Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 04:08 PM JST

PDB ID	:	7VMN
EMDB ID	:	EMD-33937
Title	:	Structure of recombinant RyR2 (EGTA dataset, class 2, closed state)
Authors	:	Kobayashi, T.; Tsutsumi, A.; Kurebayashi, N.; Kodama, M.; Kikkawa, M.; Murayama, T.; Ogawa, H.
Deposited on	:	2021-10-09
Resolution	:	3.50 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:

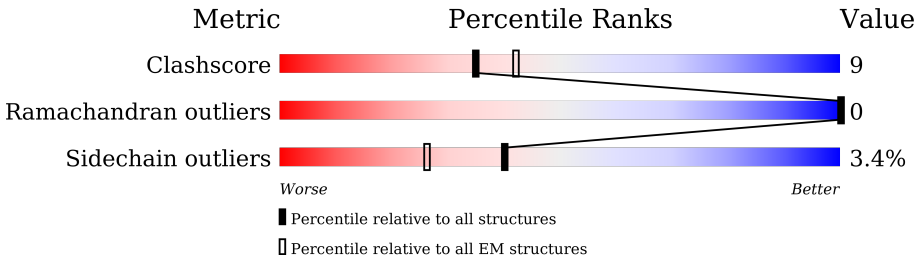
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4966	28% 65% 15% • 19%
1	B	4966	28% 65% 15% • 19%
1	C	4966	28% 65% 16% • 19%
1	D	4966	29% 65% 15% • 19%
2	G	176	9% 45% 16% 39%
2	H	176	7% 45% 16% 39%
2	I	176	7% 45% 16% 39%
2	J	176	7% 46% 15% 39%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 123564 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4044	Total	C	N	O	S	0	0
			30071	19035	5243	5617	176		
1	B	4044	Total	C	N	O	S	0	0
			30071	19035	5243	5617	176		
1	C	4044	Total	C	N	O	S	0	0
			30071	19035	5243	5617	176		
1	D	4044	Total	C	N	O	S	0	0
			30071	19035	5243	5617	176		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	I	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	J	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-67	MET	-	initiating methionine	UNP P68106
G	-66	GLY	-	expression tag	UNP P68106
G	-65	SER	-	expression tag	UNP P68106
G	-64	SER	-	expression tag	UNP P68106
G	-63	HIS	-	expression tag	UNP P68106
G	-62	HIS	-	expression tag	UNP P68106
G	-61	HIS	-	expression tag	UNP P68106
G	-60	HIS	-	expression tag	UNP P68106
G	-59	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-58	HIS	-	expression tag	UNP P68106
G	-57	SER	-	expression tag	UNP P68106
G	-56	SER	-	expression tag	UNP P68106
G	-55	GLY	-	expression tag	UNP P68106
G	-54	LEU	-	expression tag	UNP P68106
G	-53	VAL	-	expression tag	UNP P68106
G	-52	PRO	-	expression tag	UNP P68106
G	-51	ARG	-	expression tag	UNP P68106
G	-50	GLY	-	expression tag	UNP P68106
G	-49	SER	-	expression tag	UNP P68106
G	-48	HIS	-	expression tag	UNP P68106
G	-47	MET	-	expression tag	UNP P68106
G	-46	ALA	-	expression tag	UNP P68106
G	-45	SER	-	expression tag	UNP P68106
G	-44	MET	-	expression tag	UNP P68106
G	-43	ASP	-	expression tag	UNP P68106
G	-42	GLU	-	expression tag	UNP P68106
G	-41	LYS	-	expression tag	UNP P68106
G	-40	THR	-	expression tag	UNP P68106
G	-39	THR	-	expression tag	UNP P68106
G	-38	GLY	-	expression tag	UNP P68106
G	-37	TRP	-	expression tag	UNP P68106
G	-36	ARG	-	expression tag	UNP P68106
G	-35	GLY	-	expression tag	UNP P68106
G	-34	GLY	-	expression tag	UNP P68106
G	-33	HIS	-	expression tag	UNP P68106
G	-32	VAL	-	expression tag	UNP P68106
G	-31	VAL	-	expression tag	UNP P68106
G	-30	GLU	-	expression tag	UNP P68106
G	-29	GLY	-	expression tag	UNP P68106
G	-28	LEU	-	expression tag	UNP P68106
G	-27	ALA	-	expression tag	UNP P68106
G	-26	GLY	-	expression tag	UNP P68106
G	-25	GLU	-	expression tag	UNP P68106
G	-24	LEU	-	expression tag	UNP P68106
G	-23	GLU	-	expression tag	UNP P68106
G	-22	GLN	-	expression tag	UNP P68106
G	-21	LEU	-	expression tag	UNP P68106
G	-20	ARG	-	expression tag	UNP P68106
G	-19	ALA	-	expression tag	UNP P68106
G	-18	ARG	-	expression tag	UNP P68106
G	-17	LEU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	GLU	-	expression tag	UNP P68106
G	-15	HIS	-	expression tag	UNP P68106
G	-14	HIS	-	expression tag	UNP P68106
G	-13	PRO	-	expression tag	UNP P68106
G	-12	GLN	-	expression tag	UNP P68106
G	-11	GLY	-	expression tag	UNP P68106
G	-10	GLN	-	expression tag	UNP P68106
G	-9	ARG	-	expression tag	UNP P68106
G	-8	GLU	-	expression tag	UNP P68106
G	-7	PRO	-	expression tag	UNP P68106
G	-6	GLY	-	expression tag	UNP P68106
G	-5	SER	-	expression tag	UNP P68106
G	-4	GLY	-	expression tag	UNP P68106
G	-3	GLY	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	GLY	-	expression tag	UNP P68106
G	0	GLY	-	expression tag	UNP P68106
G	1	THR	-	expression tag	UNP P68106
H	-67	MET	-	initiating methionine	UNP P68106
H	-66	GLY	-	expression tag	UNP P68106
H	-65	SER	-	expression tag	UNP P68106
H	-64	SER	-	expression tag	UNP P68106
H	-63	HIS	-	expression tag	UNP P68106
H	-62	HIS	-	expression tag	UNP P68106
H	-61	HIS	-	expression tag	UNP P68106
H	-60	HIS	-	expression tag	UNP P68106
H	-59	HIS	-	expression tag	UNP P68106
H	-58	HIS	-	expression tag	UNP P68106
H	-57	SER	-	expression tag	UNP P68106
H	-56	SER	-	expression tag	UNP P68106
H	-55	GLY	-	expression tag	UNP P68106
H	-54	LEU	-	expression tag	UNP P68106
H	-53	VAL	-	expression tag	UNP P68106
H	-52	PRO	-	expression tag	UNP P68106
H	-51	ARG	-	expression tag	UNP P68106
H	-50	GLY	-	expression tag	UNP P68106
H	-49	SER	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	MET	-	expression tag	UNP P68106
H	-46	ALA	-	expression tag	UNP P68106
H	-45	SER	-	expression tag	UNP P68106
H	-44	MET	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-43	ASP	-	expression tag	UNP P68106
H	-42	GLU	-	expression tag	UNP P68106
H	-41	LYS	-	expression tag	UNP P68106
H	-40	THR	-	expression tag	UNP P68106
H	-39	THR	-	expression tag	UNP P68106
H	-38	GLY	-	expression tag	UNP P68106
H	-37	TRP	-	expression tag	UNP P68106
H	-36	ARG	-	expression tag	UNP P68106
H	-35	GLY	-	expression tag	UNP P68106
H	-34	GLY	-	expression tag	UNP P68106
H	-33	HIS	-	expression tag	UNP P68106
H	-32	VAL	-	expression tag	UNP P68106
H	-31	VAL	-	expression tag	UNP P68106
H	-30	GLU	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	LEU	-	expression tag	UNP P68106
H	-27	ALA	-	expression tag	UNP P68106
H	-26	GLY	-	expression tag	UNP P68106
H	-25	GLU	-	expression tag	UNP P68106
H	-24	LEU	-	expression tag	UNP P68106
H	-23	GLU	-	expression tag	UNP P68106
H	-22	GLN	-	expression tag	UNP P68106
H	-21	LEU	-	expression tag	UNP P68106
H	-20	ARG	-	expression tag	UNP P68106
H	-19	ALA	-	expression tag	UNP P68106
H	-18	ARG	-	expression tag	UNP P68106
H	-17	LEU	-	expression tag	UNP P68106
H	-16	GLU	-	expression tag	UNP P68106
H	-15	HIS	-	expression tag	UNP P68106
H	-14	HIS	-	expression tag	UNP P68106
H	-13	PRO	-	expression tag	UNP P68106
H	-12	GLN	-	expression tag	UNP P68106
H	-11	GLY	-	expression tag	UNP P68106
H	-10	GLN	-	expression tag	UNP P68106
H	-9	ARG	-	expression tag	UNP P68106
H	-8	GLU	-	expression tag	UNP P68106
H	-7	PRO	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	SER	-	expression tag	UNP P68106
H	-4	GLY	-	expression tag	UNP P68106
H	-3	GLY	-	expression tag	UNP P68106
H	-2	SER	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P68106
H	0	GLY	-	expression tag	UNP P68106
H	1	THR	-	expression tag	UNP P68106
I	-67	MET	-	initiating methionine	UNP P68106
I	-66	GLY	-	expression tag	UNP P68106
I	-65	SER	-	expression tag	UNP P68106
I	-64	SER	-	expression tag	UNP P68106
I	-63	HIS	-	expression tag	UNP P68106
I	-62	HIS	-	expression tag	UNP P68106
I	-61	HIS	-	expression tag	UNP P68106
I	-60	HIS	-	expression tag	UNP P68106
I	-59	HIS	-	expression tag	UNP P68106
I	-58	HIS	-	expression tag	UNP P68106
I	-57	SER	-	expression tag	UNP P68106
I	-56	SER	-	expression tag	UNP P68106
I	-55	GLY	-	expression tag	UNP P68106
I	-54	LEU	-	expression tag	UNP P68106
I	-53	VAL	-	expression tag	UNP P68106
I	-52	PRO	-	expression tag	UNP P68106
I	-51	ARG	-	expression tag	UNP P68106
I	-50	GLY	-	expression tag	UNP P68106
I	-49	SER	-	expression tag	UNP P68106
I	-48	HIS	-	expression tag	UNP P68106
I	-47	MET	-	expression tag	UNP P68106
I	-46	ALA	-	expression tag	UNP P68106
I	-45	SER	-	expression tag	UNP P68106
I	-44	MET	-	expression tag	UNP P68106
I	-43	ASP	-	expression tag	UNP P68106
I	-42	GLU	-	expression tag	UNP P68106
I	-41	LYS	-	expression tag	UNP P68106
I	-40	THR	-	expression tag	UNP P68106
I	-39	THR	-	expression tag	UNP P68106
I	-38	GLY	-	expression tag	UNP P68106
I	-37	TRP	-	expression tag	UNP P68106
I	-36	ARG	-	expression tag	UNP P68106
I	-35	GLY	-	expression tag	UNP P68106
I	-34	GLY	-	expression tag	UNP P68106
I	-33	HIS	-	expression tag	UNP P68106
I	-32	VAL	-	expression tag	UNP P68106
I	-31	VAL	-	expression tag	UNP P68106
I	-30	GLU	-	expression tag	UNP P68106
I	-29	GLY	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-28	LEU	-	expression tag	UNP P68106
I	-27	ALA	-	expression tag	UNP P68106
I	-26	GLY	-	expression tag	UNP P68106
I	-25	GLU	-	expression tag	UNP P68106
I	-24	LEU	-	expression tag	UNP P68106
I	-23	GLU	-	expression tag	UNP P68106
I	-22	GLN	-	expression tag	UNP P68106
I	-21	LEU	-	expression tag	UNP P68106
I	-20	ARG	-	expression tag	UNP P68106
I	-19	ALA	-	expression tag	UNP P68106
I	-18	ARG	-	expression tag	UNP P68106
I	-17	LEU	-	expression tag	UNP P68106
I	-16	GLU	-	expression tag	UNP P68106
I	-15	HIS	-	expression tag	UNP P68106
I	-14	HIS	-	expression tag	UNP P68106
I	-13	PRO	-	expression tag	UNP P68106
I	-12	GLN	-	expression tag	UNP P68106
I	-11	GLY	-	expression tag	UNP P68106
I	-10	GLN	-	expression tag	UNP P68106
I	-9	ARG	-	expression tag	UNP P68106
I	-8	GLU	-	expression tag	UNP P68106
I	-7	PRO	-	expression tag	UNP P68106
I	-6	GLY	-	expression tag	UNP P68106
I	-5	SER	-	expression tag	UNP P68106
I	-4	GLY	-	expression tag	UNP P68106
I	-3	GLY	-	expression tag	UNP P68106
I	-2	SER	-	expression tag	UNP P68106
I	-1	GLY	-	expression tag	UNP P68106
I	0	GLY	-	expression tag	UNP P68106
I	1	THR	-	expression tag	UNP P68106
J	-67	MET	-	initiating methionine	UNP P68106
J	-66	GLY	-	expression tag	UNP P68106
J	-65	SER	-	expression tag	UNP P68106
J	-64	SER	-	expression tag	UNP P68106
J	-63	HIS	-	expression tag	UNP P68106
J	-62	HIS	-	expression tag	UNP P68106
J	-61	HIS	-	expression tag	UNP P68106
J	-60	HIS	-	expression tag	UNP P68106
J	-59	HIS	-	expression tag	UNP P68106
J	-58	HIS	-	expression tag	UNP P68106
J	-57	SER	-	expression tag	UNP P68106
J	-56	SER	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-55	GLY	-	expression tag	UNP P68106
J	-54	LEU	-	expression tag	UNP P68106
J	-53	VAL	-	expression tag	UNP P68106
J	-52	PRO	-	expression tag	UNP P68106
J	-51	ARG	-	expression tag	UNP P68106
J	-50	GLY	-	expression tag	UNP P68106
J	-49	SER	-	expression tag	UNP P68106
J	-48	HIS	-	expression tag	UNP P68106
J	-47	MET	-	expression tag	UNP P68106
J	-46	ALA	-	expression tag	UNP P68106
J	-45	SER	-	expression tag	UNP P68106
J	-44	MET	-	expression tag	UNP P68106
J	-43	ASP	-	expression tag	UNP P68106
J	-42	GLU	-	expression tag	UNP P68106
J	-41	LYS	-	expression tag	UNP P68106
J	-40	THR	-	expression tag	UNP P68106
J	-39	THR	-	expression tag	UNP P68106
J	-38	GLY	-	expression tag	UNP P68106
J	-37	TRP	-	expression tag	UNP P68106
J	-36	ARG	-	expression tag	UNP P68106
J	-35	GLY	-	expression tag	UNP P68106
J	-34	GLY	-	expression tag	UNP P68106
J	-33	HIS	-	expression tag	UNP P68106
J	-32	VAL	-	expression tag	UNP P68106
J	-31	VAL	-	expression tag	UNP P68106
J	-30	GLU	-	expression tag	UNP P68106
J	-29	GLY	-	expression tag	UNP P68106
J	-28	LEU	-	expression tag	UNP P68106
J	-27	ALA	-	expression tag	UNP P68106
J	-26	GLY	-	expression tag	UNP P68106
J	-25	GLU	-	expression tag	UNP P68106
J	-24	LEU	-	expression tag	UNP P68106
J	-23	GLU	-	expression tag	UNP P68106
J	-22	GLN	-	expression tag	UNP P68106
J	-21	LEU	-	expression tag	UNP P68106
J	-20	ARG	-	expression tag	UNP P68106
J	-19	ALA	-	expression tag	UNP P68106
J	-18	ARG	-	expression tag	UNP P68106
J	-17	LEU	-	expression tag	UNP P68106
J	-16	GLU	-	expression tag	UNP P68106
J	-15	HIS	-	expression tag	UNP P68106
J	-14	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	PRO	-	expression tag	UNP P68106
J	-12	GLN	-	expression tag	UNP P68106
J	-11	GLY	-	expression tag	UNP P68106
J	-10	GLN	-	expression tag	UNP P68106
J	-9	ARG	-	expression tag	UNP P68106
J	-8	GLU	-	expression tag	UNP P68106
J	-7	PRO	-	expression tag	UNP P68106
J	-6	GLY	-	expression tag	UNP P68106
J	-5	SER	-	expression tag	UNP P68106
J	-4	GLY	-	expression tag	UNP P68106
J	-3	GLY	-	expression tag	UNP P68106
J	-2	SER	-	expression tag	UNP P68106
J	-1	GLY	-	expression tag	UNP P68106
J	0	GLY	-	expression tag	UNP P68106
J	1	THR	-	expression tag	UNP P68106

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

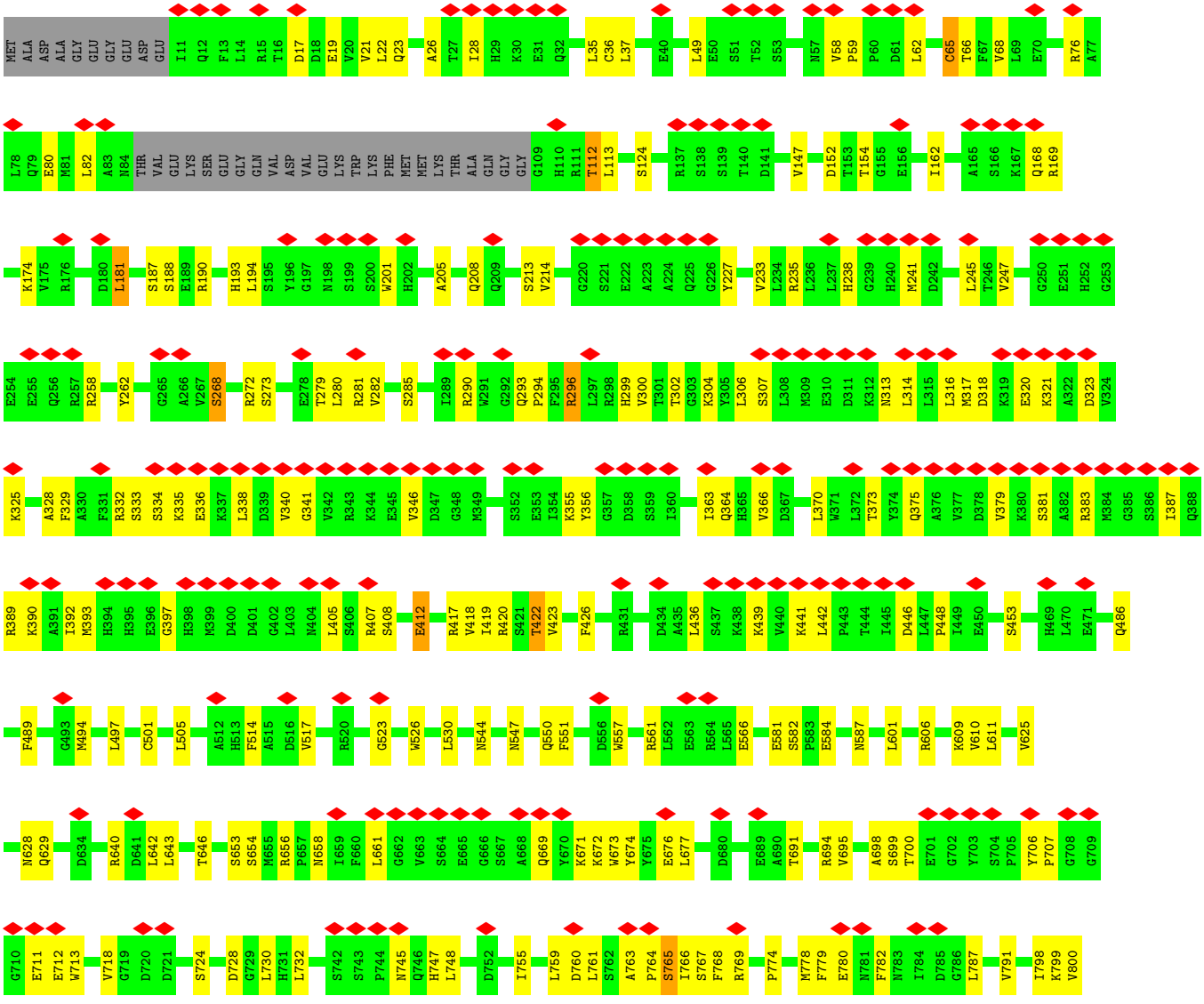
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

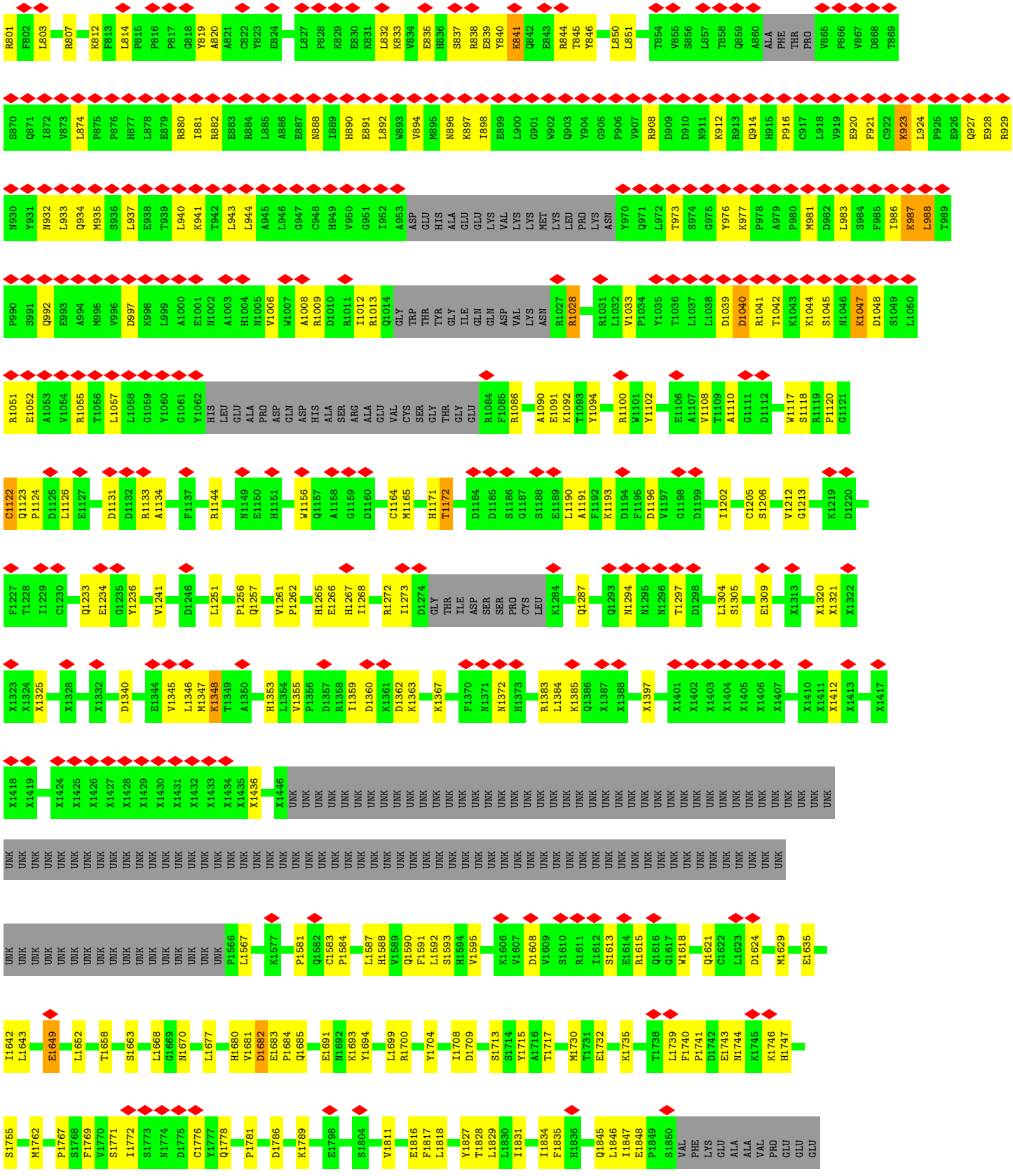
3 Residue-property plots (i)

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

- Molecule 1: Ryanodine receptor 2

Chain A:




R801 F802 L803 R807 K812 F813 L814 P815 P816 P817 G818 Y819 A820 A821 C822 Y823 E824 L827 P828 K829 E830 K831 L832 K833 V834 E835 H836 S837 R838 E839 Y840 K841 Q842 E843 R844 T845 Y846 L850 L851 T854 V855 S856 L857 T858 Q859 A860 ALA PHE THR PRO V865 P866 V867 D868 T869
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N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989
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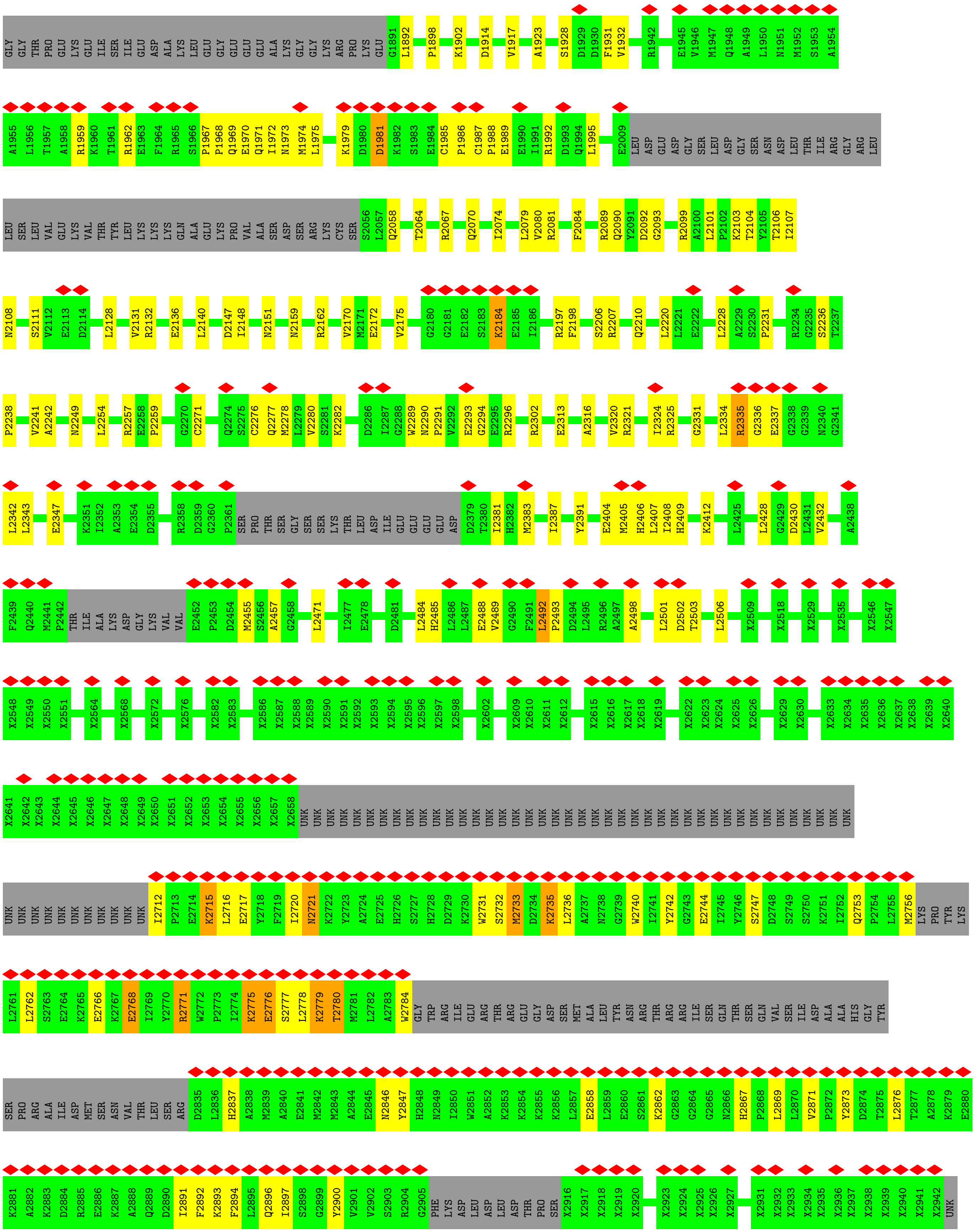
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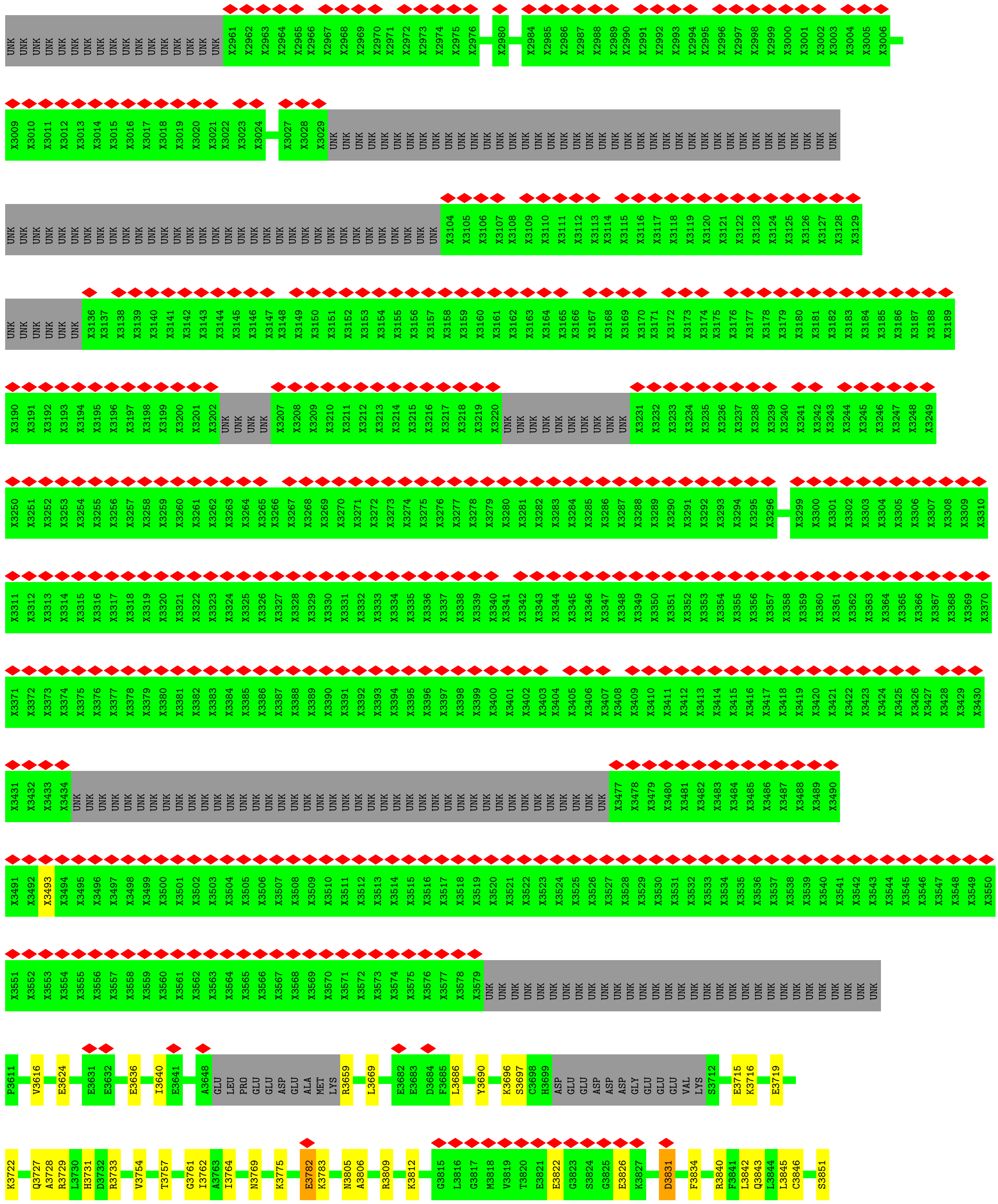
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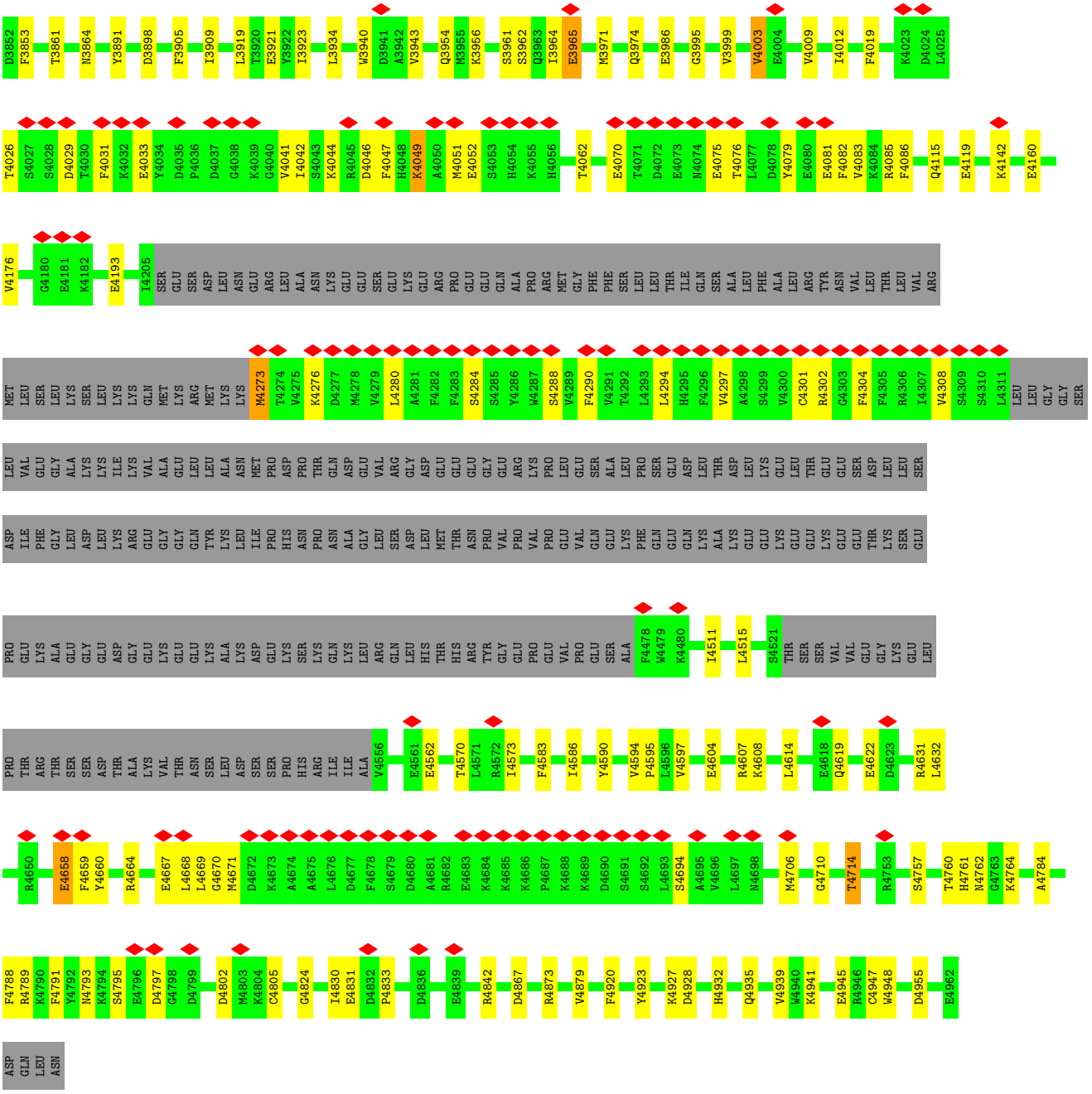
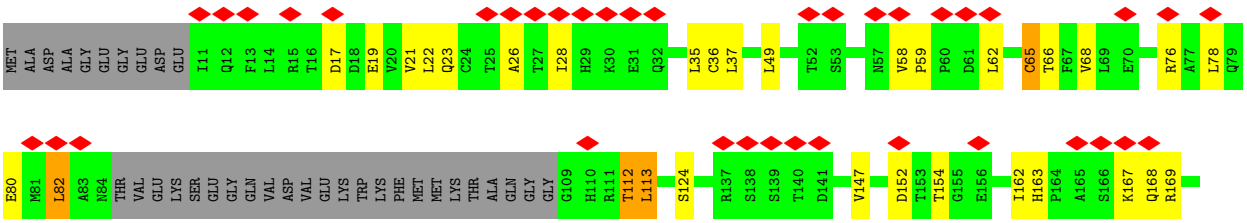
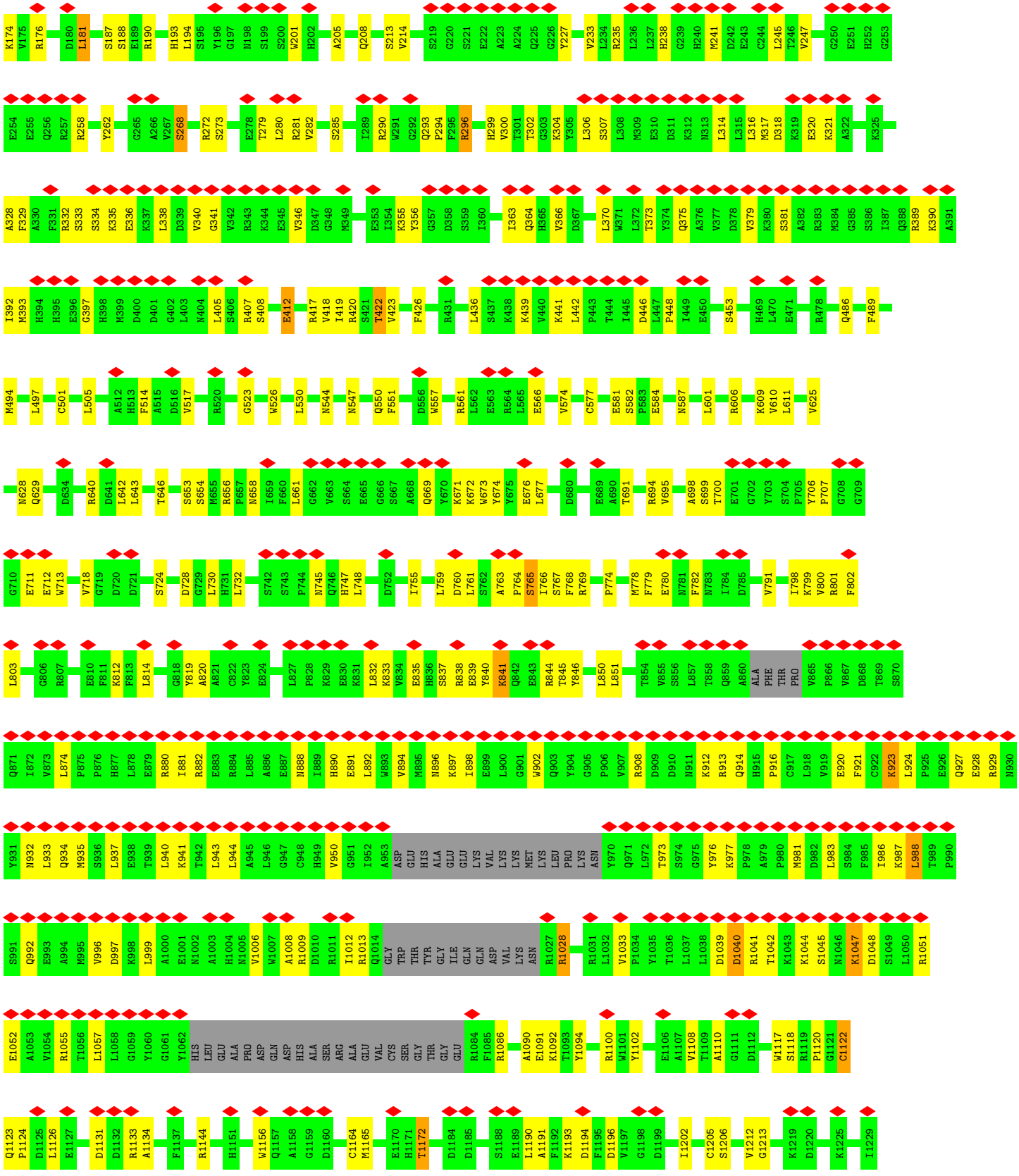


• Molecule 1: Ryanodine receptor 2

Chain B:

