Full wwPDB EM Validation Report (i)

Jun 11, 2024 – 08:06 PM JST

PDB ID	:	7VMR
EMDB ID	:	EMD-32036
Title	:	Structure of recombinant RyR2 mutant K4593A (EGTA dataset)
Authors	:	Kobayashi, T.; Tsutsumi, A.; Kurebayashi, N.; Kodama, M.; Kikkawa, M.; Murayama, T.; Ogawa, H.
Deposited on	:	2021-10-09
Resolution	:	3.30 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 (i) symbol.

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

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

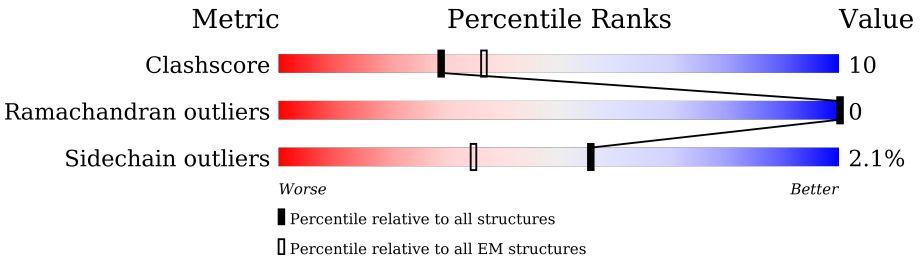
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.30 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	34% 64% 16% • 19%
1	B	4966	35% 64% 16% • 19%
1	C	4966	35% 65% 16% • 19%
1	D	4966	35% 64% 16% • 19%
2	G	176	19% 41% 18% • 39%
2	H	176	19% 40% 19% • 39%
2	I	176	18% 38% 21% • 39%
2	J	176	18% 42% 17% • 39%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 123548 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
			Total	C	N	O	S		
1	A	4044	30067	19032	5242	5617	176	0	0
1	B	4044	30067	19032	5242	5617	176	0	0
1	C	4044	30067	19032	5242	5617	176	0	0
1	D	4044	30067	19032	5242	5617	176	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4593	ALA	LYS	engineered mutation	UNP E9Q401
B	4593	ALA	LYS	engineered mutation	UNP E9Q401
C	4593	ALA	LYS	engineered mutation	UNP E9Q401
D	4593	ALA	LYS	engineered mutation	UNP E9Q401

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

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

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-67	MET	-	initiating methionine	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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).

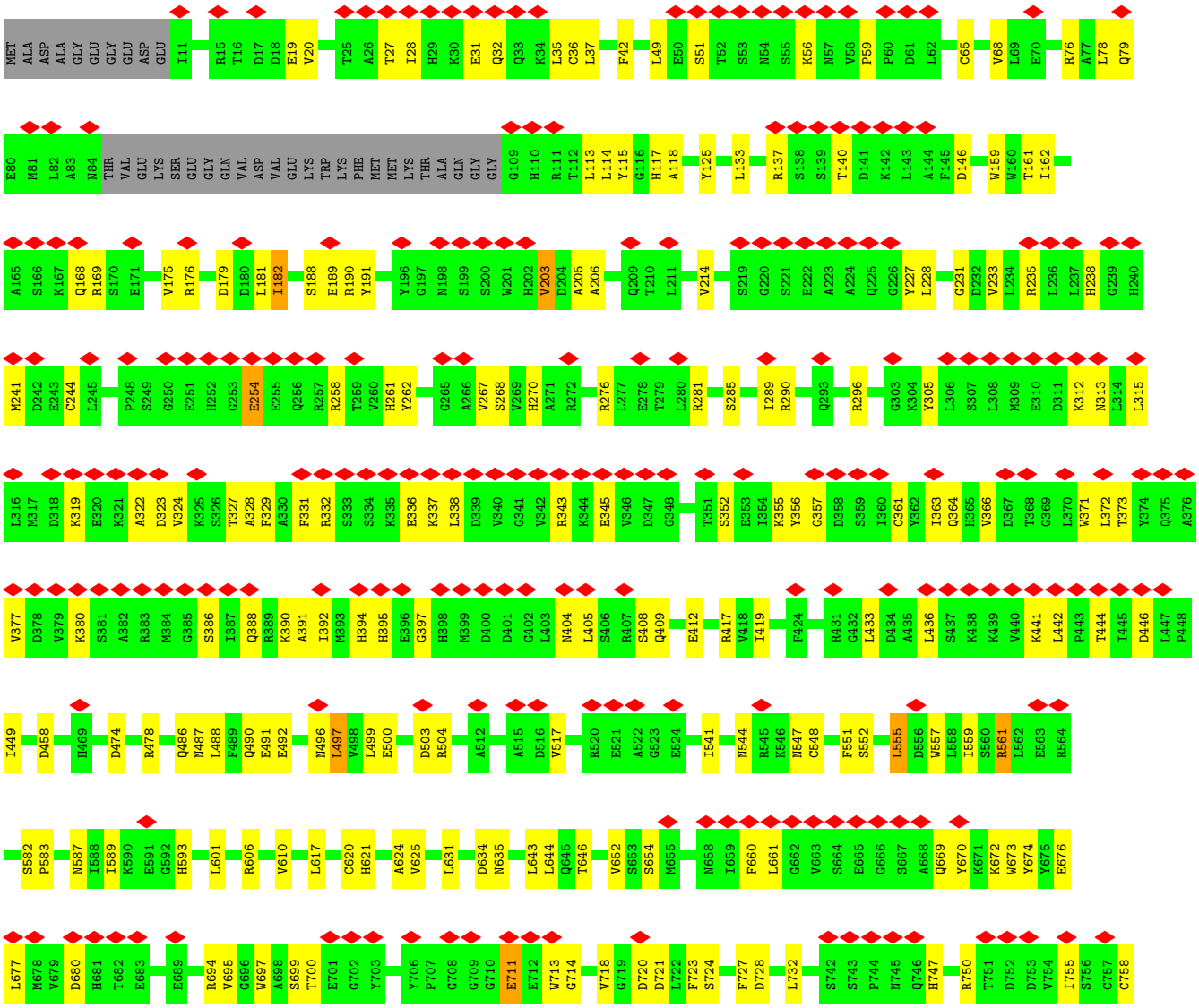
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0
3	B	1	1	1	0
3	C	1	1	1	0
3	D	1	1	1	0

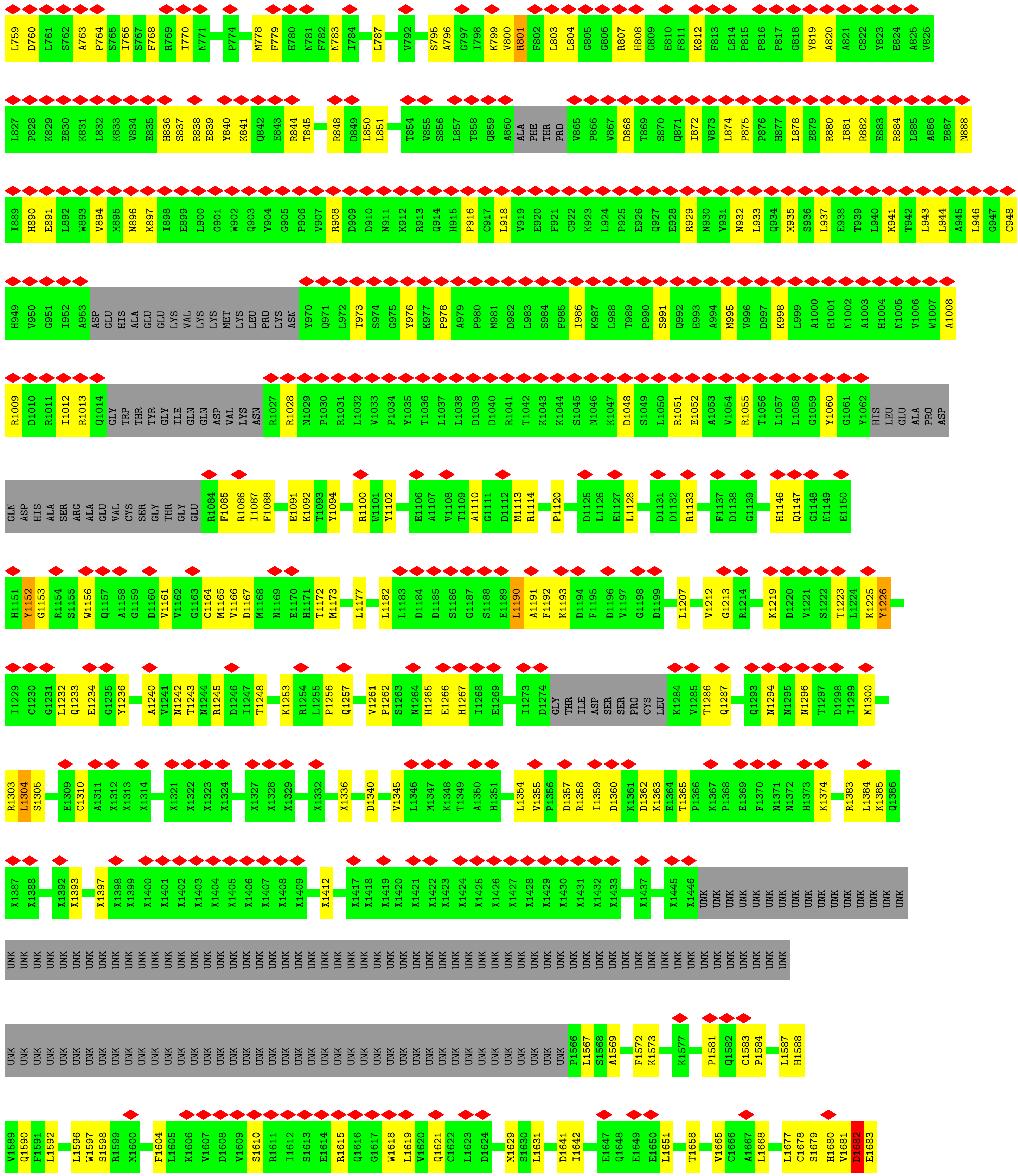
3 Residue-property plots (i)

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:

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L827 P828 K829 E830 K831 L832 K833 V834 E835 H836 S837 R838 E839 Y840 K841 Q842 E843 R844 T845 R848 D849 L850 L851 T854 V855 S856 L857 T858 Q859 A860 ALA PHE THR PRO V865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 R884 L885 A886 E887 N888
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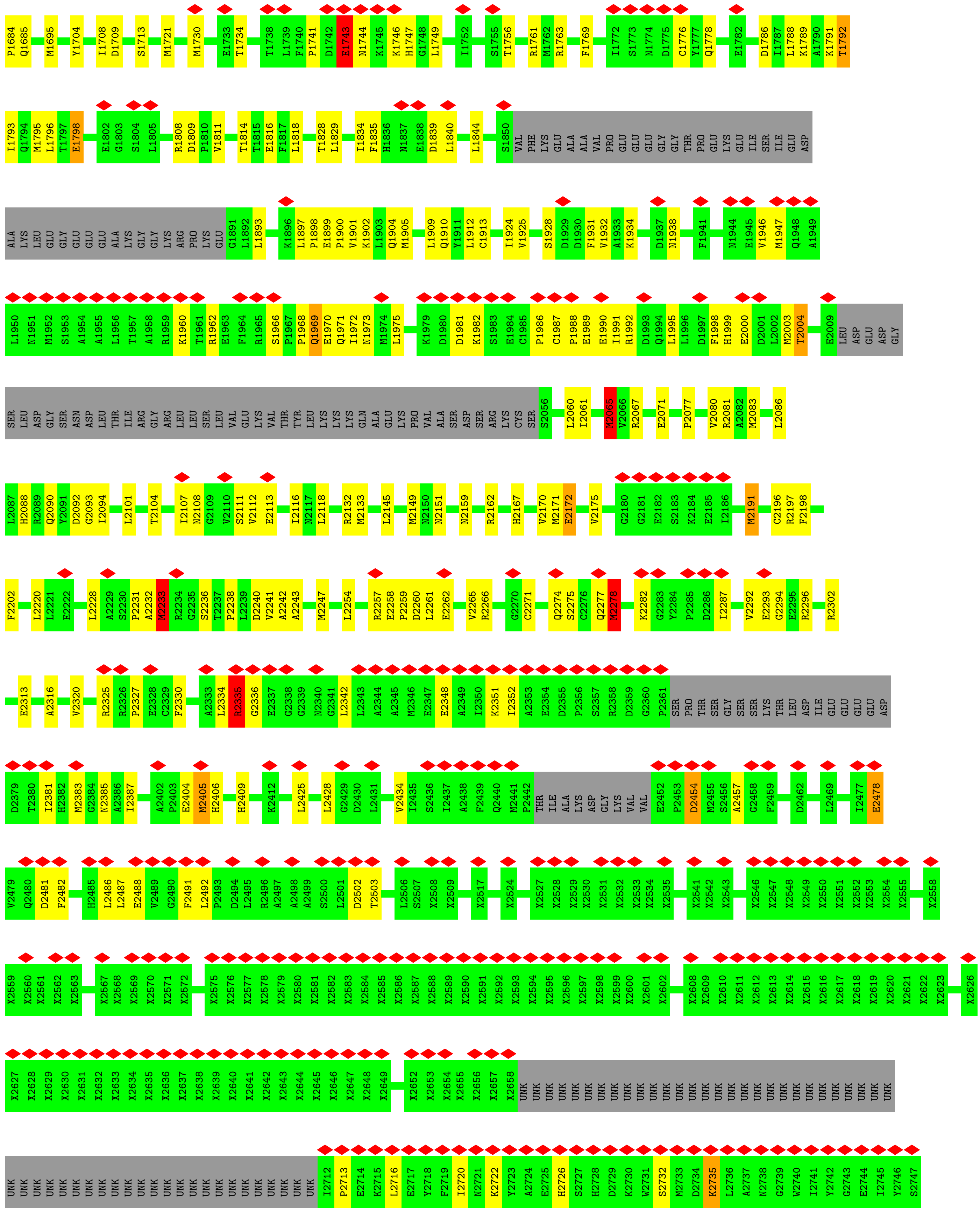
