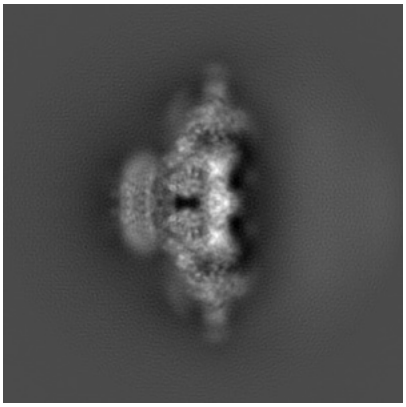
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

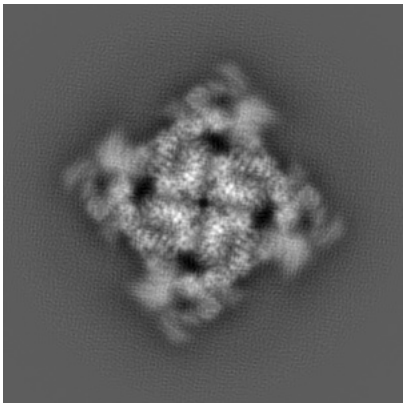
6.1.1 Primary map



X



Y

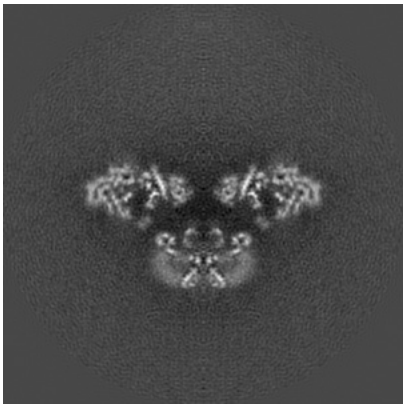


Z

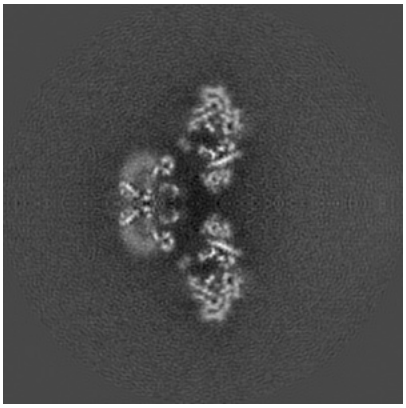
The images above show the map projected in three orthogonal directions.

6.2 Central slices

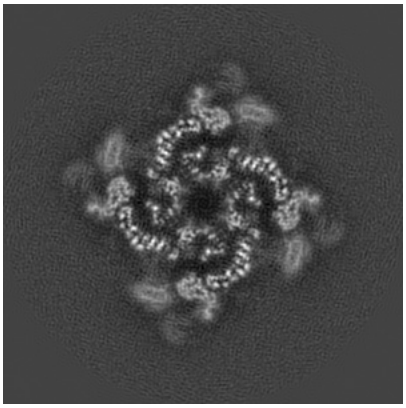
6.2.1 Primary map



X Index: 200



Y Index: 200

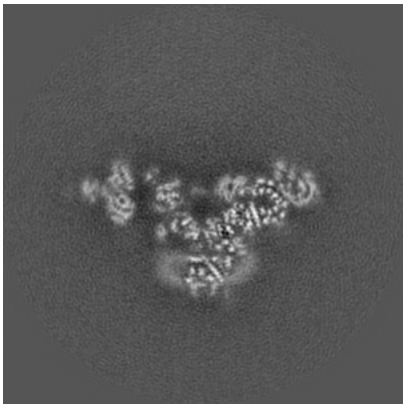


Z Index: 200

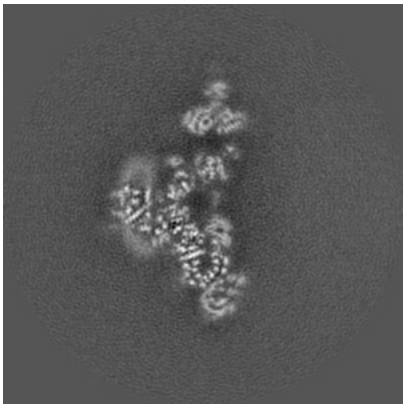
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