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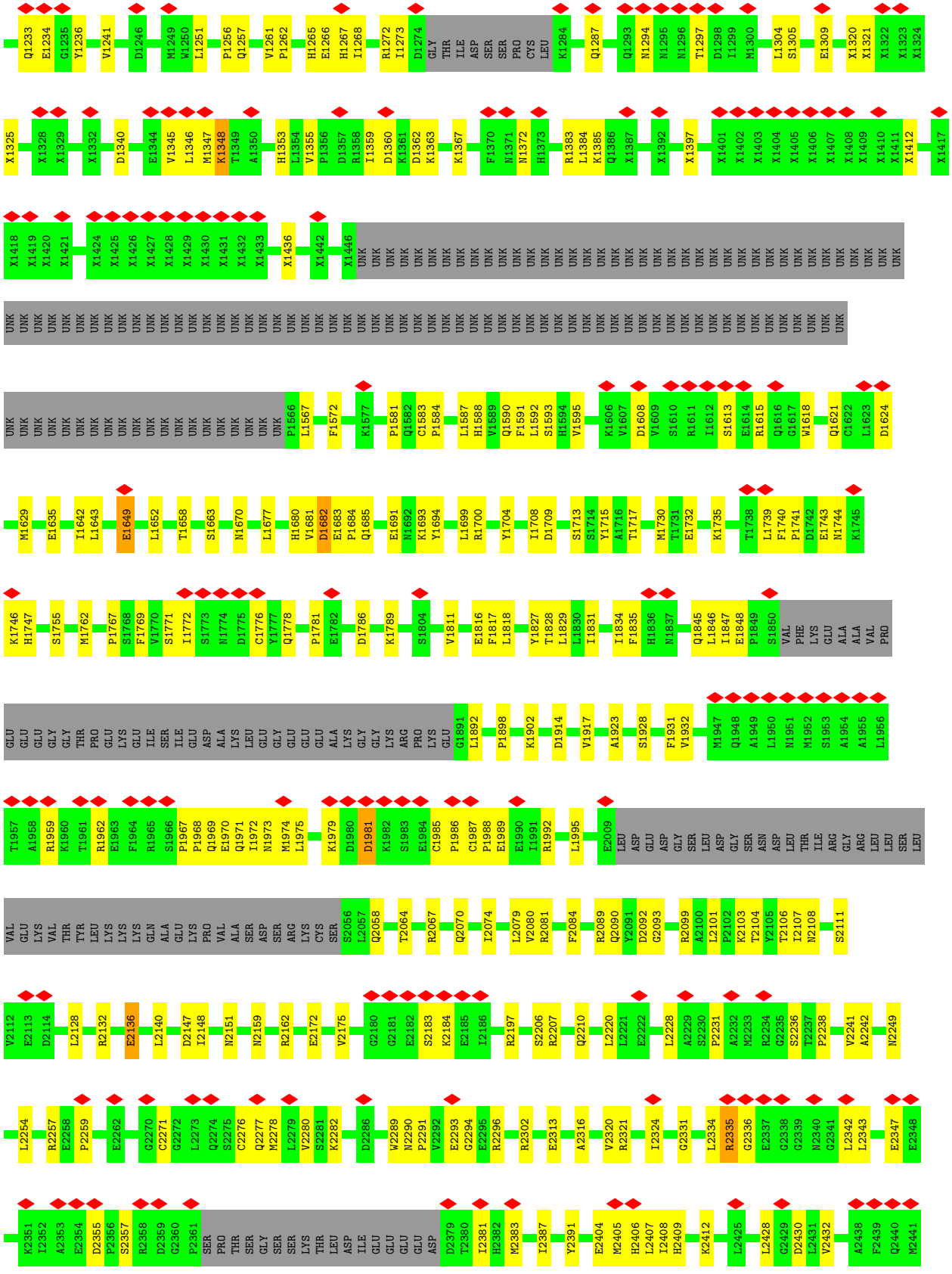
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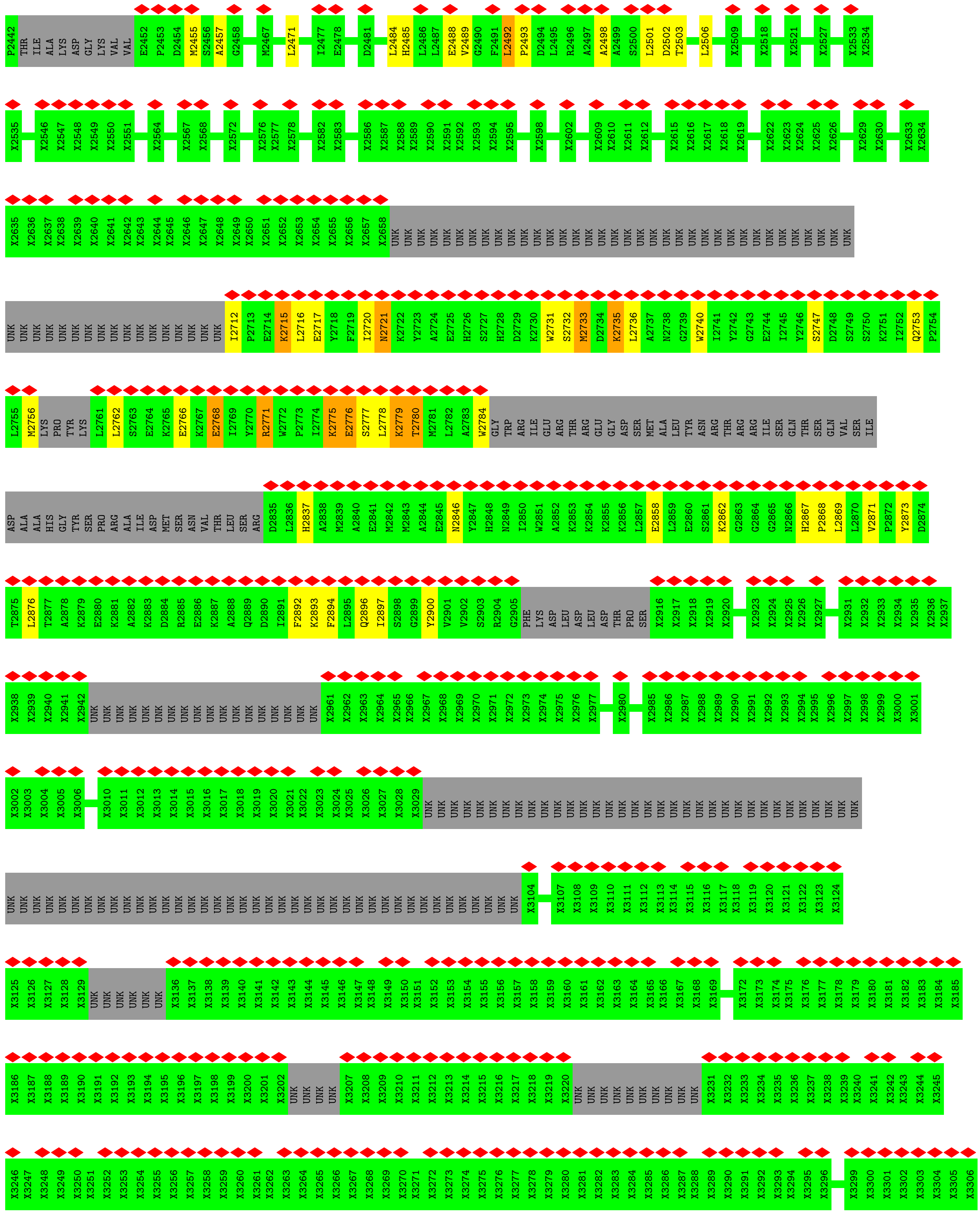
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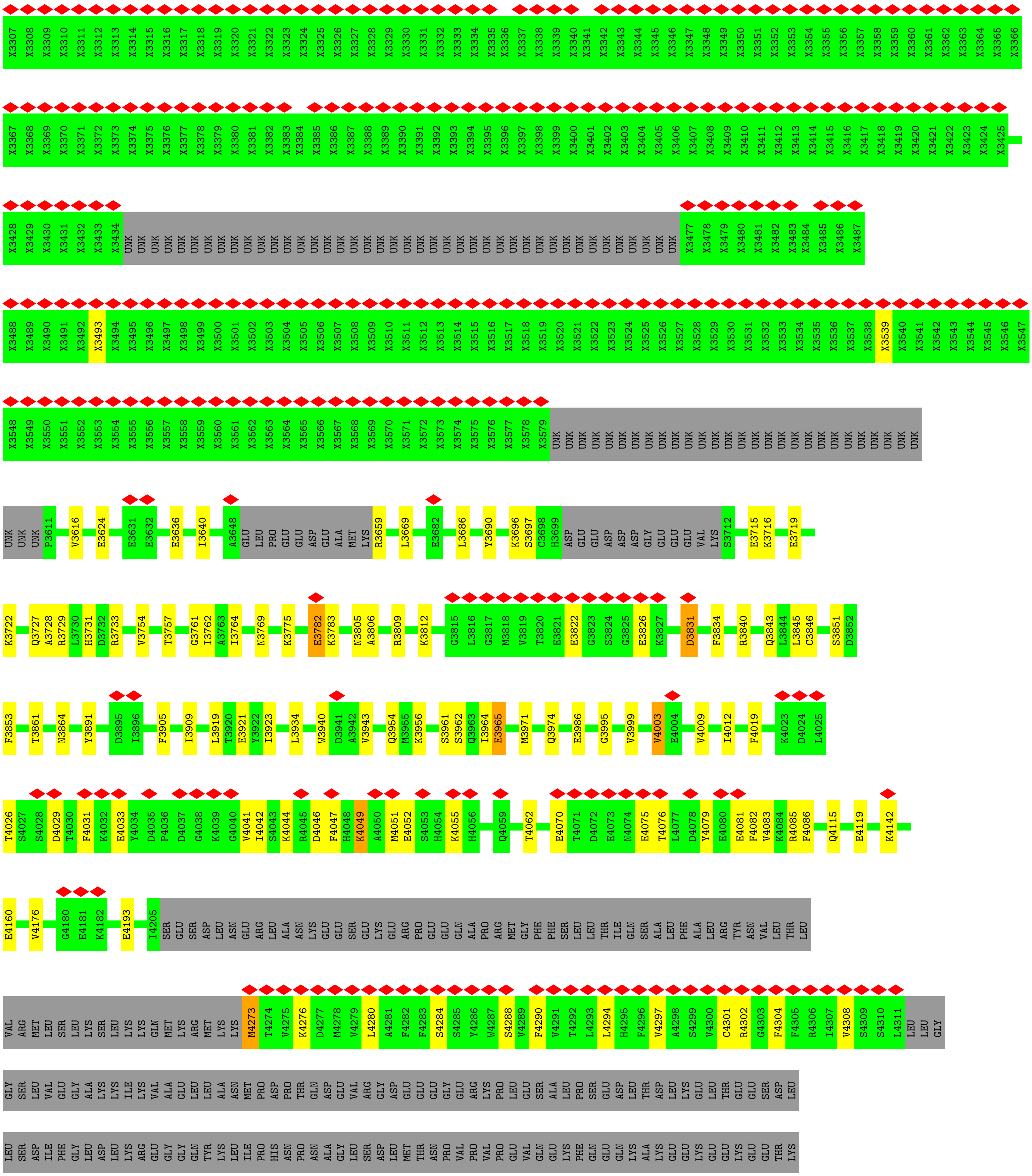
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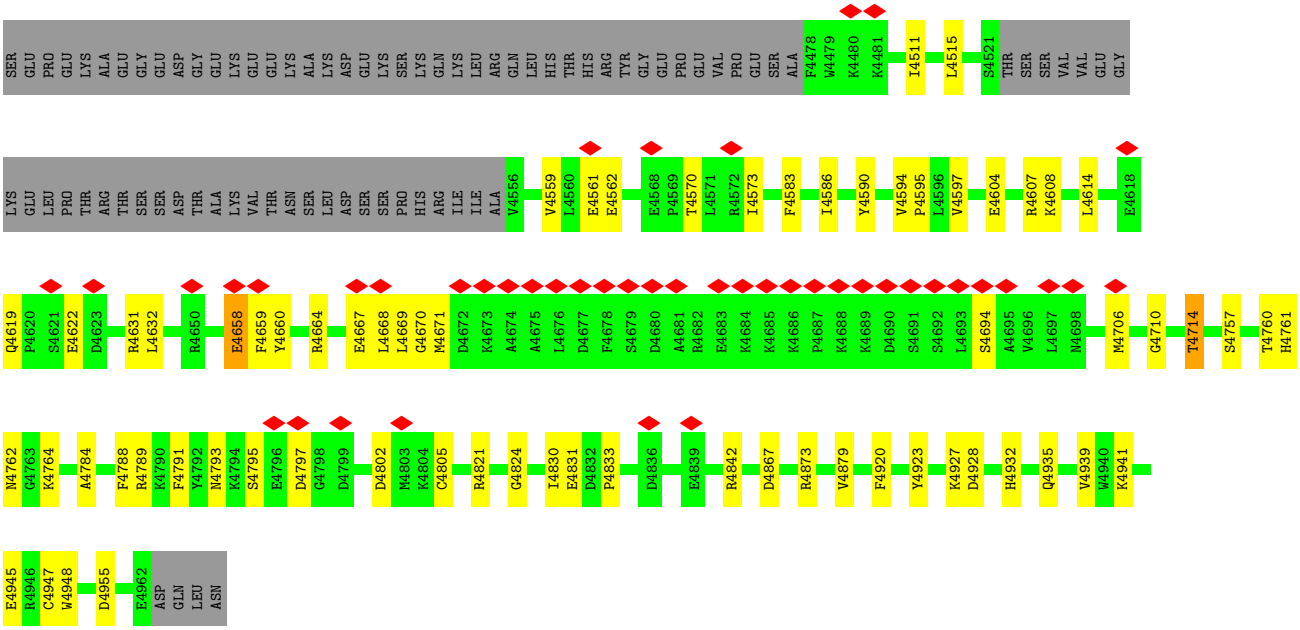
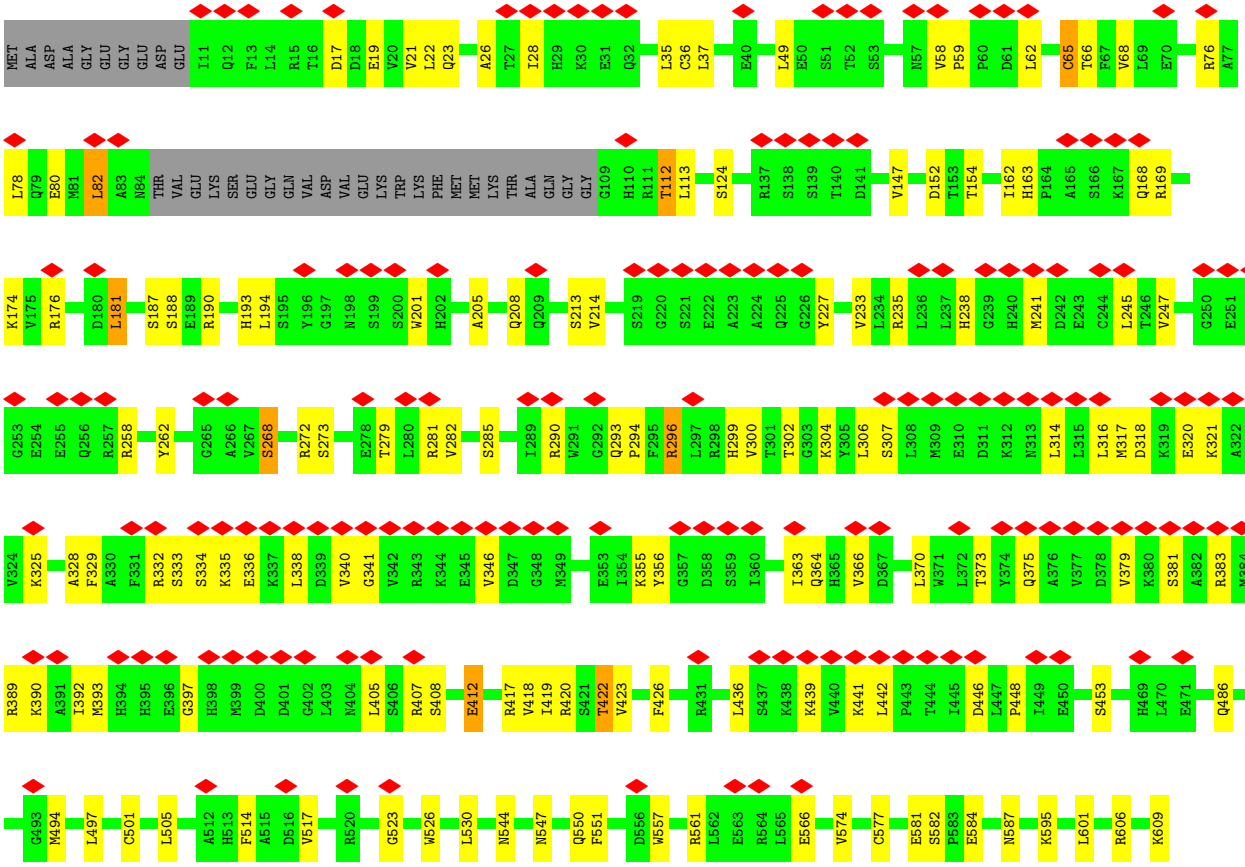
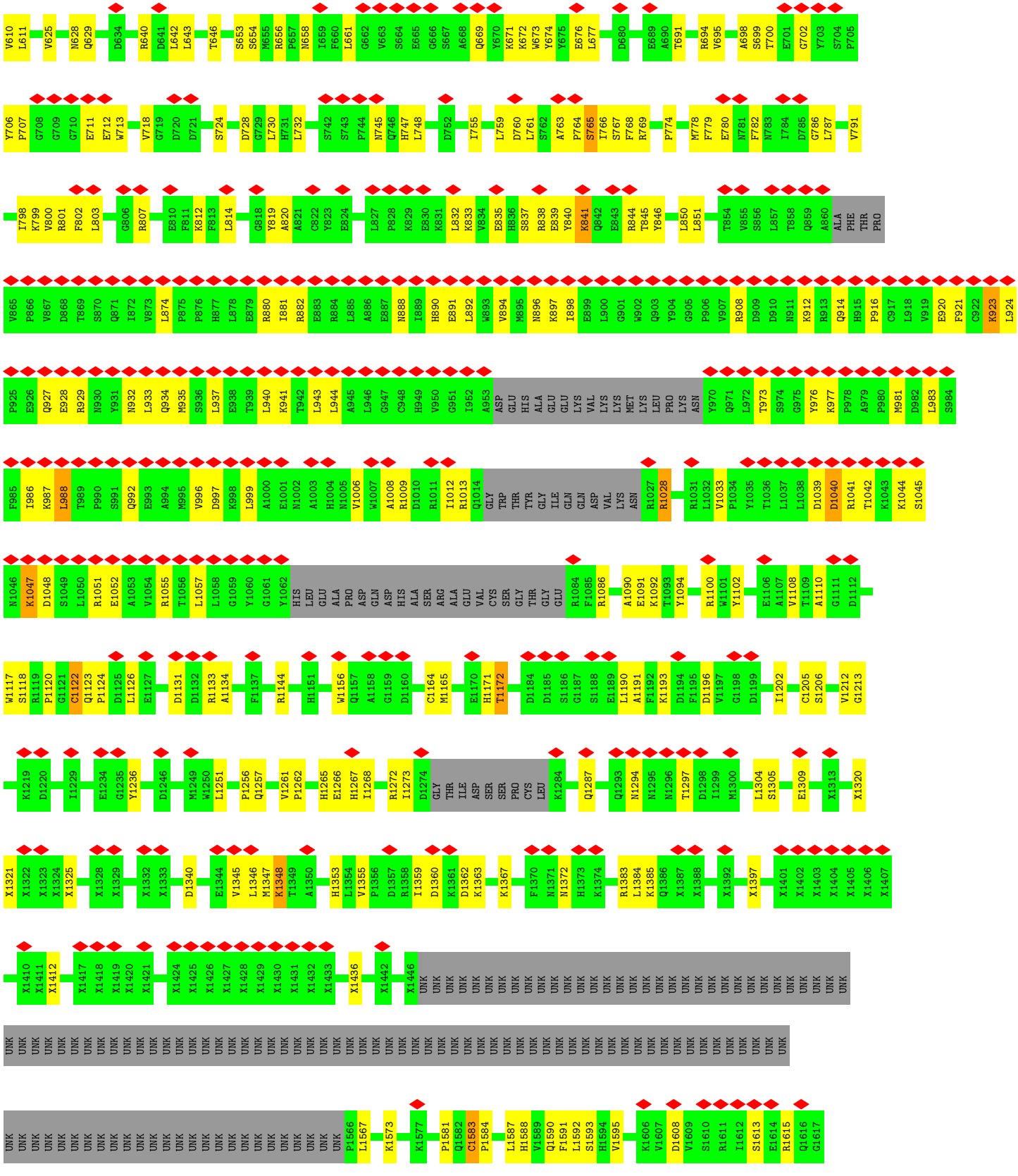
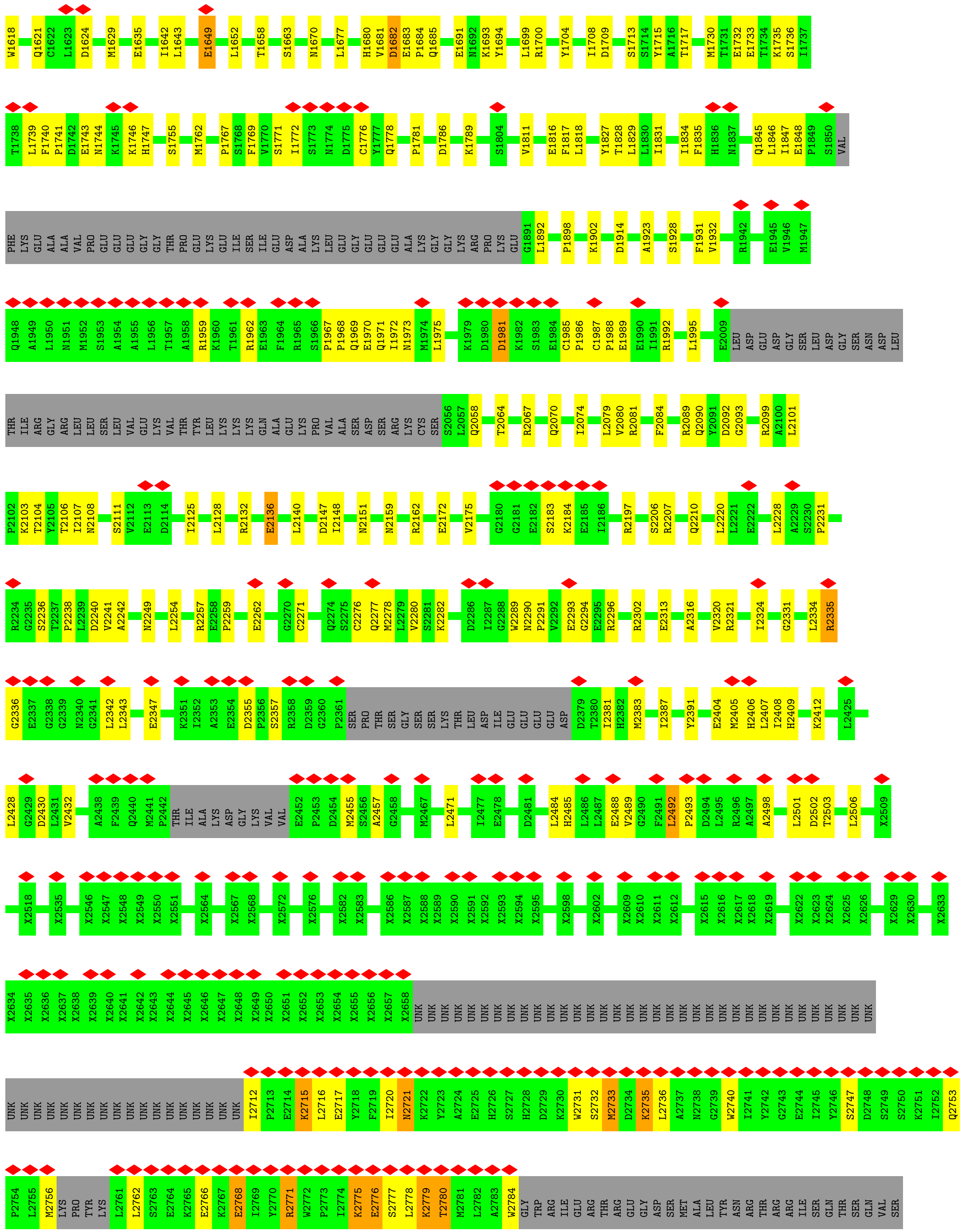


• Molecule 1: Ryanodine receptor 2

Chain C:



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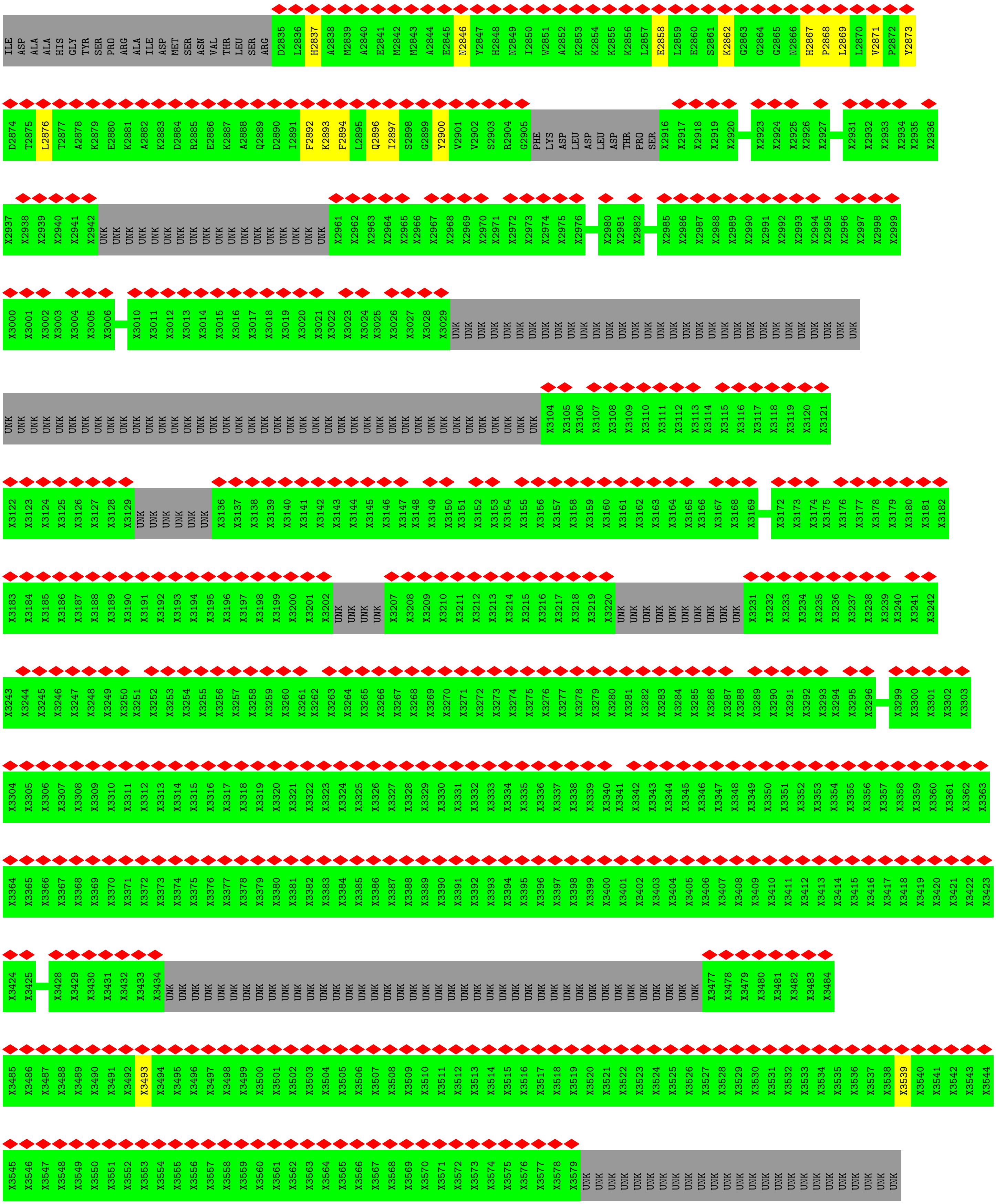
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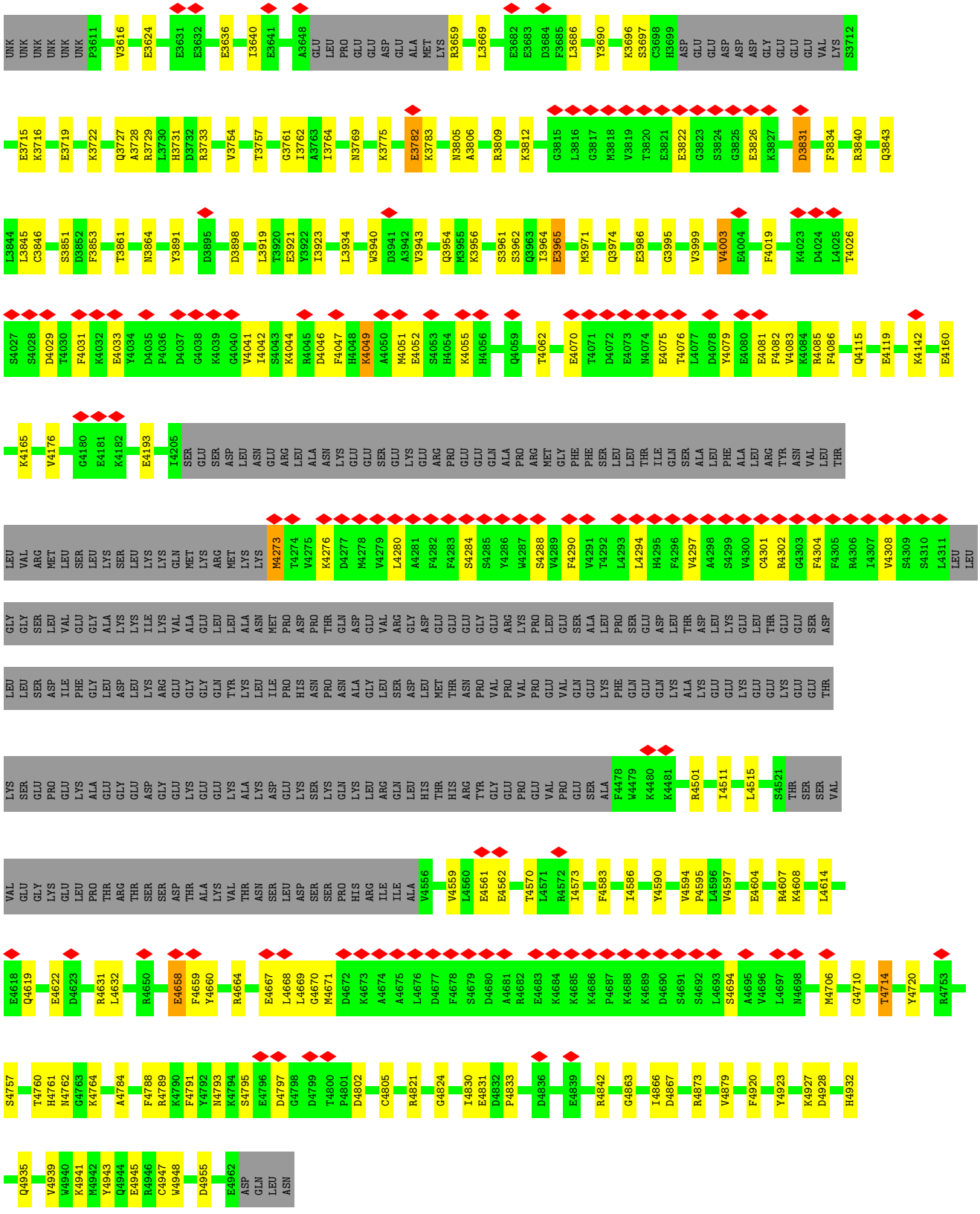
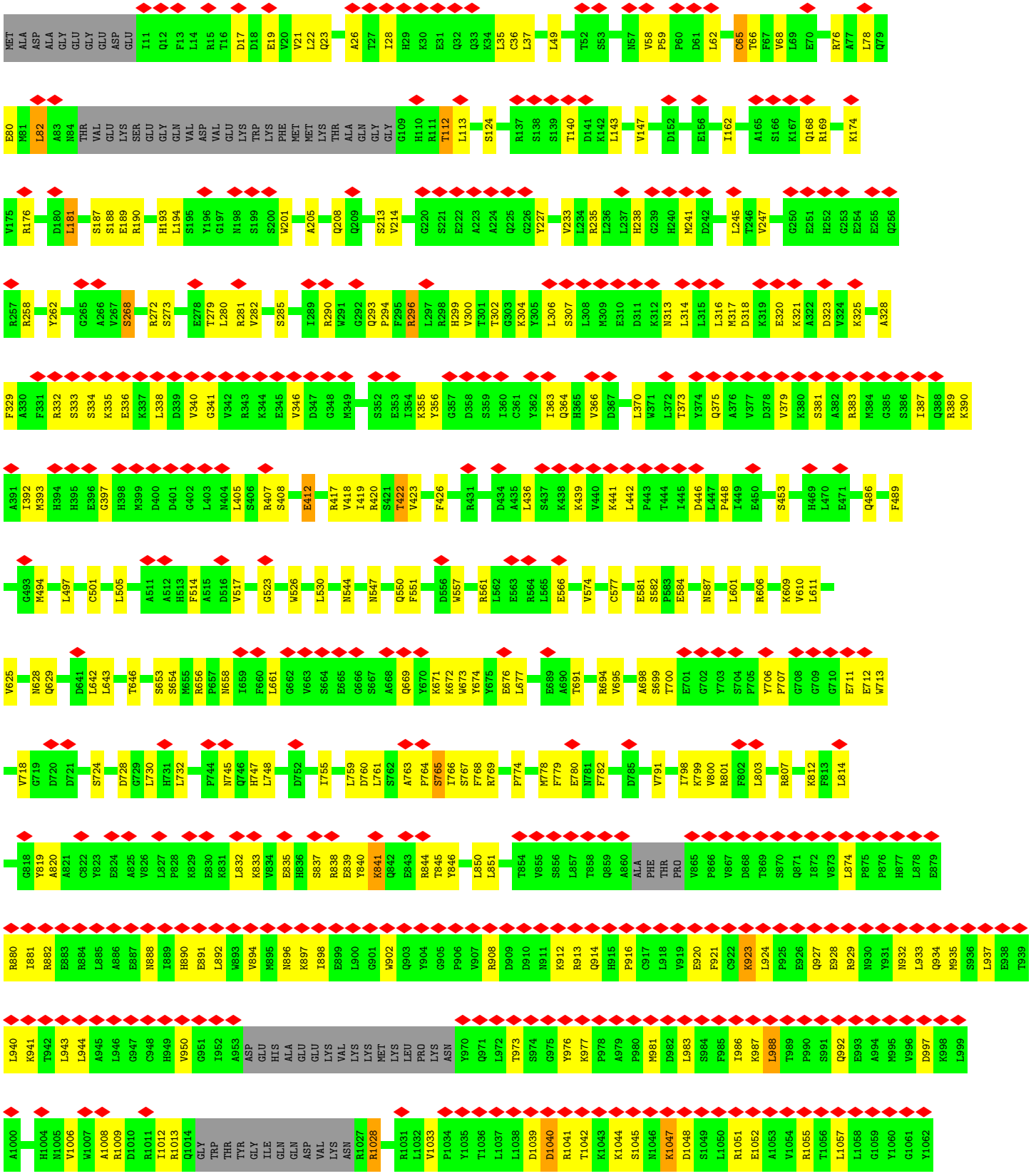