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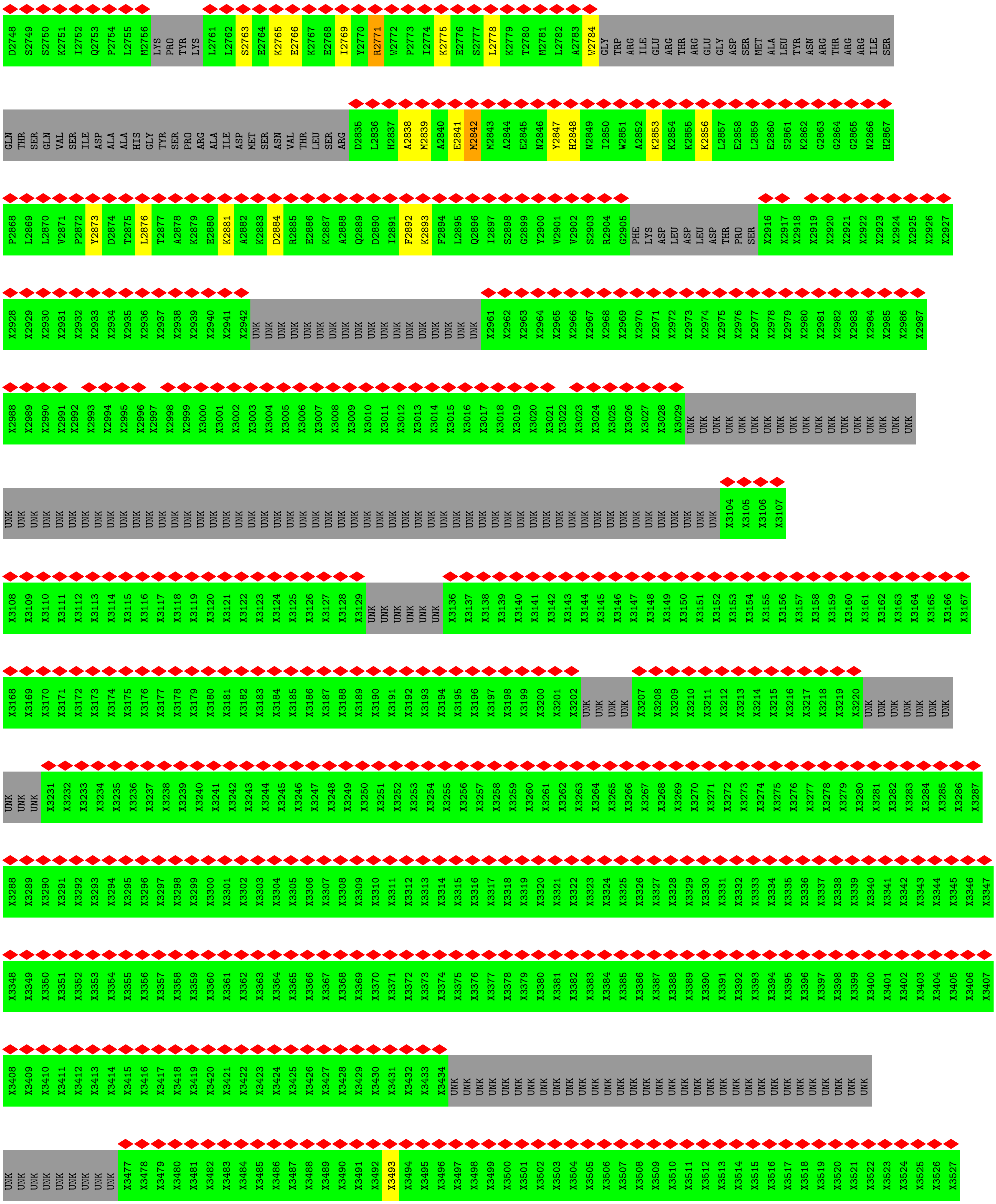
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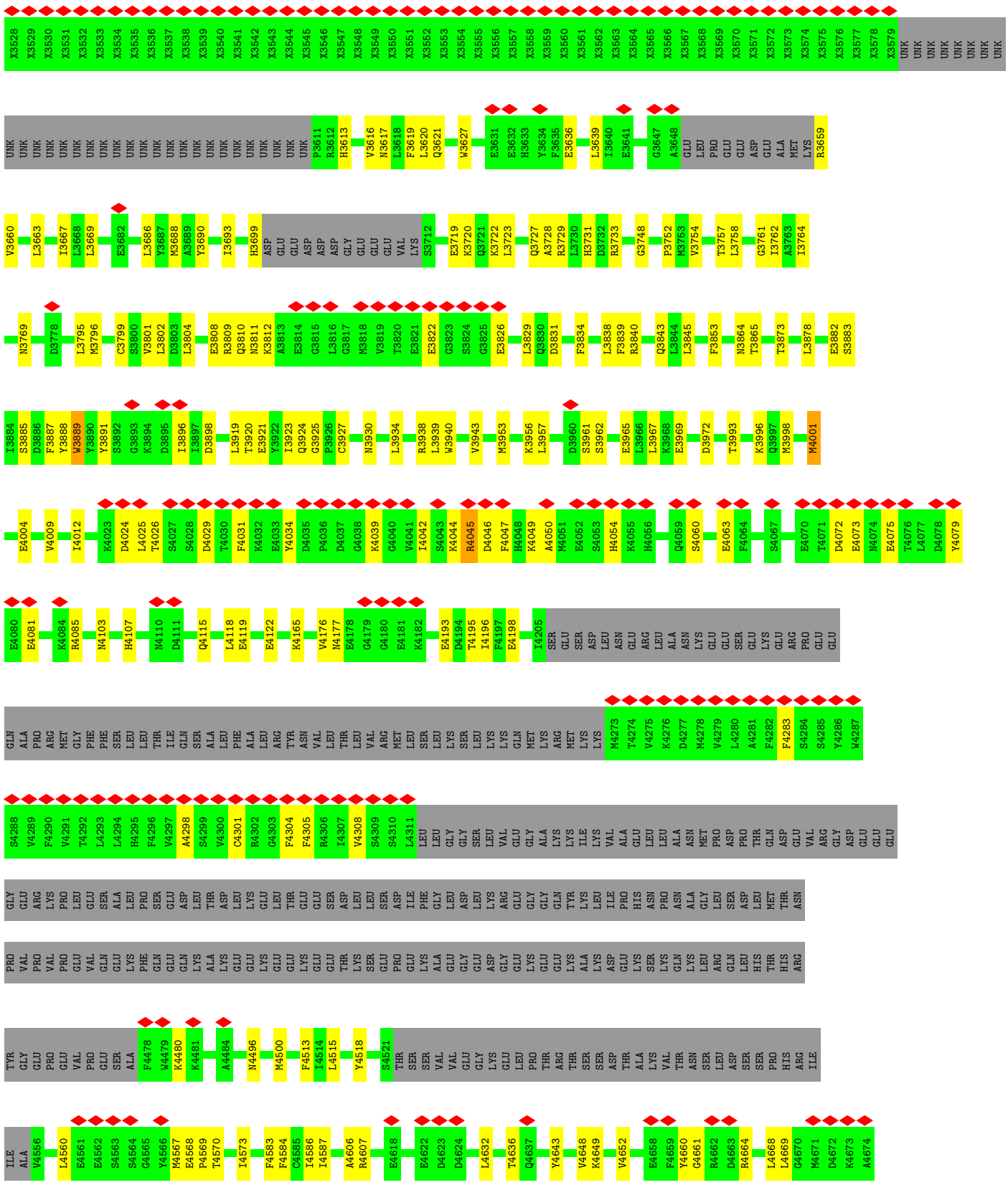
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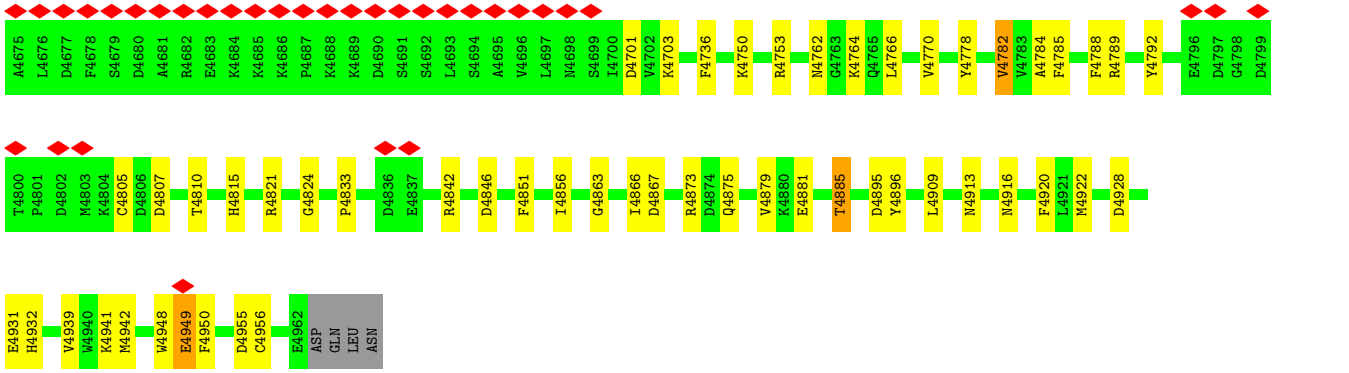
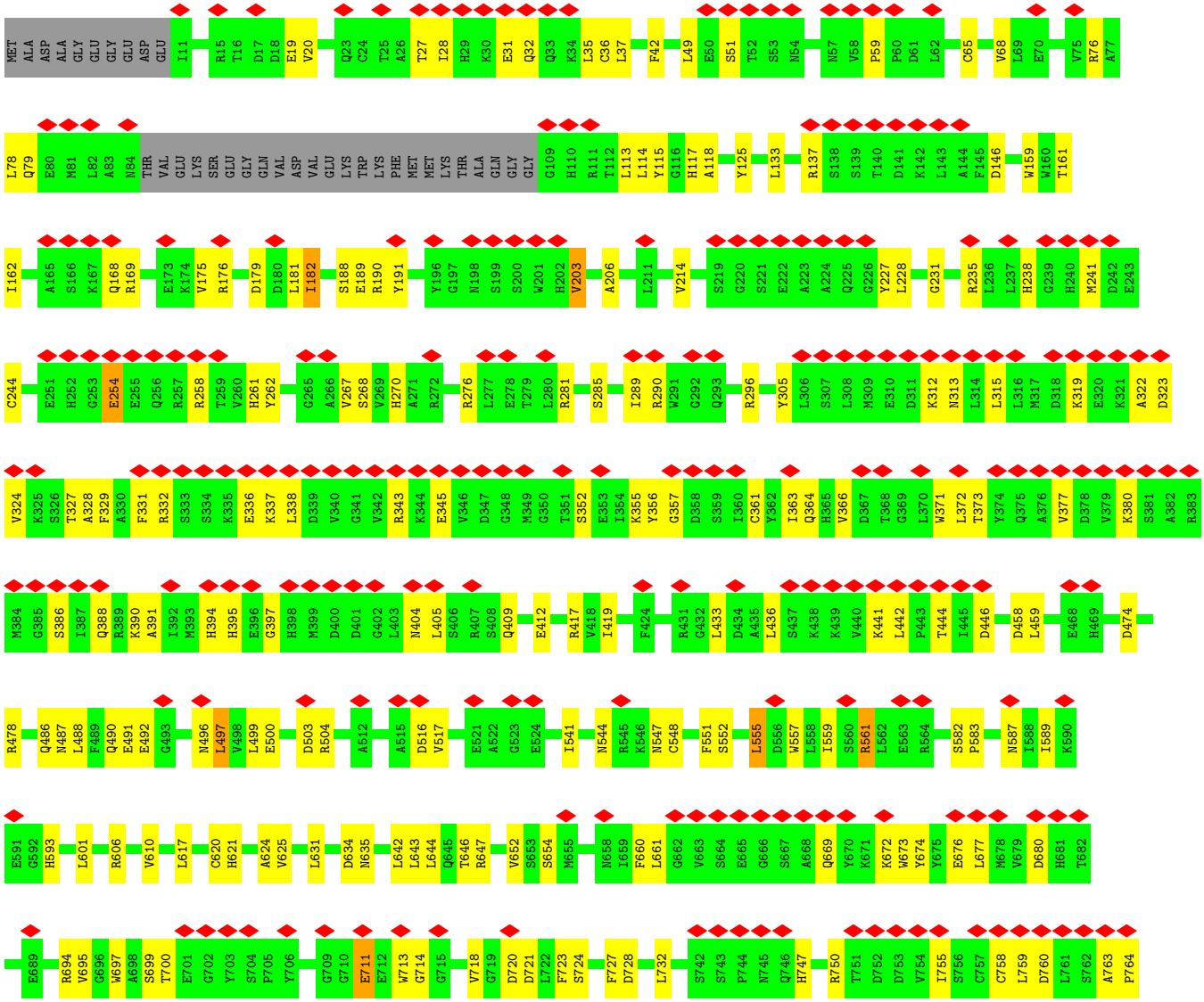
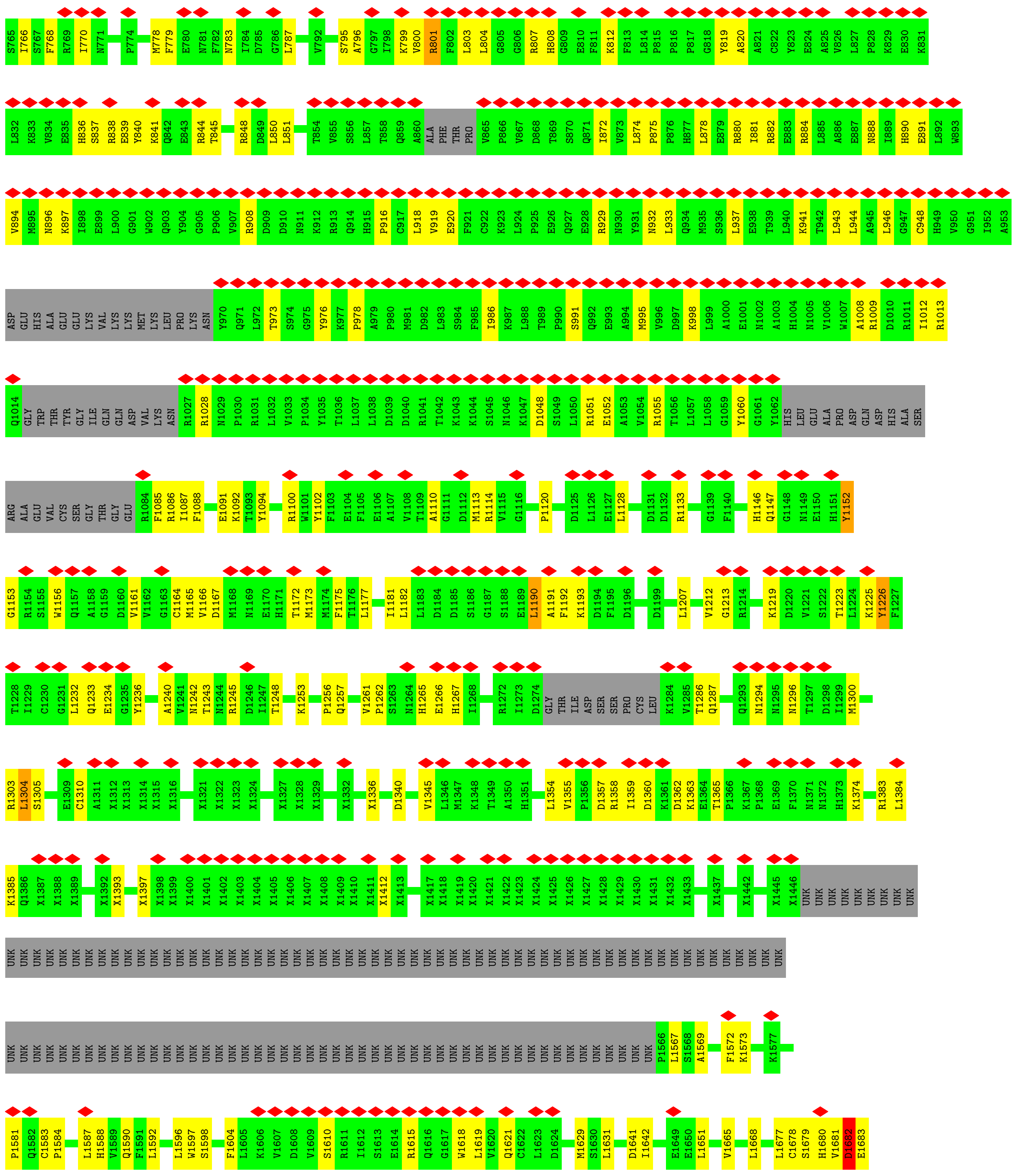