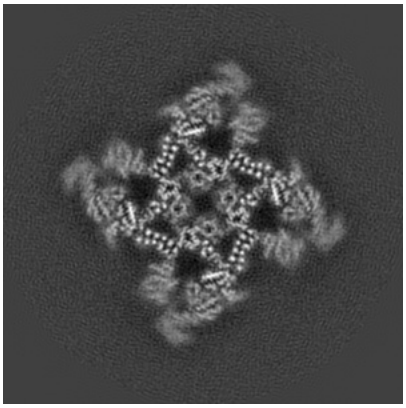
6.3.1 Primary map



X Index: 189



Y Index: 189

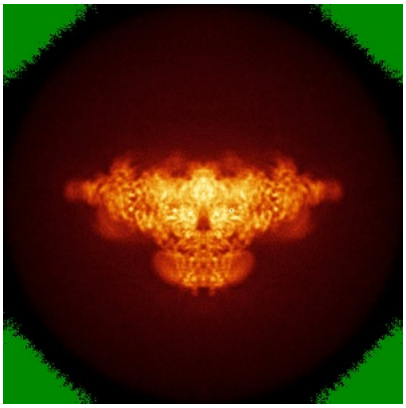


Z Index: 209

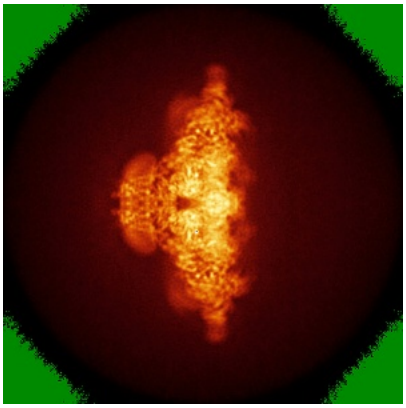
The images above show the largest variance slices of the map in three orthogonal directions.