- Molecule 1: Ryanodine receptor 2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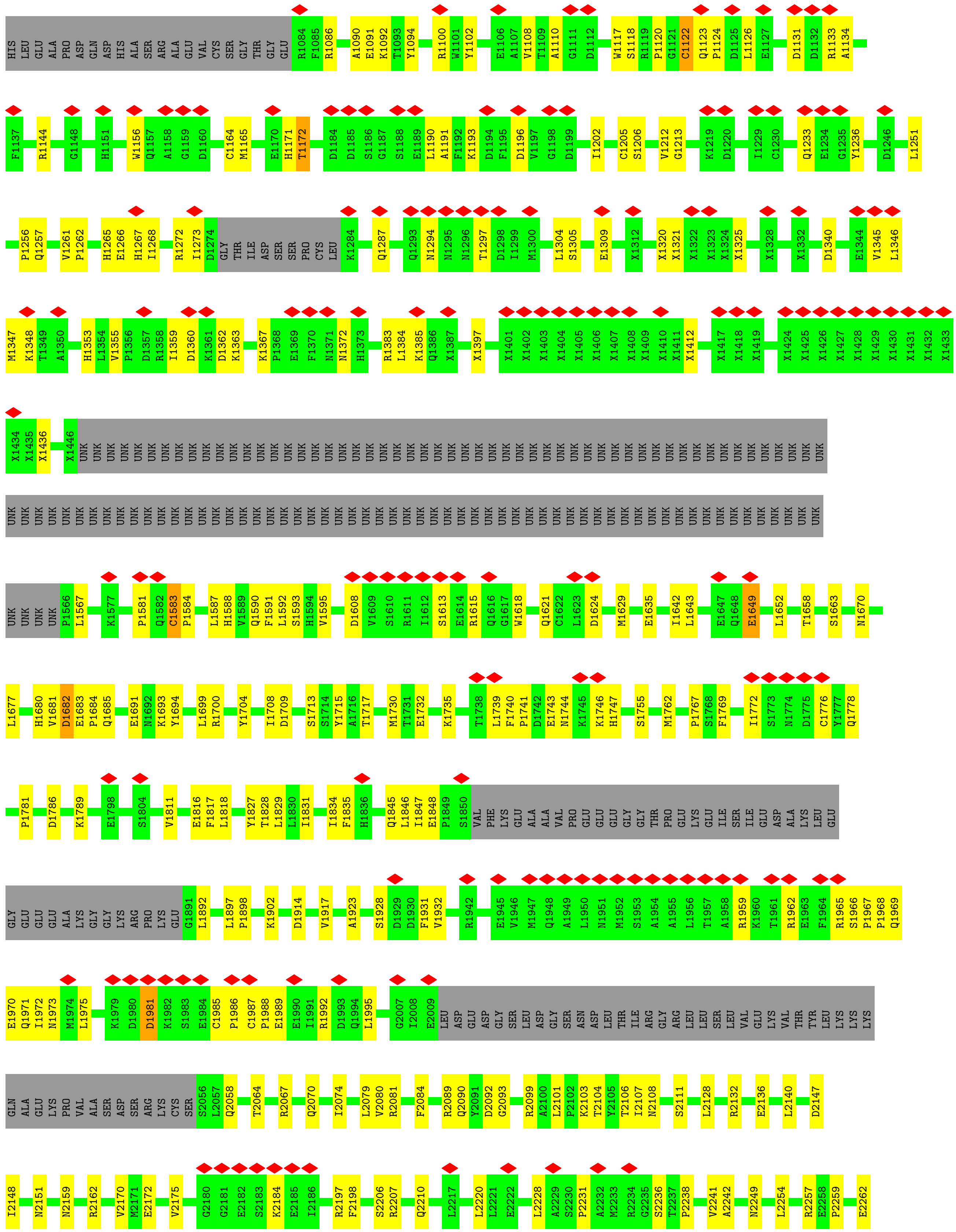
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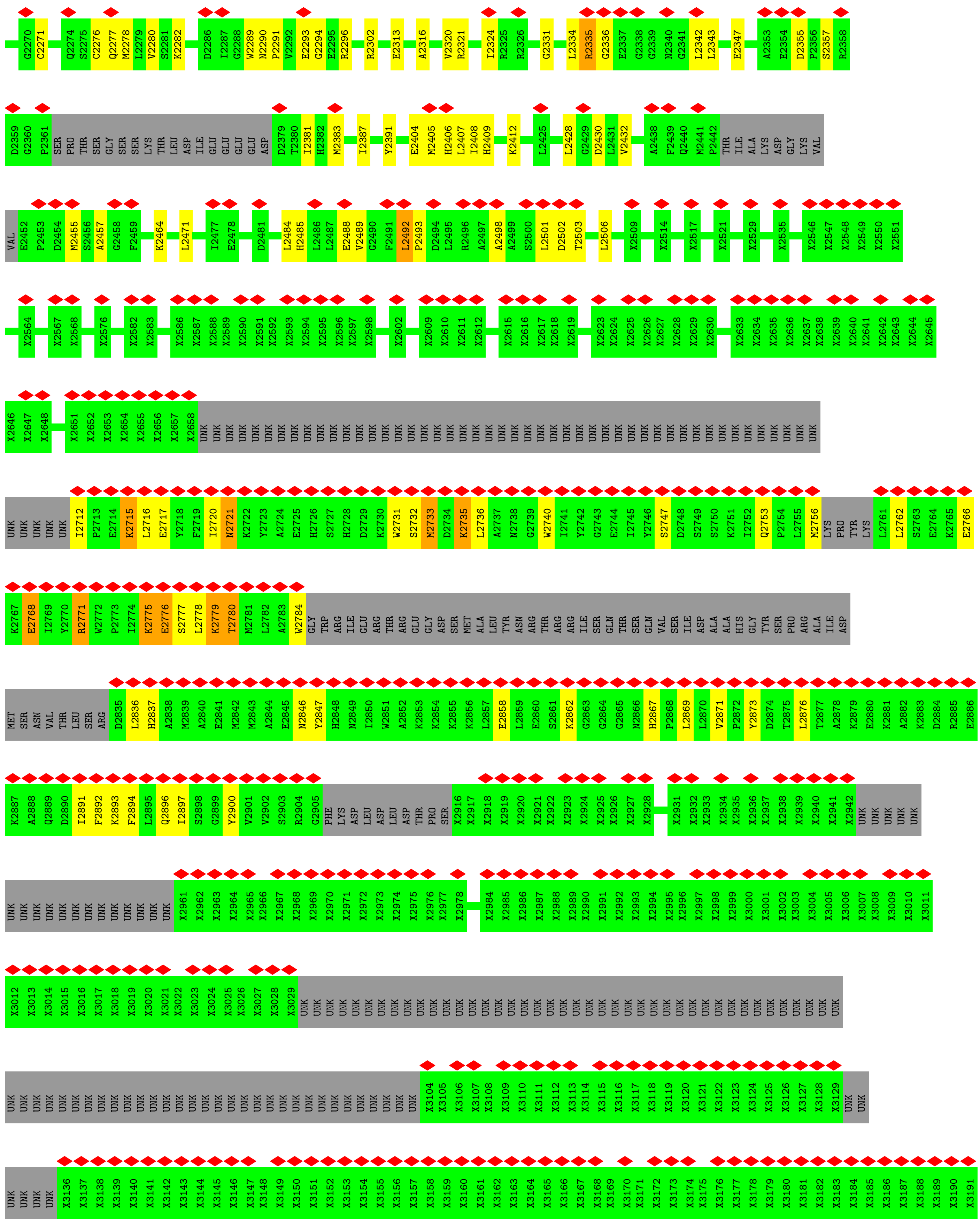
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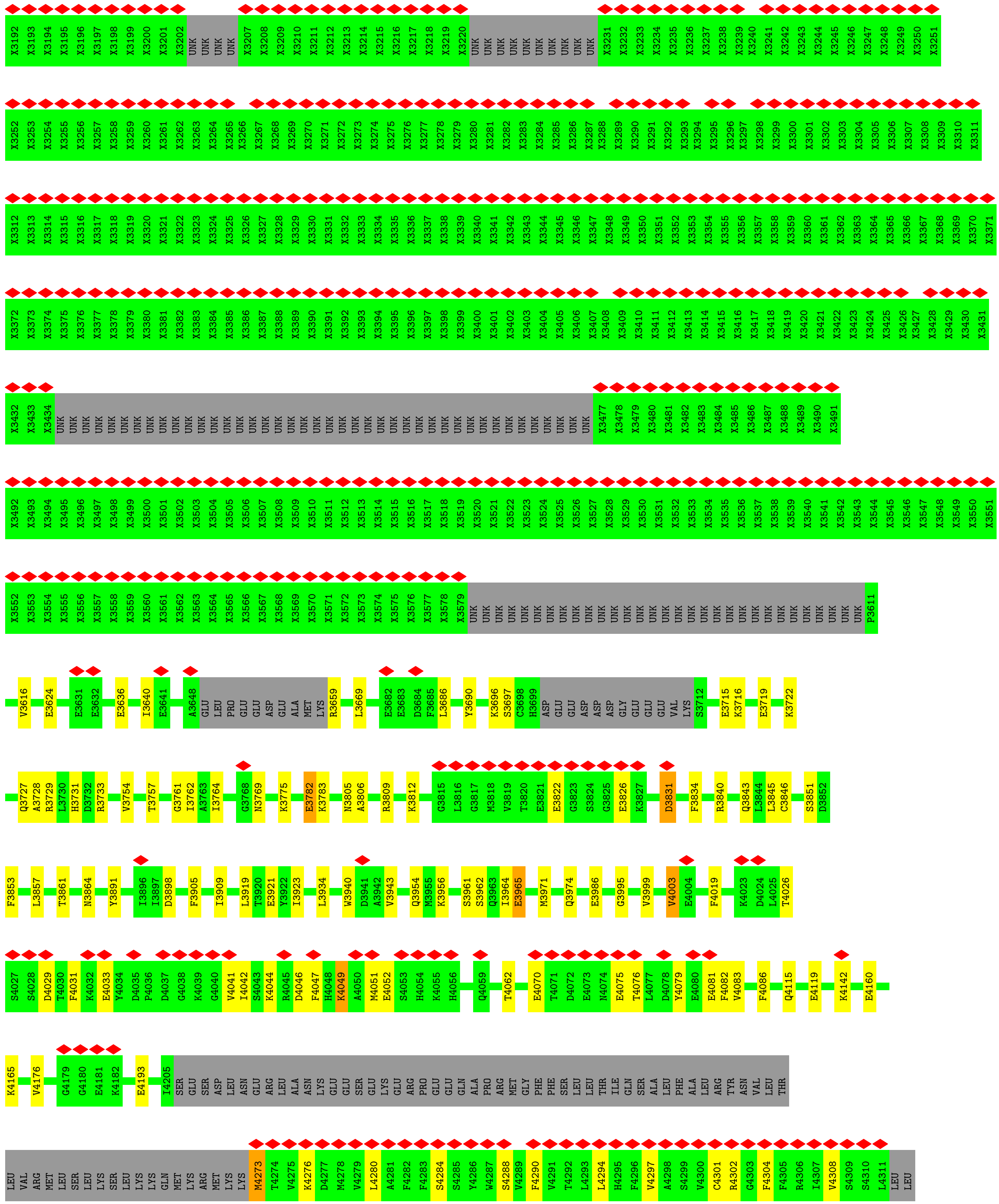
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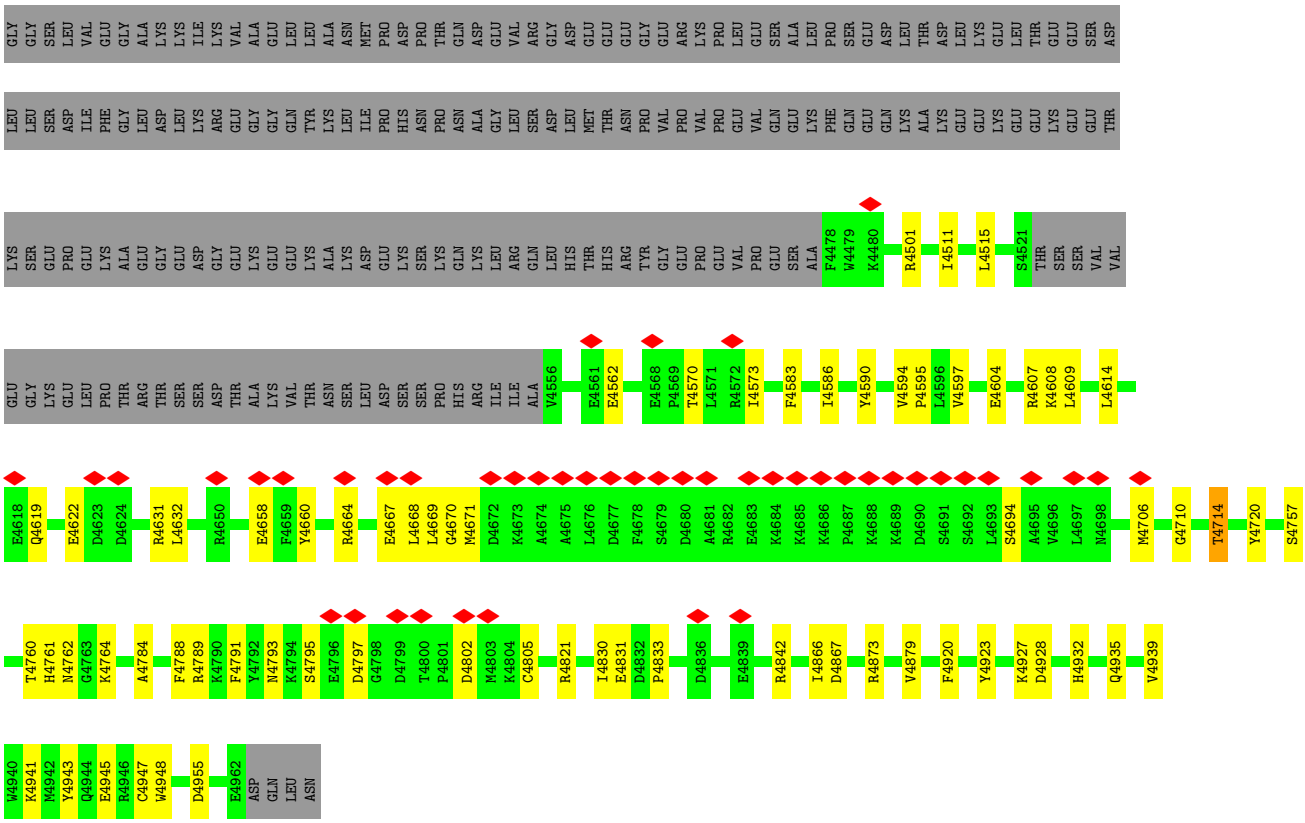
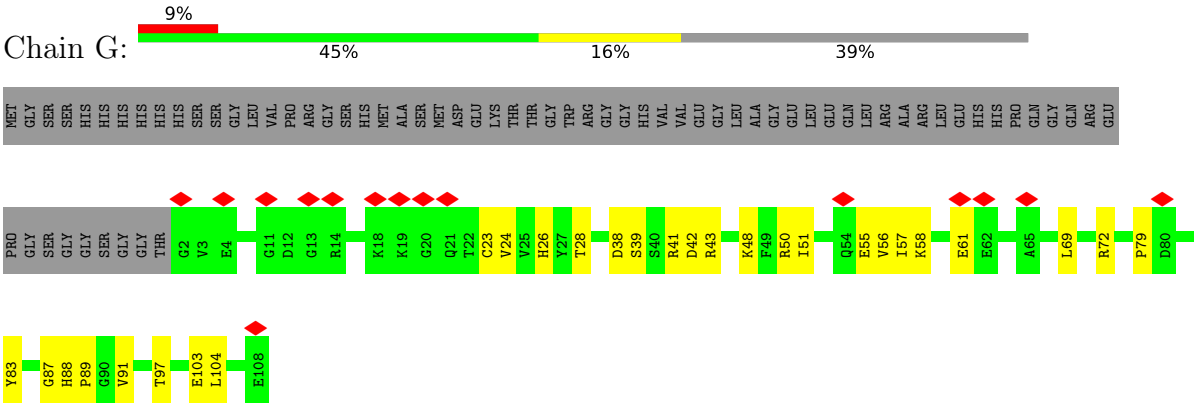
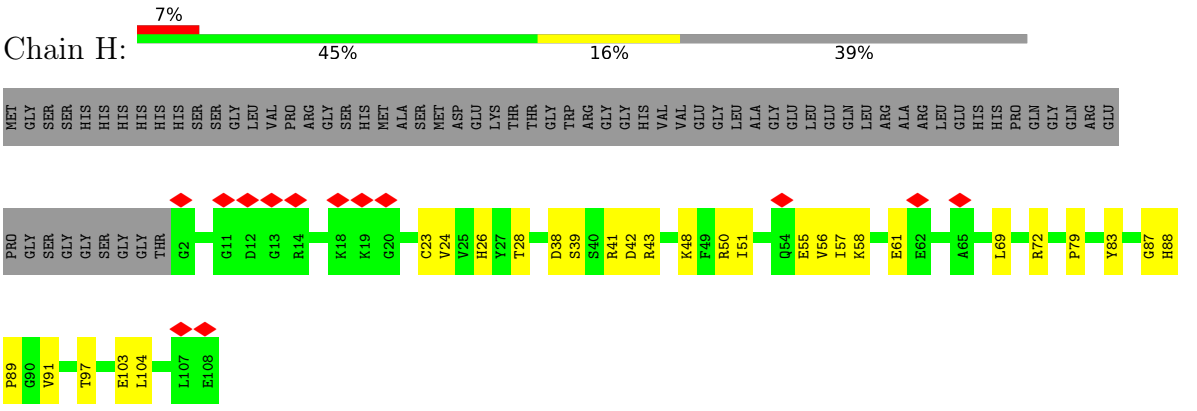
X3432 X3433 X3434 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X3477 X3478 X3479 X3480 X3481 X3482 X3483 X3484 X3485 X3486 X3487 X3488 X3489 X3490 X3491
X3492 X3493 X3494 X3495 X3496 X3497 X3498 X3499 X3500 X3501 X3502 X3503 X3504 X3505 X3506 X3507 X3508 X3509 X3510 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3519 X3520 X3521 X3522 X3523 X3524 X3525 X3526 X3527 X3528 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536 X3537 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551
X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3570 X3571 X3572 X3573 X3574 X3575 X3576 X3577 X3578 X3579 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK P3611
V3616 E3624 E3631 E3632 E3636 I3640 E3641 A3648 GLU LEU PRO GLU GLU ASP GLU ALA MET LYS R3659 L3669 E3682 E3683 D3684 F3685 L3686 Y3690 K3696 S3697 C3698 H3699 ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU VAL LYS S3712 E3715 K3716 E3719 K3722
Q3727 A3728 R3729 L3730 H3731 D3732 R3733 V3754 T3757 G3761 I3762 A3763 I3764 G3768 N3769 K3775 E3782 K3783 N3805 A3806 R3809 K3812 G3815 L3816 G3817 M3818 V3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 K3827 D3831 F3834 R3840 Q3843 L3844 L3845 C3846 S3851 D3852
F3853 L3857 T3861 N3864 Y3891 I3896 I3897 D3898 F3905 I3909 L3919 T3920 E3921 Y3922 I3923 L3934 W3940 D3941 A3942 V3943 Q3954 M3955 K3956 S3961 S3962 Q3963 I3964 E3965 M3971 Q3974 E3986 G3995 V3999 V4003 E4004 F4019 K4023 D4024 L4025 T4026
S4027 S4028 D4029 T4030 F4031 K4032 E4033 Y4034 D4035 P4036 D4037 G4038 K4039 G4040 V4041 I4042 S4043 K4044 R4045 D4046 F4047 H4048 K4049 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Q4059 T4062 E4070 T4071 D4072 E4073 N4074 E4075 T4076 L4077 D4078 Y4079 E4080 E4081 F4082 V4083 F4086 Q4115 E4119 K4142 E4160
K4165 V4176 G4179 G4180 E4181 K4182 E4193 I4205 SER GLU SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR
LEU VAL ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS M4273 T4274 V4275 K4276 D4277 M4278 V4279 L4280 A4281 F4282 F4283 S4284 S4285 Y4286 W4287 S4288 V4289 F4290 V4291 T4292 L4293 L4294 H4295 F4296 V4297 A4298 S4299 V4300 C4301 R4302 G4303 F4304 F4305 R4306 I4307 V4308 S4309 S4310 L4311 LEU LEU



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

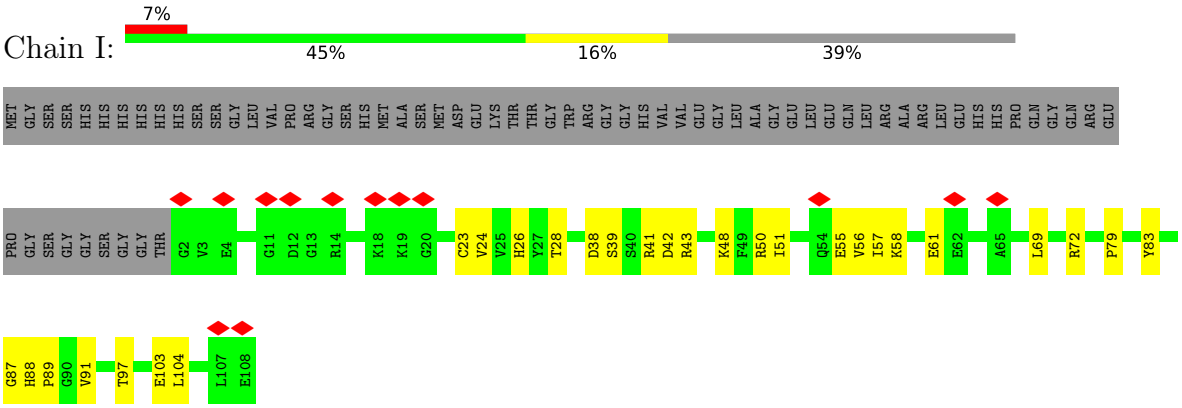


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



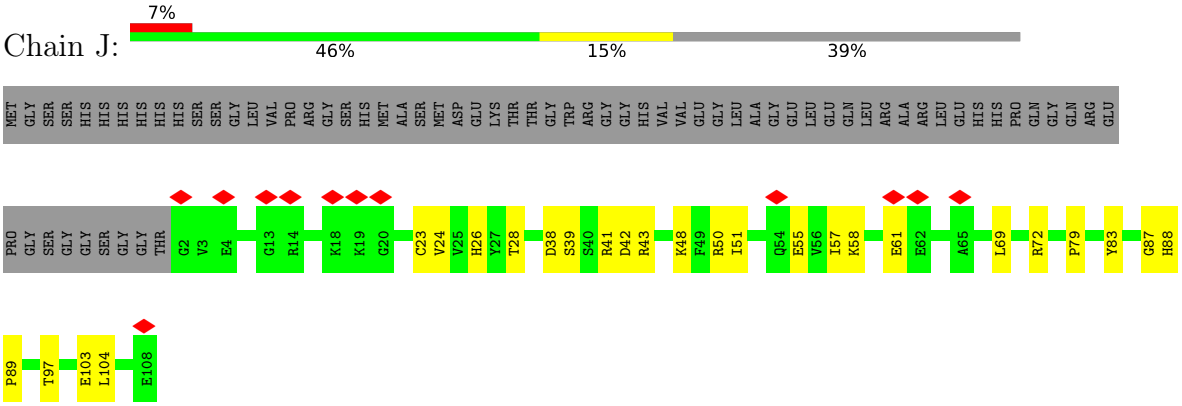
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain I:



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41197	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.076	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.284, 1.284, 1.284	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	0.26	0/26895	0.44	1/36316 (0.0%)
1	B	0.26	0/26895	0.44	1/36316 (0.0%)
1	C	0.26	0/26895	0.44	1/36316 (0.0%)
1	D	0.26	0/26895	0.44	1/36316 (0.0%)
2	G	0.27	0/835	0.47	0/1123
2	H	0.26	0/835	0.47	0/1123
2	I	0.26	0/835	0.47	0/1123
2	J	0.26	0/835	0.47	0/1123
All	All	0.26	0/110920	0.44	4/149756 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1624	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	1624	ASP	CB-CG-OD1	5.92	123.62	118.30
1	D	1624	ASP	CB-CG-OD1	5.92	123.62	118.30
1	C	1624	ASP	CB-CG-OD1	5.91	123.62	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30071	0	26711	498	0
1	B	30071	0	26711	500	0
1	C	30071	0	26711	507	0
1	D	30071	0	26711	506	0
2	G	819	0	821	19	0
2	H	819	0	821	19	0
2	I	819	0	821	19	0
2	J	819	0	821	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	123564	0	110128	2042	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2042) 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)
1:D:1772:ILE:HD11	2:J:57:ILE:HA	1.57	0.86
1:A:1233:GLN:HG3	1:B:3493:UNK:HA	1.56	0.86
1:A:4833:PRO:HB3	1:A:4842:ARG:HD3	1.61	0.82
1:C:4833:PRO:HB3	1:C:4842:ARG:HD3	1.61	0.81
1:D:76:ARG:O	1:D:80:GLU:HB2	1.81	0.81
1:D:890:HIS:HB2	1:D:932:ASN:HD22	1.46	0.81
1:B:76:ARG:O	1:B:80:GLU:HB2	1.81	0.80
1:D:4833:PRO:HB3	1:D:4842:ARG:HD3	1.61	0.80
1:B:2406:HIS:HA	1:B:2409:HIS:HB3	1.64	0.80
1:A:890:HIS:HB2	1:A:932:ASN:HD22	1.46	0.80
1:D:2406:HIS:HA	1:D:2409:HIS:HB3	1.63	0.80
1:C:76:ARG:O	1:C:80:GLU:HB2	1.81	0.80
1:A:2406:HIS:HA	1:A:2409:HIS:HB3	1.64	0.80
1:C:890:HIS:HB2	1:C:932:ASN:HD22	1.46	0.80
1:C:2406:HIS:HA	1:C:2409:HIS:HB3	1.64	0.80
1:B:4833:PRO:HB3	1:B:4842:ARG:HD3	1.61	0.79
1:B:890:HIS:HB2	1:B:932:ASN:HD22	1.46	0.79
1:A:76:ARG:O	1:A:80:GLU:HB2	1.81	0.79
1:A:1772:ILE:HD11	2:G:57:ILE:HA	1.65	0.78
1:D:1741:PRO:HB3	1:D:1746:LYS:HE3	1.68	0.75
1:A:1741:PRO:HB3	1:A:1746:LYS:HE3	1.68	0.75
1:C:1741:PRO:HB3	1:C:1746:LYS:HE3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4042:ILE:HG22	1:B:4044:LYS:H	1.53	0.73
1:D:1122:CYS:HA	1:D:1133:ARG:HD3	1.71	0.73
1:C:1122:CYS:HA	1:C:1133:ARG:HD3	1.71	0.73
1:B:1741:PRO:HB3	1:B:1746:LYS:HE3	1.68	0.73
1:C:4042:ILE:HG22	1:C:4044:LYS:H	1.53	0.73
1:A:4042:ILE:HG22	1:A:4044:LYS:H	1.53	0.73
1:D:4042:ILE:HG22	1:D:4044:LYS:H	1.53	0.72
1:B:1989:GLU:HG2	1:B:1992:ARG:HD3	1.72	0.72
1:A:1122:CYS:HA	1:A:1133:ARG:HD3	1.71	0.72
1:C:1262:PRO:HG2	1:C:1265:HIS:HB2	1.72	0.72
1:A:1262:PRO:HG2	1:A:1265:HIS:HB2	1.72	0.72
1:A:1989:GLU:HG2	1:A:1992:ARG:HD3	1.72	0.72
1:C:279:THR:HG22	1:C:281:ARG:H	1.55	0.72
1:B:1122:CYS:HA	1:B:1133:ARG:HD3	1.71	0.72
1:D:1262:PRO:HG2	1:D:1265:HIS:HB2	1.72	0.72
1:B:279:THR:HG22	1:B:281:ARG:H	1.55	0.71
1:C:1989:GLU:HG2	1:C:1992:ARG:HD3	1.72	0.71
1:B:760:ASP:HB3	1:B:764:PRO:HG2	1.73	0.71
1:D:920:GLU:HB2	1:D:923:LYS:HB2	1.73	0.71
1:A:279:THR:HG22	1:A:281:ARG:H	1.55	0.71
1:B:1262:PRO:HG2	1:B:1265:HIS:HB2	1.72	0.71
1:C:4867:ASP:OD1	1:D:4873:ARG:NH1	2.23	0.71
1:C:920:GLU:HB2	1:C:923:LYS:HB2	1.72	0.71
1:A:920:GLU:HB2	1:A:923:LYS:HB2	1.73	0.71
1:A:760:ASP:HB3	1:A:764:PRO:HG2	1.73	0.71
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.73	0.70
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.73	0.70
1:D:1989:GLU:HG2	1:D:1992:ARG:HD3	1.72	0.70
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.73	0.70
1:C:1681:VAL:HG23	1:C:1682:ASP:H	1.55	0.70
1:C:2128:LEU:HD11	1:C:2140:LEU:HD12	1.73	0.70
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.74	0.70
1:D:279:THR:HG22	1:D:281:ARG:H	1.55	0.70
1:A:162:ILE:HD11	1:A:181:LEU:HD13	1.74	0.70
1:C:4824:GLY:O	1:D:4821:ARG:NH2	2.24	0.70
1:D:2128:LEU:HD11	1:D:2140:LEU:HD12	1.73	0.70
2:J:24:VAL:HG22	2:J:48:LYS:HG2	1.74	0.70
1:A:1681:VAL:HG23	1:A:1682:ASP:H	1.55	0.70
1:A:2502:ASP:OD1	1:A:2503:THR:N	2.25	0.70
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.73	0.69
1:B:920:GLU:HB2	1:B:923:LYS:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:HD11	1:C:181:LEU:HD13	1.74	0.69
1:D:162:ILE:HD11	1:D:181:LEU:HD13	1.74	0.69
1:D:760:ASP:HB3	1:D:764:PRO:HG2	1.73	0.69
2:I:24:VAL:HG22	2:I:48:LYS:HG2	1.74	0.69
1:D:1681:VAL:HG23	1:D:1682:ASP:H	1.55	0.69
1:A:2128:LEU:HD11	1:A:2140:LEU:HD12	1.73	0.69
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.74	0.69
1:B:162:ILE:HD11	1:B:181:LEU:HD13	1.74	0.69
1:C:671:LYS:HB3	1:C:761:LEU:HB2	1.75	0.69
1:B:1233:GLN:HG3	1:C:3493:UNK:HA	1.73	0.69
1:B:671:LYS:HB3	1:B:761:LEU:HB2	1.75	0.69
1:B:1681:VAL:HG23	1:B:1682:ASP:H	1.55	0.68
1:B:2128:LEU:HD11	1:B:2140:LEU:HD12	1.73	0.68
1:A:412:GLU:OE2	1:A:412:GLU:N	2.26	0.68
1:D:671:LYS:HB3	1:D:761:LEU:HB2	1.75	0.68
1:B:2502:ASP:OD1	1:B:2503:THR:N	2.24	0.68
1:C:760:ASP:HB3	1:C:764:PRO:HG2	1.73	0.68
1:A:671:LYS:HB3	1:A:761:LEU:HB2	1.75	0.68
1:D:412:GLU:N	1:D:412:GLU:OE2	2.26	0.68
2:G:69:LEU:HA	2:G:104:LEU:HD22	1.76	0.68
1:C:412:GLU:N	1:C:412:GLU:OE2	2.26	0.67
1:B:412:GLU:N	1:B:412:GLU:OE2	2.27	0.67
2:J:69:LEU:HA	2:J:104:LEU:HD22	1.76	0.67
1:A:1044:LYS:HD2	1:A:1051:ARG:HH12	1.59	0.67
1:C:2502:ASP:OD1	1:C:2503:THR:N	2.25	0.67
1:B:1044:LYS:HD2	1:B:1051:ARG:HH12	1.59	0.67
1:D:3831:ASP:HB3	1:D:3834:PHE:HB3	1.77	0.67
1:B:908:ARG:HG2	1:B:916:PRO:HG3	1.77	0.67
1:A:486:GLN:HB3	1:A:544:ASN:HD21	1.59	0.67
1:B:486:GLN:HB3	1:B:544:ASN:HD21	1.59	0.67
1:C:3831:ASP:HB3	1:C:3834:PHE:HB3	1.77	0.66
1:D:1044:LYS:HD2	1:D:1051:ARG:HH12	1.59	0.66
1:B:1684:PRO:HD3	2:H:42:ASP:HB3	1.77	0.66
1:B:544:ASN:ND2	1:B:547:ASN:OD1	2.29	0.66
2:I:69:LEU:HA	2:I:104:LEU:HD22	1.76	0.66
1:C:486:GLN:HB3	1:C:544:ASN:HD21	1.59	0.66
1:C:1272:ARG:NH2	1:C:1584:PRO:O	2.29	0.66
1:B:1772:ILE:HD11	2:H:57:ILE:HA	1.78	0.66
1:A:544:ASN:ND2	1:A:547:ASN:OD1	2.29	0.66
1:A:940:LEU:HA	1:A:943:LEU:HD12	1.78	0.66
1:C:908:ARG:HG2	1:C:916:PRO:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:LYS:HD2	1:C:1051:ARG:HH12	1.59	0.66
1:C:2084:PHE:O	1:C:3690:TYR:OH	2.14	0.66
1:A:1272:ARG:NH2	1:A:1584:PRO:O	2.29	0.66
1:A:3831:ASP:HB3	1:A:3834:PHE:HB3	1.77	0.66
1:B:1272:ARG:NH2	1:B:1584:PRO:O	2.29	0.66
2:H:69:LEU:HA	2:H:104:LEU:HD22	1.76	0.66
1:D:908:ARG:HG2	1:D:916:PRO:HG3	1.77	0.66
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.29	0.66
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.29	0.66
1:B:2084:PHE:O	1:B:3690:TYR:OH	2.14	0.65
1:C:880:ARG:HG3	1:C:881:ILE:HD12	1.78	0.65
1:D:940:LEU:HA	1:D:943:LEU:HD12	1.78	0.65
1:A:908:ARG:HG2	1:A:916:PRO:HG3	1.77	0.65
1:B:3831:ASP:HB3	1:B:3834:PHE:HB3	1.77	0.65
1:B:4042:ILE:HG21	1:B:4047:PHE:HB2	1.79	0.65
1:A:1266:GLU:O	1:A:1267:HIS:ND1	2.30	0.65
1:C:544:ASN:ND2	1:C:547:ASN:OD1	2.29	0.65
1:C:1266:GLU:O	1:C:1267:HIS:ND1	2.30	0.65
1:D:694:ARG:HG2	1:D:728:ASP:HB3	1.78	0.65
1:A:4042:ILE:HG21	1:A:4047:PHE:HB2	1.79	0.65
1:B:1266:GLU:O	1:B:1267:HIS:ND1	2.30	0.65
1:A:4619:GLN:HE22	1:A:4631:ARG:HH12	1.43	0.65
1:D:486:GLN:HB3	1:D:544:ASN:HD21	1.59	0.65
1:D:544:ASN:ND2	1:D:547:ASN:OD1	2.29	0.65
1:B:4619:GLN:HE22	1:B:4631:ARG:HH12	1.43	0.65
1:C:694:ARG:HG2	1:C:728:ASP:HB3	1.78	0.65
1:D:880:ARG:HG3	1:D:881:ILE:HD12	1.78	0.65
1:D:1266:GLU:O	1:D:1267:HIS:ND1	2.30	0.65
1:D:2084:PHE:O	1:D:3690:TYR:OH	2.14	0.65
1:B:3954:GLN:NE2	1:B:3974:GLN:OE1	2.30	0.65
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.80	0.64
1:A:3954:GLN:NE2	1:A:3974:GLN:OE1	2.30	0.64
1:B:694:ARG:HG2	1:B:728:ASP:HB3	1.78	0.64
1:B:880:ARG:HG3	1:B:881:ILE:HD12	1.78	0.64
1:B:2074:ILE:HG21	1:B:2079:LEU:HD22	1.80	0.64
1:C:940:LEU:HA	1:C:943:LEU:HD12	1.78	0.64
1:C:4042:ILE:HG21	1:C:4047:PHE:HB2	1.79	0.64
1:B:940:LEU:HA	1:B:943:LEU:HD12	1.78	0.64
1:C:3954:GLN:NE2	1:C:3974:GLN:OE1	2.30	0.64
1:C:1684:PRO:HD3	2:I:42:ASP:HB3	1.79	0.64
1:D:1272:ARG:NH2	1:D:1584:PRO:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.29	0.64
1:D:3954:GLN:NE2	1:D:3974:GLN:OE1	2.30	0.64
1:A:3754:VAL:HA	1:A:3757:THR:HG22	1.80	0.64
1:D:1613:SER:O	1:D:1615:ARG:NH2	2.31	0.64
1:D:2074:ILE:HG21	1:D:2079:LEU:HD22	1.80	0.64
1:A:1613:SER:O	1:A:1615:ARG:NH2	2.31	0.64
1:A:2074:ILE:HG21	1:A:2079:LEU:HD22	1.80	0.64
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.79	0.64
1:D:3754:VAL:HA	1:D:3757:THR:HG22	1.80	0.64
1:A:694:ARG:HG2	1:A:728:ASP:HB3	1.78	0.64
1:A:880:ARG:HG3	1:A:881:ILE:HD12	1.78	0.64
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.29	0.64
1:A:2084:PHE:O	1:A:3690:TYR:OH	2.14	0.64
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.80	0.64
1:B:2220:LEU:HD11	1:B:2242:ALA:HB2	1.80	0.64
1:C:3754:VAL:HA	1:C:3757:THR:HG22	1.80	0.64
1:D:2502:ASP:OD1	1:D:2503:THR:N	2.24	0.64
1:C:2074:ILE:HG21	1:C:2079:LEU:HD22	1.80	0.64
1:D:4042:ILE:HG21	1:D:4047:PHE:HB2	1.79	0.64
1:C:1769:PHE:O	2:I:83:TYR:OH	2.16	0.63
1:C:4710:GLY:O	1:C:4714:THR:OG1	2.17	0.63
1:B:3754:VAL:HA	1:B:3757:THR:HG22	1.80	0.63
1:C:1902:LYS:HG3	1:C:2079:LEU:HD11	1.80	0.63
1:D:1902:LYS:HG3	1:D:2079:LEU:HD11	1.80	0.63
1:C:1092:LYS:HG2	1:C:1120:PRO:HB3	1.81	0.63
1:C:1613:SER:O	1:C:1615:ARG:NH2	2.31	0.63
1:C:2220:LEU:HD11	1:C:2242:ALA:HB2	1.80	0.63
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.80	0.63
1:C:2092:ASP:OD1	1:C:2093:GLY:N	2.31	0.63
1:C:4619:GLN:HE22	1:C:4631:ARG:HH12	1.44	0.63
1:D:2092:ASP:OD1	1:D:2093:GLY:N	2.31	0.63
1:D:4710:GLY:O	1:D:4714:THR:OG1	2.17	0.63
1:A:2220:LEU:HD11	1:A:2242:ALA:HB2	1.80	0.63
1:B:1902:LYS:HG3	1:B:2079:LEU:HD11	1.80	0.63
1:B:2092:ASP:OD1	1:B:2093:GLY:N	2.31	0.63
1:D:1092:LYS:HG2	1:D:1120:PRO:HB3	1.81	0.63
1:D:4619:GLN:HE22	1:D:4631:ARG:HH12	1.43	0.63
1:D:1359:ILE:HG13	1:D:1360:ASP:H	1.64	0.62
1:D:2099:ARG:O	1:D:2103:LYS:NZ	2.32	0.62
1:A:4710:GLY:O	1:A:4714:THR:OG1	2.16	0.62
1:B:1613:SER:O	1:B:1615:ARG:NH2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:LYS:HG2	1:A:1120:PRO:HB3	1.80	0.62
1:D:1744:ASN:HD21	1:D:1746:LYS:HE2	1.65	0.62
1:A:2335:ARG:NE	1:D:143:LEU:HD21	2.15	0.62
1:D:1588:HIS:HE1	1:D:1590:GLN:HE21	1.48	0.62
1:A:1359:ILE:HG13	1:A:1360:ASP:H	1.64	0.62
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.82	0.62
1:B:839:GLU:H	1:B:841:LYS:HZ1	1.47	0.62
1:B:1981:ASP:OD1	1:B:1981:ASP:N	2.32	0.62
1:C:988:LEU:HD23	1:C:992:GLN:HB2	1.81	0.62
1:A:1588:HIS:HE1	1:A:1590:GLN:HE21	1.48	0.62
1:A:2092:ASP:OD1	1:A:2093:GLY:N	2.31	0.62
1:B:3845:LEU:HB3	1:B:3853:PHE:CE2	2.35	0.62
1:D:1981:ASP:OD1	1:D:1981:ASP:N	2.32	0.62
1:D:3845:LEU:HB3	1:D:3853:PHE:CE2	2.35	0.62
1:A:1265:HIS:HD2	1:A:1268:ILE:HB	1.64	0.62
1:A:1902:LYS:HG3	1:A:2079:LEU:HD11	1.80	0.62
1:A:3845:LEU:HB3	1:A:3853:PHE:CE2	2.35	0.62
1:C:759:LEU:HD13	1:C:766:ILE:HG12	1.82	0.62
1:C:1359:ILE:HG13	1:C:1360:ASP:H	1.64	0.62
1:C:3845:LEU:HB3	1:C:3853:PHE:CE2	2.35	0.62
1:B:1588:HIS:HE1	1:B:1590:GLN:HE21	1.48	0.62
1:B:1297:THR:HA	1:B:1346:LEU:HD23	1.82	0.62
1:C:1297:THR:HA	1:C:1346:LEU:HD23	1.82	0.62
1:D:2220:LEU:HD11	1:D:2242:ALA:HB2	1.80	0.62
1:A:4659:PHE:O	1:B:4055:LYS:NZ	2.25	0.61
1:B:759:LEU:HD13	1:B:766:ILE:HG12	1.82	0.61
1:B:4710:GLY:O	1:B:4714:THR:OG1	2.17	0.61
1:C:1588:HIS:HE1	1:C:1590:GLN:HE21	1.48	0.61
1:D:988:LEU:HD23	1:D:992:GLN:HB2	1.81	0.61
1:A:759:LEU:HD13	1:A:766:ILE:HG12	1.82	0.61
1:A:1730:MET:SD	1:A:2106:THR:OG1	2.58	0.61
1:B:2099:ARG:O	1:B:2103:LYS:NZ	2.32	0.61
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.82	0.61
1:D:4044:LYS:HB2	1:D:4075:GLU:HG2	1.82	0.61
1:B:1092:LYS:HG2	1:B:1120:PRO:HB3	1.81	0.61
1:B:1265:HIS:HD2	1:B:1268:ILE:HB	1.64	0.61
1:C:1265:HIS:HD2	1:C:1268:ILE:HB	1.64	0.61
1:C:2099:ARG:O	1:C:2103:LYS:NZ	2.32	0.61
1:C:4044:LYS:HB2	1:C:4075:GLU:HG2	1.82	0.61
1:A:4044:LYS:HB2	1:A:4075:GLU:HG2	1.82	0.61
1:B:1744:ASN:HD21	1:B:1746:LYS:HE2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4044:LYS:HB2	1:B:4075:GLU:HG2	1.82	0.61
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.82	0.61
1:D:759:LEU:HD13	1:D:766:ILE:HG12	1.82	0.61
1:A:1684:PRO:HD3	2:G:42:ASP:HB3	1.82	0.61
1:A:1744:ASN:HD21	1:A:1746:LYS:HE2	1.65	0.61
1:B:988:LEU:HD23	1:B:992:GLN:HB2	1.82	0.61
1:B:1359:ILE:HG13	1:B:1360:ASP:H	1.64	0.61
1:D:1829:LEU:HB3	1:D:1834:ILE:HD11	1.83	0.61
1:B:235:ARG:NH1	1:B:268:SER:O	2.34	0.61
1:B:1829:LEU:HB3	1:B:1834:ILE:HD11	1.83	0.61
1:A:839:GLU:H	1:A:841:LYS:NZ	1.99	0.61
1:B:290:ARG:H	1:B:293:GLN:HE21	1.48	0.61
1:B:839:GLU:H	1:B:841:LYS:NZ	1.99	0.61
1:D:290:ARG:H	1:D:293:GLN:HE21	1.48	0.61
1:D:839:GLU:H	1:D:841:LYS:NZ	1.99	0.61
1:A:1829:LEU:HB3	1:A:1834:ILE:HD11	1.83	0.60
1:B:1847:ILE:HG23	1:B:1892:LEU:HB3	1.83	0.60
1:D:1297:THR:HA	1:D:1346:LEU:HD23	1.82	0.60
1:A:235:ARG:NH1	1:A:268:SER:O	2.34	0.60
1:A:1297:THR:HA	1:A:1346:LEU:HD23	1.82	0.60
1:B:373:THR:HG22	1:B:397:GLY:HA2	1.83	0.60
1:A:375:GLN:NE2	1:A:390:LYS:O	2.34	0.60
1:C:839:GLU:H	1:C:841:LYS:NZ	1.99	0.60
1:C:1829:LEU:HB3	1:C:1834:ILE:HD11	1.83	0.60
1:D:235:ARG:NH1	1:D:268:SER:O	2.34	0.60
1:D:2228:LEU:HD22	1:D:2296:ARG:HG3	1.83	0.60
1:A:2228:LEU:HD22	1:A:2296:ARG:HG3	1.84	0.60
1:C:375:GLN:NE2	1:C:390:LYS:O	2.34	0.60
1:C:1267:HIS:HB2	1:C:1294:ASN:HB2	1.84	0.60
1:C:1744:ASN:HD21	1:C:1746:LYS:HE2	1.65	0.60
1:D:375:GLN:NE2	1:D:390:LYS:O	2.34	0.60
1:D:1265:HIS:HD2	1:D:1268:ILE:HB	1.64	0.60
1:C:3995:GLY:O	1:C:3999:VAL:HG12	2.02	0.60
1:D:1847:ILE:HG23	1:D:1892:LEU:HB3	1.83	0.60
1:A:1267:HIS:HB2	1:A:1294:ASN:HB2	1.84	0.60
1:B:1267:HIS:HB2	1:B:1294:ASN:HB2	1.84	0.60
1:B:3995:GLY:O	1:B:3999:VAL:HG12	2.02	0.60
1:C:2228:LEU:HD22	1:C:2296:ARG:HG3	1.84	0.60
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.82	0.60
1:A:290:ARG:H	1:A:293:GLN:HE21	1.48	0.60
1:A:988:LEU:HD23	1:A:992:GLN:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:THR:HG22	1:C:397:GLY:HA2	1.83	0.60
1:D:3995:GLY:O	1:D:3999:VAL:HG12	2.02	0.60
1:B:375:GLN:NE2	1:B:390:LYS:O	2.34	0.60
1:C:379:VAL:HG13	1:C:381:SER:H	1.67	0.60
1:D:2064:THR:HG22	1:D:2067:ARG:HH12	1.67	0.60
1:C:235:ARG:NH1	1:C:268:SER:O	2.34	0.60
1:A:3995:GLY:O	1:A:3999:VAL:HG12	2.02	0.59
1:B:2228:LEU:HD22	1:B:2296:ARG:HG3	1.83	0.59
1:C:844:ARG:HE	1:C:845:THR:H	1.50	0.59
1:C:1847:ILE:HG23	1:C:1892:LEU:HB3	1.83	0.59
1:A:4784:ALA:HA	1:A:4788:PHE:HD2	1.68	0.59
1:B:426:PHE:HB3	1:B:497:LEU:HD21	1.85	0.59
1:D:379:VAL:HG13	1:D:381:SER:H	1.67	0.59
1:A:373:THR:HG22	1:A:397:GLY:HA2	1.83	0.59
1:A:1847:ILE:HG23	1:A:1892:LEU:HB3	1.83	0.59
1:A:2873:TYR:HA	1:A:2876:LEU:HD13	1.85	0.59
1:B:4784:ALA:HA	1:B:4788:PHE:HD2	1.68	0.59
1:D:1267:HIS:HB2	1:D:1294:ASN:HB2	1.84	0.59
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.68	0.59
1:B:2064:THR:HG22	1:B:2067:ARG:HH12	1.67	0.59
1:D:373:THR:HG22	1:D:397:GLY:HA2	1.83	0.59
1:B:2873:TYR:HA	1:B:2876:LEU:HD13	1.85	0.59
1:C:418:VAL:O	1:C:422:THR:HG22	2.03	0.59
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.68	0.59
1:C:2064:THR:HG22	1:C:2067:ARG:HH12	1.67	0.59
1:D:2484:LEU:O	1:D:2488:GLU:HG2	2.03	0.59
1:A:426:PHE:HB3	1:A:497:LEU:HD21	1.85	0.59
1:A:4873:ARG:NH1	1:D:4867:ASP:OD1	2.36	0.59
1:C:290:ARG:H	1:C:293:GLN:HE21	1.48	0.59
1:D:4784:ALA:HA	1:D:4788:PHE:HD2	1.67	0.59
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.68	0.58
1:A:418:VAL:O	1:A:422:THR:HG22	2.03	0.58
1:B:418:VAL:O	1:B:422:THR:HG22	2.03	0.58
1:A:2484:LEU:O	1:A:2488:GLU:HG2	2.03	0.58
1:B:2484:LEU:O	1:B:2488:GLU:HG2	2.03	0.58
1:A:1827:TYR:CZ	1:A:1831:ILE:HD11	2.39	0.58
1:B:36:CYS:SG	1:B:37:LEU:N	2.77	0.58
1:C:426:PHE:HB3	1:C:497:LEU:HD21	1.85	0.58
1:C:3731:HIS:O	1:C:3775:LYS:NZ	2.35	0.58
1:C:4784:ALA:HA	1:C:4788:PHE:HD2	1.68	0.58
1:D:1827:TYR:CZ	1:D:1831:ILE:HD11	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:VAL:HG13	1:B:381:SER:H	1.67	0.58
1:C:2873:TYR:HA	1:C:2876:LEU:HD13	1.85	0.58
1:D:844:ARG:HE	1:D:845:THR:H	1.50	0.58
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.68	0.58
1:A:2064:THR:HG22	1:A:2067:ARG:HH12	1.67	0.58
1:A:3731:HIS:O	1:A:3775:LYS:NZ	2.35	0.58
1:B:844:ARG:HE	1:B:845:THR:H	1.50	0.58
1:B:3999:VAL:O	1:B:4003:VAL:HG12	2.04	0.58
2:H:39:SER:O	2:H:43:ARG:NH1	2.37	0.58
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.68	0.58
1:D:418:VAL:O	1:D:422:THR:HG22	2.03	0.58
1:D:426:PHE:HB3	1:D:497:LEU:HD21	1.85	0.58
1:C:36:CYS:SG	1:C:37:LEU:N	2.77	0.58
1:C:1827:TYR:CZ	1:C:1831:ILE:HD11	2.38	0.58
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.68	0.58
1:B:3731:HIS:O	1:B:3775:LYS:NZ	2.35	0.58
1:C:2484:LEU:O	1:C:2488:GLU:HG2	2.03	0.58
1:D:2873:TYR:HA	1:D:2876:LEU:HD13	1.84	0.58
1:A:36:CYS:SG	1:A:37:LEU:N	2.77	0.58
1:A:844:ARG:HE	1:A:845:THR:H	1.50	0.58
1:B:934:GLN:HA	1:B:937:LEU:HD12	1.85	0.58
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.86	0.58
1:C:3999:VAL:O	1:C:4003:VAL:HG12	2.04	0.58
1:D:838:ARG:H	1:D:841:LYS:NZ	2.02	0.58
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.68	0.58
1:A:379:VAL:HG13	1:A:381:SER:H	1.67	0.57
1:A:2099:ARG:O	1:A:2103:LYS:NZ	2.32	0.57
1:C:1044:LYS:HA	1:C:1047:LYS:HZ3	1.69	0.57
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.37	0.57
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.37	0.57
1:D:934:GLN:HA	1:D:937:LEU:HD12	1.85	0.57
1:D:1044:LYS:HA	1:D:1047:LYS:HZ3	1.69	0.57
1:B:1827:TYR:CZ	1:B:1831:ILE:HD11	2.38	0.57
1:C:890:HIS:HB2	1:C:932:ASN:ND2	2.19	0.57
2:I:39:SER:O	2:I:43:ARG:NH1	2.37	0.57
1:D:2408:ILE:O	1:D:2412:LYS:HB2	2.05	0.57
1:A:700:THR:HG1	1:A:787:LEU:H	1.52	0.57
1:C:1730:MET:SD	1:C:2106:THR:OG1	2.58	0.57
1:D:36:CYS:SG	1:D:37:LEU:N	2.77	0.57
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.86	0.57
1:C:1110:ALA:HA	1:C:1156:TRP:HE1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.86	0.57
1:D:1730:MET:SD	1:D:2106:THR:OG1	2.58	0.57
1:D:2159:ASN:OD1	1:D:2162:ARG:NH2	2.37	0.57
1:B:2210:GLN:OE1	1:B:2249:ASN:ND2	2.38	0.57
1:A:838:ARG:H	1:A:841:LYS:NZ	2.02	0.57
1:A:1383:ARG:HE	1:A:1385:LYS:HE2	1.70	0.57
1:B:2867:HIS:HE2	1:B:2869:LEU:HD12	1.69	0.57
1:C:838:ARG:H	1:C:841:LYS:NZ	2.02	0.57
1:C:1383:ARG:HE	1:C:1385:LYS:HE2	1.70	0.57
1:C:2408:ILE:O	1:C:2412:LYS:HB2	2.05	0.57
1:A:934:GLN:HA	1:A:937:LEU:HD12	1.85	0.57
1:A:1981:ASP:OD1	1:A:1981:ASP:N	2.32	0.57
1:A:2867:HIS:HE2	1:A:2869:LEU:HD12	1.70	0.57
1:B:4941:LYS:O	1:B:4945:GLU:HG2	2.05	0.57
1:C:934:GLN:HA	1:C:937:LEU:HD12	1.85	0.57
1:C:2210:GLN:OE1	1:C:2249:ASN:ND2	2.38	0.57
1:D:3999:VAL:O	1:D:4003:VAL:HG12	2.04	0.57
1:B:1383:ARG:HE	1:B:1385:LYS:HE2	1.70	0.57
1:C:2276:CYS:SG	1:C:2290:ASN:ND2	2.78	0.57
1:D:2867:HIS:HE2	1:D:2869:LEU:HD12	1.70	0.57
2:J:39:SER:O	2:J:43:ARG:NH1	2.37	0.57
1:A:1110:ALA:HA	1:A:1156:TRP:HE1	1.69	0.57
1:A:3999:VAL:O	1:A:4003:VAL:HG12	2.04	0.57
1:B:2276:CYS:SG	1:B:2290:ASN:ND2	2.78	0.57
1:D:2210:GLN:OE1	1:D:2249:ASN:ND2	2.38	0.57
1:A:677:LEU:HD22	1:A:695:VAL:HG21	1.87	0.56
1:A:1190:LEU:HD11	1:A:1193:LYS:HB2	1.87	0.56
1:A:2408:ILE:O	1:A:2412:LYS:HB2	2.05	0.56
1:D:1383:ARG:HE	1:D:1385:LYS:HE2	1.70	0.56
1:B:677:LEU:HD22	1:B:695:VAL:HG21	1.87	0.56
1:B:1190:LEU:HD11	1:B:1193:LYS:HB2	1.87	0.56
1:D:1040:ASP:OD1	1:D:1040:ASP:N	2.35	0.56
1:A:4049:LYS:HA	1:A:4052:GLU:HG2	1.87	0.56
2:G:39:SER:O	2:G:43:ARG:NH1	2.37	0.56
1:B:838:ARG:H	1:B:841:LYS:NZ	2.02	0.56
1:C:1772:ILE:HD11	2:I:57:ILE:HA	1.87	0.56
1:C:2159:ASN:OD1	1:C:2162:ARG:NH2	2.37	0.56
2:I:79:PRO:HD3	2:I:97:THR:HG22	1.86	0.56
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.68	0.56
1:D:2107:ILE:HG23	1:D:2108:ASN:H	1.70	0.56
1:A:2107:ILE:HG23	1:A:2108:ASN:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:79:PRO:HD3	2:G:97:THR:HG22	1.86	0.56
1:B:1110:ALA:HA	1:B:1156:TRP:HE1	1.69	0.56
1:B:1117:TRP:HE1	1:B:1164:CYS:HB3	1.71	0.56
1:B:4049:LYS:HA	1:B:4052:GLU:HG2	1.87	0.56
1:D:227:TYR:HA	1:D:355:LYS:HA	1.88	0.56
1:D:1110:ALA:HA	1:D:1156:TRP:HE1	1.69	0.56
1:A:2210:GLN:OE1	1:A:2249:ASN:ND2	2.38	0.56
1:A:4941:LYS:O	1:A:4945:GLU:HG2	2.05	0.56
1:C:677:LEU:HD22	1:C:695:VAL:HG21	1.88	0.56
1:D:677:LEU:HD22	1:D:695:VAL:HG21	1.87	0.56
1:D:2147:ASP:O	1:D:2151:ASN:ND2	2.39	0.56
1:D:3729:ARG:O	1:D:3733:ARG:NH1	2.39	0.56
1:B:2408:ILE:O	1:B:2412:LYS:HB2	2.05	0.56
1:D:2276:CYS:SG	1:D:2290:ASN:ND2	2.78	0.56
1:D:2289:TRP:CZ2	1:D:2387:ILE:HD12	2.41	0.56
2:J:79:PRO:HD3	2:J:97:THR:HG22	1.86	0.56
1:A:1117:TRP:HE1	1:A:1164:CYS:HB3	1.71	0.56
1:A:3729:ARG:O	1:A:3733:ARG:NH1	2.39	0.56
1:A:3891:TYR:O	1:A:3956:LYS:NZ	2.39	0.56
1:B:676:GLU:HB2	1:B:803:LEU:HB2	1.86	0.56
1:C:2289:TRP:CZ2	1:C:2387:ILE:HD12	2.41	0.56
1:C:2867:HIS:HE2	1:C:2869:LEU:HD12	1.69	0.56
1:D:1190:LEU:HD11	1:D:1193:LYS:HB2	1.88	0.56
1:A:2276:CYS:SG	1:A:2290:ASN:ND2	2.78	0.56
1:B:1131:ASP:HB3	1:B:1133:ARG:HG2	1.88	0.56
1:B:2107:ILE:HG23	1:B:2108:ASN:H	1.70	0.56
1:B:2147:ASP:O	1:B:2151:ASN:ND2	2.39	0.56
1:C:2107:ILE:HG23	1:C:2108:ASN:H	1.70	0.56
1:D:890:HIS:HB2	1:D:932:ASN:ND2	2.19	0.56
1:D:3891:TYR:O	1:D:3956:LYS:NZ	2.39	0.56
1:A:227:TYR:HA	1:A:355:LYS:HA	1.87	0.55
1:C:718:VAL:HG11	1:C:791:VAL:HG13	1.88	0.55
1:C:1123:GLN:HB2	1:C:1126:LEU:HB2	1.88	0.55
1:D:1117:TRP:HE1	1:D:1164:CYS:HB3	1.71	0.55
1:D:4941:LYS:O	1:D:4945:GLU:HG2	2.05	0.55
1:A:2147:ASP:O	1:A:2151:ASN:ND2	2.39	0.55
1:B:718:VAL:HG11	1:B:791:VAL:HG13	1.88	0.55
1:C:4941:LYS:O	1:C:4945:GLU:HG2	2.05	0.55
1:B:168:GLN:HG3	1:B:169:ARG:HG3	1.88	0.55
1:B:4079:TYR:O	1:B:4083:VAL:HG23	2.07	0.55
2:H:79:PRO:HD3	2:H:97:THR:HG22	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1131:ASP:HB3	1:C:1133:ARG:HG2	1.89	0.55
1:D:769:ARG:HA	1:D:774:PRO:HA	1.89	0.55
1:A:1123:GLN:HB2	1:A:1126:LEU:HB2	1.88	0.55
1:A:1131:ASP:HB3	1:A:1133:ARG:HG2	1.88	0.55
1:A:2289:TRP:CZ2	1:A:2387:ILE:HD12	2.41	0.55
1:A:4079:TYR:O	1:A:4083:VAL:HG23	2.07	0.55
1:B:1123:GLN:HB2	1:B:1126:LEU:HB2	1.88	0.55
1:B:1730:MET:SD	1:B:2106:THR:OG1	2.58	0.55
1:C:3729:ARG:O	1:C:3733:ARG:NH1	2.39	0.55
1:D:4079:TYR:O	1:D:4083:VAL:HG23	2.07	0.55
1:A:890:HIS:HB2	1:A:932:ASN:ND2	2.19	0.55
1:A:2335:ARG:HE	1:D:143:LEU:HD21	1.72	0.55
1:B:1009:ARG:O	1:B:1013:ARG:NH1	2.40	0.55
1:C:1321:UNK:HA	1:C:1436:UNK:HA	1.89	0.55
1:C:4079:TYR:O	1:C:4083:VAL:HG23	2.07	0.55
1:D:281:ARG:NH1	1:D:346:VAL:O	2.30	0.55
1:A:844:ARG:HE	1:A:845:THR:HG22	1.72	0.55
1:A:4789:ARG:NH2	1:A:4805:CYS:SG	2.80	0.55
1:C:1190:LEU:HD11	1:C:1193:LYS:HB2	1.88	0.55
1:C:2147:ASP:O	1:C:2151:ASN:ND2	2.39	0.55
1:D:247:VAL:O	1:D:272:ARG:NH1	2.40	0.55
1:D:4789:ARG:NH2	1:D:4805:CYS:SG	2.80	0.55
1:A:168:GLN:HG3	1:A:169:ARG:HG3	1.88	0.55
1:B:227:TYR:HA	1:B:355:LYS:HA	1.87	0.55
1:B:247:VAL:O	1:B:272:ARG:NH1	2.40	0.55
1:C:1709:ASP:HA	1:C:1713:SER:HB3	1.89	0.55
1:D:1584:PRO:HD2	1:D:1587:LEU:HD23	1.89	0.55
1:A:247:VAL:O	1:A:272:ARG:NH1	2.40	0.55
1:A:2337:GLU:HG3	1:D:140:THR:O	2.06	0.55
1:A:4867:ASP:OD1	1:B:4873:ARG:NH1	2.40	0.55
1:B:1709:ASP:HA	1:B:1713:SER:HB3	1.89	0.55
1:B:2289:TRP:CZ2	1:B:2387:ILE:HD12	2.41	0.55
1:D:4049:LYS:HA	1:D:4052:GLU:HG2	1.88	0.55
1:D:4757:SER:O	1:D:4761:HIS:HB2	2.07	0.55
1:A:4142:LYS:NZ	1:A:4955:ASP:OD2	2.39	0.55
1:C:247:VAL:O	1:C:272:ARG:NH1	2.40	0.55
1:D:4142:LYS:NZ	1:D:4955:ASP:OD2	2.39	0.55
1:A:718:VAL:HG11	1:A:791:VAL:HG13	1.88	0.55
1:B:1044:LYS:HA	1:B:1047:LYS:HZ3	1.72	0.55
1:B:2277:GLN:HA	1:B:2280:VAL:HG22	1.89	0.55
1:B:3729:ARG:O	1:B:3733:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4757:SER:O	1:B:4761:HIS:HB2	2.07	0.55
1:D:1131:ASP:HB3	1:D:1133:ARG:HG2	1.89	0.55
1:A:4757:SER:O	1:A:4761:HIS:HB2	2.07	0.54
1:B:1321:UNK:HA	1:B:1436:UNK:HA	1.89	0.54
1:C:227:TYR:HA	1:C:355:LYS:HA	1.88	0.54
1:D:1321:UNK:HA	1:D:1436:UNK:HA	1.89	0.54
1:A:769:ARG:HA	1:A:774:PRO:HA	1.89	0.54
1:A:1584:PRO:HD2	1:A:1587:LEU:HD23	1.89	0.54
1:A:1709:ASP:HA	1:A:1713:SER:HB3	1.89	0.54
1:D:844:ARG:HE	1:D:845:THR:HG22	1.72	0.54
1:B:844:ARG:HE	1:B:845:THR:HG22	1.72	0.54
1:B:4789:ARG:NH2	1:B:4805:CYS:SG	2.80	0.54
1:C:4789:ARG:NH2	1:C:4805:CYS:SG	2.80	0.54
1:D:168:GLN:HG3	1:D:169:ARG:HG3	1.88	0.54
1:A:629:GLN:HE21	1:A:1670:ASN:HD22	1.56	0.54
1:C:769:ARG:HA	1:C:774:PRO:HA	1.89	0.54
1:C:1117:TRP:HE1	1:C:1164:CYS:HB3	1.71	0.54
1:D:486:GLN:CB	1:D:544:ASN:HD21	2.20	0.54
1:D:1709:ASP:HA	1:D:1713:SER:HB3	1.89	0.54
1:B:1769:PHE:O	2:H:83:TYR:OH	2.25	0.54
1:C:844:ARG:HE	1:C:845:THR:HG22	1.72	0.54
1:C:1009:ARG:O	1:C:1013:ARG:NH1	2.40	0.54
1:C:4049:LYS:HA	1:C:4052:GLU:HG2	1.88	0.54
1:D:1123:GLN:HB2	1:D:1126:LEU:HB2	1.88	0.54
1:C:168:GLN:HG3	1:C:169:ARG:HG3	1.88	0.54
1:C:838:ARG:H	1:C:841:LYS:HZ1	1.54	0.54
1:D:718:VAL:HG11	1:D:791:VAL:HG13	1.88	0.54
1:D:3731:HIS:O	1:D:3775:LYS:NZ	2.35	0.54
1:A:1009:ARG:O	1:A:1013:ARG:NH1	2.40	0.54
1:A:1044:LYS:HA	1:A:1047:LYS:HZ3	1.73	0.54
1:A:4160:GLU:OE1	1:A:4160:GLU:N	2.41	0.54
1:C:1932:VAL:HG21	1:C:3616:VAL:HA	1.90	0.54
1:D:1009:ARG:O	1:D:1013:ARG:NH1	2.40	0.54
1:D:2277:GLN:HA	1:D:2280:VAL:HG22	1.89	0.54
1:D:4046:ASP:OD1	1:D:4046:ASP:N	2.40	0.54
1:D:4160:GLU:N	1:D:4160:GLU:OE1	2.41	0.54
1:A:1040:ASP:OD1	1:A:1040:ASP:N	2.35	0.54
1:B:629:GLN:HE21	1:B:1670:ASN:HD22	1.56	0.54
1:C:4046:ASP:OD1	1:C:4046:ASP:N	2.40	0.54
1:D:1677:LEU:HA	1:D:1680:HIS:HB2	1.89	0.54
1:B:769:ARG:HA	1:B:774:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1584:PRO:HD2	1:B:1587:LEU:HD23	1.89	0.54
1:D:1932:VAL:HG21	1:D:3616:VAL:HA	1.90	0.54
1:D:2271:CYS:SG	1:D:2294:GLY:N	2.81	0.54
1:D:2747:SER:O	1:D:2753:GLN:NE2	2.39	0.54
1:A:486:GLN:CB	1:A:544:ASN:HD21	2.20	0.53
1:A:838:ARG:H	1:A:841:LYS:HZ1	1.55	0.53
1:C:1397:UNK:HA	1:C:1412:UNK:HA	1.90	0.53
1:C:2271:CYS:SG	1:C:2294:GLY:N	2.81	0.53
1:C:4757:SER:O	1:C:4761:HIS:HB2	2.07	0.53
1:D:1397:UNK:HA	1:D:1412:UNK:HA	1.90	0.53
1:C:4160:GLU:OE1	1:C:4160:GLU:N	2.41	0.53
2:I:58:LYS:HA	2:I:61:GLU:HG2	1.90	0.53
1:A:582:SER:HB2	1:A:584:GLU:OE2	2.09	0.53
1:A:1321:UNK:HA	1:A:1436:UNK:HA	1.89	0.53
1:A:2325:ARG:NH2	1:D:189:GLU:O	2.39	0.53
1:A:4830:ILE:HG22	1:A:4831:GLU:H	1.74	0.53
1:C:486:GLN:CB	1:C:544:ASN:HD21	2.20	0.53
1:D:334:SER:OG	1:D:335:LYS:N	2.41	0.53
1:A:2271:CYS:SG	1:A:2294:GLY:N	2.81	0.53
1:A:2747:SER:O	1:A:2753:GLN:NE2	2.38	0.53
1:B:1397:UNK:HA	1:B:1412:UNK:HA	1.90	0.53
1:B:1932:VAL:HG21	1:B:3616:VAL:HA	1.90	0.53
1:B:4142:LYS:NZ	1:B:4955:ASP:OD2	2.39	0.53
1:C:1677:LEU:HA	1:C:1680:HIS:HB2	1.89	0.53
1:D:582:SER:HB2	1:D:584:GLU:OE2	2.09	0.53
1:A:1677:LEU:HA	1:A:1680:HIS:HB2	1.89	0.53
1:B:2455:MET:HG3	1:B:2457:ALA:H	1.74	0.53
1:C:2277:GLN:HA	1:C:2280:VAL:HG22	1.89	0.53
1:B:59:PRO:HB3	1:B:296:ARG:HH12	1.74	0.53
1:B:4160:GLU:OE1	1:B:4160:GLU:N	2.41	0.53
1:B:4276:LYS:NZ	1:B:4562:GLU:OE1	2.42	0.53
1:A:59:PRO:HB3	1:A:296:ARG:HH12	1.74	0.53
1:B:486:GLN:CB	1:B:544:ASN:HD21	2.20	0.53
1:D:2383:MET:O	1:D:2387:ILE:HG12	2.09	0.53
1:A:1914:ASP:OD1	1:A:2089:ARG:NH1	2.40	0.53
1:A:1932:VAL:HG21	1:A:3616:VAL:HA	1.89	0.53
1:A:2277:GLN:HA	1:A:2280:VAL:HG22	1.89	0.53
1:B:2747:SER:O	1:B:2753:GLN:NE2	2.38	0.53
1:B:3891:TYR:O	1:B:3956:LYS:NZ	2.39	0.53
2:H:58:LYS:HA	2:H:61:GLU:HG2	1.90	0.53
1:C:1584:PRO:HD2	1:C:1587:LEU:HD23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2254:LEU:O	1:C:3809:ARG:HD3	2.09	0.53
2:J:58:LYS:HA	2:J:61:GLU:HG2	1.90	0.53
1:B:300:VAL:O	1:B:420:ARG:NH1	2.37	0.53
1:B:2271:CYS:SG	1:B:2294:GLY:N	2.81	0.53
1:B:4830:ILE:HG22	1:B:4831:GLU:H	1.74	0.53
1:C:672:LYS:HB3	1:C:819:TYR:HA	1.91	0.53
1:C:4276:LYS:NZ	1:C:4562:GLU:OE1	2.42	0.53
1:A:4276:LYS:NZ	1:A:4562:GLU:OE1	2.42	0.53
1:A:4824:GLY:O	1:B:4821:ARG:NH2	2.42	0.53
1:B:1677:LEU:HA	1:B:1680:HIS:HB2	1.89	0.53
1:B:2867:HIS:CD2	1:B:2869:LEU:HB2	2.44	0.53
1:C:1629:MET:HE1	1:C:1685:GLN:HE21	1.74	0.53
1:C:2455:MET:HG3	1:C:2457:ALA:H	1.74	0.53
1:C:2867:HIS:CD2	1:C:2869:LEU:HB2	2.44	0.53
1:C:4830:ILE:HG22	1:C:4831:GLU:H	1.74	0.53
1:D:59:PRO:HB3	1:D:296:ARG:HH12	1.74	0.53
1:A:1397:UNK:HA	1:A:1412:UNK:HA	1.90	0.52
1:B:2383:MET:O	1:B:2387:ILE:HG12	2.09	0.52
1:C:1972:ILE:HA	1:C:1975:LEU:HG	1.91	0.52
1:C:2383:MET:O	1:C:2387:ILE:HG12	2.09	0.52
1:D:2254:LEU:O	1:D:3809:ARG:HD3	2.09	0.52
1:A:2383:MET:O	1:A:2387:ILE:HG12	2.09	0.52
1:C:629:GLN:HE21	1:C:1670:ASN:HD22	1.56	0.52
1:C:640:ARG:HH22	2:I:91:VAL:HG13	1.74	0.52
1:C:1981:ASP:OD1	1:C:1981:ASP:N	2.32	0.52
1:D:838:ARG:H	1:D:841:LYS:HZ1	1.55	0.52
1:D:4830:ILE:HG22	1:D:4831:GLU:H	1.74	0.52
2:J:50:ARG:N	2:J:55:GLU:OE2	2.41	0.52
1:A:2148:ILE:HA	1:A:2151:ASN:HD22	1.73	0.52
1:A:2867:HIS:CD2	1:A:2869:LEU:HB2	2.44	0.52
1:B:1040:ASP:OD1	1:B:1040:ASP:N	2.35	0.52
1:C:874:LEU:HD21	1:C:941:LYS:HD3	1.92	0.52
1:C:2081:ARG:HG3	1:C:3686:LEU:HD22	1.92	0.52
1:D:1972:ILE:HA	1:D:1975:LEU:HG	1.92	0.52
1:A:334:SER:OG	1:A:335:LYS:N	2.41	0.52
1:B:1629:MET:CE	1:B:1685:GLN:HE21	2.22	0.52
1:D:629:GLN:HE21	1:D:1670:ASN:HD22	1.56	0.52
1:A:281:ARG:NH1	1:A:346:VAL:O	2.30	0.52
1:A:874:LEU:HD21	1:A:941:LYS:HD3	1.92	0.52
1:A:2455:MET:HG3	1:A:2457:ALA:H	1.74	0.52
1:B:340:VAL:HG23	1:B:341:GLY:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:SER:HB2	1:B:584:GLU:OE2	2.09	0.52
1:B:672:LYS:HB3	1:B:819:TYR:HA	1.91	0.52
1:B:874:LEU:HD21	1:B:941:LYS:HD3	1.92	0.52
1:B:3954:GLN:NE2	1:B:3971:MET:SD	2.83	0.52
1:C:1629:MET:CE	1:C:1685:GLN:HE21	2.22	0.52
1:C:3961:SER:OG	1:C:3962:SER:N	2.43	0.52
1:D:874:LEU:HD21	1:D:941:LYS:HD3	1.92	0.52
1:A:2254:LEU:O	1:A:3809:ARG:HD3	2.09	0.52
1:B:2148:ILE:HA	1:B:2151:ASN:HD22	1.73	0.52
1:D:672:LYS:HB3	1:D:819:TYR:HA	1.91	0.52
1:D:711:GLU:O	1:D:712:GLU:HG2	2.10	0.52
1:D:3640:ILE:HD12	1:D:3697:SER:HB2	1.92	0.52
1:D:3954:GLN:NE2	1:D:3971:MET:SD	2.83	0.52
1:D:4276:LYS:NZ	1:D:4562:GLU:OE1	2.42	0.52
1:A:927:GLN:HG3	1:A:928:GLU:HG3	1.92	0.52
1:B:489:PHE:HD1	1:B:494:MET:SD	2.33	0.52
1:C:3954:GLN:NE2	1:C:3971:MET:SD	2.83	0.52
1:D:375:GLN:HE22	1:D:392:ILE:H	1.58	0.52
1:A:1629:MET:CE	1:A:1685:GLN:HE21	2.22	0.52
1:A:3954:GLN:NE2	1:A:3971:MET:SD	2.83	0.52
2:G:58:LYS:HA	2:G:61:GLU:HG2	1.91	0.52
1:C:4928:ASP:O	1:C:4932:HIS:NE2	2.43	0.52
1:D:340:VAL:HG23	1:D:341:GLY:H	1.75	0.52
1:D:2148:ILE:HA	1:D:2151:ASN:HD22	1.73	0.52
1:D:2455:MET:HG3	1:D:2457:ALA:H	1.74	0.52
1:A:672:LYS:HB3	1:A:819:TYR:HA	1.91	0.52
1:C:334:SER:OG	1:C:335:LYS:N	2.41	0.52
1:C:375:GLN:HE22	1:C:392:ILE:H	1.58	0.52
1:D:4928:ASP:O	1:D:4932:HIS:NE2	2.43	0.52
1:A:2335:ARG:HH21	1:D:143:LEU:HD11	1.73	0.52
1:A:4928:ASP:O	1:A:4932:HIS:NE2	2.43	0.52
1:B:2081:ARG:HG3	1:B:3686:LEU:HD22	1.92	0.52
1:B:3961:SER:OG	1:B:3962:SER:N	2.43	0.52
1:A:489:PHE:HD1	1:A:494:MET:SD	2.33	0.51
1:C:1715:TYR:CZ	1:C:1762:MET:HB3	2.45	0.51
1:C:2148:ILE:HA	1:C:2151:ASN:HD22	1.73	0.51
1:C:2775:LYS:O	1:C:2779:LYS:HG3	2.10	0.51
1:C:2858:GLU:O	1:C:2862:LYS:HG2	2.10	0.51
1:D:2867:HIS:CD2	1:D:2869:LEU:HB2	2.44	0.51
1:A:3961:SER:OG	1:A:3962:SER:N	2.43	0.51
2:G:50:ARG:N	2:G:55:GLU:OE2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ARG:N	2:H:55:GLU:OE2	2.41	0.51
1:C:927:GLN:HG3	1:C:928:GLU:HG3	1.92	0.51
1:C:2342:LEU:HB2	1:C:2430:ASP:OD2	2.11	0.51
1:C:3846:CYS:HG	1:C:3853:PHE:HD2	1.57	0.51
1:D:1042:THR:O	1:D:1045:SER:OG	2.28	0.51
1:D:1265:HIS:CD2	1:D:1268:ILE:HB	2.45	0.51
1:D:1629:MET:CE	1:D:1685:GLN:HE21	2.22	0.51
1:D:1715:TYR:CZ	1:D:1762:MET:HB3	2.45	0.51
1:A:711:GLU:O	1:A:712:GLU:HG2	2.10	0.51
1:A:3640:ILE:HD12	1:A:3697:SER:HB2	1.91	0.51
1:B:26:ALA:HB2	1:B:194:LEU:HD21	1.93	0.51
1:B:927:GLN:HG3	1:B:928:GLU:HG3	1.92	0.51
1:B:1914:ASP:OD1	1:B:2089:ARG:NH1	2.40	0.51
1:B:2342:LEU:HB2	1:B:2430:ASP:OD2	2.11	0.51
1:B:2775:LYS:O	1:B:2779:LYS:HG3	2.10	0.51
1:B:3640:ILE:HD12	1:B:3697:SER:HB2	1.92	0.51
1:C:711:GLU:O	1:C:712:GLU:HG2	2.10	0.51
1:C:3891:TYR:O	1:C:3956:LYS:NZ	2.39	0.51
1:C:4142:LYS:NZ	1:C:4955:ASP:OD2	2.39	0.51
1:D:26:ALA:HB2	1:D:194:LEU:HD21	1.93	0.51
1:B:2254:LEU:O	1:B:3809:ARG:HD3	2.09	0.51
1:C:340:VAL:HG23	1:C:341:GLY:H	1.75	0.51
1:C:489:PHE:HD1	1:C:494:MET:SD	2.33	0.51
1:D:2081:ARG:HG3	1:D:3686:LEU:HD22	1.92	0.51
1:A:26:ALA:HB2	1:A:194:LEU:HD21	1.93	0.51
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.93	0.51
1:B:763:ALA:HB3	1:B:764:PRO:HD3	1.93	0.51
1:C:59:PRO:HB3	1:C:296:ARG:HH12	1.74	0.51
1:C:582:SER:HB2	1:C:584:GLU:OE2	2.09	0.51
1:A:1845:GLN:HA	1:A:1848:GLU:HG2	1.93	0.51
1:A:2343:LEU:O	1:A:2347:GLU:HG2	2.11	0.51
1:B:4928:ASP:O	1:B:4932:HIS:NE2	2.43	0.51
1:C:26:ALA:HB2	1:C:194:LEU:HD21	1.93	0.51
1:C:763:ALA:HB3	1:C:764:PRO:HD3	1.93	0.51
1:C:2343:LEU:O	1:C:2347:GLU:HG2	2.11	0.51
1:C:3640:ILE:HD12	1:C:3697:SER:HB2	1.92	0.51
2:I:50:ARG:N	2:I:55:GLU:OE2	2.41	0.51
1:D:489:PHE:HD1	1:D:494:MET:SD	2.33	0.51
1:D:927:GLN:HG3	1:D:928:GLU:HG3	1.92	0.51
1:D:2343:LEU:O	1:D:2347:GLU:HG2	2.11	0.51
1:D:2858:GLU:O	1:D:2862:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1265:HIS:CD2	1:B:1268:ILE:HB	2.45	0.51
1:C:1102:TYR:HA	1:C:1164:CYS:O	2.11	0.51
1:D:1845:GLN:HA	1:D:1848:GLU:HG2	1.93	0.51
1:A:375:GLN:HE22	1:A:392:ILE:H	1.58	0.51
1:A:1715:TYR:CZ	1:A:1762:MET:HB3	2.45	0.51
1:B:1845:GLN:HA	1:B:1848:GLU:HG2	1.93	0.51
1:B:4046:ASP:N	1:B:4046:ASP:OD1	2.40	0.51
1:C:238:HIS:HB2	1:C:241:MET:HB2	1.93	0.51
1:D:1914:ASP:OD1	1:D:2089:ARG:NH1	2.40	0.51
1:D:2740:TRP:HB3	1:D:2756:MET:HG3	1.93	0.51
1:D:2775:LYS:O	1:D:2779:LYS:HG3	2.10	0.51
1:A:1042:THR:O	1:A:1045:SER:OG	2.28	0.51
1:A:1972:ILE:HA	1:A:1975:LEU:HG	1.92	0.51
1:A:2081:ARG:HG3	1:A:3686:LEU:HD22	1.92	0.51
1:B:711:GLU:O	1:B:712:GLU:HG2	2.10	0.51
1:B:1811:VAL:HB	1:B:1818:LEU:HD13	1.93	0.51
1:B:1972:ILE:HA	1:B:1975:LEU:HG	1.92	0.51
1:A:640:ARG:HH22	2:G:91:VAL:HG13	1.74	0.51
1:A:732:LEU:HB3	1:A:779:PHE:CZ	2.46	0.51
1:A:2108:ASN:HD21	1:A:2111:SER:HB3	1.76	0.51
1:A:2291:PRO:HB3	1:A:2387:ILE:HD13	1.93	0.51
1:A:2740:TRP:HB3	1:A:2756:MET:HG3	1.93	0.51
1:A:2775:LYS:O	1:A:2779:LYS:HG3	2.10	0.51
1:B:1715:TYR:CZ	1:B:1762:MET:HB3	2.45	0.51
1:B:2291:PRO:HB3	1:B:2387:ILE:HD13	1.93	0.51
1:B:2740:TRP:HB3	1:B:2756:MET:HG3	1.93	0.51
1:C:765:SER:OG	1:C:780:GLU:HA	2.11	0.51
1:C:2291:PRO:HB3	1:C:2387:ILE:HD13	1.93	0.51
1:C:2498:ALA:O	1:C:2501:LEU:HD23	2.11	0.51
1:D:2291:PRO:HB3	1:D:2387:ILE:HD13	1.93	0.51
1:A:340:VAL:HG23	1:A:341:GLY:H	1.75	0.50
1:B:732:LEU:HB3	1:B:779:PHE:CZ	2.46	0.50
1:B:1102:TYR:HA	1:B:1164:CYS:O	2.11	0.50
1:C:2278:MET:N	1:C:2278:MET:SD	2.84	0.50
1:D:763:ALA:HB3	1:D:764:PRO:HD3	1.93	0.50
1:A:2342:LEU:HB2	1:A:2430:ASP:OD2	2.10	0.50
1:A:2858:GLU:O	1:A:2862:LYS:HG2	2.10	0.50
1:B:2498:ALA:O	1:B:2501:LEU:HD23	2.11	0.50
1:C:28:ILE:HG21	1:C:201:TRP:HH2	1.77	0.50
1:A:238:HIS:HB2	1:A:241:MET:HB2	1.94	0.50
1:A:765:SER:OG	1:A:780:GLU:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:765:SER:OG	1:B:780:GLU:HA	2.11	0.50
1:B:890:HIS:HB2	1:B:932:ASN:ND2	2.19	0.50
1:C:2716:LEU:O	1:C:2720:ILE:HG12	2.12	0.50
1:C:2740:TRP:HB3	1:C:2756:MET:HG3	1.93	0.50
1:D:765:SER:OG	1:D:780:GLU:HA	2.11	0.50
1:D:839:GLU:H	1:D:841:LYS:HZ1	1.58	0.50
1:D:3961:SER:OG	1:D:3962:SER:N	2.43	0.50
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.45	0.50
1:A:2278:MET:N	1:A:2278:MET:SD	2.84	0.50
1:B:28:ILE:HG21	1:B:201:TRP:HH2	1.77	0.50
1:B:1042:THR:O	1:B:1045:SER:OG	2.28	0.50
1:B:2108:ASN:HD21	1:B:2111:SER:HB3	1.76	0.50
1:B:2716:LEU:O	1:B:2720:ILE:HG12	2.12	0.50
1:C:281:ARG:NH1	1:C:346:VAL:O	2.30	0.50
1:C:732:LEU:HB3	1:C:779:PHE:CZ	2.46	0.50
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.45	0.50
1:C:1811:VAL:HB	1:C:1818:LEU:HD13	1.93	0.50
1:C:2206:SER:OG	1:C:2207:ARG:N	2.44	0.50
1:C:4866:ILE:HD12	1:D:4866:ILE:HD13	1.93	0.50
1:D:238:HIS:HB2	1:D:241:MET:HB2	1.94	0.50
1:A:281:ARG:O	1:A:285:SER:OG	2.26	0.50
1:A:300:VAL:O	1:A:420:ARG:NH1	2.37	0.50
1:A:2716:LEU:O	1:A:2720:ILE:HG12	2.12	0.50
1:B:281:ARG:O	1:B:285:SER:OG	2.26	0.50
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.44	0.50
1:B:2858:GLU:O	1:B:2862:LYS:HG2	2.10	0.50
1:C:2070:GLN:O	1:C:3659:ARG:NH1	2.44	0.50
1:A:1102:TYR:HB2	1:A:1165:MET:HG3	1.94	0.50
1:C:1845:GLN:HA	1:C:1848:GLU:HG2	1.93	0.50
1:C:1914:ASP:OD1	1:C:2089:ARG:NH1	2.40	0.50
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.94	0.50
1:D:2498:ALA:O	1:D:2501:LEU:HD23	2.11	0.50
1:A:851:LEU:HB3	1:A:1212:VAL:HG12	1.94	0.50
1:A:1985:CYS:SG	1:A:1992:ARG:HD2	2.52	0.50
1:A:2498:ALA:O	1:A:2501:LEU:HD23	2.11	0.50
1:B:281:ARG:NH1	1:B:346:VAL:O	2.30	0.50
1:B:851:LEU:HB3	1:B:1212:VAL:HG12	1.94	0.50
1:B:2206:SER:OG	1:B:2207:ARG:N	2.44	0.50
1:B:2721:ASN:C	1:B:2721:ASN:HD22	2.15	0.50
1:C:1985:CYS:SG	1:C:1992:ARG:HD2	2.52	0.50
1:C:2108:ASN:HD21	1:C:2111:SER:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ILE:HG21	1:D:201:TRP:HH2	1.77	0.50
1:D:1171:HIS:HB2	1:D:1193:LYS:HZ2	1.76	0.50
1:D:2108:ASN:HD21	1:D:2111:SER:HB3	1.76	0.50
1:D:2278:MET:SD	1:D:2278:MET:N	2.84	0.50
1:A:839:GLU:H	1:A:841:LYS:HZ1	1.59	0.50
1:A:1265:HIS:CD2	1:A:1268:ILE:HB	2.45	0.50
1:B:375:GLN:HE22	1:B:392:ILE:H	1.58	0.50
1:B:640:ARG:HH22	2:H:91:VAL:HG13	1.76	0.50
1:B:1986:PRO:HB2	1:B:1988:PRO:HD2	1.94	0.50
1:B:2343:LEU:O	1:B:2347:GLU:HG2	2.11	0.50
1:C:1102:TYR:HB2	1:C:1165:MET:HG3	1.94	0.50
1:A:28:ILE:HG21	1:A:201:TRP:HH2	1.77	0.50
1:A:1008:ALA:O	1:A:1012:ILE:HG23	2.12	0.50
1:A:1102:TYR:HA	1:A:1164:CYS:O	2.11	0.50
1:B:238:HIS:HB2	1:B:241:MET:HB2	1.93	0.50
1:B:1345:VAL:HG13	1:B:1347:MET:SD	2.52	0.50
1:C:851:LEU:HB3	1:C:1212:VAL:HG12	1.94	0.50
1:C:1986:PRO:HB2	1:C:1988:PRO:HD2	1.94	0.50
1:C:2721:ASN:C	1:C:2721:ASN:HD22	2.15	0.50
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.94	0.49
1:B:2278:MET:N	1:B:2278:MET:SD	2.84	0.49
1:B:2894:PHE:HA	1:B:2897:ILE:HG12	1.94	0.49
1:D:851:LEU:HB3	1:D:1212:VAL:HG12	1.94	0.49
1:D:1102:TYR:HA	1:D:1164:CYS:O	2.11	0.49
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.45	0.49
1:D:1359:ILE:HG12	1:D:1363:LYS:HD2	1.94	0.49
1:D:1811:VAL:HB	1:D:1818:LEU:HD13	1.93	0.49
1:D:1986:PRO:HB2	1:D:1988:PRO:HD2	1.94	0.49
1:A:1345:VAL:HG13	1:A:1347:MET:SD	2.52	0.49
1:C:23:GLN:HG3	1:C:213:SER:HB3	1.94	0.49
1:C:2334:LEU:HD13	1:C:2342:LEU:HD12	1.95	0.49
1:D:2206:SER:OG	1:D:2207:ARG:N	2.44	0.49
1:D:2334:LEU:HD13	1:D:2342:LEU:HD12	1.95	0.49
1:C:1040:ASP:N	1:C:1040:ASP:OD1	2.35	0.49
1:C:2080:VAL:HG13	1:C:3669:LEU:HD22	1.94	0.49
1:C:2747:SER:O	1:C:2753:GLN:NE2	2.38	0.49
1:C:4570:THR:HA	1:C:4573:ILE:HG12	1.95	0.49
1:D:1102:TYR:HB2	1:D:1165:MET:HG3	1.94	0.49
1:A:441:LYS:HG2	1:A:442:LEU:HD23	1.94	0.49
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.94	0.49
1:B:2080:VAL:HG13	1:B:3669:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1345:VAL:HG13	1:C:1347:MET:SD	2.52	0.49
1:D:1008:ALA:O	1:D:1012:ILE:HG23	2.12	0.49
1:D:2342:LEU:HB2	1:D:2430:ASP:OD2	2.11	0.49
1:A:1811:VAL:HB	1:A:1818:LEU:HD13	1.93	0.49
1:B:1359:ILE:HG12	1:B:1363:LYS:HD2	1.94	0.49
1:B:2717:GLU:HA	1:B:2720:ILE:HG12	1.95	0.49
1:B:3728:ALA:HA	1:B:3731:HIS:ND1	2.28	0.49
1:D:732:LEU:HB3	1:D:779:PHE:CZ	2.46	0.49
1:D:1345:VAL:HG13	1:D:1347:MET:SD	2.52	0.49
1:A:2070:GLN:O	1:A:3659:ARG:NH1	2.44	0.49
1:A:3493:UNK:HA	1:D:1233:GLN:HG3	1.95	0.49
1:B:4079:TYR:HA	1:B:4082:PHE:HB3	1.95	0.49
1:C:1700:ARG:NH1	1:C:1817:PHE:O	2.46	0.49
1:A:436:LEU:HD21	1:A:517:VAL:HG12	1.95	0.49
1:A:1700:ARG:NH1	1:A:1817:PHE:O	2.46	0.49
1:A:1986:PRO:HB2	1:A:1988:PRO:HD2	1.94	0.49
1:B:441:LYS:HG2	1:B:442:LEU:HD23	1.94	0.49
1:B:1102:TYR:HB2	1:B:1165:MET:HG3	1.94	0.49
1:C:1042:THR:O	1:C:1045:SER:OG	2.28	0.49
1:C:2894:PHE:HA	1:C:2897:ILE:HG12	1.94	0.49
1:D:1266:GLU:OE1	1:D:1267:HIS:HB3	2.12	0.49
1:D:1985:CYS:SG	1:D:1992:ARG:HD2	2.52	0.49
1:D:4660:TYR:HB3	1:D:4664:ARG:HH21	1.78	0.49
1:A:2717:GLU:HA	1:A:2720:ILE:HG12	1.95	0.49
1:A:2721:ASN:HD22	1:A:2721:ASN:C	2.15	0.49
1:B:1970:GLU:HA	1:B:1973:ASN:HB2	1.95	0.49
1:C:658:ASN:HD22	1:C:833:LYS:H	1.61	0.49
1:C:1266:GLU:OE1	1:C:1267:HIS:HB3	2.12	0.49
1:C:2183:SER:O	1:C:2183:SER:OG	2.31	0.49
1:D:658:ASN:HD22	1:D:833:LYS:H	1.61	0.49
1:D:4757:SER:HA	1:D:4760:THR:HG22	1.95	0.49
1:A:1266:GLU:OE1	1:A:1267:HIS:HB3	2.12	0.49
1:A:2334:LEU:HD13	1:A:2342:LEU:HD12	1.95	0.49
1:A:4079:TYR:HA	1:A:4082:PHE:HB3	1.95	0.49
1:A:4757:SER:HA	1:A:4760:THR:HG22	1.95	0.49
1:B:699:SER:OG	1:B:700:THR:N	2.46	0.49
1:B:1266:GLU:OE1	1:B:1267:HIS:HB3	2.12	0.49
1:B:1985:CYS:SG	1:B:1992:ARG:HD2	2.52	0.49
1:B:4660:TYR:HB3	1:B:4664:ARG:HH21	1.78	0.49
1:C:300:VAL:O	1:C:420:ARG:NH1	2.37	0.49
1:C:4079:TYR:HA	1:C:4082:PHE:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:HG3	1:A:213:SER:HB3	1.94	0.49
1:A:2206:SER:OG	1:A:2207:ARG:N	2.44	0.49
1:B:112:THR:HG21	1:B:174:LYS:HD3	1.95	0.49
1:B:1649:GLU:HA	1:B:1649:GLU:OE2	2.13	0.49
1:C:1359:ILE:HG12	1:C:1363:LYS:HD2	1.94	0.49
1:C:3728:ALA:HA	1:C:3731:HIS:ND1	2.28	0.49
1:A:2080:VAL:HG13	1:A:3669:LEU:HD22	1.94	0.48
1:A:4570:THR:HA	1:A:4573:ILE:HG12	1.95	0.48
1:B:1008:ALA:O	1:B:1012:ILE:HG23	2.12	0.48
1:B:2334:LEU:HD13	1:B:2342:LEU:HD12	1.95	0.48
1:C:700:THR:HG1	1:C:787:LEU:H	1.59	0.48
1:C:1970:GLU:HA	1:C:1973:ASN:HB2	1.95	0.48
1:C:4608:LYS:HG3	1:C:4614:LEU:HB2	1.95	0.48
1:D:329:PHE:HB3	1:D:363:ILE:HD11	1.95	0.48
1:D:2717:GLU:HA	1:D:2720:ILE:HG12	1.95	0.48
1:D:2721:ASN:HD22	1:D:2721:ASN:C	2.15	0.48
1:A:890:HIS:O	1:A:894:VAL:HG23	2.13	0.48
1:D:23:GLN:HG3	1:D:213:SER:HB3	1.94	0.48
1:D:2070:GLN:O	1:D:3659:ARG:NH1	2.44	0.48
1:D:2716:LEU:O	1:D:2720:ILE:HG12	2.12	0.48
1:D:2894:PHE:HA	1:D:2897:ILE:HG12	1.94	0.48
1:D:3728:ALA:HA	1:D:3731:HIS:ND1	2.28	0.48
1:A:112:THR:HG21	1:A:174:LYS:HD3	1.95	0.48
1:A:1241:VAL:HG21	1:B:3539:UNK:HA	1.94	0.48
1:A:1359:ILE:HG12	1:A:1363:LYS:HD2	1.94	0.48
1:A:2894:PHE:HA	1:A:2897:ILE:HG12	1.94	0.48
1:A:3728:ALA:HA	1:A:3731:HIS:ND1	2.28	0.48
1:B:4608:LYS:HG3	1:B:4614:LEU:HB2	1.95	0.48
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.94	0.48
1:C:3636:GLU:HG2	1:C:3696:LYS:HE3	1.94	0.48
1:D:4570:THR:HA	1:D:4573:ILE:HG12	1.95	0.48
2:J:88:HIS:HD2	2:J:89:PRO:HD2	1.78	0.48
1:A:1649:GLU:HA	1:A:1649:GLU:OE2	2.13	0.48
1:C:890:HIS:O	1:C:894:VAL:HG23	2.13	0.48
1:C:1649:GLU:HA	1:C:1649:GLU:OE2	2.13	0.48
1:C:2717:GLU:HA	1:C:2720:ILE:HG12	1.95	0.48
2:I:72:ARG:HG2	2:I:103:GLU:HB2	1.95	0.48
1:D:19:GLU:HG2	1:D:68:VAL:HG22	1.96	0.48
1:D:1567:LEU:HD22	1:D:1581:PRO:HB3	1.95	0.48
1:D:1629:MET:HE1	1:D:1685:GLN:HE21	1.79	0.48
1:A:699:SER:OG	1:A:700:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4046:ASP:OD1	1:A:4046:ASP:N	2.40	0.48
1:B:258:ARG:NH1	1:B:316:LEU:O	2.47	0.48
1:B:334:SER:OG	1:B:335:LYS:N	2.41	0.48
1:B:730:LEU:HD23	1:B:748:LEU:HD23	1.96	0.48
2:H:72:ARG:HG2	2:H:103:GLU:HB2	1.95	0.48
2:H:88:HIS:HD2	2:H:89:PRO:HD2	1.79	0.48
1:C:112:THR:HG21	1:C:174:LYS:HD3	1.95	0.48
1:C:329:PHE:HB3	1:C:363:ILE:HD11	1.95	0.48
1:C:1567:LEU:HD22	1:C:1581:PRO:HB3	1.95	0.48
1:D:112:THR:HG21	1:D:174:LYS:HD3	1.95	0.48
1:D:1649:GLU:HA	1:D:1649:GLU:OE2	2.13	0.48
1:D:1700:ARG:NH1	1:D:1817:PHE:O	2.46	0.48
1:D:2080:VAL:HG13	1:D:3669:LEU:HD22	1.94	0.48
1:D:4079:TYR:HA	1:D:4082:PHE:HB3	1.95	0.48
2:J:72:ARG:HG2	2:J:103:GLU:HB2	1.95	0.48
1:B:1165:MET:HB3	1:B:1236:TYR:CE2	2.49	0.48
1:B:1700:ARG:NH1	1:B:1817:PHE:O	2.46	0.48
1:B:2070:GLN:O	1:B:3659:ARG:NH1	2.44	0.48
1:C:1090:ALA:HB3	1:C:1202:ILE:HD11	1.95	0.48
1:C:1171:HIS:HB2	1:C:1193:LYS:HZ2	1.78	0.48
1:C:1968:PRO:HA	1:C:1971:GLN:HB3	1.96	0.48
1:A:19:GLU:HG2	1:A:68:VAL:HG22	1.96	0.48
1:A:1567:LEU:HD22	1:A:1581:PRO:HB3	1.95	0.48
1:A:1970:GLU:HA	1:A:1973:ASN:HB2	1.95	0.48
1:A:3923:ILE:HD13	1:A:3934:LEU:HD12	1.96	0.48
1:B:658:ASN:HD22	1:B:833:LYS:H	1.61	0.48
1:B:3636:GLU:HG2	1:B:3696:LYS:HE3	1.94	0.48
1:B:4570:THR:HA	1:B:4573:ILE:HG12	1.95	0.48
1:C:1165:MET:HB3	1:C:1236:TYR:CE2	2.49	0.48
1:C:1642:ILE:HD11	1:C:1699:LEU:HD23	1.96	0.48
1:D:258:ARG:NH1	1:D:316:LEU:O	2.47	0.48
1:D:932:ASN:OD1	1:D:933:LEU:N	2.47	0.48
1:A:329:PHE:HB3	1:A:363:ILE:HD11	1.95	0.48
1:A:1629:MET:HE1	1:A:1685:GLN:HE21	1.79	0.48
1:B:329:PHE:HB3	1:B:363:ILE:HD11	1.95	0.48
1:B:1567:LEU:HD22	1:B:1581:PRO:HB3	1.95	0.48
1:C:839:GLU:H	1:C:841:LYS:HZ1	1.60	0.48
1:D:882:ARG:HD2	1:D:937:LEU:HD23	1.96	0.48
1:D:3636:GLU:HG2	1:D:3696:LYS:HE3	1.94	0.48
1:A:932:ASN:OD1	1:A:933:LEU:N	2.47	0.48
1:A:3636:GLU:HG2	1:A:3696:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:72:ARG:HG2	2:G:103:GLU:HB2	1.96	0.48
1:B:4273:MET:HE2	1:B:4273:MET:N	2.29	0.48
1:C:258:ARG:NH1	1:C:316:LEU:O	2.47	0.48
1:D:436:LEU:HD21	1:D:517:VAL:HG12	1.95	0.48
1:D:1118:SER:HA	1:D:1134:ALA:HA	1.96	0.48
1:A:730:LEU:HD23	1:A:748:LEU:HD23	1.96	0.48
1:A:4660:TYR:HB3	1:A:4664:ARG:HH21	1.78	0.48
1:B:23:GLN:HG3	1:B:213:SER:HB3	1.94	0.48
1:B:642:LEU:HD12	1:B:643:LEU:HA	1.96	0.48
1:B:4757:SER:HA	1:B:4760:THR:HG22	1.95	0.48
1:C:436:LEU:HD21	1:C:517:VAL:HG12	1.95	0.48
1:C:441:LYS:HG2	1:C:442:LEU:HD23	1.94	0.48
1:C:1008:ALA:O	1:C:1012:ILE:HG23	2.12	0.48
1:C:1257:GLN:HA	1:C:1384:LEU:HD22	1.95	0.48
1:C:1273:ILE:HD11	1:C:1287:GLN:HB2	1.95	0.48
1:C:4290:PHE:HZ	1:C:4573:ILE:HD11	1.79	0.48
1:D:812:LYS:O	1:D:812:LYS:NZ	2.35	0.48
1:D:2784:TRP:HH2	1:D:2846:ASN:HB2	1.78	0.48
1:A:1090:ALA:HB3	1:A:1202:ILE:HD11	1.95	0.47
1:A:4029:ASP:OD1	1:A:4029:ASP:N	2.47	0.47
1:B:3923:ILE:HD13	1:B:3934:LEU:HD12	1.96	0.47
1:D:706:TYR:HA	1:D:838:ARG:HG2	1.97	0.47
1:D:890:HIS:O	1:D:894:VAL:HG23	2.13	0.47
1:D:1052:GLU:HA	1:D:1055:ARG:HB2	1.96	0.47
1:A:1257:GLN:HA	1:A:1384:LEU:HD22	1.95	0.47
1:A:4608:LYS:HG3	1:A:4614:LEU:HB2	1.95	0.47
1:B:606:ARG:NH2	1:B:1635:GLU:OE1	2.34	0.47
1:B:713:TRP:NE1	1:B:841:LYS:HG2	2.30	0.47
1:B:1052:GLU:HA	1:B:1055:ARG:HB2	1.96	0.47
1:B:2784:TRP:HH2	1:B:2846:ASN:HB2	1.79	0.47
1:C:3728:ALA:HA	1:C:3731:HIS:CE1	2.49	0.47
1:C:4757:SER:HA	1:C:4760:THR:HG22	1.95	0.47
1:C:4863:GLY:CA	1:D:4866:ILE:HG12	2.44	0.47
2:I:88:HIS:HD2	2:I:89:PRO:HD2	1.79	0.47
1:D:441:LYS:HG2	1:D:442:LEU:HD23	1.94	0.47
1:D:4273:MET:HE2	1:D:4273:MET:N	2.29	0.47
1:D:4608:LYS:HG3	1:D:4614:LEU:HB2	1.95	0.47
1:A:258:ARG:NH1	1:A:316:LEU:O	2.47	0.47
1:A:658:ASN:HD22	1:A:833:LYS:H	1.61	0.47
1:A:807:ARG:O	1:A:1615:ARG:NE	2.46	0.47
1:B:19:GLU:HG2	1:B:68:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1642:ILE:HD11	1:B:1699:LEU:HD23	1.96	0.47
1:C:713:TRP:NE1	1:C:841:LYS:HG2	2.30	0.47
1:C:4029:ASP:OD1	1:C:4029:ASP:N	2.47	0.47
1:D:1642:ILE:HD11	1:D:1699:LEU:HD23	1.96	0.47
1:D:1970:GLU:HA	1:D:1973:ASN:HB2	1.95	0.47
1:D:1972:ILE:HD12	1:D:1975:LEU:HD11	1.96	0.47
1:A:882:ARG:HD2	1:A:937:LEU:HD23	1.96	0.47
1:A:1273:ILE:HD11	1:A:1287:GLN:HB2	1.95	0.47
1:A:2784:TRP:HH2	1:A:2846:ASN:HB2	1.79	0.47
1:B:2485:HIS:O	1:B:2489:VAL:HG12	2.14	0.47
1:B:4290:PHE:HZ	1:B:4573:ILE:HD11	1.79	0.47
1:B:4694:SER:O	1:B:4694:SER:OG	2.32	0.47
1:C:19:GLU:HG2	1:C:68:VAL:HG22	1.96	0.47
1:C:606:ARG:NH2	1:C:1635:GLU:OE1	2.34	0.47
1:C:1265:HIS:CD2	1:C:1268:ILE:HB	2.45	0.47
1:C:2776:GLU:O	1:C:2780:THR:HG22	2.15	0.47
1:D:713:TRP:NE1	1:D:841:LYS:HG2	2.29	0.47
1:D:4762:ASN:O	1:D:4764:LYS:N	2.48	0.47
1:A:606:ARG:NH2	1:A:1635:GLU:OE1	2.34	0.47
1:A:706:TYR:HA	1:A:838:ARG:HG2	1.96	0.47
1:A:2197:ARG:HB3	1:A:2236:SER:OG	2.15	0.47
1:A:4290:PHE:HZ	1:A:4573:ILE:HD11	1.79	0.47
1:B:1100:ARG:HB3	1:B:1236:TYR:CD2	2.49	0.47
1:B:1118:SER:HA	1:B:1134:ALA:HA	1.96	0.47
1:B:1968:PRO:HA	1:B:1971:GLN:HB3	1.96	0.47
1:C:1118:SER:HA	1:C:1134:ALA:HA	1.96	0.47
1:C:3923:ILE:HD13	1:C:3934:LEU:HD12	1.96	0.47
1:D:699:SER:OG	1:D:700:THR:N	2.46	0.47
1:D:921:PHE:HE1	1:D:932:ASN:HD21	1.63	0.47
1:D:3728:ALA:HA	1:D:3731:HIS:CE1	2.49	0.47
1:D:3846:CYS:HG	1:D:3853:PHE:HD2	1.60	0.47
1:A:642:LEU:HD12	1:A:643:LEU:HA	1.96	0.47
2:G:88:HIS:HD2	2:G:89:PRO:HD2	1.78	0.47
1:B:882:ARG:HD2	1:B:937:LEU:HD23	1.96	0.47
1:B:932:ASN:OD1	1:B:933:LEU:N	2.47	0.47
1:B:1652:LEU:HD12	1:B:1699:LEU:HD13	1.97	0.47
1:B:3728:ALA:HA	1:B:3731:HIS:CE1	2.49	0.47
1:C:730:LEU:HD23	1:C:748:LEU:HD23	1.96	0.47
1:C:1100:ARG:HB3	1:C:1236:TYR:CD2	2.49	0.47
1:D:1100:ARG:HB3	1:D:1236:TYR:CD2	2.49	0.47
1:D:1273:ILE:HD11	1:D:1287:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2231:PRO:HD3	1:D:2381:ILE:HD11	1.96	0.47
1:D:4290:PHE:HZ	1:D:4573:ILE:HD11	1.79	0.47
1:A:336:GLU:HG3	1:A:338:LEU:HD22	1.97	0.47
1:A:713:TRP:NE1	1:A:841:LYS:HG2	2.30	0.47
1:A:921:PHE:HE1	1:A:932:ASN:HD21	1.63	0.47
1:A:1165:MET:HB3	1:A:1236:TYR:CE2	2.49	0.47
1:A:1171:HIS:HB2	1:A:1193:LYS:HZ2	1.80	0.47