• Molecule 1: Ryanodine receptor 2

Chain B:

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L832 K833 V834 E835 H836 S837 R838 E839 Y840 K841 Q842 E843 R844 T845 R848 D849 L850 L851 T854 V855 S856 L857 T858 Q859 A860 ALA PHE THR PRO V865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 R884 L885 A886 E887 N888 I889 H890 E891 L892 W893
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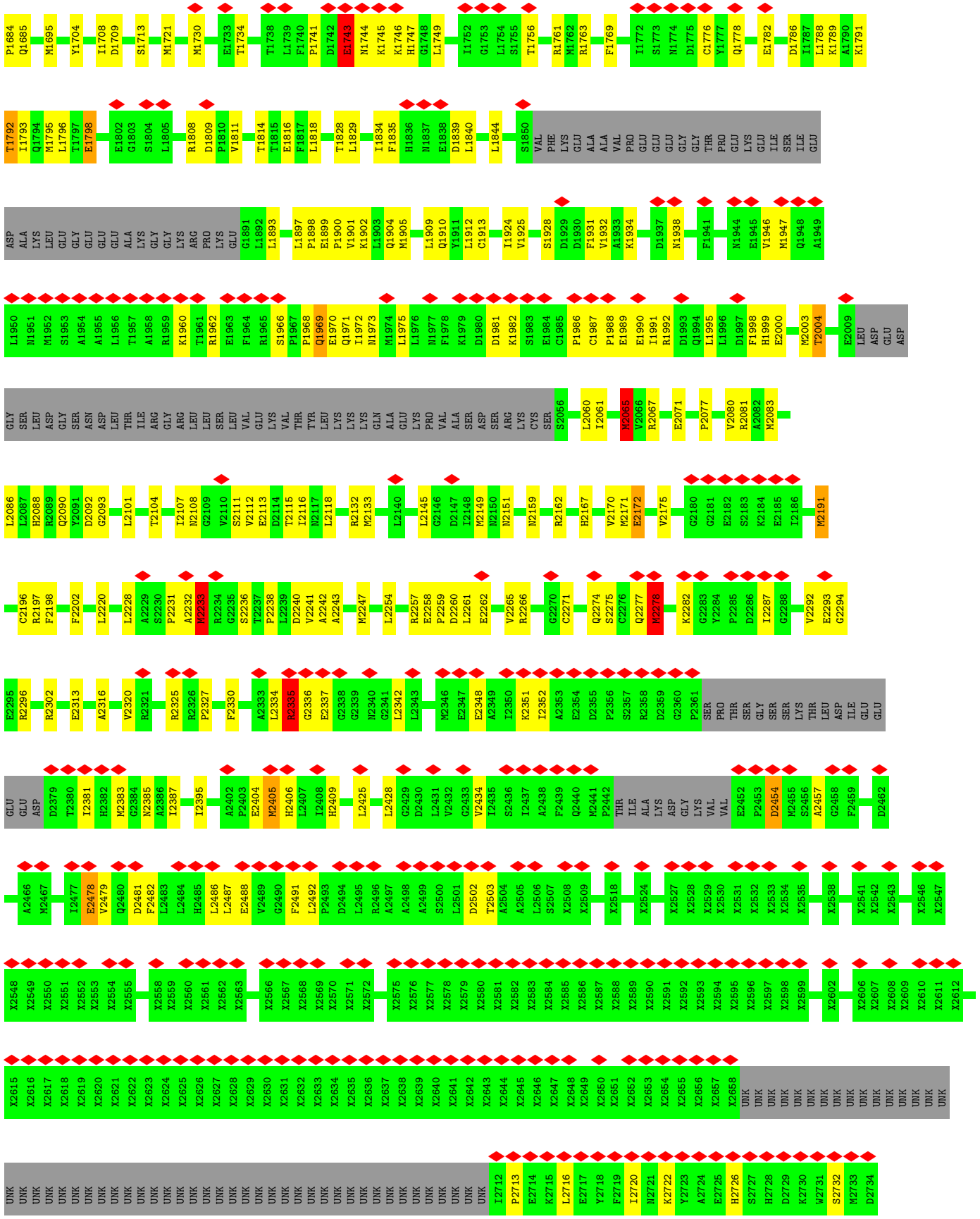
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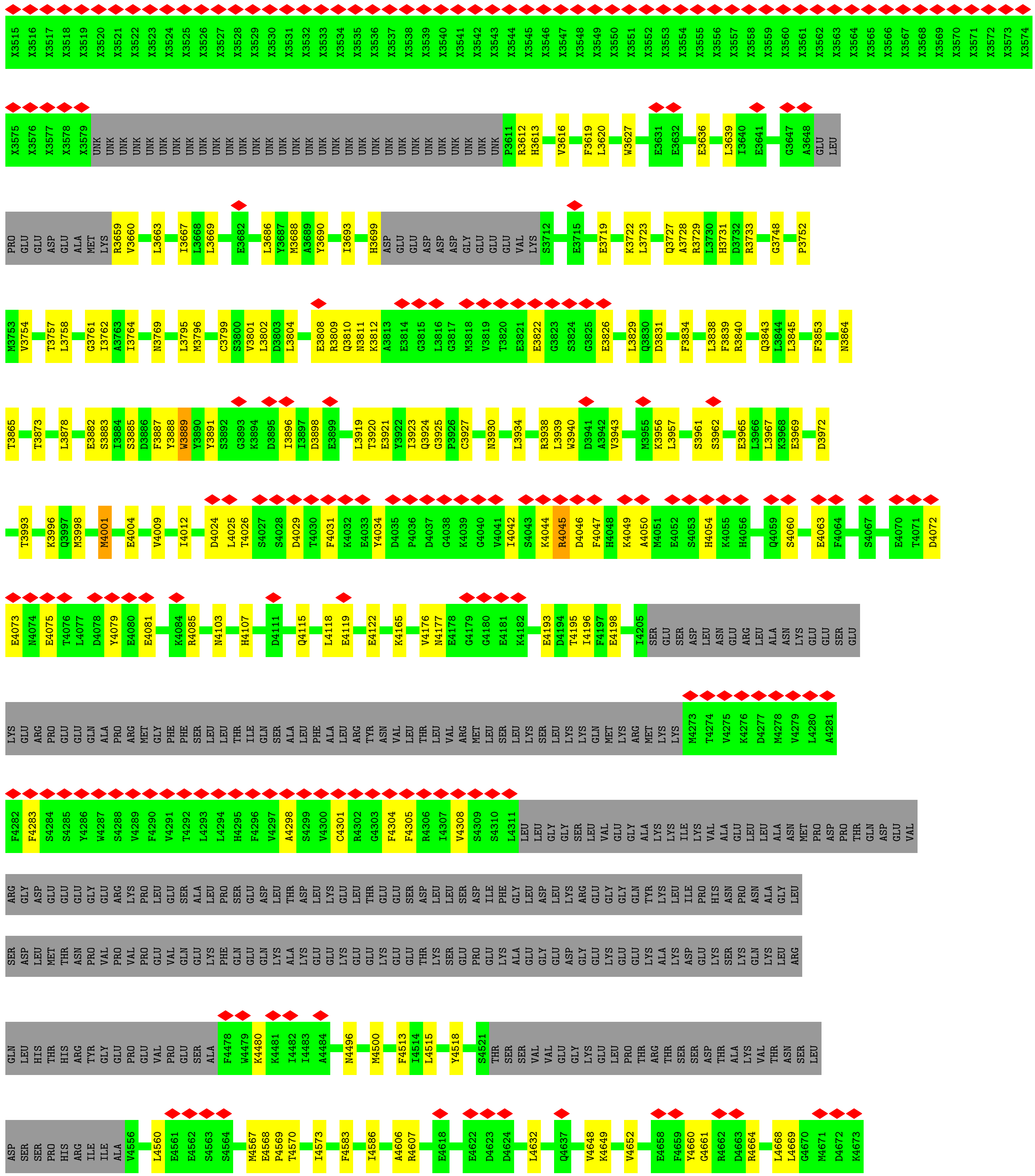
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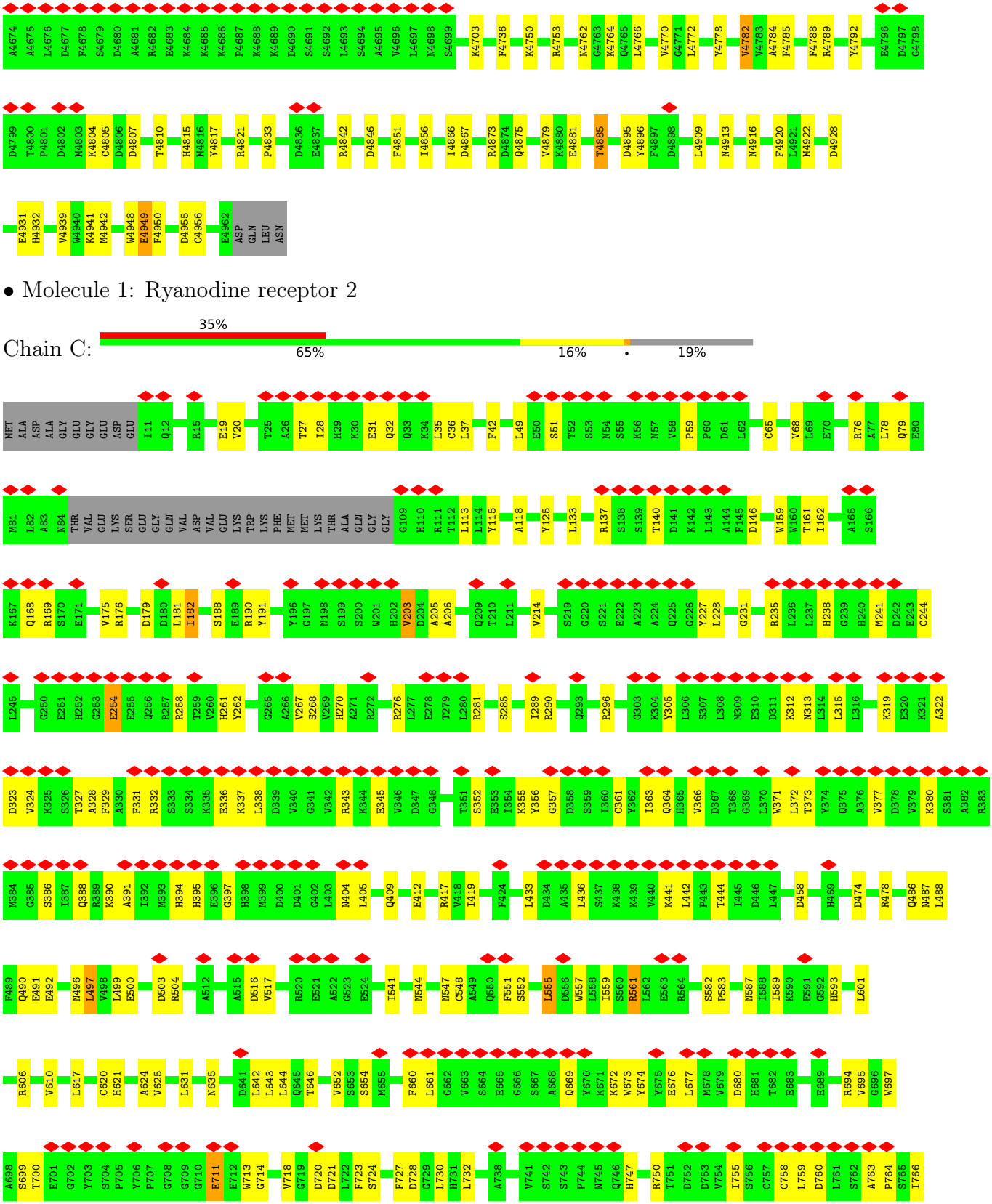
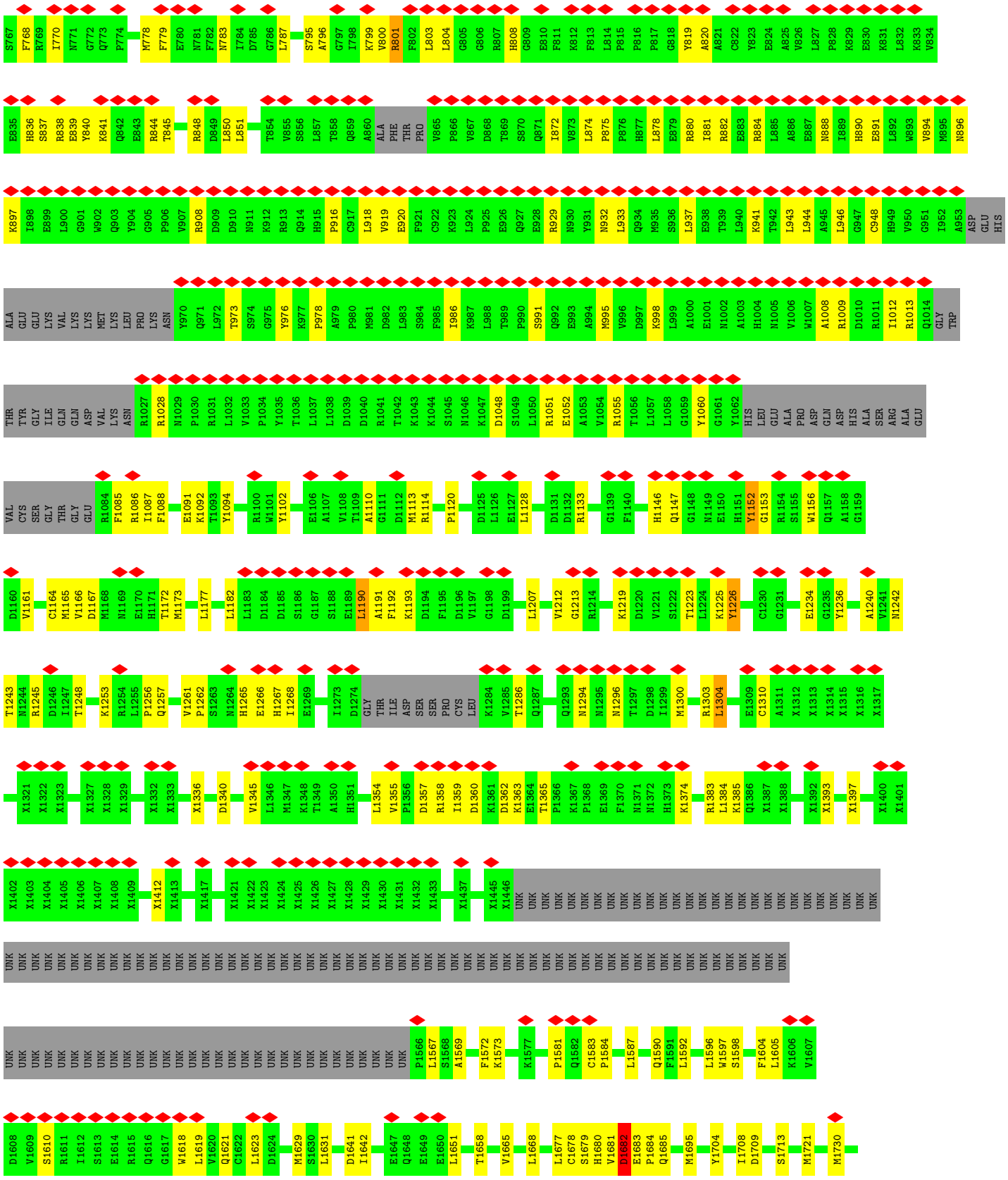