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

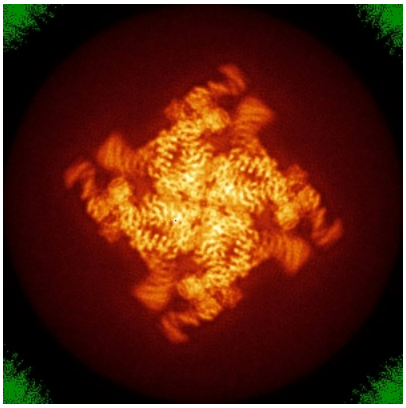
6.4.1 Primary map



X



Y

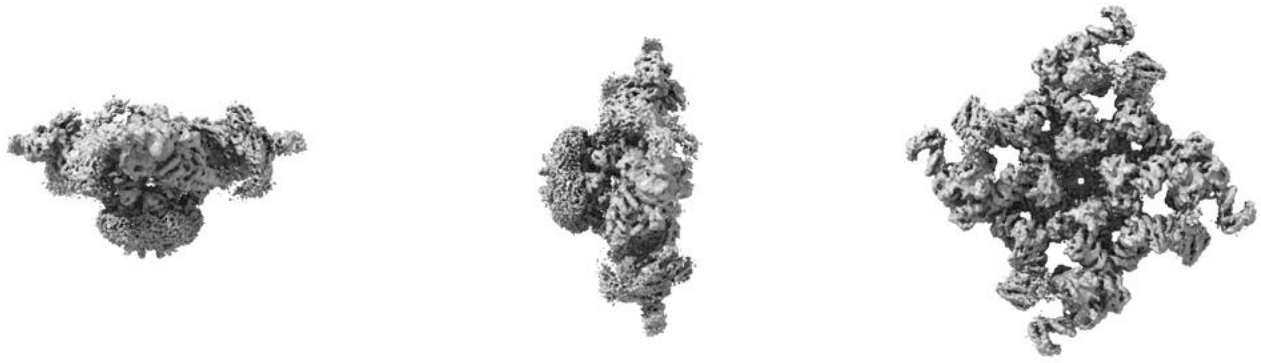


Z

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

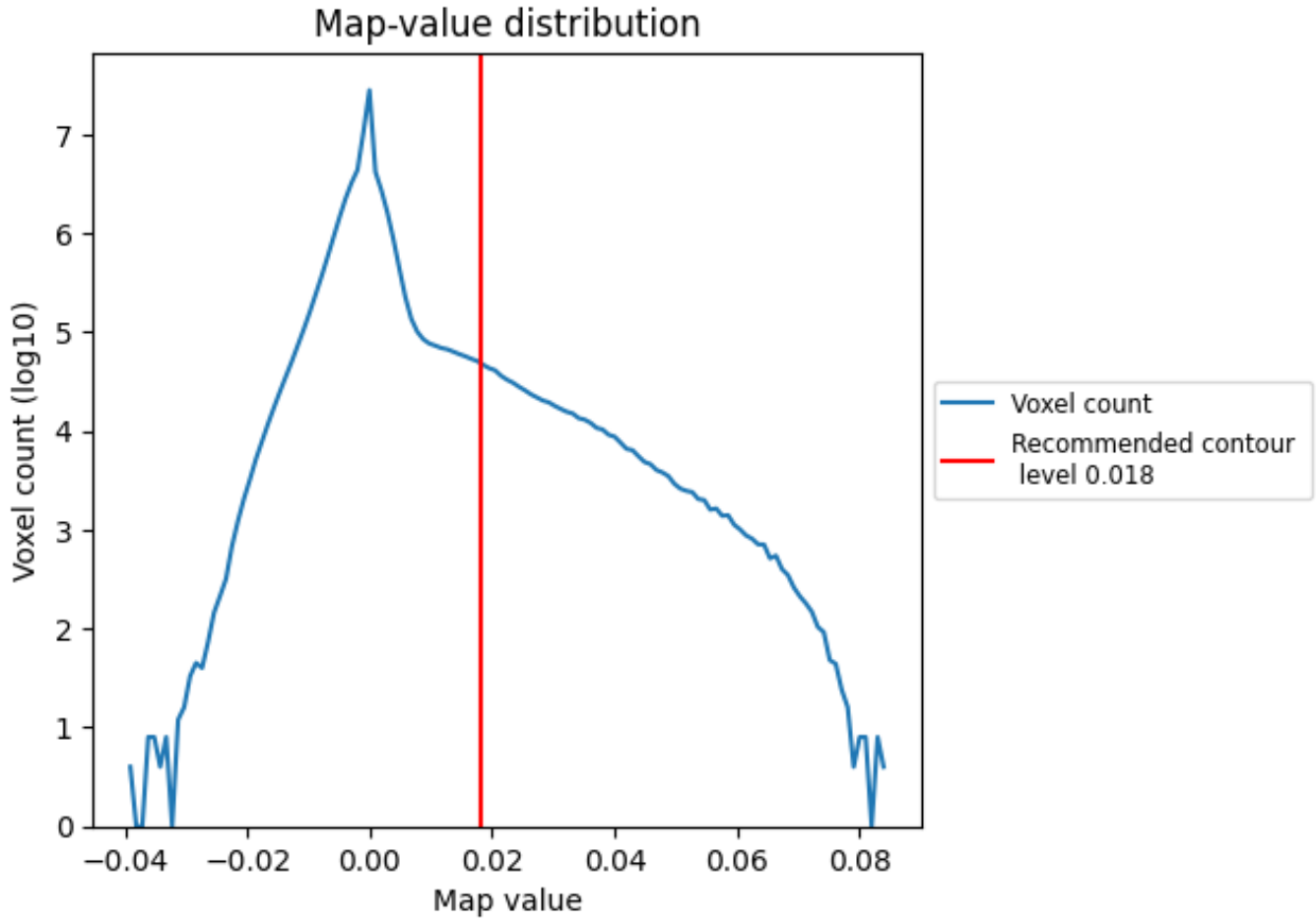
6.6 Mask visualisation (i)