1:A:1972:ILE:HD12	1:A:1975:LEU:HD11	1.96	0.47
1:A:2780:THR:HG21	1:A:2846:ASN:ND2	2.30	0.47
1:A:4830:ILE:HB	1:A:4842:ARG:NH2	2.30	0.47
1:B:486:GLN:HB3	1:B:544:ASN:ND2	2.30	0.47
1:B:921:PHE:HE1	1:B:932:ASN:HD21	1.63	0.47
1:B:1090:ALA:HB3	1:B:1202:ILE:HD11	1.95	0.47
1:B:1273:ILE:HD11	1:B:1287:GLN:HB2	1.95	0.47
1:B:2197:ARG:HB3	1:B:2236:SER:OG	2.15	0.47
1:B:4830:ILE:HB	1:B:4842:ARG:NH2	2.30	0.47
1:C:642:LEU:HD12	1:C:643:LEU:HA	1.96	0.47
1:C:699:SER:OG	1:C:700:THR:N	2.46	0.47
1:C:921:PHE:HE1	1:C:932:ASN:HD21	1.63	0.47
1:C:932:ASN:OD1	1:C:933:LEU:N	2.47	0.47
1:C:1052:GLU:HA	1:C:1055:ARG:HB2	1.96	0.47
1:C:2784:TRP:HH2	1:C:2846:ASN:HB2	1.78	0.47
1:C:4660:TYR:HB3	1:C:4664:ARG:HH21	1.78	0.47
1:C:4863:GLY:HA2	1:D:4866:ILE:HG12	1.97	0.47
1:D:1257:GLN:HA	1:D:1384:LEU:HD22	1.95	0.47
2:J:26:HIS:CE1	2:J:41:ARG:HG2	2.50	0.47
1:A:1052:GLU:HA	1:A:1055:ARG:HB2	1.96	0.47
1:A:1100:ARG:HB3	1:A:1236:TYR:CD2	2.49	0.47
1:A:3728:ALA:HA	1:A:3731:HIS:CE1	2.49	0.47
1:A:3805:ASN:OD1	1:A:3806:ALA:N	2.48	0.47
1:B:436:LEU:HD21	1:B:517:VAL:HG12	1.95	0.47
1:B:888:ASN:O	1:B:892:LEU:HG	2.15	0.47
1:B:1257:GLN:HA	1:B:1384:LEU:HD22	1.95	0.47
1:C:706:TYR:HA	1:C:838:ARG:HG2	1.97	0.47
2:I:26:HIS:CE1	2:I:41:ARG:HG2	2.50	0.47
1:D:2776:GLU:O	1:D:2780:THR:HG22	2.15	0.47
1:A:2485:HIS:O	1:A:2489:VAL:HG12	2.14	0.47
1:B:2506:LEU:HD23	1:B:2506:LEU:H	1.80	0.47
1:B:4029:ASP:OD1	1:B:4029:ASP:N	2.48	0.47
1:C:888:ASN:O	1:C:892:LEU:HG	2.15	0.47
1:D:730:LEU:HD23	1:D:748:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1165:MET:HB3	1:D:1236:TYR:CE2	2.49	0.47
1:D:2197:ARG:HB3	1:D:2236:SER:OG	2.15	0.47
1:D:3923:ILE:HD13	1:D:3934:LEU:HD12	1.96	0.47
1:A:2101:LEU:O	1:A:2104:THR:HG22	2.15	0.47
1:A:2231:PRO:HD3	1:A:2381:ILE:HD11	1.96	0.47
1:B:890:HIS:O	1:B:894:VAL:HG23	2.13	0.47
1:C:235:ARG:NH1	1:C:273:SER:OG	2.48	0.47
1:C:2780:THR:HG21	1:C:2846:ASN:ND2	2.30	0.47
1:C:4273:MET:N	1:C:4273:MET:HE2	2.30	0.47
1:D:888:ASN:O	1:D:892:LEU:HG	2.15	0.47
1:D:1090:ALA:HB3	1:D:1202:ILE:HD11	1.95	0.47
1:D:1305:SER:OG	1:D:1588:HIS:O	2.33	0.47
1:A:1287:GLN:HG2	1:A:1355:VAL:HG13	1.97	0.46
1:A:1652:LEU:HD12	1:A:1699:LEU:HD13	1.97	0.46
1:A:2058:GLN:HA	1:A:2090:GLN:HE21	1.81	0.46
1:B:2776:GLU:O	1:B:2780:THR:HG22	2.15	0.46
1:B:2780:THR:HG21	1:B:2846:ASN:ND2	2.30	0.46
1:B:3761:GLY:HA2	1:B:3764:ILE:HG22	1.97	0.46
1:B:3805:ASN:OD1	1:B:3806:ALA:N	2.48	0.46
1:C:336:GLU:HG3	1:C:338:LEU:HD22	1.97	0.46
1:C:2485:HIS:O	1:C:2489:VAL:HG12	2.14	0.46
1:D:1968:PRO:HA	1:D:1971:GLN:HB3	1.96	0.46
1:D:2506:LEU:HD23	1:D:2506:LEU:H	1.80	0.46
1:A:486:GLN:HB3	1:A:544:ASN:ND2	2.30	0.46
1:A:973:THR:OG1	1:A:976:TYR:O	2.19	0.46
1:A:1118:SER:HA	1:A:1134:ALA:HA	1.96	0.46
1:A:1642:ILE:HD11	1:A:1699:LEU:HD23	1.96	0.46
1:A:1713:SER:O	1:A:1717:THR:HG23	2.16	0.46
1:A:2257:ARG:HG3	1:A:2259:PRO:HD3	1.97	0.46
1:B:235:ARG:NH1	1:B:273:SER:OG	2.48	0.46
1:D:300:VAL:O	1:D:420:ARG:NH1	2.37	0.46
1:D:2780:THR:HG21	1:D:2846:ASN:ND2	2.30	0.46
1:D:4830:ILE:HB	1:D:4842:ARG:NH2	2.30	0.46
1:A:1305:SER:OG	1:A:1588:HIS:O	2.33	0.46
1:A:2506:LEU:HD23	1:A:2506:LEU:H	1.80	0.46
1:B:706:TYR:HA	1:B:838:ARG:HG2	1.96	0.46
1:B:921:PHE:O	1:B:929:ARG:NH1	2.45	0.46
1:B:1287:GLN:HG2	1:B:1355:VAL:HG13	1.97	0.46
1:B:2058:GLN:HA	1:B:2090:GLN:HE21	1.81	0.46
1:B:4659:PHE:O	1:C:4055:LYS:NZ	2.39	0.46
1:C:629:GLN:NE2	1:C:1670:ASN:HD22	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2231:PRO:HD3	1:C:2381:ILE:HD11	1.96	0.46
1:C:4830:ILE:HB	1:C:4842:ARG:NH2	2.30	0.46
1:D:235:ARG:NH1	1:D:273:SER:OG	2.48	0.46
1:D:1684:PRO:HD3	2:J:42:ASP:HB3	1.98	0.46
1:D:2485:HIS:O	1:D:2489:VAL:HG12	2.14	0.46
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.18	0.46
1:A:2776:GLU:O	1:A:2780:THR:HG22	2.15	0.46
2:G:38:ASP:OD1	2:G:39:SER:N	2.49	0.46
1:B:336:GLU:HG3	1:B:338:LEU:HD22	1.97	0.46
1:C:882:ARG:HD2	1:C:937:LEU:HD23	1.96	0.46
1:C:4193:GLU:OE2	1:C:4943:TYR:OH	2.28	0.46
1:D:642:LEU:HD12	1:D:643:LEU:HA	1.96	0.46
1:D:1287:GLN:HG2	1:D:1355:VAL:HG13	1.97	0.46
1:D:4294:LEU:HA	1:D:4297:VAL:HG12	1.97	0.46
1:A:547:ASN:O	1:A:551:PHE:HD1	1.99	0.46
1:B:587:ASN:OD1	1:B:2132:ARG:NH1	2.49	0.46
1:B:629:GLN:NE2	1:B:1670:ASN:HD22	2.13	0.46
1:B:2101:LEU:O	1:B:2104:THR:HG22	2.15	0.46
1:C:547:ASN:O	1:C:551:PHE:HD1	1.99	0.46
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.98	0.46
1:D:547:ASN:O	1:D:551:PHE:HD1	1.99	0.46
1:D:587:ASN:OD1	1:D:2132:ARG:NH1	2.49	0.46
1:A:1968:PRO:HA	1:A:1971:GLN:HB3	1.96	0.46
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.18	0.46
1:B:547:ASN:O	1:B:551:PHE:HD1	1.99	0.46
1:B:1969:GLN:O	1:B:1973:ASN:ND2	2.49	0.46
2:H:38:ASP:OD1	2:H:39:SER:N	2.49	0.46
1:C:193:HIS:CE1	1:C:208:GLN:HE21	2.34	0.46
1:C:1287:GLN:HG2	1:C:1355:VAL:HG13	1.97	0.46
1:C:4947:CYS:SG	1:C:4948:TRP:N	2.89	0.46
1:D:629:GLN:NE2	1:D:1670:ASN:HD22	2.13	0.46
1:D:1969:GLN:O	1:D:1973:ASN:ND2	2.49	0.46
1:A:235:ARG:NH1	1:A:273:SER:OG	2.48	0.46
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.98	0.46
1:B:654:SER:HB2	1:B:837:SER:OG	2.16	0.46
1:B:981:MET:HG3	1:B:983:LEU:HG	1.98	0.46
1:B:1124:PRO:HD2	1:B:1595:VAL:HG23	1.98	0.46
2:H:26:HIS:CE1	2:H:41:ARG:HG2	2.50	0.46
1:C:812:LYS:O	1:C:812:LYS:NZ	2.35	0.46
1:C:1972:ILE:HD12	1:C:1975:LEU:HD11	1.96	0.46
1:C:2058:GLN:HA	1:C:2090:GLN:HE21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2197:ARG:HB3	1:C:2236:SER:OG	2.15	0.46
1:D:2058:GLN:HA	1:D:2090:GLN:HE21	1.81	0.46
1:D:4947:CYS:SG	1:D:4948:TRP:N	2.89	0.46
1:A:888:ASN:O	1:A:892:LEU:HG	2.14	0.46
1:A:1969:GLN:O	1:A:1973:ASN:ND2	2.49	0.46
1:A:4273:MET:HE2	1:A:4273:MET:N	2.31	0.46
2:G:26:HIS:CE1	2:G:41:ARG:HG2	2.50	0.46
1:B:1241:VAL:HG21	1:C:3539:UNK:HA	1.98	0.46
1:B:4947:CYS:SG	1:B:4948:TRP:N	2.89	0.46
2:H:28:THR:O	2:H:28:THR:OG1	2.34	0.46
1:C:281:ARG:O	1:C:285:SER:OG	2.26	0.46
1:C:587:ASN:OD1	1:C:2132:ARG:NH1	2.49	0.46
1:D:1362:ASP:OD1	1:D:1362:ASP:N	2.49	0.46
1:A:21:VAL:HG13	1:A:65:CYS:O	2.16	0.46
1:A:700:THR:HA	1:A:707:PRO:HB3	1.98	0.46
1:A:3898:ASP:OD1	1:A:3898:ASP:N	2.46	0.46
1:A:4294:LEU:HA	1:A:4297:VAL:HG12	1.97	0.46
1:B:530:LEU:HD23	1:B:530:LEU:HA	1.78	0.46
1:B:1362:ASP:N	1:B:1362:ASP:OD1	2.49	0.46
1:B:1967:PRO:HD2	1:B:1970:GLU:OE1	2.16	0.46
1:B:3986:GLU:O	1:B:4935:GLN:NE2	2.49	0.46
1:B:4294:LEU:HA	1:B:4297:VAL:HG12	1.97	0.46
1:C:486:GLN:HB3	1:C:544:ASN:ND2	2.30	0.46
1:C:1305:SER:OG	1:C:1588:HIS:O	2.33	0.46
1:C:1743:GLU:CD	1:C:1744:ASN:HD22	2.20	0.46
1:C:1969:GLN:O	1:C:1973:ASN:ND2	2.49	0.46
1:D:2492:LEU:N	1:D:2493:PRO:HD2	2.31	0.46
1:D:3986:GLU:O	1:D:4935:GLN:NE2	2.49	0.46
1:D:4115:GLN:O	1:D:4119:GLU:HG3	2.16	0.46
1:A:193:HIS:CE1	1:A:208:GLN:HE21	2.34	0.46
1:A:629:GLN:NE2	1:A:1670:ASN:HD22	2.13	0.46
1:A:2334:LEU:HD13	1:A:2342:LEU:CD1	2.46	0.46
1:A:2732:SER:O	1:A:2735:LYS:HG3	2.16	0.46
1:B:2231:PRO:HD3	1:B:2381:ILE:HD11	1.96	0.46
1:C:505:LEU:HD22	1:C:526:TRP:HD1	1.81	0.46
1:C:1713:SER:O	1:C:1717:THR:HG23	2.16	0.46
1:C:2506:LEU:HD23	1:C:2506:LEU:H	1.80	0.46
1:D:700:THR:HA	1:D:707:PRO:HB3	1.98	0.46
1:D:981:MET:HG3	1:D:983:LEU:HG	1.98	0.46
1:D:1786:ASP:O	1:D:1789:LYS:HG2	2.16	0.46
1:D:2101:LEU:O	1:D:2104:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3761:GLY:HA2	1:A:3764:ILE:HG22	1.98	0.45
1:A:4632:LEU:H	1:A:4632:LEU:HD23	1.81	0.45
1:B:706:TYR:HA	1:B:838:ARG:CG	2.46	0.45
1:B:2732:SER:O	1:B:2735:LYS:HG3	2.16	0.45
1:B:4632:LEU:HD23	1:B:4632:LEU:H	1.81	0.45
1:B:4762:ASN:O	1:B:4764:LYS:N	2.48	0.45
1:C:671:LYS:HA	1:C:761:LEU:HD12	1.99	0.45
1:C:2101:LEU:O	1:C:2104:THR:HG22	2.15	0.45
1:C:3805:ASN:OD1	1:C:3806:ALA:N	2.48	0.45
1:C:4632:LEU:HD23	1:C:4632:LEU:H	1.81	0.45
1:D:21:VAL:HG13	1:D:65:CYS:O	2.16	0.45
1:D:3761:GLY:HA2	1:D:3764:ILE:HG22	1.97	0.45
1:D:4632:LEU:HD23	1:D:4632:LEU:H	1.81	0.45
2:J:38:ASP:OD1	2:J:39:SER:N	2.49	0.45
1:A:654:SER:HB2	1:A:837:SER:OG	2.16	0.45
1:A:706:TYR:HA	1:A:838:ARG:CG	2.46	0.45
1:A:1786:ASP:O	1:A:1789:LYS:HG2	2.16	0.45
1:A:4304:PHE:O	1:A:4308:VAL:HG22	2.16	0.45
1:B:1713:SER:O	1:B:1717:THR:HG23	2.16	0.45
1:C:318:ASP:OD1	1:C:318:ASP:N	2.50	0.45
1:C:1362:ASP:N	1:C:1362:ASP:OD1	2.49	0.45
1:C:2257:ARG:HG3	1:C:2259:PRO:HD3	1.97	0.45
1:C:2732:SER:HA	1:C:2735:LYS:HG3	1.99	0.45
1:D:2732:SER:O	1:D:2735:LYS:HG3	2.16	0.45
1:A:3986:GLU:O	1:A:4935:GLN:NE2	2.49	0.45
1:A:4115:GLN:O	1:A:4119:GLU:HG3	2.16	0.45
1:B:505:LEU:HD22	1:B:526:TRP:HD1	1.81	0.45
1:B:1972:ILE:HD12	1:B:1975:LEU:HD11	1.96	0.45
1:B:4115:GLN:O	1:B:4119:GLU:HG3	2.16	0.45
1:B:4304:PHE:O	1:B:4308:VAL:HG22	2.16	0.45
1:C:700:THR:HA	1:C:707:PRO:HB3	1.98	0.45
1:C:1124:PRO:HD2	1:C:1595:VAL:HG23	1.98	0.45
1:C:1652:LEU:HD12	1:C:1699:LEU:HD13	1.97	0.45
1:C:1967:PRO:HD2	1:C:1970:GLU:OE1	2.16	0.45
1:C:2732:SER:O	1:C:2735:LYS:HG3	2.16	0.45
1:C:4304:PHE:O	1:C:4308:VAL:HG22	2.16	0.45
1:D:281:ARG:O	1:D:285:SER:OG	2.26	0.45
1:D:1652:LEU:HD12	1:D:1699:LEU:HD13	1.97	0.45
1:D:3805:ASN:OD1	1:D:3806:ALA:N	2.48	0.45
1:D:4304:PHE:O	1:D:4308:VAL:HG22	2.16	0.45
1:A:1767:PRO:HG3	1:A:1781:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:HIS:CE1	1:B:208:GLN:HE21	2.34	0.45
1:B:1359:ILE:HG13	1:B:1360:ASP:N	2.31	0.45
1:B:4070:GLU:OE1	1:B:4070:GLU:N	2.47	0.45
1:C:3761:GLY:HA2	1:C:3764:ILE:HG22	1.97	0.45
1:C:3845:LEU:HD13	1:C:3853:PHE:CZ	2.52	0.45
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.18	0.45
1:D:336:GLU:HG3	1:D:338:LEU:HD22	1.97	0.45
1:D:973:THR:OG1	1:D:976:TYR:O	2.19	0.45
1:A:2732:SER:HA	1:A:2735:LYS:HG3	1.99	0.45
1:B:1305:SER:OG	1:B:1588:HIS:O	2.33	0.45
1:B:1608:ASP:OD1	1:B:1608:ASP:N	2.49	0.45
1:C:706:TYR:CD1	1:C:838:ARG:HB3	2.52	0.45
2:I:38:ASP:OD1	2:I:39:SER:N	2.49	0.45
1:D:2320:VAL:O	1:D:2324:ILE:HG12	2.17	0.45
1:A:4947:CYS:SG	1:A:4948:TRP:N	2.89	0.45
1:B:700:THR:HA	1:B:707:PRO:HB3	1.98	0.45
1:B:745:ASN:O	1:B:747:HIS:ND1	2.47	0.45
1:B:1743:GLU:CD	1:B:1744:ASN:HD22	2.20	0.45
1:B:2257:ARG:HG3	1:B:2259:PRO:HD3	1.97	0.45
1:B:2334:LEU:HD13	1:B:2342:LEU:CD1	2.46	0.45
1:C:981:MET:HG3	1:C:983:LEU:HG	1.98	0.45
1:D:486:GLN:HB3	1:D:544:ASN:ND2	2.29	0.45
1:D:530:LEU:HD23	1:D:530:LEU:HA	1.78	0.45
1:D:706:TYR:CD1	1:D:838:ARG:HB3	2.52	0.45
1:D:1713:SER:O	1:D:1717:THR:HG23	2.16	0.45
1:D:1967:PRO:HD2	1:D:1970:GLU:OE1	2.16	0.45
1:D:2058:GLN:HG3	1:D:2090:GLN:NE2	2.32	0.45
1:D:2732:SER:HA	1:D:2735:LYS:HG3	1.99	0.45
1:D:4273:MET:HE3	1:D:4273:MET:HB2	1.85	0.45
1:A:587:ASN:OD1	1:A:2132:ARG:NH1	2.49	0.45
1:A:669:GLN:HB3	1:A:673:TRP:HZ2	1.82	0.45
1:A:1743:GLU:CD	1:A:1744:ASN:HD22	2.20	0.45
1:A:4670:GLY:O	1:A:4671:MET:HG2	2.17	0.45
1:B:21:VAL:HG13	1:B:65:CYS:O	2.16	0.45
1:B:671:LYS:HA	1:B:761:LEU:HD12	1.99	0.45
1:B:2058:GLN:HG3	1:B:2090:GLN:NE2	2.32	0.45
1:B:2320:VAL:O	1:B:2324:ILE:HG12	2.17	0.45
1:B:4670:GLY:O	1:B:4671:MET:HG2	2.17	0.45
1:C:1786:ASP:O	1:C:1789:LYS:HG2	2.16	0.45
1:C:4294:LEU:HA	1:C:4297:VAL:HG12	1.97	0.45
1:D:299:HIS:HD2	1:D:302:THR:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:GLN:HB3	1:D:673:TRP:HZ2	1.82	0.45
1:D:671:LYS:HA	1:D:761:LEU:HD12	1.99	0.45
1:D:2257:ARG:HG3	1:D:2259:PRO:HD3	1.97	0.45
1:A:981:MET:HG3	1:A:983:LEU:HG	1.98	0.45
1:A:1967:PRO:HD2	1:A:1970:GLU:OE1	2.16	0.45
1:B:318:ASP:OD1	1:B:318:ASP:N	2.50	0.45
1:B:1086:ARG:HH21	1:B:1251:LEU:HD13	1.82	0.45
1:C:1086:ARG:HH21	1:C:1251:LEU:HD13	1.82	0.45
1:C:4115:GLN:O	1:C:4119:GLU:HG3	2.16	0.45
1:D:193:HIS:CE1	1:D:208:GLN:HE21	2.34	0.45
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.98	0.45
1:D:654:SER:HB2	1:D:837:SER:OG	2.16	0.45
1:D:706:TYR:HA	1:D:838:ARG:CG	2.46	0.45
1:D:1608:ASP:OD1	1:D:1608:ASP:N	2.49	0.45
1:A:299:HIS:HD2	1:A:302:THR:H	1.65	0.45
1:A:1608:ASP:OD1	1:A:1608:ASP:N	2.49	0.45
1:A:2762:LEU:HD22	1:A:2766:GLU:O	2.17	0.45
1:A:3845:LEU:HD13	1:A:3853:PHE:CZ	2.52	0.45
1:A:4762:ASN:O	1:A:4764:LYS:N	2.48	0.45
1:B:2257:ARG:CG	1:B:2259:PRO:HD3	2.47	0.45
1:B:2732:SER:HA	1:B:2735:LYS:HG3	1.99	0.45
1:C:654:SER:HB2	1:C:837:SER:OG	2.16	0.45
1:C:669:GLN:HB3	1:C:673:TRP:HZ2	1.82	0.45
1:C:976:TYR:O	1:C:977:LYS:HD2	2.17	0.45
1:C:2320:VAL:O	1:C:2324:ILE:HG12	2.17	0.45
1:D:1124:PRO:HD2	1:D:1595:VAL:HG23	1.98	0.45
1:D:1743:GLU:CD	1:D:1744:ASN:HD22	2.19	0.45
1:D:2334:LEU:HD13	1:D:2342:LEU:CD1	2.46	0.45
1:D:3845:LEU:HD13	1:D:3853:PHE:CZ	2.52	0.45
1:A:845:THR:OG1	1:A:846:TYR:N	2.50	0.45
1:A:2257:ARG:CG	1:A:2259:PRO:HD3	2.47	0.45
1:A:2405:MET:SD	1:A:2407:LEU:HB2	2.57	0.45
1:B:656:ARG:NH2	1:B:835:GLU:OE2	2.50	0.45
1:B:2172:GLU:HA	1:B:2175:VAL:HG12	1.99	0.45
1:B:2405:MET:SD	1:B:2407:LEU:HB2	2.57	0.45
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.18	0.45
1:C:924:LEU:HB2	1:C:929:ARG:HD3	1.99	0.45
1:C:1320:UNK:HA	1:C:1325:UNK:HA	1.99	0.45
1:C:1359:ILE:HG13	1:C:1360:ASP:N	2.31	0.45
1:C:3986:GLU:O	1:C:4935:GLN:NE2	2.49	0.45
1:C:4594:VAL:HA	1:C:4597:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1320:UNK:HA	1:D:1325:UNK:HA	1.99	0.45
1:D:1629:MET:HG3	1:D:1642:ILE:HG21	1.99	0.45
1:A:671:LYS:HA	1:A:761:LEU:HD12	1.98	0.44
1:A:745:ASN:O	1:A:747:HIS:ND1	2.47	0.44
1:A:1353:HIS:CE1	1:A:1367:LYS:HE3	2.52	0.44
1:B:706:TYR:OH	1:B:851:LEU:HD11	2.18	0.44
1:B:1353:HIS:CE1	1:B:1367:LYS:HE3	2.52	0.44
1:B:1767:PRO:HG3	1:B:1781:PRO:HB3	1.98	0.44
1:B:4594:VAL:HA	1:B:4597:VAL:HG12	1.99	0.44
1:C:807:ARG:O	1:C:1615:ARG:NE	2.46	0.44
1:C:1353:HIS:CE1	1:C:1367:LYS:HE3	2.52	0.44
1:C:1591:PHE:CZ	1:C:1593:SER:HB2	2.52	0.44
1:C:1629:MET:HG3	1:C:1642:ILE:HG21	1.98	0.44
1:C:2405:MET:SD	1:C:2407:LEU:HB2	2.57	0.44
1:D:976:TYR:O	1:D:977:LYS:HD2	2.17	0.44
1:D:1591:PHE:CZ	1:D:1593:SER:HB2	2.52	0.44
1:D:1677:LEU:O	1:D:1681:VAL:HG22	2.18	0.44
1:D:4176:VAL:HG11	1:D:4879:VAL:HA	1.99	0.44
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.98	0.44
1:A:706:TYR:CD1	1:A:838:ARG:HB3	2.52	0.44
1:A:706:TYR:OH	1:A:851:LEU:HD11	2.18	0.44
1:A:921:PHE:O	1:A:929:ARG:NH1	2.45	0.44
1:A:1124:PRO:HD2	1:A:1595:VAL:HG23	1.98	0.44
1:A:1196:ASP:OD1	1:A:1196:ASP:N	2.50	0.44
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.49	0.44
1:A:2172:GLU:HA	1:A:2175:VAL:HG12	1.99	0.44
1:B:674:TYR:N	1:B:820:ALA:O	2.51	0.44
1:B:1629:MET:HE2	1:B:1642:ILE:HD13	1.99	0.44
1:B:1629:MET:HG3	1:B:1642:ILE:HG21	1.99	0.44
1:B:2492:LEU:N	1:B:2493:PRO:HD2	2.31	0.44
2:H:83:TYR:HB3	2:H:87:GLY:HA2	2.00	0.44
1:C:299:HIS:HD2	1:C:302:THR:H	1.65	0.44
1:C:674:TYR:N	1:C:820:ALA:O	2.51	0.44
1:C:706:TYR:HA	1:C:838:ARG:CG	2.46	0.44
1:C:2257:ARG:CG	1:C:2259:PRO:HD3	2.47	0.44
1:C:3898:ASP:OD1	1:C:3898:ASP:N	2.46	0.44
1:D:656:ARG:NH2	1:D:835:GLU:OE2	2.50	0.44
1:D:845:THR:OG1	1:D:846:TYR:N	2.50	0.44
1:D:1767:PRO:HG3	1:D:1781:PRO:HB3	1.99	0.44
1:A:896:ASN:OD1	1:A:897:LYS:N	2.51	0.44
1:A:2492:LEU:N	1:A:2493:PRO:HD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4594:VAL:HA	1:A:4597:VAL:HG12	1.99	0.44
1:C:845:THR:OG1	1:C:846:TYR:N	2.50	0.44
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.83	0.44
1:D:924:LEU:HB2	1:D:929:ARG:HD3	1.99	0.44
1:D:2405:MET:SD	1:D:2407:LEU:HB2	2.57	0.44
1:D:4594:VAL:HA	1:D:4597:VAL:HG12	1.99	0.44
1:A:318:ASP:OD1	1:A:318:ASP:N	2.50	0.44
1:A:924:LEU:HB2	1:A:929:ARG:HD3	1.99	0.44
1:A:2058:GLN:HG3	1:A:2090:GLN:NE2	2.32	0.44
1:A:2320:VAL:O	1:A:2324:ILE:HG12	2.17	0.44
1:B:706:TYR:CD1	1:B:838:ARG:HB3	2.52	0.44
1:B:1591:PHE:CZ	1:B:1593:SER:HB2	2.52	0.44
1:B:1786:ASP:O	1:B:1789:LYS:HG2	2.16	0.44
1:B:2731:TRP:CE2	1:B:2762:LEU:HD12	2.53	0.44
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.87	0.44
1:C:1733:GLU:O	1:C:1736:SER:OG	2.30	0.44
1:C:2058:GLN:HG3	1:C:2090:GLN:NE2	2.32	0.44
1:C:2334:LEU:HD13	1:C:2342:LEU:CD1	2.46	0.44
1:C:2492:LEU:N	1:C:2493:PRO:HD2	2.31	0.44
1:D:2316:ALA:O	1:D:2320:VAL:HG23	2.18	0.44
1:A:888:ASN:O	1:A:891:GLU:HG2	2.18	0.44
1:A:1256:PRO:HG2	1:A:1592:LEU:HD21	1.99	0.44
2:G:83:TYR:HB3	2:G:87:GLY:HA2	2.00	0.44
1:B:669:GLN:HB3	1:B:673:TRP:HZ2	1.82	0.44
1:B:888:ASN:O	1:B:891:GLU:HG2	2.18	0.44
1:B:2282:LYS:HA	1:B:2282:LYS:HD2	1.89	0.44
1:B:4051:MET:HE1	1:B:4062:THR:HA	2.00	0.44
1:C:850:LEU:HD23	1:C:1213:GLY:O	2.18	0.44
1:C:4694:SER:O	1:C:4694:SER:OG	2.32	0.44
1:D:807:ARG:O	1:D:1615:ARG:NE	2.46	0.44
1:D:888:ASN:O	1:D:891:GLU:HG2	2.18	0.44
1:D:4670:GLY:O	1:D:4671:MET:HG2	2.17	0.44
2:J:83:TYR:HB3	2:J:87:GLY:HA2	2.00	0.44
1:A:976:TYR:O	1:A:977:LYS:HD2	2.17	0.44
1:A:1086:ARG:HH21	1:A:1251:LEU:HD13	1.82	0.44
1:A:2316:ALA:O	1:A:2320:VAL:HG23	2.18	0.44
1:B:896:ASN:OD1	1:B:897:LYS:N	2.51	0.44
1:B:1196:ASP:N	1:B:1196:ASP:OD1	2.50	0.44
1:B:2316:ALA:O	1:B:2320:VAL:HG23	2.18	0.44
1:B:2331:GLY:HA3	1:B:2391:TYR:HE1	1.83	0.44
1:C:21:VAL:HG13	1:C:65:CYS:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:LEU:HD11	1:C:643:LEU:HD21	2.00	0.44
1:C:1767:PRO:HG3	1:C:1781:PRO:HB3	1.98	0.44
1:C:2731:TRP:CE2	1:C:2762:LEU:HD12	2.53	0.44
1:C:4670:GLY:O	1:C:4671:MET:HG2	2.17	0.44
1:D:674:TYR:N	1:D:820:ALA:O	2.51	0.44
1:D:4044:LYS:HE2	1:D:4044:LYS:HB3	1.81	0.44
1:A:233:VAL:O	1:A:408:SER:OG	2.36	0.44
1:A:674:TYR:N	1:A:820:ALA:O	2.51	0.44
2:G:23:CYS:SG	2:G:51:ILE:HD11	2.58	0.44
1:B:850:LEU:HD23	1:B:1213:GLY:O	2.18	0.44
1:C:896:ASN:OD1	1:C:897:LYS:N	2.51	0.44
1:C:1608:ASP:N	1:C:1608:ASP:OD1	2.49	0.44
2:I:23:CYS:SG	2:I:51:ILE:HD11	2.58	0.44
1:D:706:TYR:OH	1:D:851:LEU:HD11	2.18	0.44
1:D:1048:ASP:OD1	1:D:1051:ARG:NH1	2.48	0.44
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.83	0.44
1:A:1591:PHE:CZ	1:A:1593:SER:HB2	2.52	0.44
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.84	0.44
1:B:2892:PHE:O	1:B:2896:GLN:HG2	2.18	0.44
1:C:557:TRP:CE2	1:C:561:ARG:HG3	2.53	0.44
1:C:4762:ASN:O	1:C:4764:LYS:N	2.48	0.44
2:J:23:CYS:SG	2:J:51:ILE:HD11	2.58	0.44
1:A:1359:ILE:HG13	1:A:1360:ASP:N	2.31	0.44
1:A:1677:LEU:O	1:A:1681:VAL:HG22	2.18	0.44
1:A:2731:TRP:CE2	1:A:2762:LEU:HD12	2.53	0.44
1:B:924:LEU:HB2	1:B:929:ARG:HD3	1.99	0.44
1:B:1028:ARG:O	1:B:1028:ARG:HD3	2.18	0.44
1:B:1677:LEU:O	1:B:1681:VAL:HG22	2.18	0.44
1:B:2762:LEU:HD22	1:B:2766:GLU:O	2.17	0.44
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.83	0.44
1:C:2331:GLY:HA3	1:C:2391:TYR:HE1	1.83	0.44
1:C:2404:GLU:HG3	1:C:2405:MET:H	1.83	0.44
2:I:83:TYR:HB3	2:I:87:GLY:HA2	2.00	0.44
1:D:505:LEU:HD22	1:D:526:TRP:HD1	1.81	0.44
1:D:1086:ARG:HH21	1:D:1251:LEU:HD13	1.82	0.44
1:D:1196:ASP:OD1	1:D:1196:ASP:N	2.50	0.44
1:D:1304:LEU:HD12	1:D:1340:ASP:HB2	2.00	0.44
1:A:712:GLU:HB3	1:A:713:TRP:CE3	2.53	0.43
1:A:850:LEU:HD23	1:A:1213:GLY:O	2.18	0.43
1:A:997:ASP:HB2	1:A:1047:LYS:HD3	2.00	0.43
1:A:1304:LEU:HD12	1:A:1340:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1629:MET:HG3	1:A:1642:ILE:HG21	1.99	0.43
1:A:1704:TYR:O	1:A:1708:ILE:HG12	2.18	0.43
1:A:2733:MET:O	1:A:2736:LEU:HG	2.18	0.43
1:A:3719:GLU:HA	1:A:3722:LYS:HG2	2.00	0.43
1:B:2183:SER:O	1:B:2183:SER:OG	2.31	0.43
2:H:23:CYS:SG	2:H:51:ILE:HD11	2.58	0.43
1:C:712:GLU:HB3	1:C:713:TRP:CE3	2.53	0.43
1:C:1028:ARG:O	1:C:1028:ARG:HD3	2.18	0.43
1:C:1256:PRO:HG2	1:C:1592:LEU:HD21	1.99	0.43
1:C:1747:HIS:O	1:C:1747:HIS:ND1	2.51	0.43
1:D:557:TRP:CE2	1:D:561:ARG:HG3	2.53	0.43
1:D:707:PRO:HD2	1:D:838:ARG:HD2	2.00	0.43
1:D:712:GLU:HB3	1:D:713:TRP:CE3	2.53	0.43
1:D:986:ILE:O	1:D:1055:ARG:NH1	2.51	0.43
1:D:1172:THR:HB	1:D:1190:LEU:HD12	2.00	0.43
1:D:1747:HIS:ND1	1:D:1747:HIS:O	2.51	0.43
1:A:4594:VAL:N	1:A:4595:PRO:HD2	2.33	0.43
1:B:986:ILE:O	1:B:1055:ARG:NH1	2.51	0.43
1:B:1320:UNK:HA	1:B:1325:UNK:HA	1.99	0.43
1:B:2715:LYS:HG3	1:B:2900:TYR:OH	2.17	0.43
1:B:3845:LEU:HD13	1:B:3853:PHE:CZ	2.52	0.43
1:B:4594:VAL:N	1:B:4595:PRO:HD2	2.33	0.43
1:C:656:ARG:NH2	1:C:835:GLU:OE2	2.50	0.43
1:C:1704:TYR:O	1:C:1708:ILE:HG12	2.18	0.43
1:C:2101:LEU:HD13	1:C:3624:GLU:HB3	2.00	0.43
1:D:1353:HIS:CE1	1:D:1367:LYS:HE3	2.52	0.43
1:A:611:LEU:HD11	1:A:643:LEU:HD21	2.00	0.43
1:A:986:ILE:O	1:A:1055:ARG:NH1	2.51	0.43
1:A:2892:PHE:O	1:A:2896:GLN:HG2	2.18	0.43
1:B:544:ASN:O	1:B:581:GLU:HG2	2.19	0.43
1:B:845:THR:OG1	1:B:846:TYR:N	2.50	0.43
1:B:976:TYR:O	1:B:977:LYS:HD2	2.17	0.43
1:B:2101:LEU:HD13	1:B:3624:GLU:HB3	2.00	0.43
1:B:2404:GLU:HG3	1:B:2405:MET:H	1.83	0.43
1:B:2733:MET:O	1:B:2736:LEU:HG	2.18	0.43
1:C:233:VAL:O	1:C:408:SER:OG	2.36	0.43
1:C:888:ASN:O	1:C:891:GLU:HG2	2.18	0.43
1:C:2172:GLU:HA	1:C:2175:VAL:HG12	1.99	0.43
1:C:2240:ASP:OD1	1:C:2296:ARG:NH2	2.43	0.43
1:C:2316:ALA:O	1:C:2320:VAL:HG23	2.18	0.43
1:C:2715:LYS:HG3	1:C:2900:TYR:OH	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2733:MET:O	1:C:2736:LEU:HG	2.18	0.43
1:C:4294:LEU:HA	1:C:4294:LEU:HD12	1.88	0.43
1:C:4590:TYR:HA	1:C:4594:VAL:CG2	2.49	0.43
1:D:646:THR:OG1	1:D:1685:GLN:NE2	2.52	0.43
1:D:745:ASN:O	1:D:747:HIS:ND1	2.47	0.43
1:D:850:LEU:HD23	1:D:1213:GLY:O	2.18	0.43
1:D:896:ASN:OD1	1:D:897:LYS:N	2.51	0.43
1:D:1928:SER:OG	1:D:3616:VAL:HG23	2.19	0.43
1:D:2172:GLU:HA	1:D:2175:VAL:HG12	1.99	0.43
1:D:2257:ARG:CG	1:D:2259:PRO:HD3	2.47	0.43
1:D:2715:LYS:HG3	1:D:2900:TYR:OH	2.17	0.43
1:D:4594:VAL:N	1:D:4595:PRO:HD2	2.33	0.43
1:A:290:ARG:H	1:A:293:GLN:NE2	2.16	0.43
1:A:707:PRO:HD2	1:A:838:ARG:HD2	2.00	0.43
1:A:2715:LYS:HG3	1:A:2900:TYR:OH	2.17	0.43
1:B:1304:LEU:HD12	1:B:1340:ASP:HB2	2.00	0.43
1:B:1747:HIS:ND1	1:B:1747:HIS:O	2.51	0.43
1:B:2335:ARG:HD3	1:B:2336:GLY:N	2.34	0.43
1:C:544:ASN:O	1:C:581:GLU:HG2	2.19	0.43
1:C:1677:LEU:O	1:C:1681:VAL:HG22	2.18	0.43
1:D:544:ASN:O	1:D:581:GLU:HG2	2.19	0.43
1:D:3719:GLU:HA	1:D:3722:LYS:HG2	2.00	0.43
1:D:4051:MET:HE1	1:D:4062:THR:HA	2.00	0.43
1:A:505:LEU:HD22	1:A:526:TRP:HD1	1.82	0.43
1:A:544:ASN:O	1:A:581:GLU:HG2	2.19	0.43
1:A:557:TRP:CE2	1:A:561:ARG:HG3	2.53	0.43
1:A:2331:GLY:HA3	1:A:2391:TYR:HE1	1.83	0.43
1:B:4793:ASN:O	1:B:4795:SER:N	2.50	0.43
1:D:407:ARG:HH21	1:D:3864:ASN:HB3	1.84	0.43
1:D:611:LEU:HD11	1:D:643:LEU:HD21	2.00	0.43
1:D:1028:ARG:O	1:D:1028:ARG:HD3	2.18	0.43
1:D:2355:ASP:OD2	1:D:2357:SER:OG	2.30	0.43
1:A:601:LEU:HG	1:A:642:LEU:HD21	2.00	0.43
1:A:656:ARG:NH2	1:A:835:GLU:OE2	2.50	0.43
1:A:4176:VAL:HG11	1:A:4879:VAL:HA	1.99	0.43
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.83	0.43
1:B:557:TRP:CE2	1:B:561:ARG:HG3	2.53	0.43
1:B:1987:CYS:N	1:B:1988:PRO:HD2	2.34	0.43
1:B:4176:VAL:HG11	1:B:4879:VAL:HA	1.99	0.43
1:C:646:THR:OG1	1:C:1685:GLN:NE2	2.52	0.43
1:C:986:ILE:O	1:C:1055:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1928:SER:OG	1:C:3616:VAL:HG23	2.19	0.43
1:C:2762:LEU:HD22	1:C:2766:GLU:O	2.17	0.43
1:C:4594:VAL:N	1:C:4595:PRO:HD2	2.33	0.43
1:D:921:PHE:O	1:D:929:ARG:NH1	2.45	0.43
1:D:1704:TYR:O	1:D:1708:ILE:HG12	2.18	0.43
1:D:2731:TRP:CE2	1:D:2762:LEU:HD12	2.53	0.43
1:D:2762:LEU:HD22	1:D:2766:GLU:O	2.17	0.43
1:D:2892:PHE:O	1:D:2896:GLN:HG2	2.18	0.43
1:D:4830:ILE:HG22	1:D:4831:GLU:N	2.34	0.43
1:A:1172:THR:HB	1:A:1190:LEU:HD12	2.00	0.43
1:A:1320:UNK:HA	1:A:1325:UNK:HA	1.99	0.43
1:B:407:ARG:HH21	1:B:3864:ASN:HB3	1.84	0.43
1:B:712:GLU:HB3	1:B:713:TRP:CE3	2.53	0.43
1:B:997:ASP:HB2	1:B:1047:LYS:HD3	2.00	0.43
1:B:1256:PRO:HG2	1:B:1592:LEU:HD21	1.99	0.43
1:B:4019:PHE:CD1	1:B:4086:PHE:HB3	2.54	0.43
1:B:4867:ASP:OD1	1:C:4873:ARG:NH1	2.51	0.43
1:C:1172:THR:HB	1:C:1190:LEU:HD12	2.00	0.43
1:D:233:VAL:O	1:D:408:SER:OG	2.36	0.43
1:D:1256:PRO:HG2	1:D:1592:LEU:HD21	1.99	0.43
1:D:1769:PHE:O	2:J:83:TYR:OH	2.33	0.43
1:A:765:SER:HB3	1:A:782:PHE:CE1	2.54	0.43
1:A:778:MET:HG3	1:A:780:GLU:OE2	2.19	0.43
1:A:2712:ILE:HG21	1:A:2717:GLU:OE2	2.19	0.43
1:B:299:HIS:HD2	1:B:302:THR:H	1.65	0.43
1:B:698:ALA:HA	1:B:724:SER:HA	2.01	0.43
1:C:765:SER:HB3	1:C:782:PHE:CE1	2.54	0.43
1:C:4176:VAL:HG11	1:C:4879:VAL:HA	1.99	0.43
1:D:765:SER:HB3	1:D:782:PHE:CE1	2.54	0.43
1:D:3715:GLU:OE2	1:D:3716:LYS:NZ	2.52	0.43
1:D:4590:TYR:HA	1:D:4594:VAL:CG2	2.49	0.43
1:A:66:THR:HG1	1:A:124:SER:HG	1.62	0.43
1:A:245:LEU:HD13	1:A:262:TYR:CE1	2.54	0.43
1:A:1028:ARG:O	1:A:1028:ARG:HD3	2.18	0.43
1:A:1789:LYS:HB2	1:A:1835:PHE:CE1	2.54	0.43
1:A:4830:ILE:HG22	1:A:4831:GLU:N	2.33	0.43
1:B:1704:TYR:O	1:B:1708:ILE:HG12	2.18	0.43
1:B:3846:CYS:HG	1:B:3853:PHE:HD2	1.67	0.43
1:C:152:ASP:OD2	1:C:154:THR:OG1	2.37	0.43
1:C:1205:CYS:SG	1:C:1206:SER:N	2.92	0.43
1:C:1789:LYS:HB2	1:C:1835:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2712:ILE:HG21	1:C:2717:GLU:OE2	2.19	0.43
1:C:2892:PHE:O	1:C:2896:GLN:HG2	2.18	0.43
1:C:3715:GLU:OE2	1:C:3716:LYS:NZ	2.52	0.43
1:C:3719:GLU:HA	1:C:3722:LYS:HG2	2.00	0.43
1:D:997:ASP:HB2	1:D:1047:LYS:HD3	2.00	0.43
1:D:1789:LYS:HB2	1:D:1835:PHE:CE1	2.54	0.43
1:D:3898:ASP:OD1	1:D:3898:ASP:N	2.46	0.43
1:D:4019:PHE:CD1	1:D:4086:PHE:HB3	2.54	0.43
1:A:1205:CYS:SG	1:A:1206:SER:N	2.92	0.43
1:A:4694:SER:O	1:A:4694:SER:OG	2.32	0.43
1:B:643:LEU:HD13	1:B:1658:THR:HG23	2.01	0.43
1:B:765:SER:HB3	1:B:782:PHE:CE1	2.54	0.43
1:B:1172:THR:HB	1:B:1190:LEU:HD12	2.00	0.43
1:B:2753:GLN:HB2	1:B:2756:MET:HG2	2.01	0.43
1:B:3719:GLU:HA	1:B:3722:LYS:HG2	2.00	0.43
1:C:706:TYR:OH	1:C:851:LEU:HD11	2.18	0.43
1:C:983:LEU:O	1:C:1055:ARG:HD2	2.19	0.43
1:C:1304:LEU:HD12	1:C:1340:ASP:HB2	2.00	0.43
1:C:4019:PHE:CD1	1:C:4086:PHE:HB3	2.54	0.43
1:C:4830:ILE:HG22	1:C:4831:GLU:N	2.34	0.43
1:C:4923:TYR:CZ	1:C:4927:LYS:HD2	2.54	0.43
1:D:245:LEU:HD13	1:D:262:TYR:CE1	2.54	0.43
1:D:317:MET:HE3	1:D:321:LYS:O	2.19	0.43
1:D:601:LEU:HG	1:D:642:LEU:HD21	2.00	0.43
1:D:2282:LYS:HA	1:D:2282:LYS:HD2	1.89	0.43
1:D:2712:ILE:HG21	1:D:2717:GLU:OE2	2.19	0.43
1:D:4294:LEU:HA	1:D:4294:LEU:HD12	1.88	0.43
1:A:983:LEU:O	1:A:1055:ARG:HD2	2.19	0.42
1:A:1771:SER:HA	2:G:56:VAL:HA	2.00	0.42
1:A:2101:LEU:HD13	1:A:3624:GLU:HB3	2.00	0.42
1:A:4019:PHE:CD1	1:A:4086:PHE:HB3	2.54	0.42
1:A:4793:ASN:O	1:A:4795:SER:N	2.50	0.42
1:B:58:VAL:HG12	1:B:320:GLU:HA	2.01	0.42
1:B:245:LEU:HD13	1:B:262:TYR:CE1	2.54	0.42
1:B:294:PRO:HA	1:B:329:PHE:O	2.19	0.42
1:B:317:MET:HE3	1:B:321:LYS:O	2.19	0.42
1:B:799:LYS:HG2	1:B:1621:GLN:NE2	2.34	0.42
1:B:812:LYS:O	1:B:812:LYS:NZ	2.35	0.42
1:B:1928:SER:OG	1:B:3616:VAL:HG23	2.19	0.42
1:C:245:LEU:HD13	1:C:262:TYR:CE1	2.54	0.42
1:C:245:LEU:HD13	1:C:262:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2335:ARG:HD3	1:C:2336:GLY:N	2.34	0.42
1:C:2768:GLU:OE2	1:C:2771:ARG:HD2	2.19	0.42
1:D:1205:CYS:SG	1:D:1206:SER:N	2.92	0.42
1:D:1359:ILE:HG13	1:D:1360:ASP:N	2.31	0.42
1:D:1629:MET:HE2	1:D:1642:ILE:HD13	2.02	0.42
1:A:58:VAL:HG12	1:A:320:GLU:HA	2.01	0.42
1:A:245:LEU:HD13	1:A:262:TYR:HE1	1.84	0.42
1:A:407:ARG:HH21	1:A:3864:ASN:HB3	1.84	0.42
1:A:646:THR:OG1	1:A:1685:GLN:NE2	2.52	0.42
1:B:2712:ILE:HG21	1:B:2717:GLU:OE2	2.19	0.42
1:B:4830:ILE:HG22	1:B:4831:GLU:N	2.33	0.42
1:C:66:THR:OG1	1:C:124:SER:OG	2.33	0.42
1:C:745:ASN:O	1:C:747:HIS:ND1	2.47	0.42
1:C:778:MET:HG3	1:C:780:GLU:OE2	2.19	0.42
1:C:1987:CYS:N	1:C:1988:PRO:HD2	2.34	0.42
1:C:2753:GLN:HB2	1:C:2756:MET:HG2	2.01	0.42
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.87	0.42
1:D:2404:GLU:HG3	1:D:2405:MET:H	1.83	0.42
1:D:2768:GLU:OE2	1:D:2771:ARG:HD2	2.19	0.42
1:D:4923:TYR:CZ	1:D:4927:LYS:HD2	2.54	0.42
1:A:294:PRO:HA	1:A:329:PHE:O	2.19	0.42
1:A:3822:GLU:HB2	1:A:3826:GLU:HA	2.01	0.42
1:A:4590:TYR:HA	1:A:4594:VAL:CG2	2.49	0.42
1:B:245:LEU:HD13	1:B:262:TYR:HE1	1.84	0.42
1:B:601:LEU:HG	1:B:642:LEU:HD21	2.00	0.42
1:B:755:ILE:HD11	1:B:768:PHE:HB3	2.01	0.42
1:B:801:ARG:HA	1:B:1618:TRP:O	2.20	0.42
1:B:1643:LEU:HD22	1:B:1694:TYR:O	2.19	0.42
1:B:1732:GLU:OE2	1:B:1735:LYS:HB2	2.20	0.42
1:B:4294:LEU:HA	1:B:4294:LEU:HD12	1.88	0.42
1:B:4590:TYR:HA	1:B:4594:VAL:CG2	2.49	0.42
1:C:707:PRO:HD2	1:C:838:ARG:HD2	2.00	0.42
1:C:799:LYS:HG2	1:C:1621:GLN:NE2	2.34	0.42
1:C:1771:SER:HA	2:I:56:VAL:HA	2.01	0.42
1:C:1959:ARG:HH21	1:C:1962:ARG:HH12	1.67	0.42
1:D:983:LEU:O	1:D:1055:ARG:HD2	2.19	0.42
1:D:2733:MET:O	1:D:2736:LEU:HG	2.18	0.42
1:D:4070:GLU:OE1	1:D:4070:GLU:N	2.47	0.42
1:D:4694:SER:O	1:D:4694:SER:OG	2.32	0.42
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.52	0.42
1:A:530:LEU:HA	1:A:530:LEU:HD23	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:LEU:HD13	1:A:673:TRP:CD1	2.55	0.42
1:A:1928:SER:OG	1:A:3616:VAL:HG23	2.19	0.42
1:A:2404:GLU:HG3	1:A:2405:MET:H	1.83	0.42
1:A:3715:GLU:OE2	1:A:3716:LYS:NZ	2.52	0.42
1:A:3919:LEU:O	1:A:3923:ILE:HG12	2.20	0.42
1:B:66:THR:OG1	1:B:124:SER:OG	2.32	0.42
1:B:290:ARG:H	1:B:293:GLN:NE2	2.16	0.42
1:B:611:LEU:HD11	1:B:643:LEU:HD21	2.00	0.42
1:B:4668:LEU:HG	1:B:4669:LEU:HD12	2.02	0.42
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.52	0.42
1:C:601:LEU:HG	1:C:642:LEU:HD21	2.00	0.42
1:C:997:ASP:HB2	1:C:1047:LYS:HD3	2.00	0.42
1:C:1196:ASP:N	1:C:1196:ASP:OD1	2.50	0.42
1:C:2313:GLU:OE1	1:C:3812:LYS:HE2	2.20	0.42
1:D:940:LEU:O	1:D:944:LEU:HG	2.20	0.42
1:D:2331:GLY:HA3	1:D:2391:TYR:HE1	1.83	0.42
1:D:3964:ILE:HG13	1:D:3965:GLU:OE1	2.20	0.42
1:A:152:ASP:OD2	1:A:154:THR:OG1	2.37	0.42
1:A:190:ARG:HD3	1:A:205:ALA:O	2.20	0.42
1:A:4070:GLU:OE1	1:A:4070:GLU:N	2.47	0.42
1:A:4923:TYR:CZ	1:A:4927:LYS:HD2	2.54	0.42
1:B:514:PHE:HD2	1:B:523:GLY:HA2	1.84	0.42
1:B:707:PRO:HD2	1:B:838:ARG:HD2	2.00	0.42
1:B:1959:ARG:HH21	1:B:1962:ARG:HH12	1.67	0.42
1:B:2768:GLU:OE2	1:B:2771:ARG:HD2	2.19	0.42
1:B:3919:LEU:O	1:B:3923:ILE:HG12	2.20	0.42
1:C:328:ALA:HB3	1:C:366:VAL:HG11	2.02	0.42
1:C:940:LEU:O	1:C:944:LEU:HG	2.20	0.42
1:C:2355:ASP:OD2	1:C:2357:SER:OG	2.30	0.42
1:C:4791:PHE:HE1	1:C:4833:PRO:HA	1.84	0.42
1:D:66:THR:OG1	1:D:124:SER:OG	2.33	0.42
1:D:778:MET:HG3	1:D:780:GLU:OE2	2.19	0.42
1:D:799:LYS:HG2	1:D:1621:GLN:NE2	2.34	0.42
1:D:1643:LEU:HD22	1:D:1694:TYR:O	2.19	0.42
1:D:2101:LEU:HD13	1:D:3624:GLU:HB3	2.00	0.42
1:D:2335:ARG:HD3	1:D:2336:GLY:N	2.34	0.42
1:A:625:VAL:HG23	1:A:628:ASN:HB2	2.02	0.42
1:A:643:LEU:HD13	1:A:1658:THR:HG23	2.01	0.42
1:A:2716:LEU:HG	1:A:2900:TYR:HE2	1.84	0.42
1:B:28:ILE:HG21	1:B:201:TRP:CH2	2.55	0.42
1:B:328:ALA:HB3	1:B:366:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:LEU:HD13	1:B:673:TRP:CD1	2.55	0.42
1:B:1776:CYS:SG	1:B:1778:GLN:HB2	2.60	0.42
1:B:3715:GLU:OE2	1:B:3716:LYS:NZ	2.52	0.42
1:C:28:ILE:HG21	1:C:201:TRP:CH2	2.55	0.42
1:C:1372:ASN:OD1	1:C:1372:ASN:N	2.53	0.42
1:C:2428:LEU:O	1:C:2432:VAL:HG23	2.20	0.42
1:C:4070:GLU:OE1	1:C:4070:GLU:N	2.47	0.42
2:I:28:THR:HA	2:I:39:SER:HA	2.02	0.42
1:D:698:ALA:HA	1:D:724:SER:HA	2.01	0.42
1:D:1987:CYS:N	1:D:1988:PRO:HD2	2.34	0.42
1:D:2428:LEU:O	1:D:2432:VAL:HG23	2.20	0.42
1:A:514:PHE:HD2	1:A:523:GLY:HA2	1.84	0.42
1:A:1732:GLU:OE2	1:A:1735:LYS:HB2	2.20	0.42
1:A:1747:HIS:ND1	1:A:1747:HIS:O	2.51	0.42
1:A:2753:GLN:HB2	1:A:2756:MET:HG2	2.01	0.42
1:A:3846:CYS:HG	1:A:3853:PHE:HD2	1.65	0.42
1:A:3964:ILE:HG13	1:A:3965:GLU:OE1	2.20	0.42
1:B:317:MET:HB2	1:B:321:LYS:HE3	2.01	0.42
1:B:840:TYR:CE2	1:B:850:LEU:HA	2.55	0.42
1:B:1205:CYS:SG	1:B:1206:SER:N	2.92	0.42
1:B:1789:LYS:HB2	1:B:1835:PHE:CE1	2.54	0.42
1:B:1789:LYS:HZ1	1:B:1835:PHE:H	1.67	0.42
2:H:28:THR:HA	2:H:39:SER:HA	2.02	0.42
1:C:290:ARG:H	1:C:293:GLN:NE2	2.16	0.42
1:C:514:PHE:HD2	1:C:523:GLY:HA2	1.84	0.42
1:C:801:ARG:HA	1:C:1618:TRP:O	2.20	0.42
1:C:2238:PRO:O	1:C:2241:VAL:HG12	2.19	0.42
1:C:2716:LEU:HG	1:C:2900:TYR:HE2	1.85	0.42
1:D:28:ILE:HG21	1:D:201:TRP:CH2	2.55	0.42
1:D:318:ASP:OD1	1:D:318:ASP:N	2.50	0.42
1:D:1732:GLU:OE2	1:D:1735:LYS:HB2	2.20	0.42
1:A:799:LYS:HG2	1:A:1621:GLN:NE2	2.34	0.42
1:A:1009:ARG:O	1:A:1012:ILE:HG12	2.20	0.42
1:A:1643:LEU:HD22	1:A:1694:TYR:O	2.19	0.42
1:A:2313:GLU:OE1	1:A:3812:LYS:HE2	2.20	0.42
1:B:233:VAL:O	1:B:408:SER:OG	2.36	0.42
1:B:778:MET:HG3	1:B:780:GLU:OE2	2.19	0.42
1:B:1771:SER:HA	2:H:56:VAL:HA	2.01	0.42
1:B:4791:PHE:HE1	1:B:4833:PRO:HA	1.84	0.42
1:C:1643:LEU:HD22	1:C:1694:TYR:O	2.19	0.42
1:C:1683:GLU:HB3	2:I:42:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:LEU:HB2	1:D:393:MET:HB2	2.02	0.42
1:D:661:LEU:HD13	1:D:673:TRP:CD1	2.55	0.42
1:D:3940:TRP:HA	1:D:3943:VAL:HG12	2.01	0.42
1:A:417:ARG:NH1	1:A:420:ARG:HH22	2.18	0.42
1:A:2335:ARG:HD3	1:A:2336:GLY:N	2.34	0.42
1:A:2768:GLU:OE2	1:A:2771:ARG:HD2	2.20	0.42
1:B:280:LEU:H	1:B:280:LEU:HD12	1.85	0.42
1:B:370:LEU:HB2	1:B:393:MET:HB2	2.02	0.42
1:B:1193:LYS:HZ2	1:B:1194:ASP:H	1.68	0.42
1:B:1979:LYS:HD3	1:B:1979:LYS:HA	1.95	0.42
1:B:2238:PRO:O	1:B:2241:VAL:HG12	2.19	0.42
1:C:417:ARG:NH1	1:C:420:ARG:HH22	2.18	0.42
1:C:4026:THR:O	1:C:4031:PHE:HB3	2.20	0.42
1:D:328:ALA:HB3	1:D:366:VAL:HG11	2.02	0.42
1:D:417:ARG:NH1	1:D:420:ARG:HH22	2.18	0.42
1:D:419:ILE:O	1:D:423:VAL:HG13	2.20	0.42
1:D:514:PHE:HD2	1:D:523:GLY:HA2	1.84	0.42
1:D:1009:ARG:O	1:D:1012:ILE:HG12	2.20	0.42
1:D:2716:LEU:HG	1:D:2900:TYR:HE2	1.85	0.42
1:D:4791:PHE:HE1	1:D:4833:PRO:HA	1.84	0.42
1:A:446:ASP:O	1:A:448:PRO:HD3	2.20	0.42
1:A:1048:ASP:HA	1:A:1051:ARG:HD2	2.02	0.42
1:A:1769:PHE:O	2:G:83:TYR:OH	2.37	0.42
1:A:1979:LYS:HD3	1:A:1979:LYS:HA	1.95	0.42
1:A:1987:CYS:N	1:A:1988:PRO:HD2	2.34	0.42
1:B:307:SER:OG	1:B:317:MET:HG2	2.20	0.42
1:B:1048:ASP:HA	1:B:1051:ARG:HD2	2.02	0.42
1:B:4923:TYR:CZ	1:B:4927:LYS:HD2	2.54	0.42
1:C:307:SER:OG	1:C:317:MET:HG2	2.20	0.42
1:C:370:LEU:HB2	1:C:393:MET:HB2	2.02	0.42
1:C:407:ARG:HH21	1:C:3864:ASN:HB3	1.84	0.42
1:A:28:ILE:HG21	1:A:201:TRP:CH2	2.55	0.41
1:A:419:ILE:O	1:A:423:VAL:HG13	2.20	0.41
1:A:698:ALA:HA	1:A:724:SER:HA	2.01	0.41
1:A:841:LYS:HE2	1:A:841:LYS:HB2	1.79	0.41
1:A:1776:CYS:SG	1:A:1778:GLN:HB2	2.60	0.41
1:A:4026:THR:O	1:A:4031:PHE:HB3	2.20	0.41
1:B:152:ASP:OD2	1:B:154:THR:OG1	2.37	0.41
1:B:417:ARG:NH1	1:B:420:ARG:HH22	2.18	0.41
1:B:419:ILE:O	1:B:423:VAL:HG13	2.20	0.41
1:B:798:ILE:HG13	1:B:800:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2716:LEU:HG	1:B:2900:TYR:HE2	1.85	0.41
1:C:62:LEU:HA	1:C:65:CYS:SG	2.60	0.41
1:C:698:ALA:HA	1:C:724:SER:HA	2.01	0.41
1:D:446:ASP:O	1:D:448:PRO:HD3	2.20	0.41
1:D:2278:MET:O	1:D:2282:LYS:HG2	2.20	0.41
1:D:2464:LYS:HE3	1:D:2464:LYS:HB3	1.93	0.41
1:A:801:ARG:HA	1:A:1618:TRP:O	2.20	0.41
1:A:890:HIS:NE2	1:A:924:LEU:HD11	2.35	0.41
1:A:1629:MET:HE2	1:A:1642:ILE:HD13	2.02	0.41
1:A:2238:PRO:O	1:A:2241:VAL:HG12	2.19	0.41
2:G:28:THR:HA	2:G:39:SER:HA	2.02	0.41
1:B:983:LEU:O	1:B:1055:ARG:HD2	2.19	0.41
1:C:317:MET:HE3	1:C:321:LYS:O	2.20	0.41
1:C:661:LEU:HD13	1:C:673:TRP:CD1	2.55	0.41
1:C:1740:PHE:CD1	1:C:1923:ALA:HB1	2.56	0.41
1:C:3822:GLU:HB2	1:C:3826:GLU:HA	2.01	0.41
1:D:1372:ASN:OD1	1:D:1372:ASN:N	2.53	0.41
1:D:3822:GLU:HB2	1:D:3826:GLU:HA	2.01	0.41
1:D:4668:LEU:HG	1:D:4669:LEU:HD12	2.02	0.41
2:J:28:THR:HA	2:J:39:SER:HA	2.02	0.41
1:A:328:ALA:HB3	1:A:366:VAL:HG11	2.02	0.41
1:A:1931:PHE:CE1	1:A:1995:LEU:HB2	2.55	0.41
1:A:2278:MET:O	1:A:2282:LYS:HG2	2.20	0.41
1:A:4583:PHE:HA	1:A:4586:ILE:HG22	2.02	0.41
1:A:4791:PHE:HE1	1:A:4833:PRO:HA	1.84	0.41
1:B:4511:ILE:O	1:B:4515:LEU:HG	2.20	0.41
1:C:294:PRO:HA	1:C:329:PHE:O	2.19	0.41
1:C:643:LEU:HD13	1:C:1658:THR:HG23	2.01	0.41
1:C:973:THR:OG1	1:C:976:TYR:O	2.19	0.41
1:C:1776:CYS:SG	1:C:1778:GLN:HB2	2.60	0.41
1:D:190:ARG:HD3	1:D:205:ALA:O	2.20	0.41
1:D:317:MET:HB2	1:D:321:LYS:HE3	2.01	0.41
1:D:755:ILE:HD11	1:D:768:PHE:HB3	2.01	0.41
1:D:801:ARG:HA	1:D:1618:TRP:O	2.20	0.41
1:D:1776:CYS:SG	1:D:1778:GLN:HB2	2.60	0.41
1:D:3919:LEU:O	1:D:3923:ILE:HG12	2.20	0.41
1:D:4029:ASP:OD1	1:D:4029:ASP:N	2.47	0.41
1:A:940:LEU:O	1:A:944:LEU:HG	2.20	0.41
1:A:2742:TYR:OH	1:A:2744:GLU:OE2	2.33	0.41
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.52	0.41
1:B:646:THR:OG1	1:B:1685:GLN:NE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:VAL:HA	1:B:999:LEU:HD12	2.02	0.41
1:B:1931:PHE:CE1	1:B:1995:LEU:HB2	2.55	0.41
1:B:3940:TRP:HA	1:B:3943:VAL:HG12	2.01	0.41
1:B:4026:THR:O	1:B:4031:PHE:HB3	2.20	0.41
1:B:4583:PHE:HA	1:B:4586:ILE:HG22	2.03	0.41
1:C:190:ARG:HD3	1:C:205:ALA:O	2.20	0.41
1:C:317:MET:HB2	1:C:321:LYS:HE3	2.01	0.41
1:C:658:ASN:HB2	1:C:832:LEU:HD12	2.03	0.41
1:C:890:HIS:NE2	1:C:924:LEU:HD11	2.36	0.41
1:C:3940:TRP:HA	1:C:3943:VAL:HG12	2.01	0.41
1:C:4165:LYS:HE3	1:C:4165:LYS:HB2	1.84	0.41
1:C:4583:PHE:HA	1:C:4586:ILE:HG22	2.03	0.41
1:C:4668:LEU:HG	1:C:4669:LEU:HD12	2.02	0.41
1:C:4793:ASN:O	1:C:4795:SER:N	2.50	0.41
1:D:606:ARG:NH2	1:D:1635:GLU:OE1	2.34	0.41
1:D:643:LEU:HD13	1:D:1658:THR:HG23	2.01	0.41
1:D:1048:ASP:HA	1:D:1051:ARG:HD2	2.02	0.41
1:D:1091:GLU:HB3	1:D:1094:TYR:CD2	2.53	0.41
1:D:1931:PHE:CE1	1:D:1995:LEU:HB2	2.55	0.41
1:D:2313:GLU:OE1	1:D:3812:LYS:HE2	2.20	0.41
1:D:2753:GLN:HB2	1:D:2756:MET:HG2	2.01	0.41
1:D:4026:THR:O	1:D:4031:PHE:HB3	2.20	0.41
1:A:62:LEU:HA	1:A:65:CYS:SG	2.60	0.41
1:A:755:ILE:HD11	1:A:768:PHE:HB3	2.01	0.41
1:A:840:TYR:CE2	1:A:850:LEU:HA	2.55	0.41
1:A:1959:ARG:HH21	1:A:1962:ARG:HH12	1.67	0.41
1:B:190:ARG:HD3	1:B:205:ALA:O	2.20	0.41
1:B:3822:GLU:HB2	1:B:3826:GLU:HA	2.01	0.41
1:C:58:VAL:HG12	1:C:320:GLU:HA	2.01	0.41
1:C:530:LEU:HA	1:C:530:LEU:HD23	1.77	0.41
1:C:912:LYS:O	1:C:914:GLN:HG3	2.21	0.41
1:C:1009:ARG:O	1:C:1012:ILE:HG12	2.20	0.41
1:C:1048:ASP:HA	1:C:1051:ARG:HD2	2.02	0.41
1:C:1732:GLU:OE2	1:C:1735:LYS:HB2	2.20	0.41
1:D:245:LEU:HD13	1:D:262:TYR:HE1	1.84	0.41
1:D:294:PRO:HA	1:D:329:PHE:O	2.19	0.41
1:D:840:TYR:CE2	1:D:850:LEU:HA	2.55	0.41
1:D:898:ILE:HD13	1:D:973:THR:HB	2.02	0.41
1:D:1959:ARG:HH21	1:D:1962:ARG:HH12	1.66	0.41
1:D:3762:ILE:HD12	1:D:3840:ARG:HG3	2.01	0.41
1:D:3857:LEU:HD23	1:D:3857:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4511:ILE:O	1:D:4515:LEU:HG	2.21	0.41
1:A:798:ILE:HG13	1:A:800:VAL:HG23	2.02	0.41
1:A:3762:ILE:HD12	1:A:3840:ARG:HG3	2.01	0.41
1:A:3964:ILE:HG21	1:A:4085:ARG:HH11	1.86	0.41
1:B:625:VAL:HG23	1:B:628:ASN:HB2	2.02	0.41
1:B:890:HIS:NE2	1:B:924:LEU:HD11	2.36	0.41
1:C:446:ASP:O	1:C:448:PRO:HD3	2.20	0.41
1:C:755:ILE:HD11	1:C:768:PHE:HB3	2.01	0.41
1:C:798:ILE:HG13	1:C:800:VAL:HG23	2.03	0.41
1:C:1100:ARG:HB2	1:C:1236:TYR:HA	2.03	0.41
1:C:1931:PHE:CE1	1:C:1995:LEU:HB2	2.55	0.41
1:C:2125:ILE:HD13	1:C:2125:ILE:HA	1.91	0.41
1:C:2238:PRO:HA	1:C:2241:VAL:HG12	2.03	0.41
1:C:3782:GLU:OE2	1:C:3783:LYS:HG3	2.21	0.41
1:D:58:VAL:HG12	1:D:320:GLU:HA	2.01	0.41
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.52	0.41
1:D:1740:PHE:CD1	1:D:1923:ALA:HB1	2.55	0.41
1:D:4165:LYS:HE3	1:D:4165:LYS:HB2	1.84	0.41
1:A:898:ILE:HD13	1:A:973:THR:HB	2.02	0.41
1:A:1683:GLU:HB3	2:G:42:ASP:HB3	2.02	0.41
1:A:2238:PRO:HA	1:A:2241:VAL:HG12	2.03	0.41
1:A:2428:LEU:O	1:A:2432:VAL:HG23	2.20	0.41
1:A:3940:TRP:HA	1:A:3943:VAL:HG12	2.01	0.41
1:B:304:LYS:HB2	1:B:316:LEU:HD12	2.03	0.41
1:B:1372:ASN:OD1	1:B:1372:ASN:N	2.53	0.41
1:B:2278:MET:O	1:B:2282:LYS:HG2	2.20	0.41
1:B:2313:GLU:OE1	1:B:3812:LYS:HE2	2.19	0.41
1:B:2867:HIS:ND1	1:B:2868:PRO:HD2	2.36	0.41
1:B:3905:PHE:O	1:B:3909:ILE:HG12	2.21	0.41
1:C:304:LYS:HB2	1:C:316:LEU:HD12	2.03	0.41
1:C:595:LYS:HE2	1:C:595:LYS:HB3	1.89	0.41
1:C:802:PHE:HB2	1:C:1618:TRP:HB2	2.02	0.41
1:C:3762:ILE:HD12	1:C:3840:ARG:HG3	2.01	0.41
1:C:3919:LEU:O	1:C:3923:ILE:HG12	2.20	0.41
1:D:356:TYR:HA	1:D:405:LEU:HB2	2.03	0.41
1:D:383:ARG:HH21	1:D:387:ILE:HD12	1.86	0.41
1:D:625:VAL:HG23	1:D:628:ASN:HB2	2.02	0.41
1:D:4193:GLU:OE2	1:D:4943:TYR:OH	2.28	0.41
1:A:307:SER:OG	1:A:317:MET:HG2	2.20	0.41
1:A:323:ASP:OD2	1:A:325:LYS:HB2	2.21	0.41
1:A:912:LYS:O	1:A:914:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1740:PHE:CD1	1:A:1923:ALA:HB1	2.55	0.41
1:A:3842:LEU:HD23	1:A:3842:LEU:HA	1.96	0.41
1:A:4051:MET:HE1	1:A:4062:THR:HA	2.02	0.41
1:A:4668:LEU:HG	1:A:4669:LEU:HD12	2.02	0.41
1:B:62:LEU:HA	1:B:65:CYS:SG	2.60	0.41
1:B:838:ARG:H	1:B:841:LYS:HZ1	1.66	0.41
1:B:898:ILE:HD13	1:B:973:THR:HB	2.02	0.41
1:B:3762:ILE:HD12	1:B:3840:ARG:HG3	2.01	0.41
1:C:78:LEU:O	1:C:82:LEU:HB2	2.21	0.41
1:C:323:ASP:OD2	1:C:325:LYS:HB2	2.21	0.41
1:C:419:ILE:O	1:C:423:VAL:HG13	2.20	0.41
1:C:840:TYR:CE2	1:C:850:LEU:HA	2.55	0.41
1:C:4044:LYS:HE2	1:C:4044:LYS:HB3	1.81	0.41
1:D:304:LYS:HB2	1:D:316:LEU:HD12	2.03	0.41
1:D:306:LEU:HD22	1:D:314:LEU:HD13	2.02	0.41
1:D:658:ASN:HB2	1:D:832:LEU:HD12	2.03	0.41
1:D:2238:PRO:HA	1:D:2241:VAL:HG12	2.03	0.41
1:D:4583:PHE:HA	1:D:4586:ILE:HG22	2.02	0.41
1:A:304:LYS:HB2	1:A:316:LEU:HD12	2.03	0.41
1:A:306:LEU:HD22	1:A:314:LEU:HD13	2.02	0.41
1:A:317:MET:HB2	1:A:321:LYS:HE3	2.02	0.41
1:A:370:LEU:HB2	1:A:393:MET:HB2	2.02	0.41
1:A:3905:PHE:O	1:A:3909:ILE:HG12	2.21	0.41
1:A:4294:LEU:HA	1:A:4294:LEU:HD12	1.88	0.41
1:A:4511:ILE:O	1:A:4515:LEU:HG	2.20	0.41
1:A:4658:GLU:OE1	1:A:4659:PHE:N	2.54	0.41
1:B:169:ARG:HH12	1:B:176:ARG:NH1	2.19	0.41
1:B:802:PHE:HB2	1:B:1618:TRP:HB2	2.02	0.41
1:B:912:LYS:O	1:B:914:GLN:HG3	2.21	0.41
1:B:940:LEU:O	1:B:944:LEU:HG	2.20	0.41
1:B:1009:ARG:O	1:B:1012:ILE:HG12	2.20	0.41
1:B:1100:ARG:HB2	1:B:1236:TYR:HA	2.03	0.41
1:B:1629:MET:HE1	1:B:1685:GLN:HE21	1.85	0.41
1:B:2408:ILE:O	1:B:2412:LYS:CB	2.69	0.41
1:B:3964:ILE:HG13	1:B:3965:GLU:OE1	2.20	0.41
1:B:4658:GLU:OE1	1:B:4659:PHE:N	2.54	0.41
1:C:921:PHE:O	1:C:929:ARG:NH1	2.45	0.41
1:C:1294:ASN:O	1:C:1348:LYS:HE3	2.21	0.41
1:C:1595:VAL:O	1:C:1595:VAL:HG13	2.21	0.41
1:C:1691:GLU:OE2	1:C:1693:LYS:NZ	2.54	0.41
1:C:2278:MET:O	1:C:2282:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3964:ILE:HG13	1:C:3965:GLU:OE1	2.20	0.41
1:C:4301:CYS:SG	1:C:4302:ARG:HG3	2.61	0.41
1:D:78:LEU:O	1:D:82:LEU:HB2	2.21	0.41
1:D:307:SER:OG	1:D:317:MET:HG2	2.20	0.41
1:D:323:ASP:OD2	1:D:325:LYS:HB2	2.21	0.41
1:D:798:ILE:HG13	1:D:800:VAL:HG23	2.02	0.41
1:D:912:LYS:O	1:D:914:GLN:HG3	2.21	0.41
1:D:3782:GLU:OE2	1:D:3783:LYS:HG3	2.21	0.41
1:D:3905:PHE:O	1:D:3909:ILE:HG12	2.21	0.41
1:A:2847:TYR:OH	1:A:2891:ILE:HD13	2.21	0.41
1:A:4608:LYS:HG2	1:A:4614:LEU:HD22	2.03	0.41
1:B:306:LEU:HD22	1:B:314:LEU:HD13	2.02	0.41
1:B:356:TYR:HA	1:B:405:LEU:HB2	2.03	0.41
1:B:658:ASN:HB2	1:B:832:LEU:HD12	2.03	0.41
1:B:1294:ASN:O	1:B:1348:LYS:HE3	2.21	0.41
1:B:2428:LEU:O	1:B:2432:VAL:HG23	2.20	0.41
1:C:306:LEU:HD22	1:C:314:LEU:HD13	2.02	0.41
1:C:356:TYR:HA	1:C:405:LEU:HB2	2.03	0.41
1:C:383:ARG:HH21	1:C:387:ILE:HD12	1.86	0.41
1:C:574:VAL:HA	1:C:577:CYS:SG	2.61	0.41
1:C:996:VAL:HA	1:C:999:LEU:HD12	2.02	0.41
1:C:1898:PRO:O	1:C:1902:LYS:HG2	2.21	0.41
1:C:4051:MET:HE1	1:C:4062:THR:HA	2.03	0.41
1:C:4608:LYS:HG2	1:C:4614:LEU:HD22	2.03	0.41
1:D:574:VAL:HA	1:D:577:CYS:SG	2.61	0.41
1:D:755:ILE:HD12	1:D:769:ARG:O	2.21	0.41
1:D:1595:VAL:HG13	1:D:1595:VAL:O	2.21	0.41
1:D:1691:GLU:OE2	1:D:1693:LYS:NZ	2.54	0.41
1:D:1897:LEU:HA	1:D:1898:PRO:HD3	1.97	0.41
1:D:4301:CYS:SG	1:D:4302:ARG:HG3	2.61	0.41
1:D:4608:LYS:HG2	1:D:4614:LEU:HD22	2.03	0.41
1:A:280:LEU:HD12	1:A:280:LEU:H	1.85	0.40
1:A:383:ARG:HH21	1:A:387:ILE:HD12	1.86	0.40
1:A:658:ASN:HB2	1:A:832:LEU:HD12	2.03	0.40
1:A:812:LYS:O	1:A:812:LYS:NZ	2.35	0.40
1:A:987:LYS:HA	1:A:987:LYS:HD2	1.90	0.40
1:A:1294:ASN:O	1:A:1348:LYS:HE3	2.21	0.40
1:A:1372:ASN:OD1	1:A:1372:ASN:N	2.53	0.40
1:A:1789:LYS:HZ1	1:A:1835:PHE:H	1.70	0.40
1:A:2184:LYS:HZ3	1:A:2184:LYS:HG2	1.71	0.40
1:B:446:ASP:O	1:B:448:PRO:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:VAL:HA	1:B:577:CYS:SG	2.61	0.40
1:B:1100:ARG:NH1	1:B:1234:GLU:O	2.54	0.40
1:B:1740:PHE:CD1	1:B:1923:ALA:HB1	2.56	0.40
1:B:4824:GLY:O	1:C:4821:ARG:NH2	2.54	0.40
1:C:169:ARG:HH12	1:C:176:ARG:NH1	2.19	0.40
1:C:1573:LYS:HZ2	1:C:1584:PRO:HG2	1.86	0.40
1:C:4511:ILE:O	1:C:4515:LEU:HG	2.20	0.40
1:C:4559:VAL:HG22	1:C:4561:GLU:HG2	2.03	0.40
1:C:4658:GLU:OE1	1:C:4659:PHE:N	2.54	0.40
1:D:62:LEU:HA	1:D:65:CYS:SG	2.60	0.40
1:D:902:TRP:HA	1:D:913:ARG:O	2.21	0.40
1:D:1965:ARG:O	1:D:1966:SER:OG	2.38	0.40
1:D:2238:PRO:O	1:D:2241:VAL:HG12	2.19	0.40
1:D:2271:CYS:SG	1:D:2293:GLU:HB2	2.61	0.40
1:D:2836:LEU:HD13	1:D:2836:LEU:HA	1.97	0.40
1:A:1190:LEU:HD21	1:A:1193:LYS:HB2	2.03	0.40
1:A:1898:PRO:O	1:A:1902:LYS:HG2	2.22	0.40
1:A:1970:GLU:O	1:A:1974:MET:HG2	2.22	0.40
1:A:3782:GLU:OE2	1:A:3783:LYS:HG3	2.21	0.40
1:A:4046:ASP:O	1:A:4049:LYS:HG3	2.22	0.40
1:B:78:LEU:O	1:B:82:LEU:HB2	2.21	0.40
1:B:755:ILE:HD12	1:B:769:ARG:O	2.22	0.40
1:B:1572:PHE:HE1	1:B:1587:LEU:HD21	1.87	0.40
1:B:1898:PRO:O	1:B:1902:LYS:HG2	2.22	0.40
1:B:2331:GLY:HA3	1:B:2391:TYR:CE1	2.57	0.40
1:B:2355:ASP:OD2	1:B:2357:SER:OG	2.30	0.40
1:B:4301:CYS:SG	1:B:4302:ARG:HG3	2.61	0.40
1:B:4559:VAL:HG22	1:B:4561:GLU:HG2	2.03	0.40
1:C:2262:GLU:OE1	1:C:2262:GLU:N	2.48	0.40
1:C:3964:ILE:HG21	1:C:4085:ARG:HH11	1.86	0.40
1:D:280:LEU:H	1:D:280:LEU:HD12	1.85	0.40
1:D:313:ASN:HD21	1:D:392:ILE:HA	1.87	0.40
1:D:799:LYS:HG2	1:D:1621:GLN:HE22	1.86	0.40
1:D:2262:GLU:OE1	1:D:2262:GLU:N	2.48	0.40
1:D:4501:ARG:HH12	1:D:4720:TYR:HE2	1.69	0.40
1:A:313:ASN:HD21	1:A:392:ILE:HA	1.87	0.40
1:A:356:TYR:HA	1:A:405:LEU:HB2	2.03	0.40
1:A:1691:GLU:OE2	1:A:1693:LYS:NZ	2.54	0.40
1:A:2271:CYS:SG	1:A:2293:GLU:HB2	2.61	0.40
1:A:4009:VAL:HA	1:A:4012:ILE:HG12	2.03	0.40
1:B:902:TRP:HA	1:B:913:ARG:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1048:ASP:OD1	1:B:1051:ARG:NH1	2.48	0.40
1:B:1683:GLU:HB3	1:B:1684:PRO:HD3	2.04	0.40
1:B:1917:VAL:HG21	1:B:2089:ARG:HH21	1.86	0.40
1:B:2136:GLU:O	1:B:2140:LEU:HG	2.21	0.40
1:B:3782:GLU:OE2	1:B:3783:LYS:HG3	2.21	0.40
1:B:3964:ILE:HG21	1:B:4085:ARG:HH11	1.86	0.40
1:B:4009:VAL:HA	1:B:4012:ILE:HG12	2.03	0.40
1:C:625:VAL:HG23	1:C:628:ASN:HB2	2.02	0.40
1:C:799:LYS:HG2	1:C:1621:GLN:HE22	1.87	0.40
1:C:898:ILE:HD13	1:C:973:THR:HB	2.02	0.40
1:C:2136:GLU:O	1:C:2140:LEU:HG	2.21	0.40
1:C:4501:ARG:NH1	1:C:4720:TYR:HE2	2.19	0.40
1:C:4830:ILE:HB	1:C:4842:ARG:HH21	1.87	0.40
1:D:940:LEU:HD11	1:D:950:VAL:HG11	2.04	0.40
1:D:1898:PRO:O	1:D:1902:LYS:HG2	2.22	0.40
1:D:1917:VAL:HG21	1:D:2089:ARG:HH21	1.86	0.40
1:D:2170:VAL:HG21	1:D:2198:PHE:CD2	2.57	0.40
1:A:755:ILE:HD12	1:A:769:ARG:O	2.22	0.40
1:A:1100:ARG:NH1	1:A:1234:GLU:O	2.55	0.40
1:A:4301:CYS:SG	1:A:4302:ARG:HG3	2.61	0.40
1:B:167:LYS:HA	1:B:167:LYS:HD3	1.97	0.40
1:B:799:LYS:HG2	1:B:1621:GLN:HE22	1.86	0.40
1:B:2271:CYS:SG	1:B:2293:GLU:HB2	2.61	0.40
1:C:162:ILE:O	1:C:163:HIS:ND1	2.55	0.40
1:C:755:ILE:HD12	1:C:769:ARG:O	2.22	0.40
1:C:1048:ASP:OD1	1:C:1051:ARG:NH1	2.48	0.40
1:C:2867:HIS:ND1	1:C:2868:PRO:HD2	2.36	0.40
1:D:674:TYR:HB2	1:D:819:TYR:HB3	2.04	0.40
1:D:890:HIS:NE2	1:D:924:LEU:HD11	2.36	0.40
1:D:1100:ARG:HB2	1:D:1236:TYR:HA	2.03	0.40
1:D:1190:LEU:HD21	1:D:1193:LYS:HB2	2.03	0.40
1:D:2847:TYR:OH	1:D:2891:ILE:HD13	2.21	0.40
1:D:4501:ARG:NH1	1:D:4720:TYR:HE2	2.19	0.40
1:D:4609:LEU:HD23	1:D:4609:LEU:HA	1.96	0.40
1:D:4793:ASN:O	1:D:4795:SER:N	2.50	0.40
1:A:1668:LEU:HD23	1:A:2131:VAL:HG22	2.04	0.40
1:A:1917:VAL:HG21	1:A:2089:ARG:HH21	1.86	0.40
1:A:2170:VAL:HG21	1:A:2198:PHE:CD2	2.57	0.40
1:A:2331:GLY:HA3	1:A:2391:TYR:CE1	2.57	0.40
1:B:162:ILE:O	1:B:163:HIS:ND1	2.55	0.40
1:B:940:LEU:HD11	1:B:950:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1595:VAL:O	1:B:1595:VAL:HG13	2.21	0.40
1:B:1691:GLU:OE2	1:B:1693:LYS:NZ	2.54	0.40
1:B:1970:GLU:O	1:B:1974:MET:HG2	2.22	0.40
1:C:332:ARG:HH21	1:C:340:VAL:HG12	1.87	0.40
1:C:702:GLY:O	1:C:786:GLY:HA2	2.22	0.40
1:C:1629:MET:HE2	1:C:1642:ILE:HD13	2.04	0.40
1:C:1683:GLU:HB3	1:C:1684:PRO:HD3	2.04	0.40
1:C:2271:CYS:SG	1:C:2293:GLU:HB2	2.61	0.40
1:D:169:ARG:HH12	1:D:176:ARG:NH1	2.19	0.40
1:D:1683:GLU:HB3	2:J:42:ASP:HB3	2.04	0.40
1:D:4046:ASP:O	1:D:4049:LYS:HG3	2.22	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	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100	100
1	B	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100	100
1	C	3255/4966 (66%)	3046 (94%)	209 (6%)	0	100	100
1	D	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100	100
2	G	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	H	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	I	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	J	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
All	All	13440/20568 (65%)	12595 (94%)	845 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	2862/3387 (84%)	2762 (96%)	100 (4%)	36 67
1	B	2862/3387 (84%)	2762 (96%)	100 (4%)	36 67
1	C	2862/3387 (84%)	2762 (96%)	100 (4%)	36 67
1	D	2862/3387 (84%)	2762 (96%)	100 (4%)	36 67
2	G	88/140 (63%)	88 (100%)	0	100 100
2	H	88/140 (63%)	88 (100%)	0	100 100
2	I	88/140 (63%)	88 (100%)	0	100 100
2	J	88/140 (63%)	88 (100%)	0	100 100
All	All	11800/14108 (84%)	11400 (97%)	400 (3%)	40 68