• Molecule 1: Ryanodine receptor 2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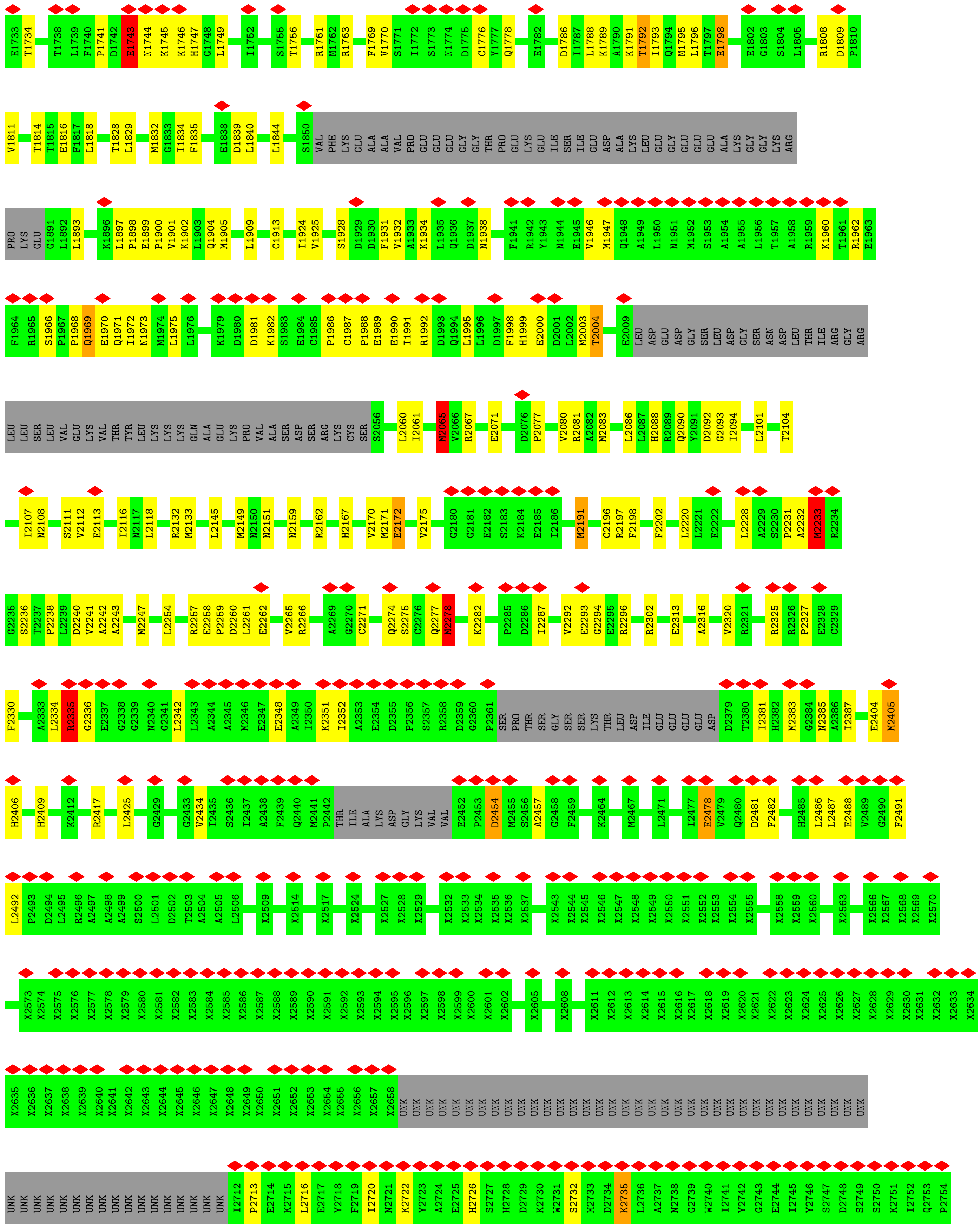
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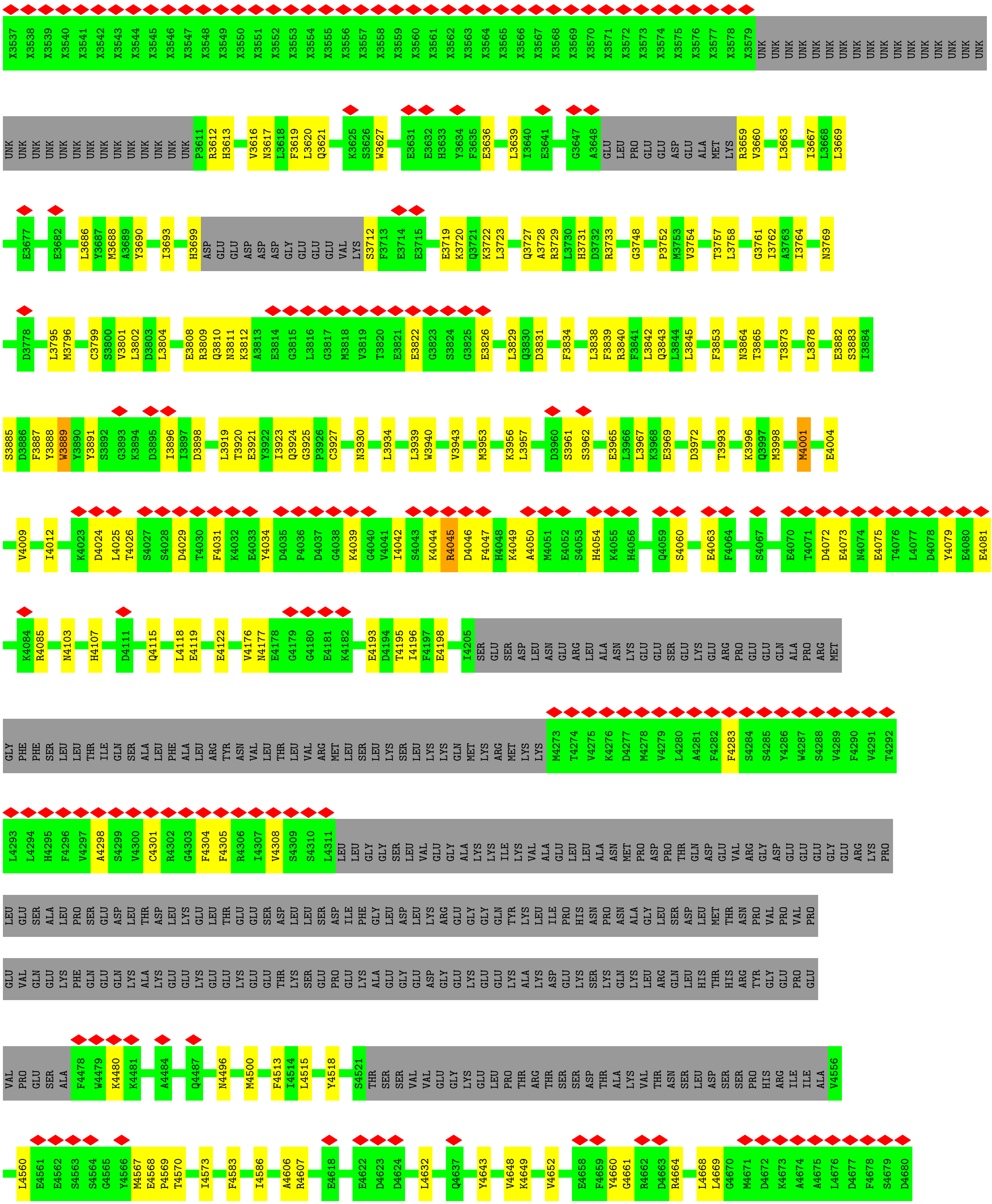
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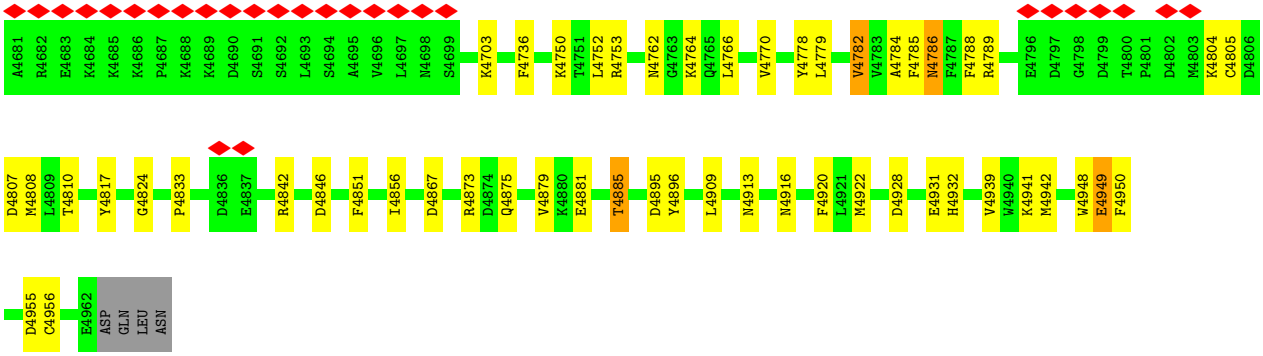