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

7 Map analysis

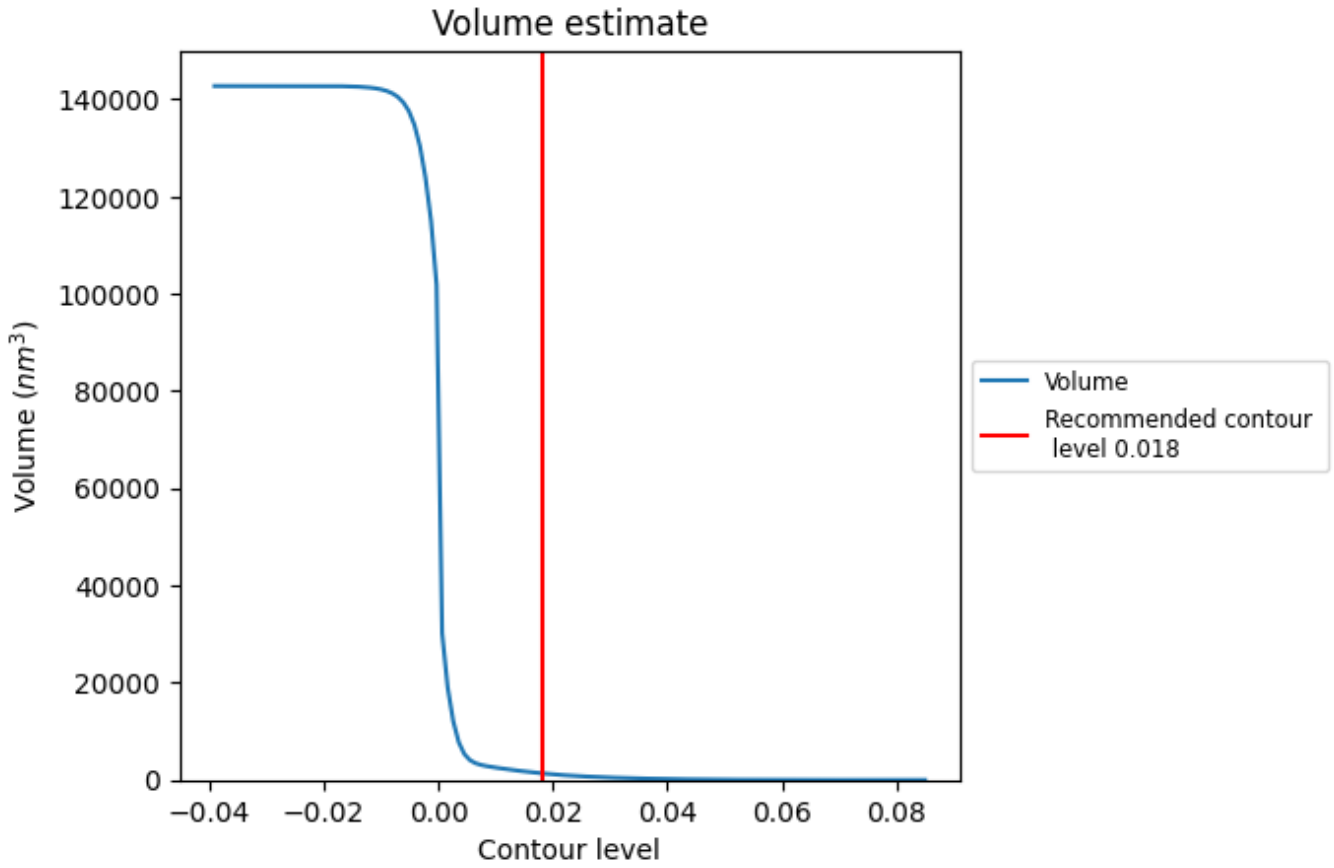
This section contains the results of statistical analysis of the map.

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.