All (400) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	22	LEU
1	A	65	CYS
1	A	82	LEU
1	A	112	THR
1	A	113	LEU
1	A	147	VAL
1	A	181	LEU
1	A	187	SER
1	A	214	VAL
1	A	268	SER
1	A	282	VAL
1	A	296	ARG
1	A	333	SER
1	A	412	GLU
1	A	422	THR
1	A	439	LYS
1	A	453	SER
1	A	501	CYS

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Mol	Chain	Res	Type
1	A	550	GLN
1	A	566	GLU
1	A	609	LYS
1	A	653	SER
1	A	691	THR
1	A	765	SER
1	A	767	SER
1	A	814	LEU
1	A	841	LYS
1	A	923	LYS
1	A	935	MET
1	A	987	LYS
1	A	988	LEU
1	A	1006	VAL
1	A	1028	ARG
1	A	1033	VAL
1	A	1039	ASP
1	A	1040	ASP
1	A	1041	ARG
1	A	1047	LYS
1	A	1057	LEU
1	A	1108	VAL
1	A	1122	CYS
1	A	1172	THR
1	A	1261	VAL
1	A	1309	GLU
1	A	1348	LYS
1	A	1583	CYS
1	A	1649	GLU
1	A	1663	SER
1	A	1682	ASP
1	A	1739	LEU
1	A	1755	SER
1	A	1816	GLU
1	A	1846	LEU
1	A	1981	ASP
1	A	2136	GLU
1	A	2184	LYS
1	A	2302	ARG
1	A	2321	ARG
1	A	2335	ARG
1	A	2471	LEU