• Molecule 1: Ryanodine receptor 2

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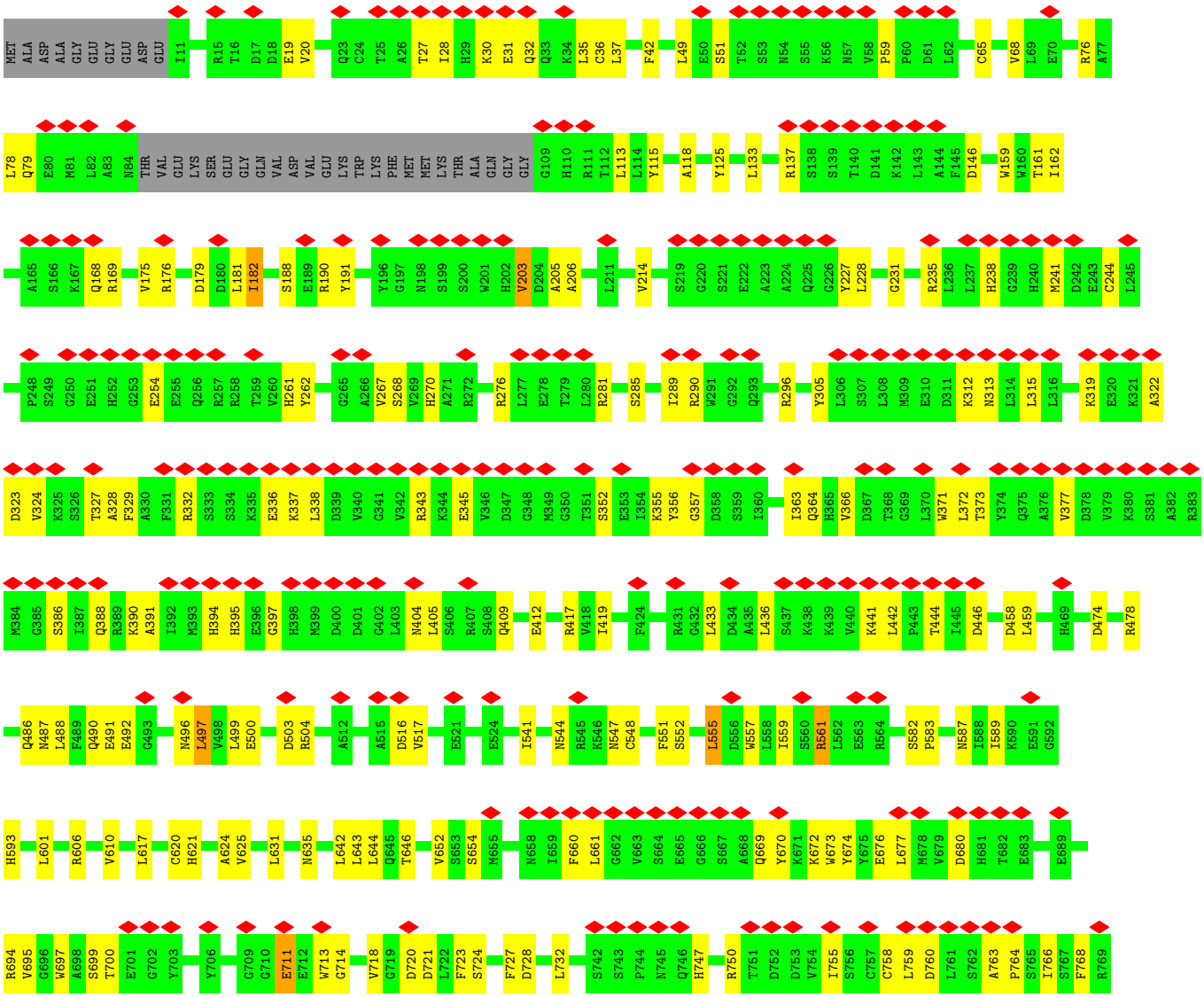