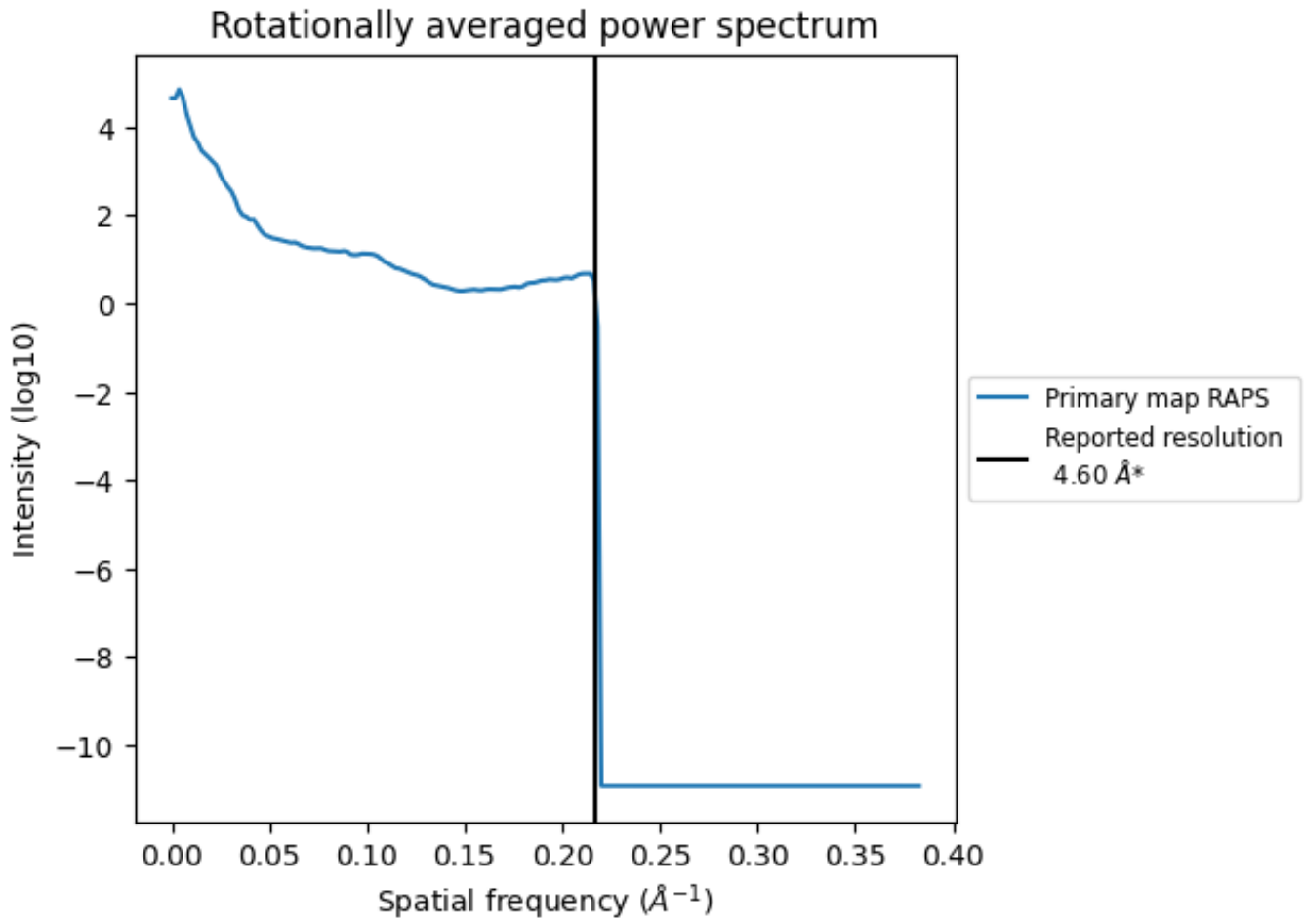
7.2 Volume estimate



The volume at the recommended contour level is 1373 nm^3; this corresponds to an approximate mass of 1240 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)