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Mol	Chain	Res	Type
1	A	2492	LEU
1	A	2715	LYS
1	A	2721	ASN
1	A	2733	MET
1	A	2735	LYS
1	A	2768	GLU
1	A	2771	ARG
1	A	2775	LYS
1	A	2776	GLU
1	A	2777	SER
1	A	2778	LEU
1	A	2779	LYS
1	A	2780	THR
1	A	2837	HIS
1	A	2871	VAL
1	A	2893	LYS
1	A	3782	GLU
1	A	3831	ASP
1	A	3851	SER
1	A	3861	THR
1	A	3965	GLU
1	A	4003	VAL
1	A	4033	GLU
1	A	4041	VAL
1	A	4049	LYS
1	A	4076	THR
1	A	4081	GLU
1	A	4273	MET
1	A	4280	LEU
1	A	4284	SER
1	A	4288	SER
1	A	4604	GLU
1	A	4622	GLU
1	A	4658	GLU
1	A	4667	GLU
1	A	4706	MET
1	A	4714	THR
1	A	4797	ASP
1	A	4802	ASP
1	B	17	ASP
1	B	22	LEU
1	B	65	CYS

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Mol	Chain	Res	Type
1	B	82	LEU
1	B	112	THR
1	B	113	LEU
1	B	147	VAL
1	B	181	LEU
1	B	187	SER
1	B	214	VAL
1	B	268	SER
1	B	282	VAL
1	B	296	ARG
1	B	333	SER
1	B	412	GLU
1	B	422	THR
1	B	439	LYS
1	B	453	SER
1	B	501	CYS
1	B	550	GLN
1	B	566	GLU
1	B	609	LYS
1	B	653	SER
1	B	691	THR
1	B	765	SER
1	B	767	SER
1	B	814	LEU
1	B	841	LYS
1	B	923	LYS
1	B	935	MET
1	B	987	LYS
1	B	988	LEU
1	B	1006	VAL
1	B	1028	ARG
1	B	1033	VAL
1	B	1039	ASP
1	B	1040	ASP
1	B	1041	ARG
1	B	1047	LYS
1	B	1057	LEU
1	B	1108	VAL
1	B	1122	CYS
1	B	1172	THR
1	B	1261	VAL
1	B	1309	GLU

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Mol	Chain	Res	Type
1	B	1348	LYS
1	B	1583	CYS
1	B	1649	GLU
1	B	1663	SER
1	B	1682	ASP
1	B	1739	LEU
1	B	1755	SER
1	B	1816	GLU
1	B	1846	LEU
1	B	1981	ASP
1	B	2136	GLU
1	B	2184	LYS
1	B	2302	ARG
1	B	2321	ARG
1	B	2335	ARG
1	B	2471	LEU
1	B	2492	LEU
1	B	2715	LYS
1	B	2721	ASN
1	B	2733	MET
1	B	2735	LYS
1	B	2768	GLU
1	B	2771	ARG
1	B	2775	LYS
1	B	2776	GLU
1	B	2777	SER
1	B	2778	LEU
1	B	2779	LYS
1	B	2780	THR
1	B	2837	HIS
1	B	2871	VAL
1	B	2893	LYS
1	B	3782	GLU
1	B	3831	ASP
1	B	3851	SER
1	B	3861	THR
1	B	3965	GLU
1	B	4003	VAL
1	B	4033	GLU
1	B	4041	VAL
1	B	4049	LYS
1	B	4076	THR

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Mol	Chain	Res	Type
1	B	4081	GLU
1	B	4273	MET
1	B	4280	LEU
1	B	4284	SER
1	B	4288	SER
1	B	4604	GLU
1	B	4622	GLU
1	B	4658	GLU
1	B	4667	GLU
1	B	4706	MET
1	B	4714	THR
1	B	4797	ASP
1	B	4802	ASP
1	C	17	ASP
1	C	22	LEU
1	C	65	CYS
1	C	82	LEU
1	C	112	THR
1	C	113	LEU
1	C	147	VAL
1	C	181	LEU
1	C	187	SER
1	C	214	VAL
1	C	268	SER
1	C	282	VAL
1	C	296	ARG
1	C	333	SER
1	C	412	GLU
1	C	422	THR
1	C	439	LYS
1	C	453	SER
1	C	501	CYS
1	C	550	GLN
1	C	566	GLU
1	C	609	LYS
1	C	653	SER
1	C	691	THR
1	C	765	SER
1	C	767	SER
1	C	814	LEU
1	C	841	LYS
1	C	923	LYS

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Mol	Chain	Res	Type
1	C	935	MET
1	C	987	LYS
1	C	988	LEU
1	C	1006	VAL
1	C	1028	ARG
1	C	1033	VAL
1	C	1039	ASP
1	C	1040	ASP
1	C	1041	ARG
1	C	1047	LYS
1	C	1057	LEU
1	C	1108	VAL
1	C	1122	CYS
1	C	1172	THR
1	C	1261	VAL
1	C	1309	GLU
1	C	1348	LYS
1	C	1583	CYS
1	C	1649	GLU
1	C	1663	SER
1	C	1682	ASP
1	C	1739	LEU
1	C	1755	SER
1	C	1816	GLU
1	C	1846	LEU
1	C	1981	ASP
1	C	2136	GLU
1	C	2184	LYS
1	C	2302	ARG
1	C	2321	ARG
1	C	2335	ARG
1	C	2471	LEU
1	C	2492	LEU
1	C	2715	LYS
1	C	2721	ASN
1	C	2733	MET
1	C	2735	LYS
1	C	2768	GLU
1	C	2771	ARG
1	C	2775	LYS
1	C	2776	GLU
1	C	2777	SER

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Mol	Chain	Res	Type
1	C	2778	LEU
1	C	2779	LYS
1	C	2780	THR
1	C	2837	HIS
1	C	2871	VAL
1	C	2893	LYS
1	C	3782	GLU
1	C	3831	ASP
1	C	3851	SER
1	C	3861	THR
1	C	3965	GLU
1	C	4003	VAL
1	C	4033	GLU
1	C	4041	VAL
1	C	4049	LYS
1	C	4076	THR
1	C	4081	GLU
1	C	4273	MET
1	C	4280	LEU
1	C	4284	SER
1	C	4288	SER
1	C	4604	GLU
1	C	4622	GLU
1	C	4658	GLU
1	C	4667	GLU
1	C	4706	MET
1	C	4714	THR
1	C	4797	ASP
1	C	4802	ASP
1	D	17	ASP
1	D	22	LEU
1	D	65	CYS
1	D	82	LEU
1	D	112	THR
1	D	113	LEU
1	D	147	VAL
1	D	181	LEU
1	D	187	SER
1	D	214	VAL
1	D	268	SER
1	D	282	VAL
1	D	296	ARG

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Mol	Chain	Res	Type
1	D	333	SER
1	D	412	GLU
1	D	422	THR
1	D	439	LYS
1	D	453	SER
1	D	501	CYS
1	D	550	GLN
1	D	566	GLU
1	D	609	LYS
1	D	653	SER
1	D	691	THR
1	D	765	SER
1	D	767	SER
1	D	814	LEU
1	D	841	LYS
1	D	923	LYS
1	D	935	MET
1	D	987	LYS
1	D	988	LEU
1	D	1006	VAL
1	D	1028	ARG
1	D	1033	VAL
1	D	1039	ASP
1	D	1040	ASP
1	D	1041	ARG
1	D	1047	LYS
1	D	1057	LEU
1	D	1108	VAL
1	D	1122	CYS
1	D	1172	THR
1	D	1261	VAL
1	D	1309	GLU
1	D	1348	LYS
1	D	1583	CYS
1	D	1649	GLU
1	D	1663	SER
1	D	1682	ASP
1	D	1739	LEU
1	D	1755	SER
1	D	1816	GLU
1	D	1846	LEU
1	D	1981	ASP

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Mol	Chain	Res	Type
1	D	2136	GLU
1	D	2184	LYS
1	D	2302	ARG
1	D	2321	ARG
1	D	2335	ARG
1	D	2471	LEU
1	D	2492	LEU
1	D	2715	LYS
1	D	2721	ASN
1	D	2733	MET
1	D	2735	LYS
1	D	2768	GLU
1	D	2771	ARG
1	D	2775	LYS
1	D	2776	GLU
1	D	2777	SER
1	D	2778	LEU
1	D	2779	LYS
1	D	2780	THR
1	D	2837	HIS
1	D	2871	VAL
1	D	2893	LYS
1	D	3782	GLU
1	D	3831	ASP
1	D	3851	SER
1	D	3861	THR
1	D	3965	GLU
1	D	4003	VAL
1	D	4033	GLU
1	D	4041	VAL
1	D	4049	LYS
1	D	4076	THR
1	D	4081	GLU
1	D	4273	MET
1	D	4280	LEU
1	D	4284	SER
1	D	4288	SER
1	D	4604	GLU
1	D	4622	GLU
1	D	4658	GLU
1	D	4667	GLU
1	D	4706	MET

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Mol	Chain	Res	Type
1	D	4714	THR
1	D	4797	ASP
1	D	4802	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	150	GLN
1	A	193	HIS
1	A	293	GLN
1	A	299	HIS
1	A	544	ASN
1	A	593	HIS
1	A	629	GLN
1	A	658	ASN
1	A	808	HIS
1	A	888	ASN
1	A	971	GLN
1	A	992	GLN
1	A	1178	ASN
1	A	1265	HIS
1	A	1588	HIS
1	A	1616	GLN
1	A	1627	GLN
1	A	1685	GLN
1	A	1744	ASN
1	A	1944	ASN
1	A	1973	ASN
1	A	2090	GLN
1	A	2150	ASN
1	A	2151	ASN
1	A	2317	ASN
1	A	2721	ASN
1	A	2726	HIS
1	A	2837	HIS
1	A	2846	ASN
1	A	3952	HIS
1	A	3954	GLN
1	A	3959	GLN
1	A	3974	GLN
1	A	4008	ASN

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Mol	Chain	Res	Type
1	A	4295	HIS
1	A	4487	GLN
1	A	4491	ASN
1	A	4496	ASN
1	A	4619	GLN
1	A	4786	ASN
1	A	4960	GLN
2	G	32	GLN
2	G	44	ASN
2	G	88	HIS
1	B	123	HIS
1	B	150	GLN
1	B	193	HIS
1	B	270	HIS
1	B	293	GLN
1	B	299	HIS
1	B	544	ASN
1	B	593	HIS
1	B	629	GLN
1	B	658	ASN
1	B	808	HIS
1	B	888	ASN
1	B	971	GLN
1	B	992	GLN
1	B	1178	ASN
1	B	1265	HIS
1	B	1588	HIS
1	B	1616	GLN
1	B	1627	GLN
1	B	1685	GLN
1	B	1744	ASN
1	B	1944	ASN
1	B	1973	ASN
1	B	2090	GLN
1	B	2150	ASN
1	B	2151	ASN
1	B	2317	ASN
1	B	2721	ASN
1	B	2726	HIS
1	B	2837	HIS
1	B	2846	ASN
1	B	3952	HIS

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Mol	Chain	Res	Type
1	B	3954	GLN
1	B	3959	GLN
1	B	3974	GLN
1	B	4008	ASN
1	B	4295	HIS
1	B	4487	GLN
1	B	4491	ASN
1	B	4496	ASN
1	B	4619	GLN
1	B	4960	GLN
2	H	32	GLN
2	H	44	ASN
2	H	88	HIS
1	C	123	HIS
1	C	150	GLN
1	C	193	HIS
1	C	270	HIS
1	C	293	GLN
1	C	299	HIS
1	C	544	ASN
1	C	593	HIS
1	C	629	GLN
1	C	658	ASN
1	C	808	HIS
1	C	888	ASN
1	C	971	GLN
1	C	992	GLN
1	C	1178	ASN
1	C	1265	HIS
1	C	1588	HIS
1	C	1627	GLN
1	C	1685	GLN
1	C	1744	ASN
1	C	1944	ASN
1	C	1973	ASN
1	C	2090	GLN
1	C	2150	ASN
1	C	2151	ASN
1	C	2317	ASN
1	C	2721	ASN
1	C	2726	HIS
1	C	2837	HIS

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Mol	Chain	Res	Type
1	C	2846	ASN
1	C	3952	HIS
1	C	3954	GLN
1	C	3959	GLN
1	C	3974	GLN
1	C	4008	ASN
1	C	4295	HIS
1	C	4487	GLN
1	C	4491	ASN
1	C	4496	ASN
1	C	4619	GLN
1	C	4960	GLN
2	I	44	ASN
2	I	88	HIS
1	D	123	HIS
1	D	150	GLN
1	D	193	HIS
1	D	293	GLN
1	D	299	HIS
1	D	544	ASN
1	D	593	HIS
1	D	629	GLN
1	D	658	ASN
1	D	808	HIS
1	D	888	ASN
1	D	971	GLN
1	D	992	GLN
1	D	1178	ASN
1	D	1265	HIS
1	D	1588	HIS
1	D	1616	GLN
1	D	1627	GLN
1	D	1685	GLN
1	D	1744	ASN
1	D	1944	ASN
1	D	1973	ASN
1	D	2090	GLN
1	D	2150	ASN
1	D	2151	ASN
1	D	2317	ASN
1	D	2721	ASN
1	D	2726	HIS

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Mol	Chain	Res	Type
1	D	2837	HIS
1	D	2846	ASN
1	D	3952	HIS
1	D	3954	GLN
1	D	3959	GLN
1	D	3974	GLN
1	D	4008	ASN
1	D	4295	HIS
1	D	4487	GLN
1	D	4491	ASN
1	D	4496	ASN
1	D	4619	GLN
1	D	4960	GLN
2	J	44	ASN
2	J	88	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

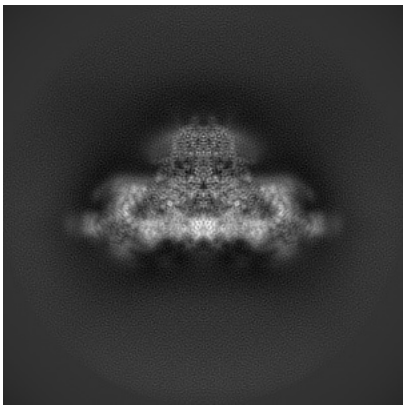
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33937. These allow visual inspection of the internal detail of the map and identification of artifacts.