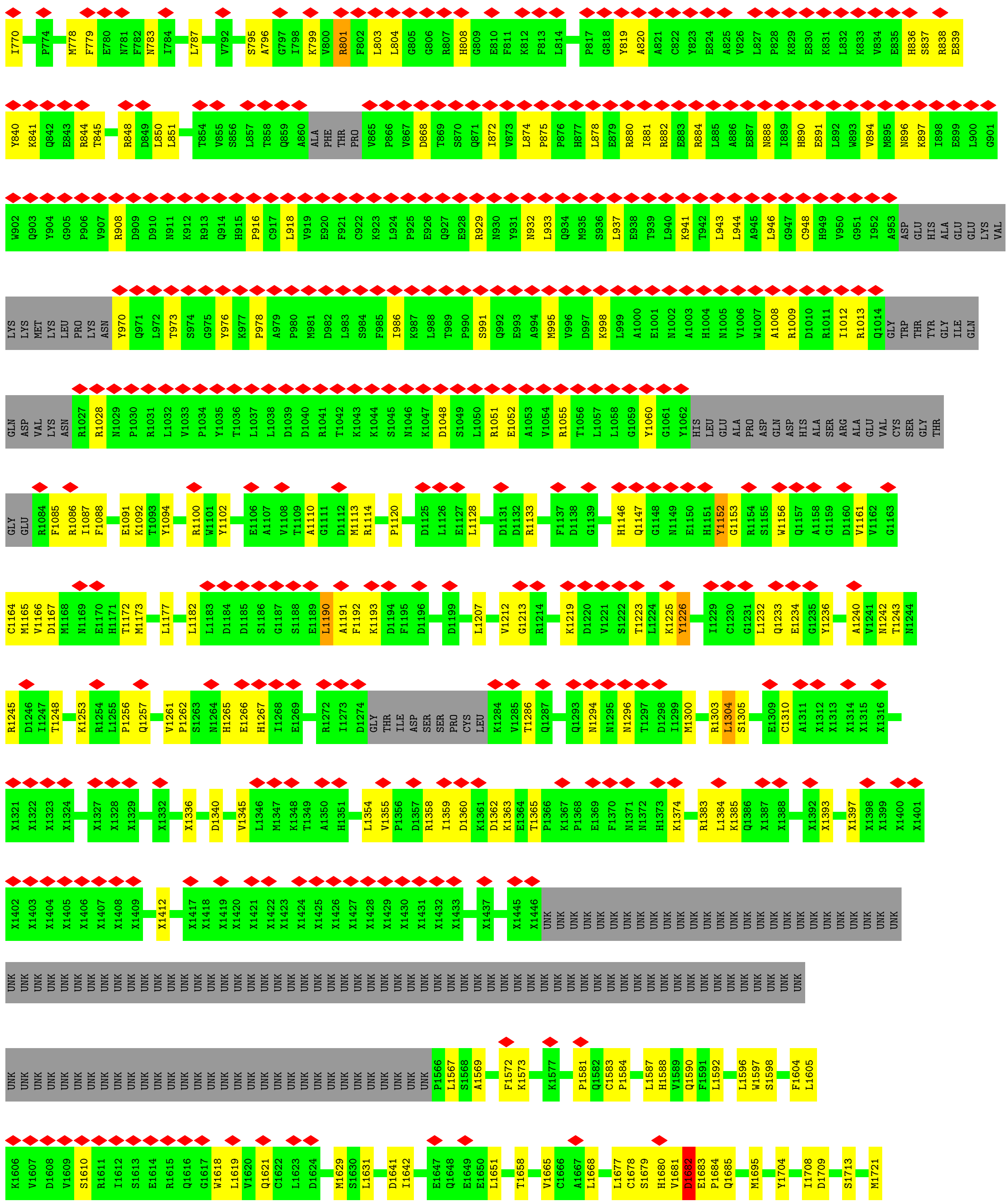
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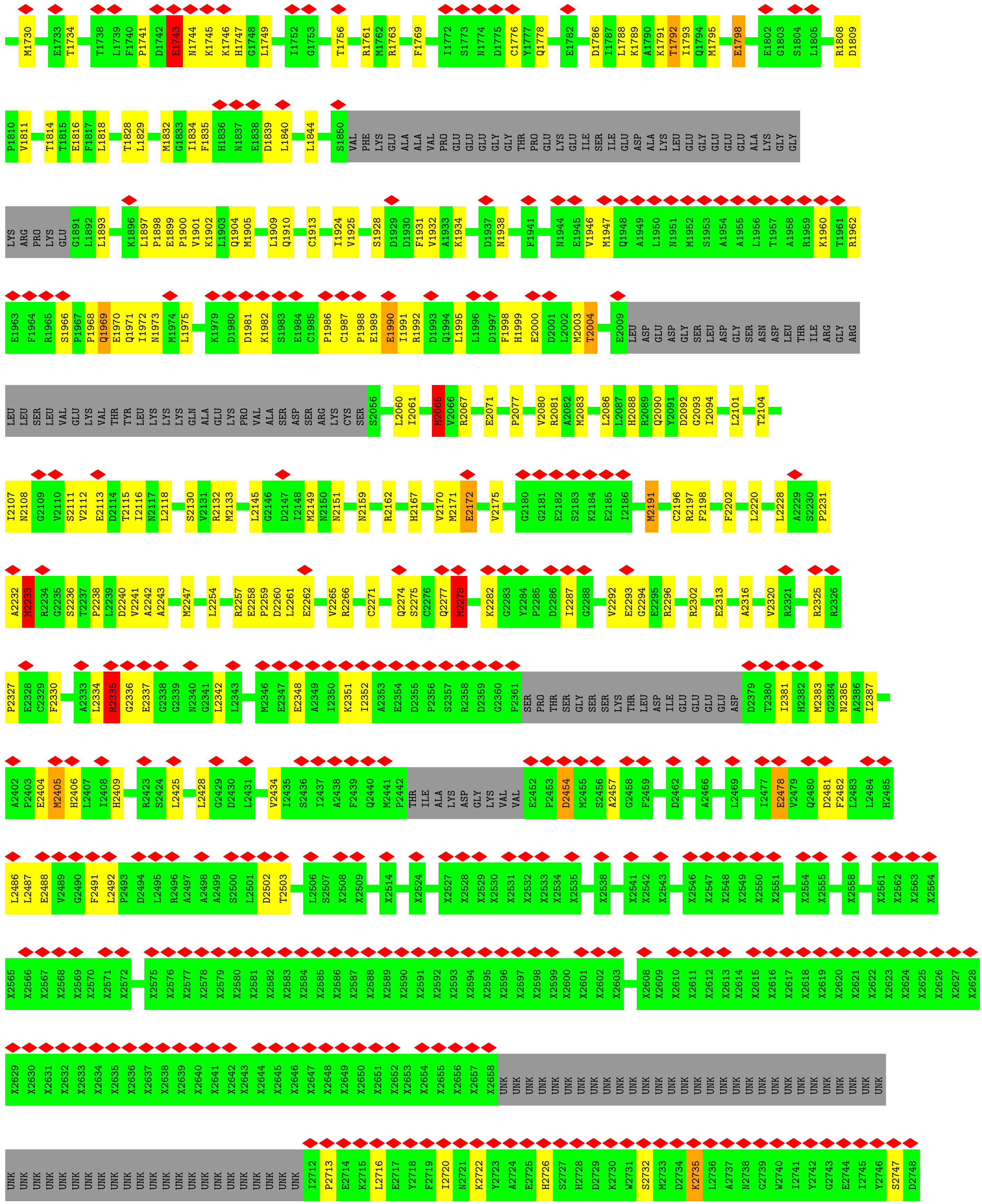
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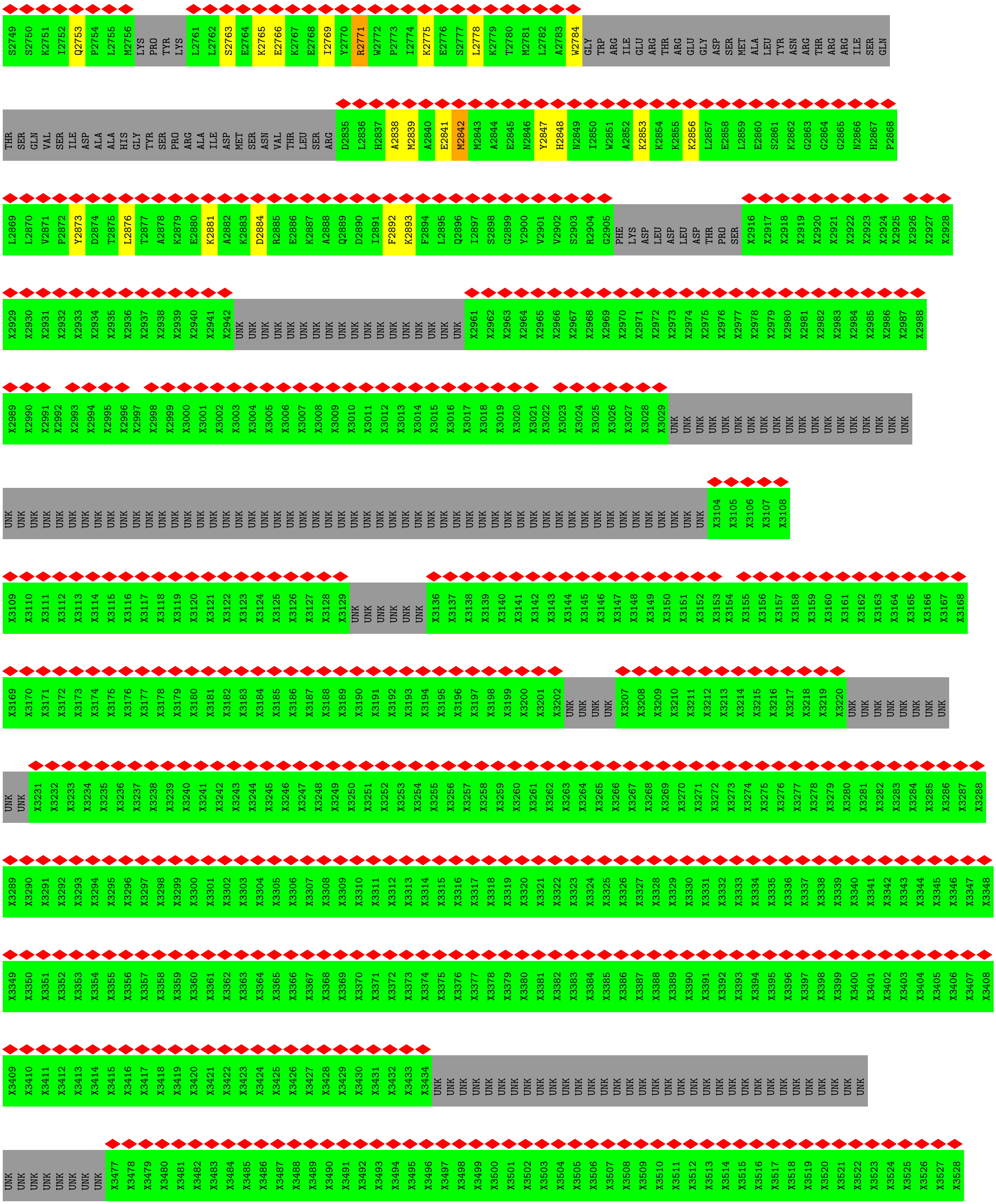
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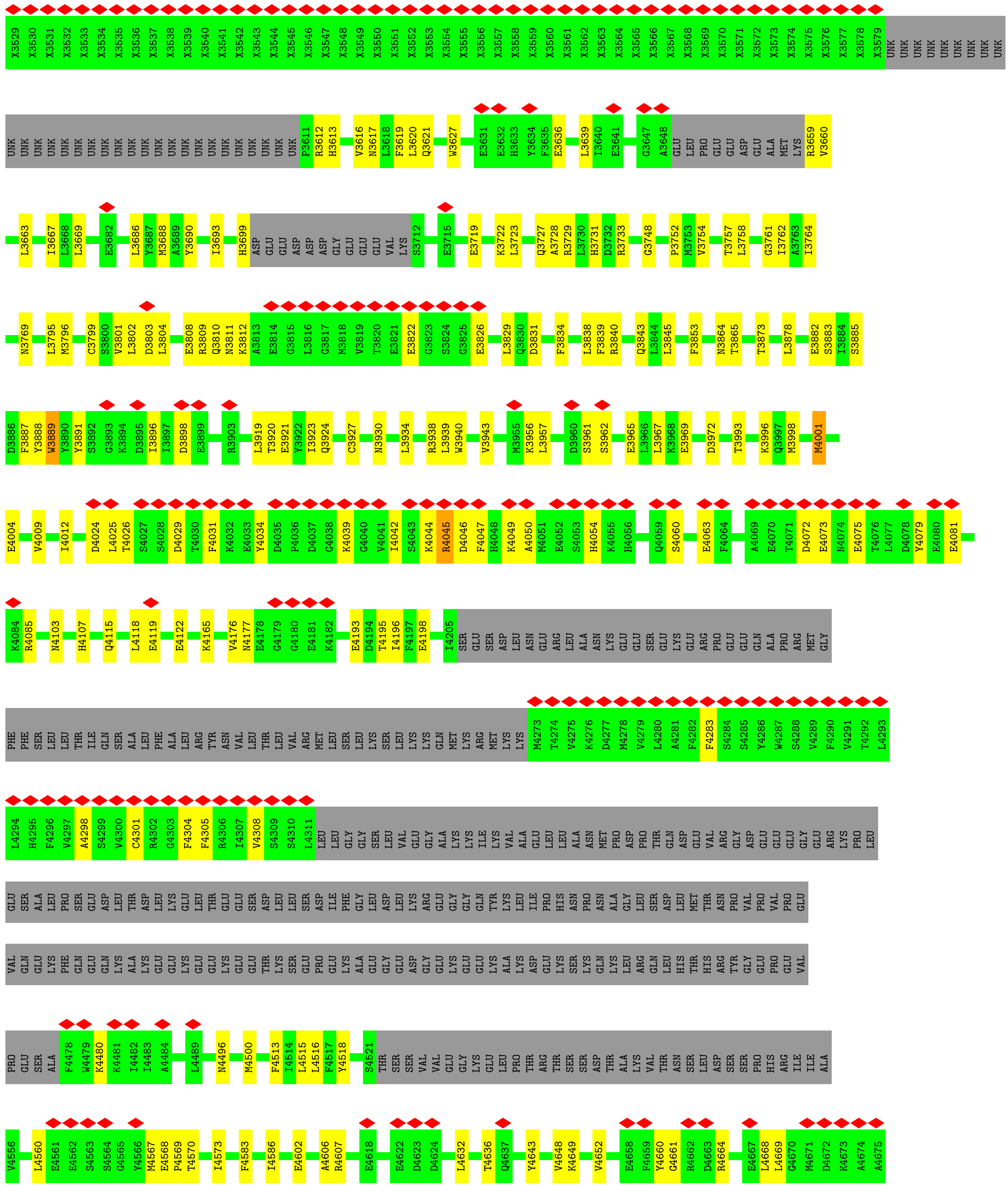
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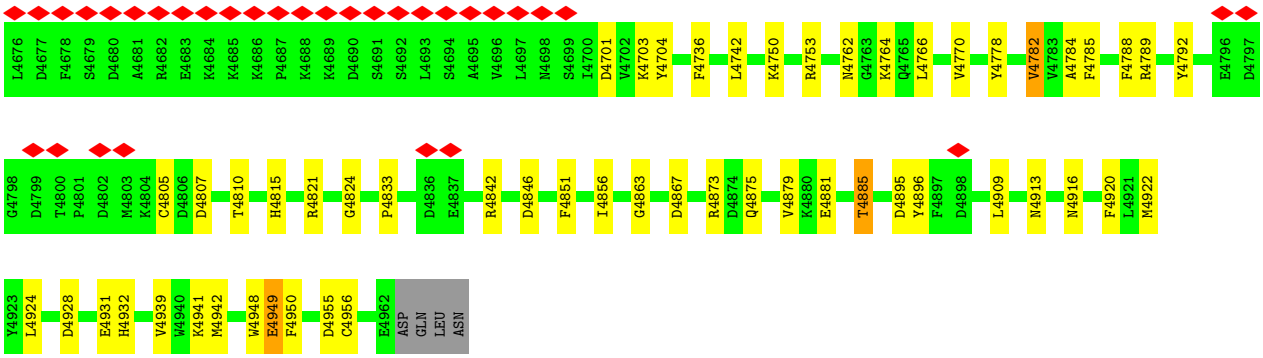
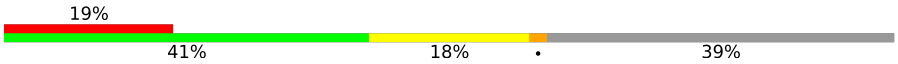
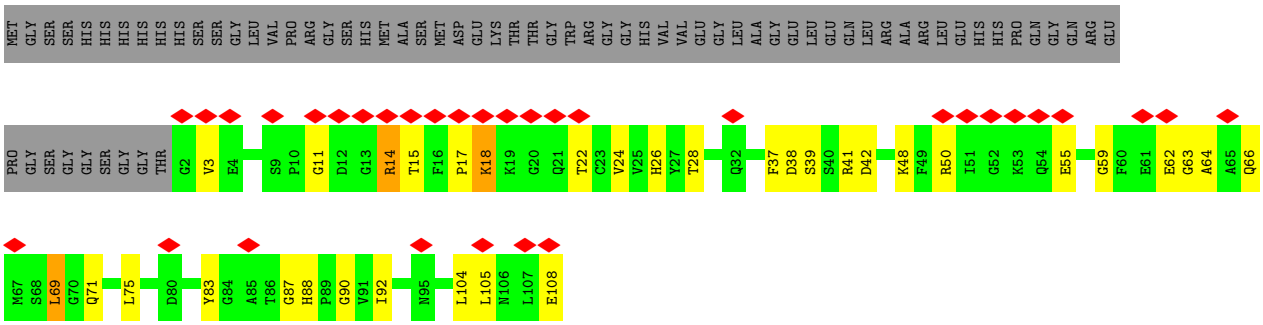
PRO GLU SER ALA F4478 W4479 K4480 K4481 I4482 I4483 A4484 L4489 N4496 M4500 F4513 I4514 L4515 L4516 F4517 Y4518 S4521 THR SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG THR SER SER ASP THR ALA LYS VAL THR ASN SER LEU ASP SER SER PRO HIS ARG ILE ILE ALA
V4556 L4560 E4561 E4562 S4563 S4564 G4565 Y4566 M4567 E4568 P4569 T4570 I4573 F4583 I4586 E4602 A4606 R4607 E4618 E4622 D4623 D4624 L4632 T4636 Q4637 Y4643 V4648 K4649 V4652 E4658 F4659 Y4660 G4661 R4662 D4663 R4664 E4667 L4668 L4669 G4670 M4671 D4672 K4673 A4674 A4675