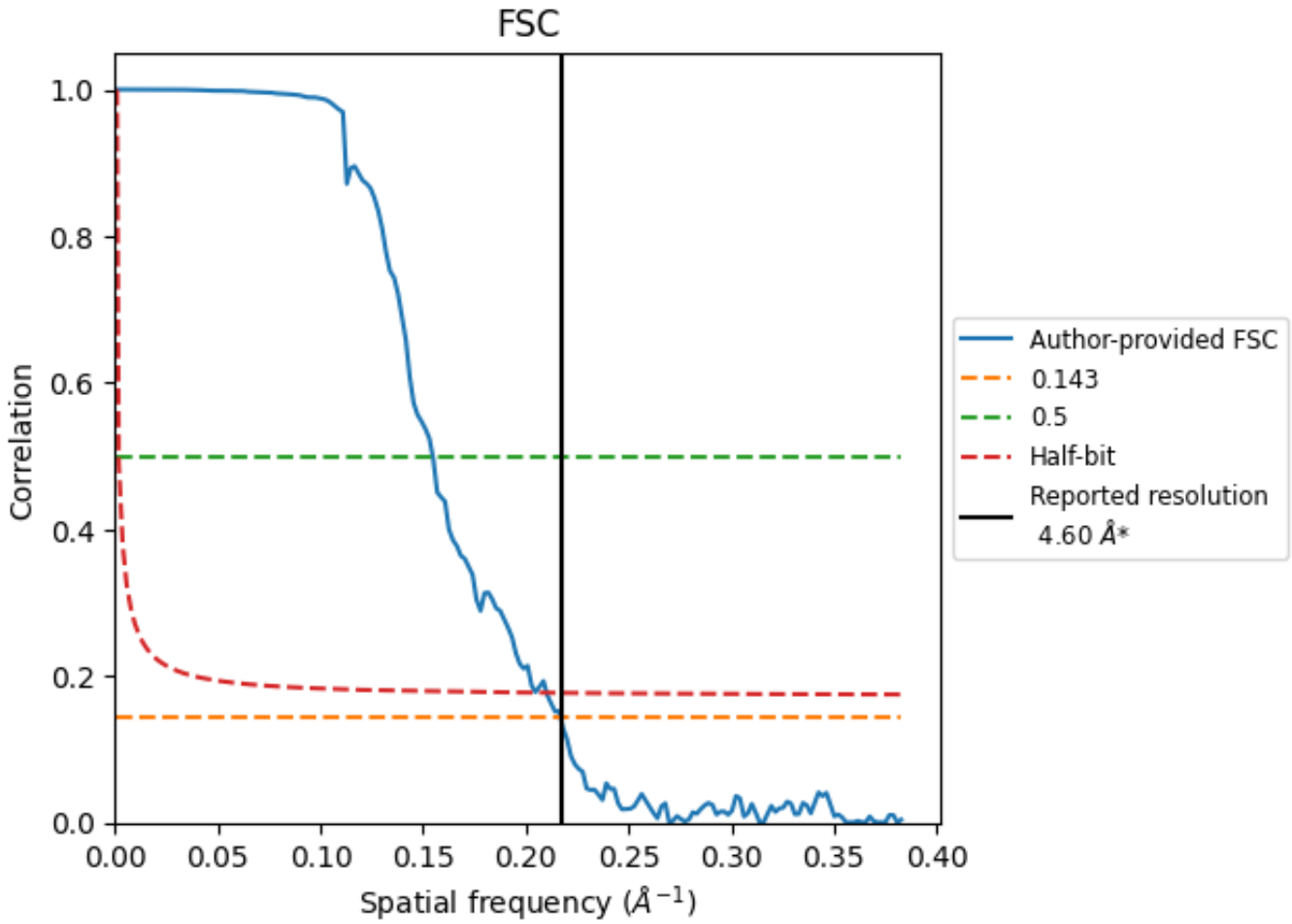


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

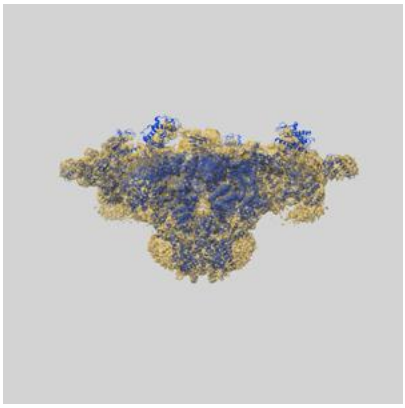
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	6.46	4.76
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

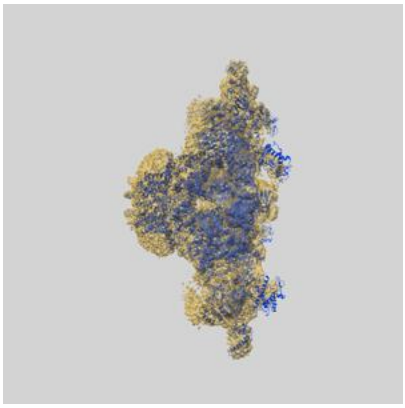
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9824 and PDB model 6JGZ. Per-residue inclusion information can be found in section 3 on page 4.