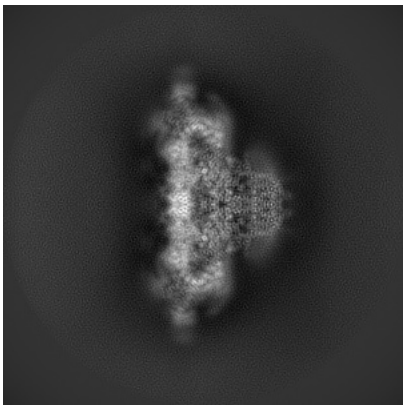
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

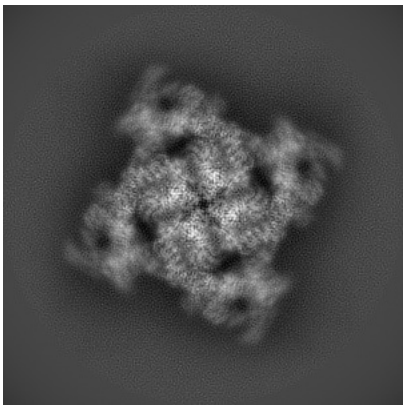
6.1.1 Primary map



X

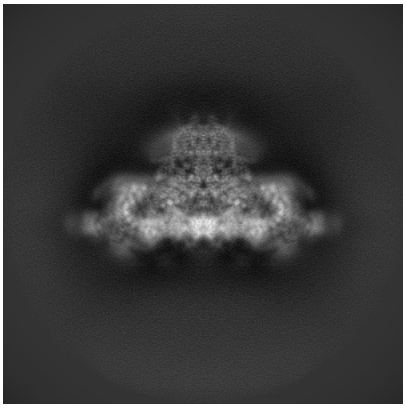


Y

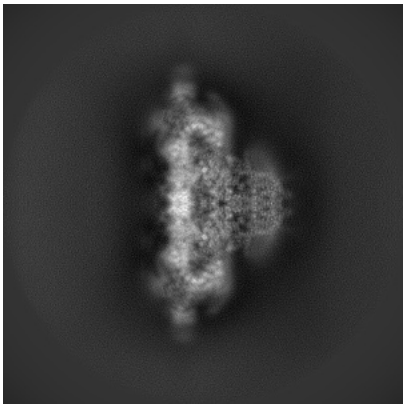


Z

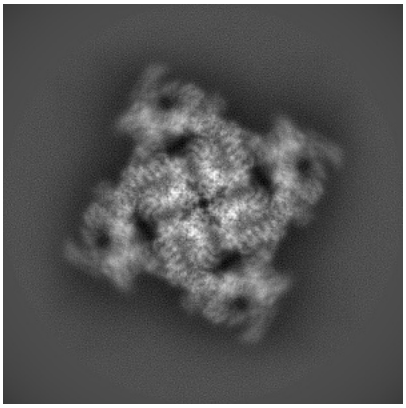
6.1.2 Raw map



X



Y

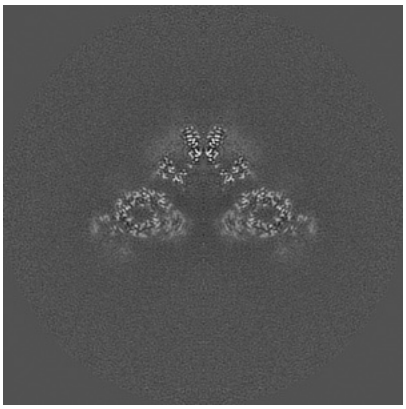


Z

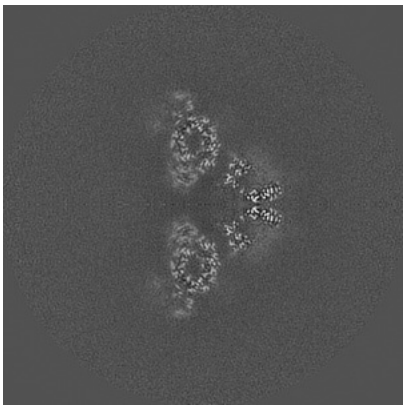
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

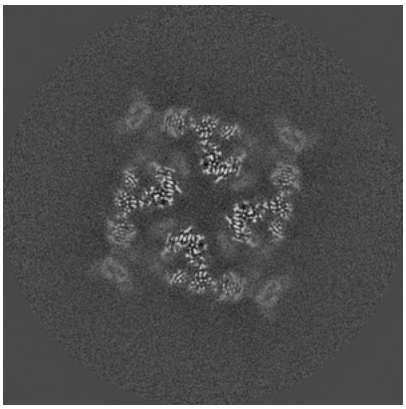
6.2.1 Primary map



X Index: 200

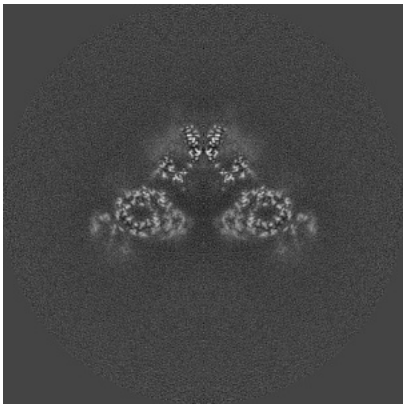


Y Index: 200

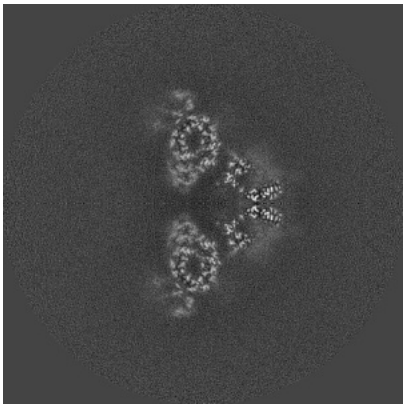


Z Index: 200

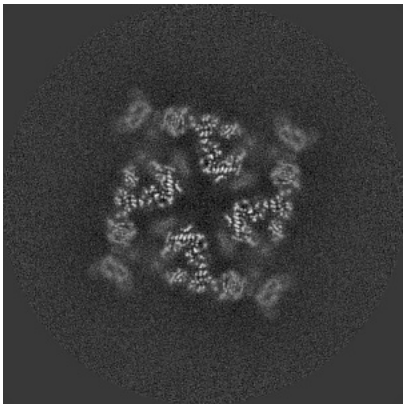
6.2.2 Raw map



X Index: 200



Y Index: 200

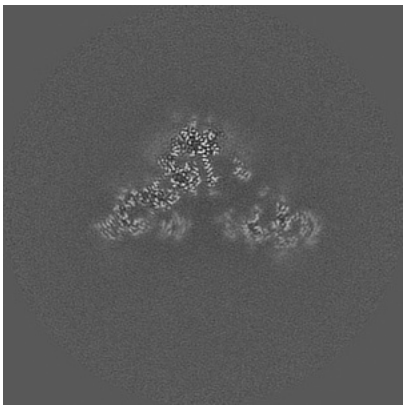


Z Index: 200

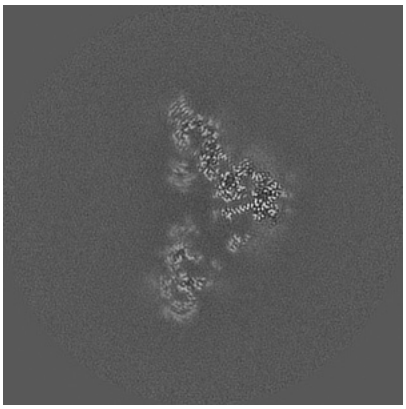
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

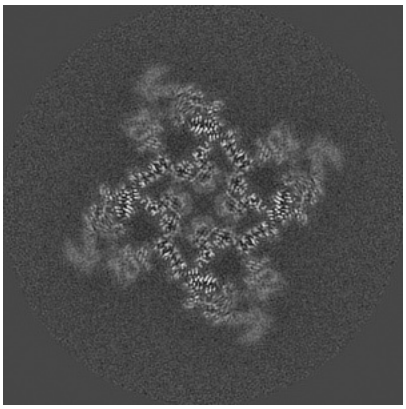
6.3.1 Primary map



X Index: 193

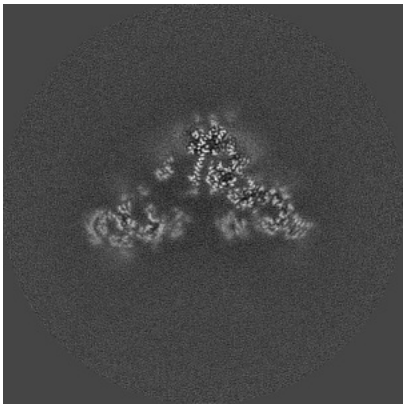


Y Index: 193

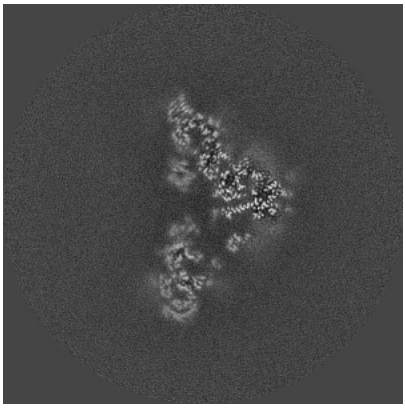


Z Index: 183

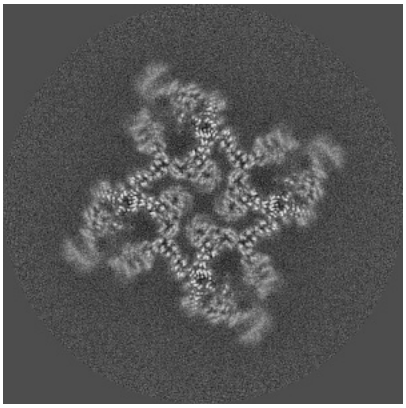
6.3.2 Raw map



X Index: 207



Y Index: 193

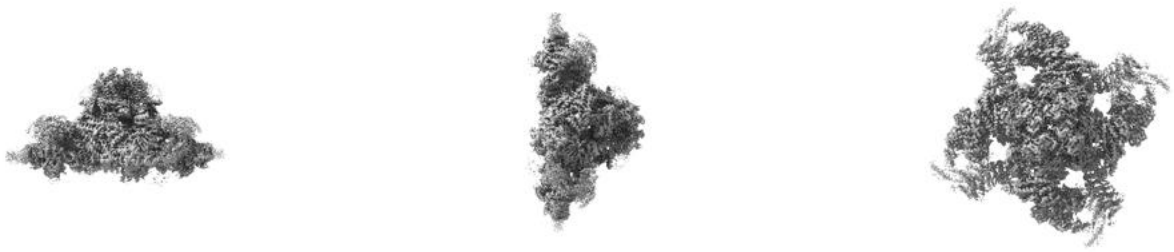


Z Index: 180

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

6.4 Orthogonal surface views (i)

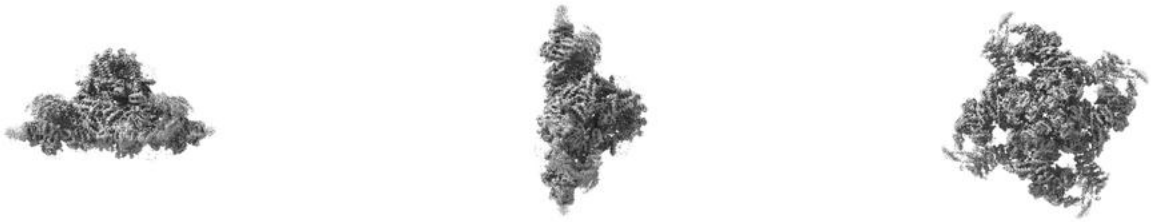
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

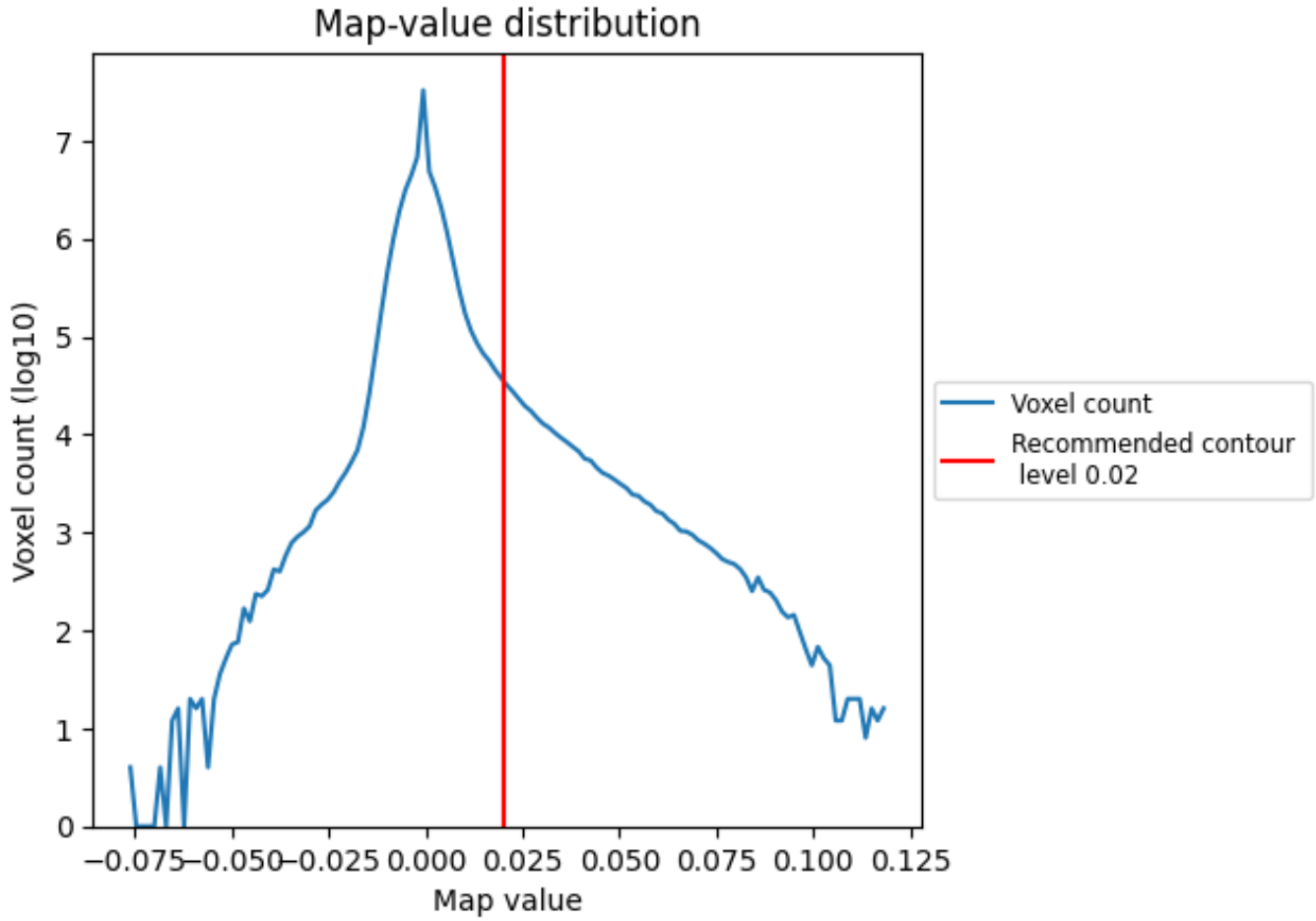
6.5 Mask visualisation (i)

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

7 Map analysis

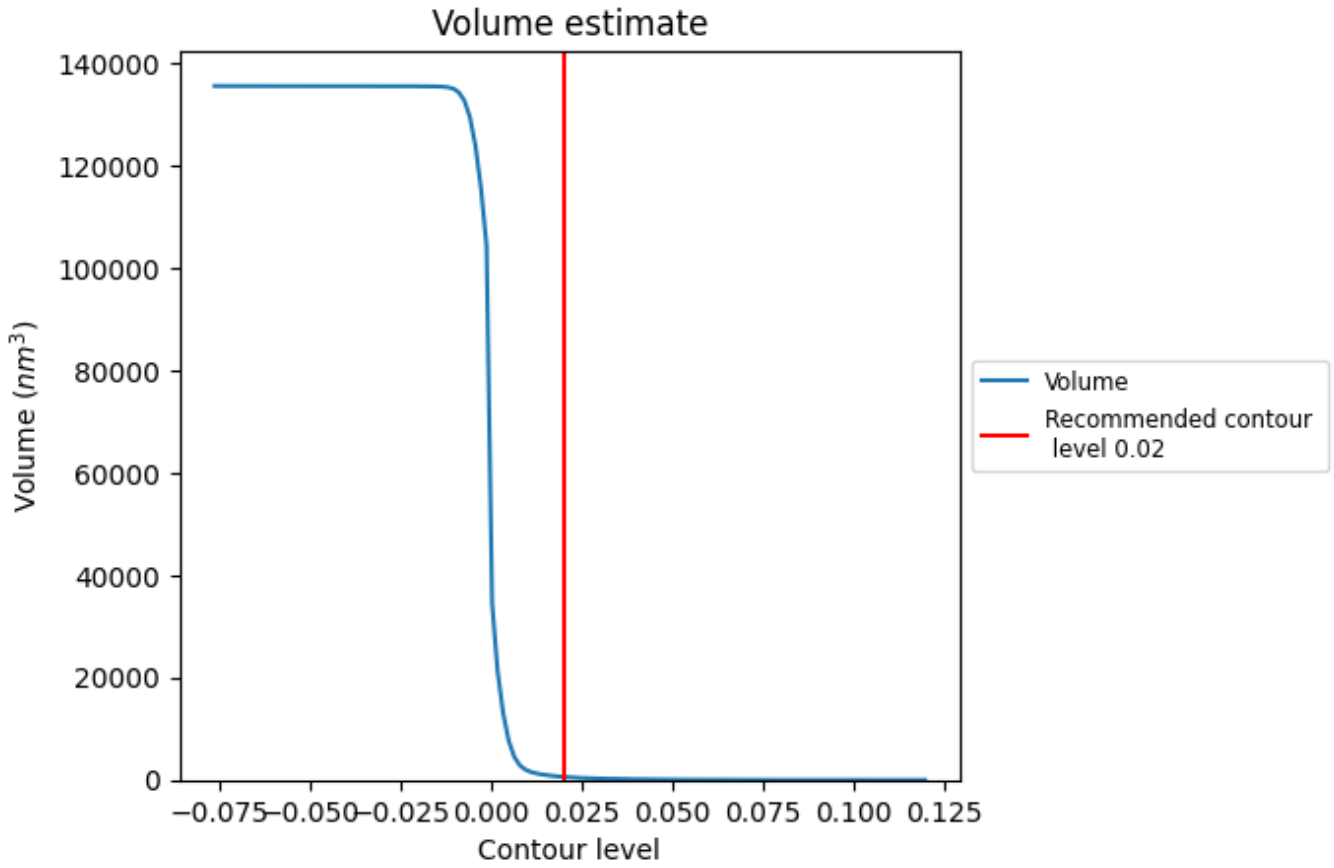
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

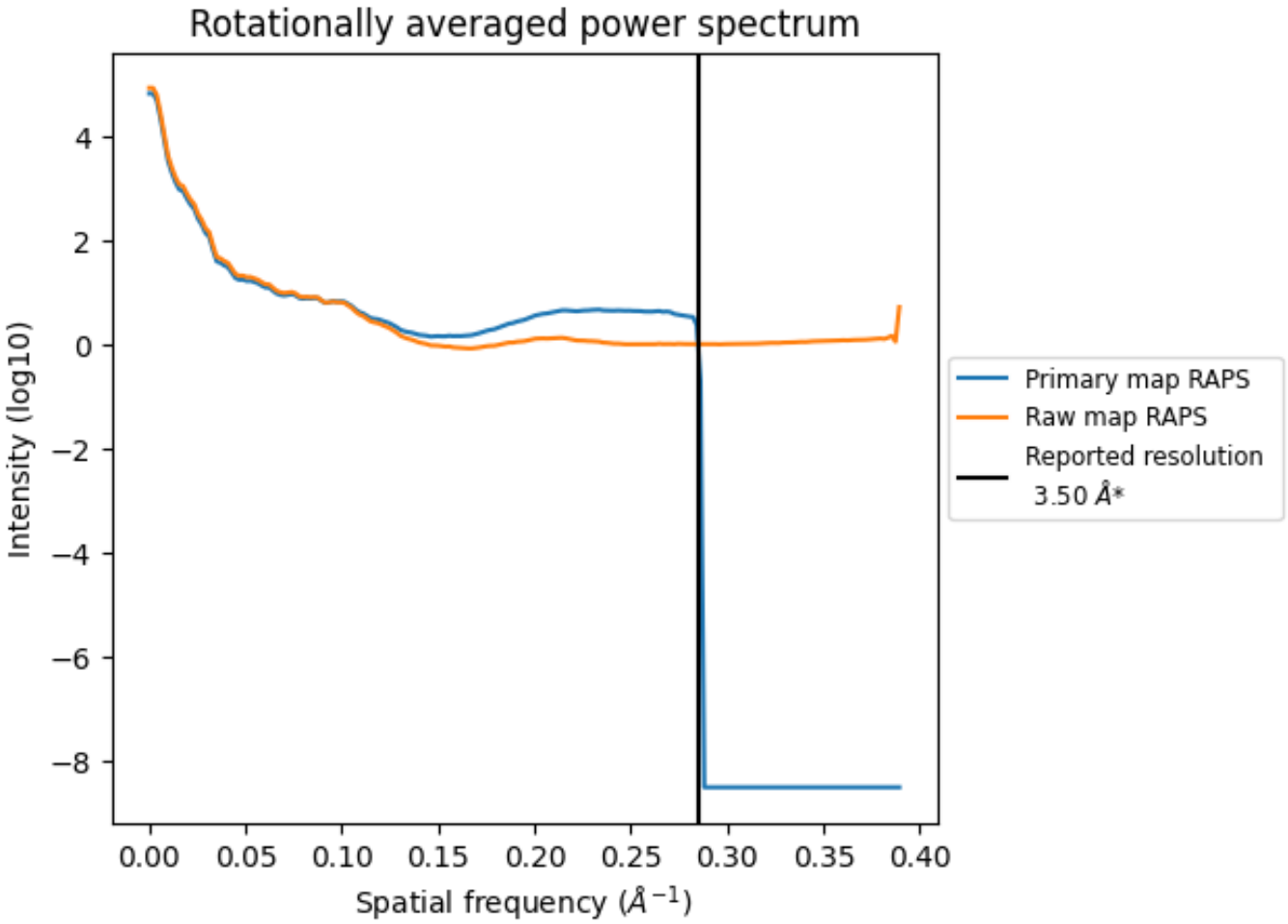
7.2 Volume estimate



The volume at the recommended contour level is 601 nm^3; this corresponds to an approximate mass of 542 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)

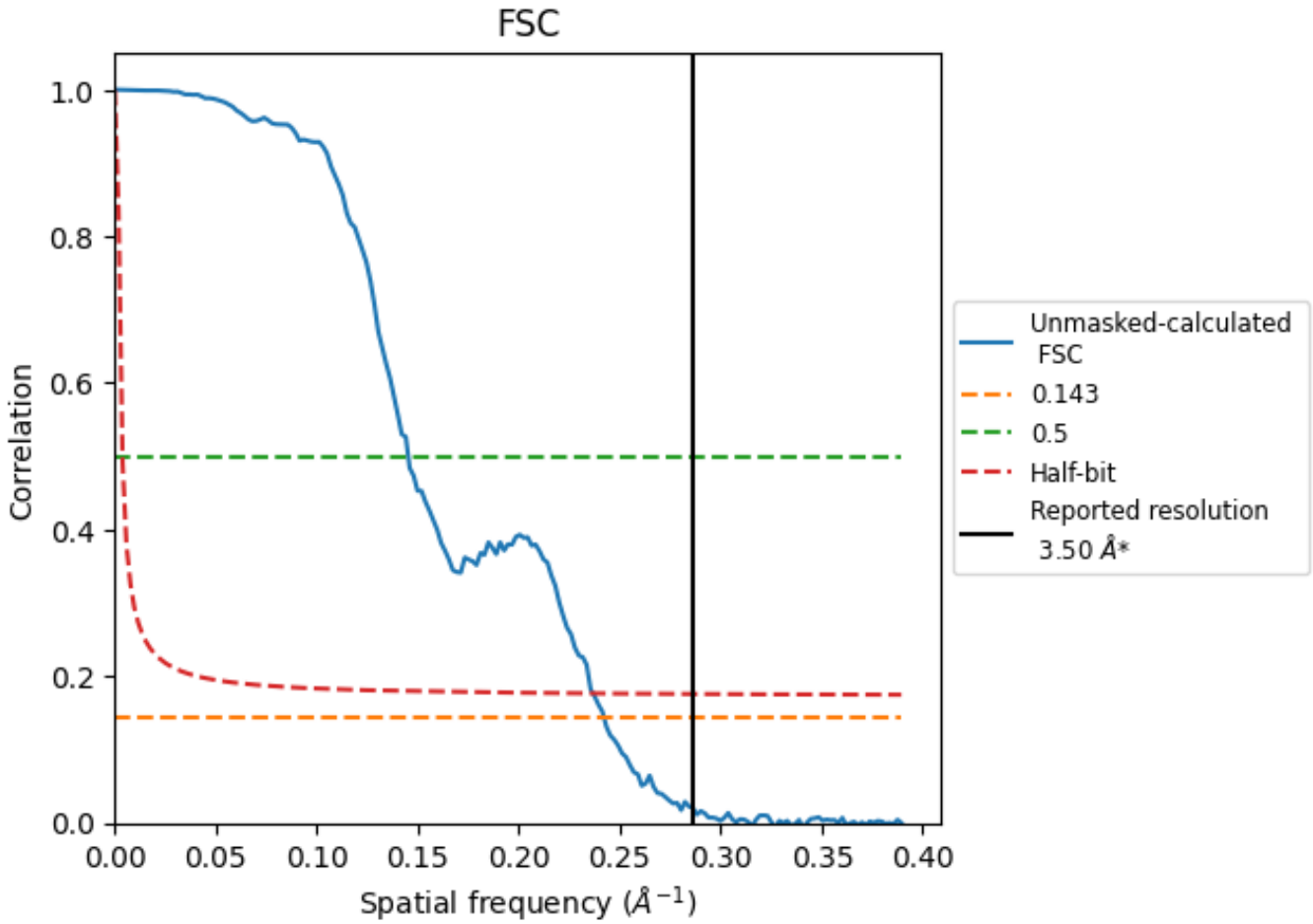


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

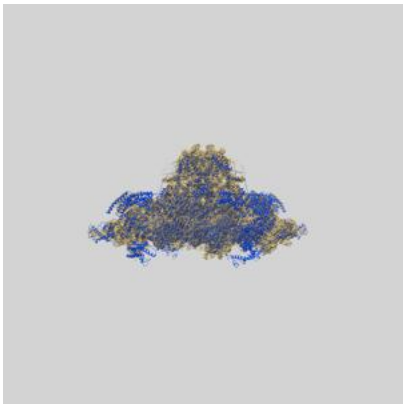
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	6.88	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.5 by more than 10 %

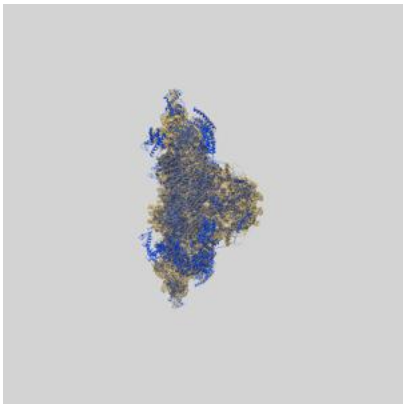
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33937 and PDB model 7VMN. Per-residue inclusion information can be found in section 3 on page 11.

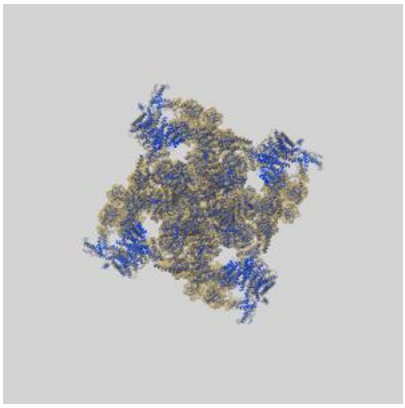
9.1 Map-model overlay



X



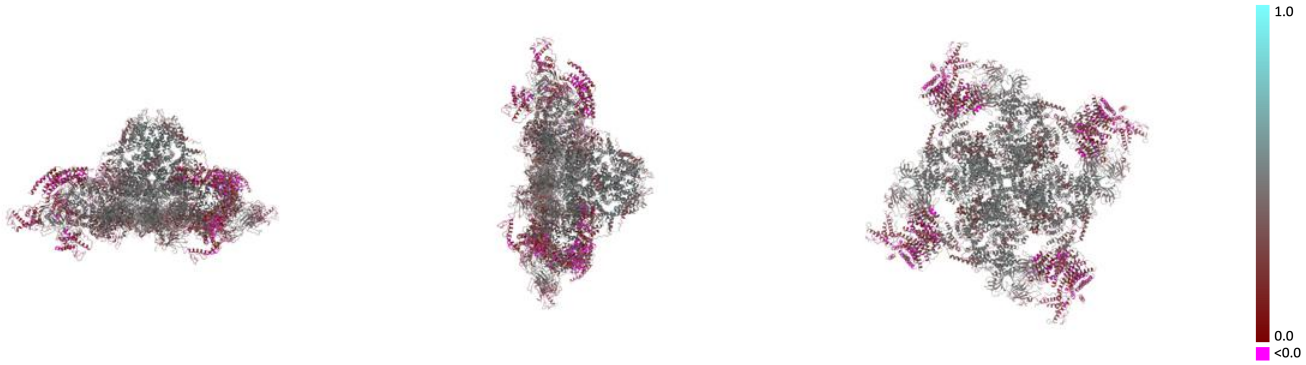
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

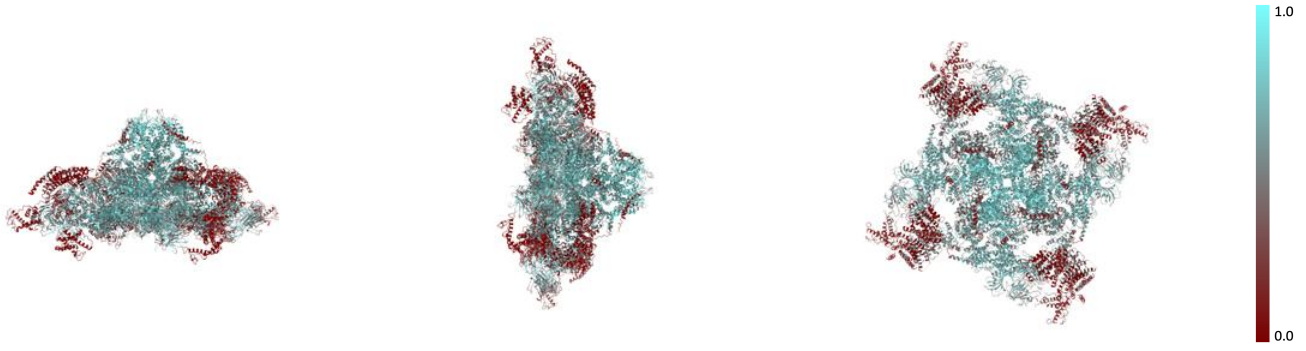
9.2 Q-score mapped to coordinate model



X Y Z

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

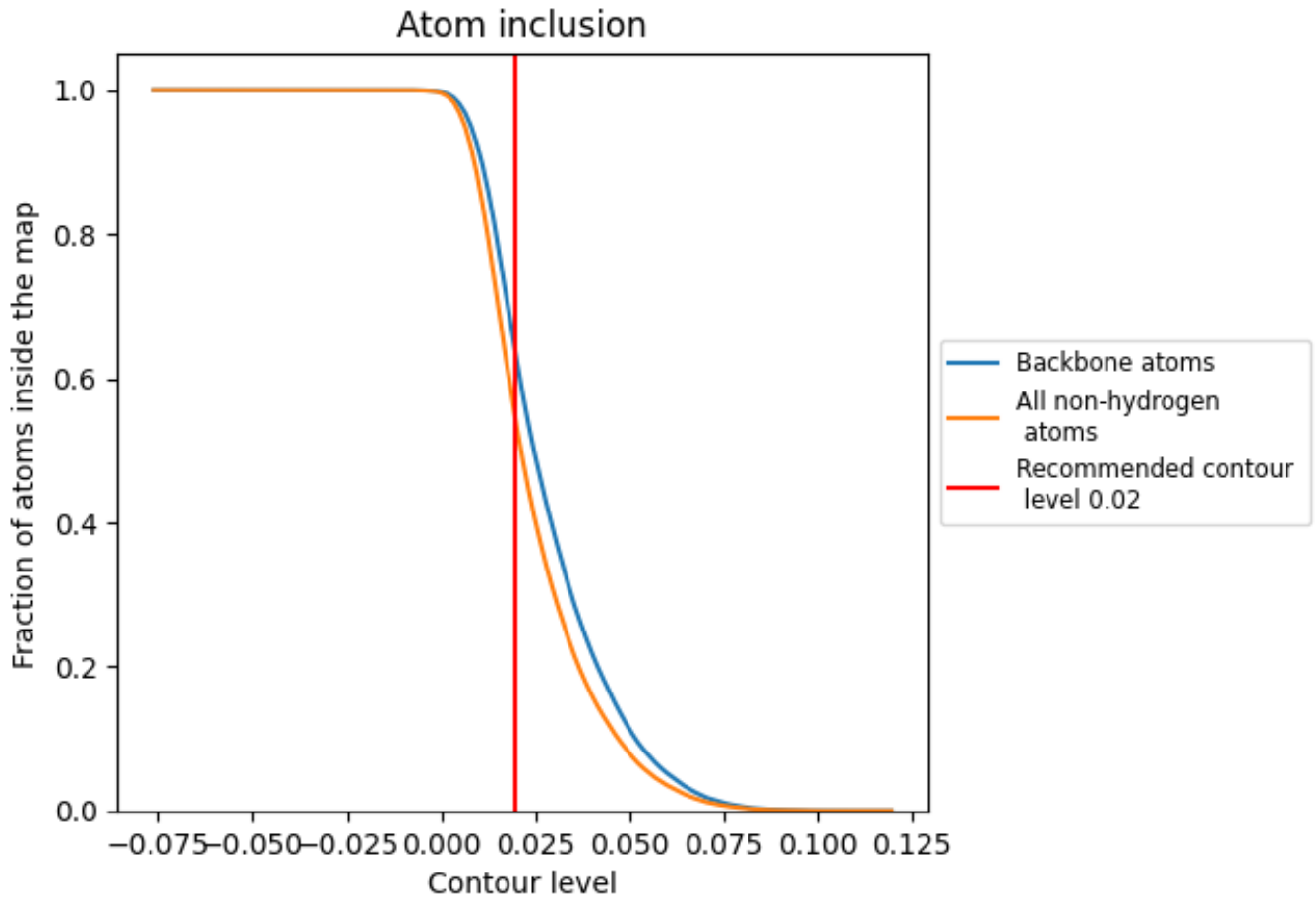
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 54% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5384	0.3770
A	0.5349	0.3750
B	0.5370	0.3760
C	0.5358	0.3760
D	0.5360	0.3740
G	0.6295	0.4370
H	0.6307	0.4350
I	0.6320	0.4300
J	0.6295	0.4350