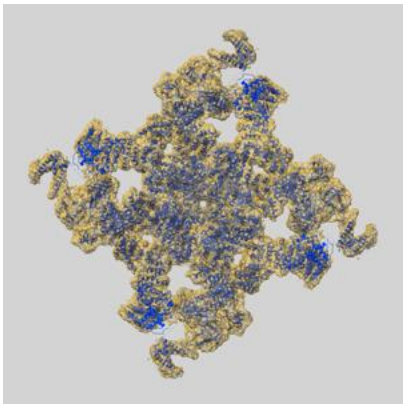
9.1 Map-model overlay



X



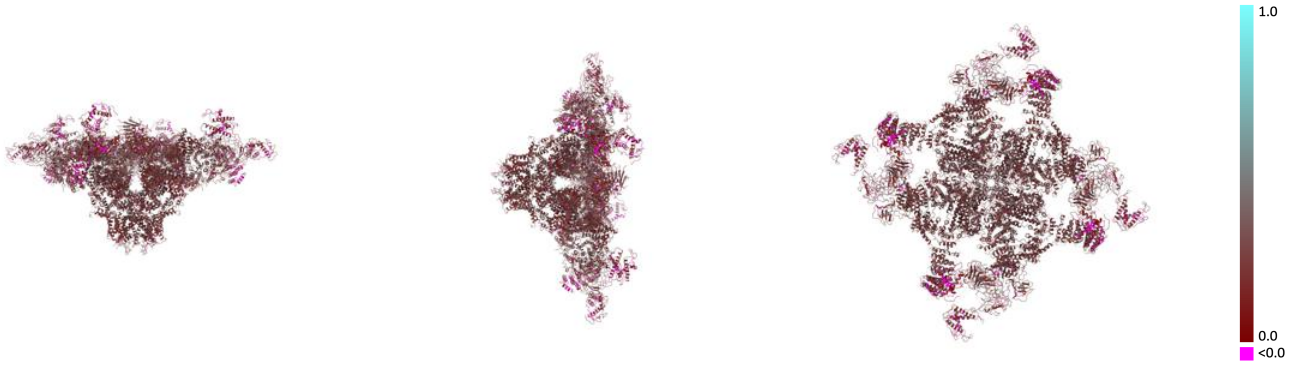
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

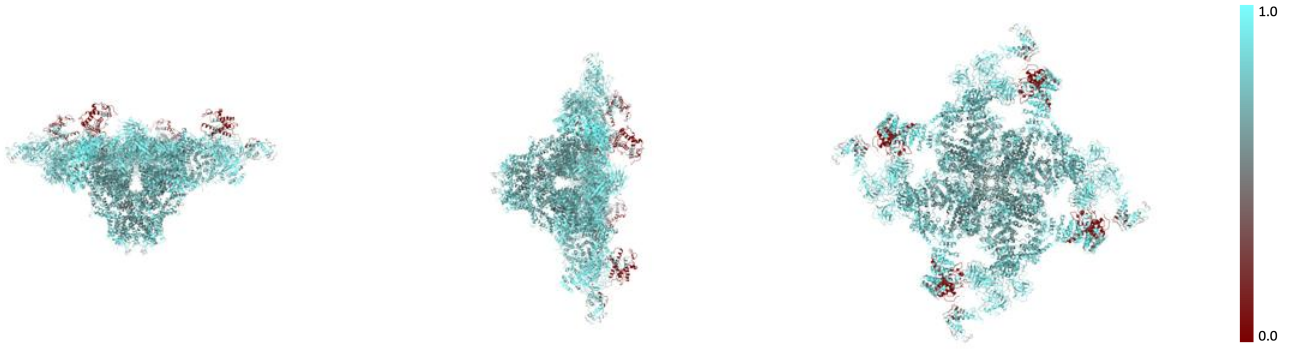
9.2 Q-score mapped to coordinate model (i)



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.

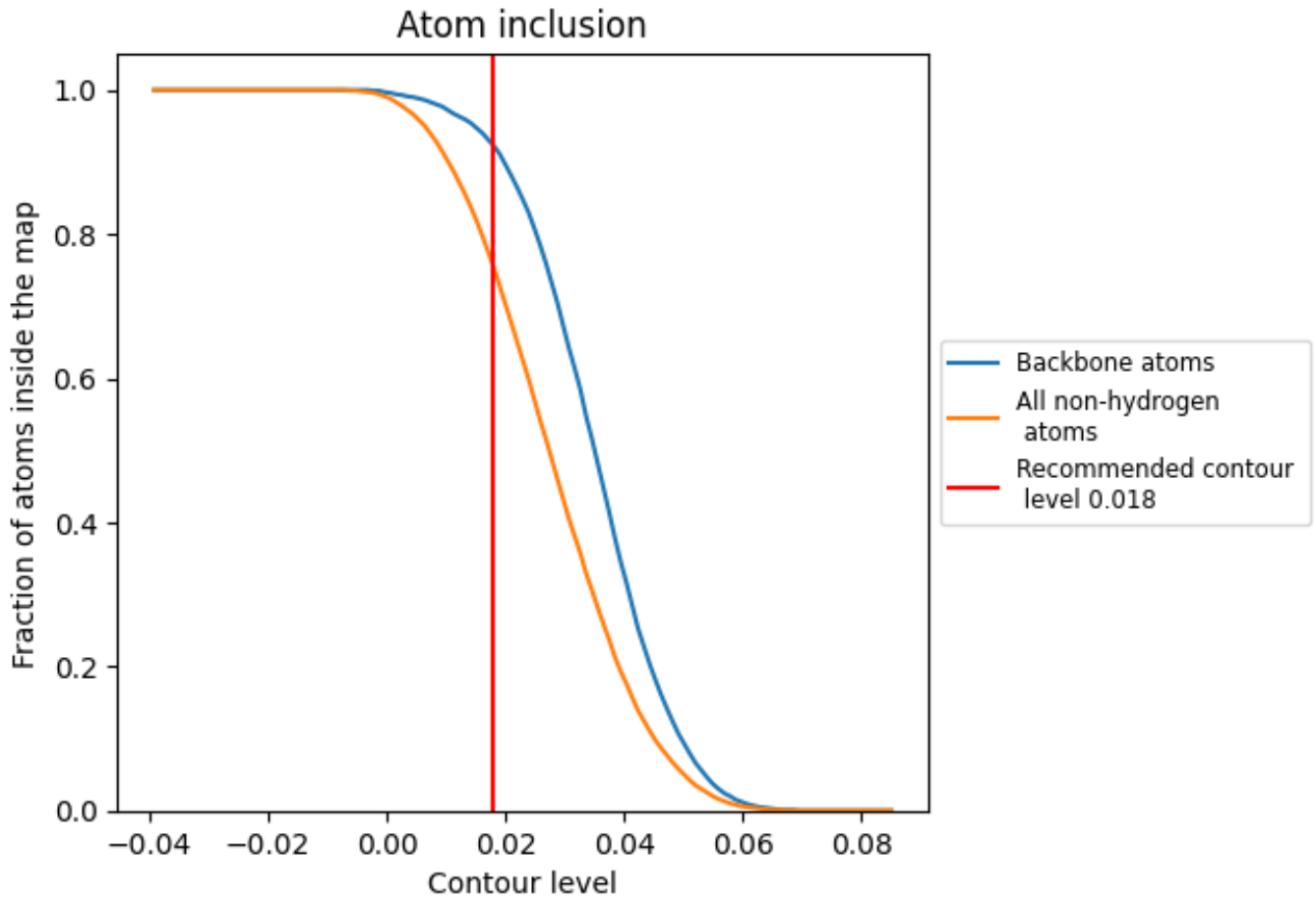
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 76% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.2490
A	0.8170	0.2650
B	0.7530	0.2480
C	0.8190	0.2650
D	0.7530	0.2490
E	0.8170	0.2650
F	0.7530	0.2480
G	0.8140	0.2650
H	0.7530	0.2480