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

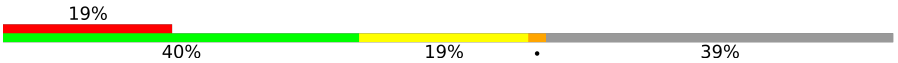
Chain G:

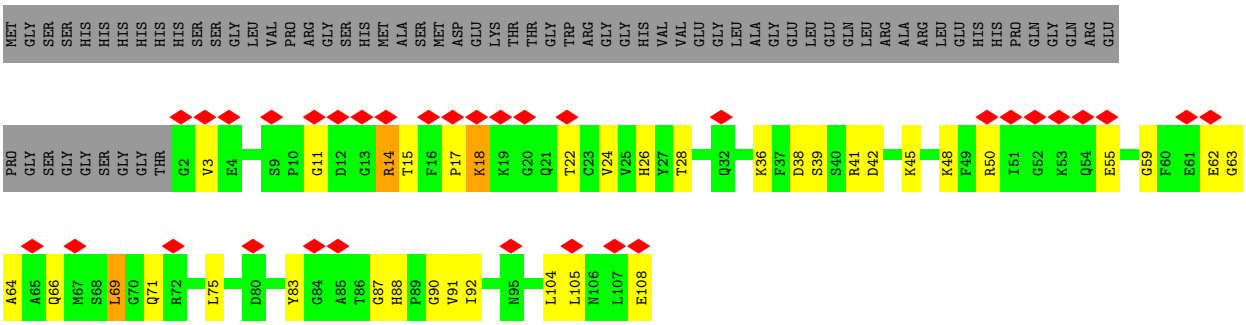




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

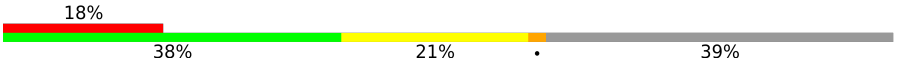
Chain H:

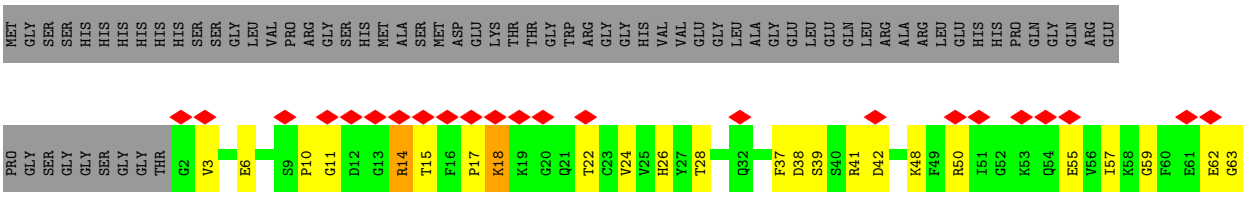


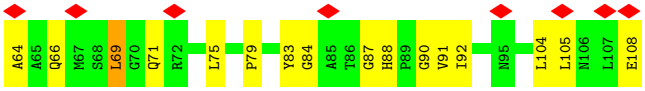


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

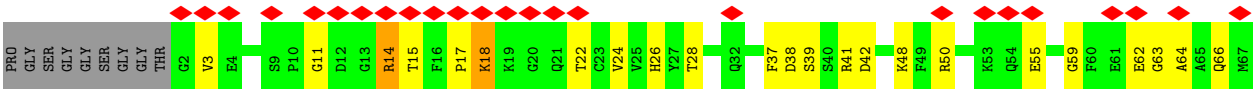
Chain I:

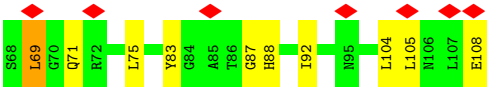






- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68394	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 ($e^-/Å^2$)	60	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	0.192	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.328, 1.328, 1.328	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0/26891	0.52	9/36312 (0.0%)
1	B	0.26	0/26891	0.52	9/36312 (0.0%)
1	C	0.26	0/26891	0.52	9/36312 (0.0%)
1	D	0.26	0/26891	0.52	9/36312 (0.0%)
2	G	0.27	0/835	0.57	0/1123
2	H	0.27	0/835	0.57	0/1123
2	I	0.27	0/835	0.57	0/1123
2	J	0.27	0/835	0.57	0/1123
All	All	0.26	0/110904	0.52	36/149740 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2233	MET	CB-CG-SD	9.46	140.78	112.40
1	D	2233	MET	CB-CG-SD	9.46	140.78	112.40
1	C	2233	MET	CB-CG-SD	9.45	140.76	112.40
1	B	2233	MET	CB-CG-SD	9.45	140.75	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2233	MET	CA-CB-CG	9.14	128.83	113.30
1	A	2233	MET	CA-CB-CG	9.14	128.83	113.30
1	C	2233	MET	CA-CB-CG	9.13	128.82	113.30
1	D	2233	MET	CA-CB-CG	9.12	128.81	113.30
1	C	2478	GLU	CA-CB-CG	6.95	128.70	113.40
1	A	2478	GLU	CA-CB-CG	6.92	128.63	113.40
1	B	2478	GLU	CA-CB-CG	6.92	128.63	113.40
1	D	2478	GLU	CA-CB-CG	6.91	128.61	113.40
1	A	1743	GLU	CA-CB-CG	6.89	128.56	113.40
1	D	1743	GLU	CA-CB-CG	6.87	128.51	113.40
1	C	1743	GLU	CA-CB-CG	6.86	128.50	113.40
1	B	1743	GLU	CA-CB-CG	6.85	128.48	113.40
1	D	1743	GLU	CB-CA-C	5.64	121.69	110.40
1	B	1743	GLU	CB-CA-C	5.64	121.68	110.40
1	C	1743	GLU	CB-CA-C	5.64	121.67	110.40
1	A	1743	GLU	CB-CA-C	5.61	121.62	110.40
1	D	1682	ASP	N-CA-CB	5.26	120.07	110.60
1	B	1682	ASP	N-CA-CB	5.25	120.05	110.60
1	C	1682	ASP	N-CA-CB	5.25	120.05	110.60
1	A	1682	ASP	N-CA-CB	5.24	120.03	110.60
1	A	2278	MET	CB-CG-SD	5.17	127.92	112.40
1	C	2278	MET	CB-CG-SD	5.17	127.91	112.40
1	D	2278	MET	CB-CG-SD	5.15	127.86	112.40
1	B	2278	MET	CB-CG-SD	5.14	127.83	112.40
1	D	2065	MET	CB-CG-SD	5.07	127.60	112.40
1	B	2065	MET	CB-CG-SD	5.06	127.59	112.40
1	A	2065	MET	CB-CG-SD	5.06	127.58	112.40
1	C	2065	MET	CB-CG-SD	5.06	127.58	112.40
1	D	2335	ARG	CB-CA-C	5.04	120.48	110.40
1	A	2335	ARG	CB-CA-C	5.04	120.47	110.40
1	C	2335	ARG	CB-CA-C	5.03	120.46	110.40
1	B	2335	ARG	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2172	GLU	Peptide
1	B	2172	GLU	Peptide
1	C	2172	GLU	Peptide
1	D	2172	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30067	0	26708	587	0
1	B	30067	0	26708	594	0
1	C	30067	0	26708	595	0
1	D	30067	0	26708	584	0
2	G	819	0	821	27	0
2	H	819	0	821	29	0
2	I	819	0	821	35	0
2	J	819	0	821	26	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	123548	0	110116	2409	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 10.

All (2409) 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:B:3845:LEU:HB3	1:B:3853:PHE:HE2	1.40	0.87
1:C:3845:LEU:HB3	1:C:3853:PHE:HE2	1.40	0.87
1:A:3845:LEU:HB3	1:A:3853:PHE:HE2	1.40	0.86
1:D:3845:LEU:HB3	1:D:3853:PHE:HE2	1.40	0.85
1:D:2327:PRO:HB2	1:D:2335:ARG:HD3	1.60	0.84
1:C:2327:PRO:HB2	1:C:2335:ARG:HD3	1.60	0.84
1:A:2327:PRO:HB2	1:A:2335:ARG:HD3	1.60	0.83
1:B:2327:PRO:HB2	1:B:2335:ARG:HD3	1.60	0.83
1:C:1913:CYS:SG	1:C:2090:GLN:NE2	2.53	0.82
2:I:26:HIS:HB2	2:I:105:LEU:HD11	1.61	0.82
1:A:1913:CYS:SG	1:A:2090:GLN:NE2	2.53	0.82
1:D:1913:CYS:SG	1:D:2090:GLN:NE2	2.53	0.81
2:J:26:HIS:HB2	2:J:105:LEU:HD11	1.61	0.81
1:D:1682:ASP:HB3	1:D:1684:PRO:HD2	1.62	0.81
2:G:26:HIS:HB2	2:G:105:LEU:HD11	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:HIS:HB2	2:H:105:LEU:HD11	1.61	0.80
1:C:1682:ASP:HB3	1:C:1684:PRO:HD2	1.62	0.80
1:B:1913:CYS:SG	1:B:2090:GLN:NE2	2.53	0.80
1:A:1682:ASP:HB3	1:A:1684:PRO:HD2	1.62	0.80
1:B:1682:ASP:HB3	1:B:1684:PRO:HD2	1.62	0.80
1:C:4833:PRO:HB3	1:C:4842:ARG:HD3	1.64	0.80
1:D:4833:PRO:HB3	1:D:4842:ARG:HD3	1.64	0.79
1:B:4833:PRO:HB3	1:B:4842:ARG:HD3	1.64	0.78
1:B:4042:ILE:HG22	1:B:4044:LYS:H	1.49	0.78
1:D:1262:PRO:HG2	1:D:1265:HIS:HB2	1.66	0.78
1:A:4833:PRO:HB3	1:A:4842:ARG:HD3	1.64	0.78
1:D:4042:ILE:HG22	1:D:4044:LYS:H	1.49	0.78
1:B:1233:GLN:HG2	1:C:3493:UNK:HA	1.64	0.77
1:B:1684:PRO:HD3	2:H:42:ASP:HB3	1.67	0.77
1:A:1743:GLU:OE1	1:A:1744:ASN:N	2.18	0.77
1:B:1262:PRO:HG2	1:B:1265:HIS:HB2	1.66	0.77
1:A:1262:PRO:HG2	1:A:1265:HIS:HB2	1.66	0.77
1:A:3889:TRP:HE3	1:D:76:ARG:HH12	1.32	0.77
1:A:3493:UNK:HA	1:D:1233:GLN:HG2	1.67	0.77
1:A:4042:ILE:HG22	1:A:4044:LYS:H	1.49	0.77
1:C:4042:ILE:HG22	1:C:4044:LYS:H	1.49	0.77
1:C:1743:GLU:OE1	1:C:1744:ASN:N	2.18	0.76
2:I:69:LEU:HA	2:I:104:LEU:HD22	1.67	0.76
1:D:1743:GLU:OE1	1:D:1744:ASN:N	2.18	0.76
1:B:4867:ASP:OD1	1:C:4873:ARG:NH1	2.18	0.76
2:G:69:LEU:HA	2:G:104:LEU:HD22	1.67	0.76
1:C:1262:PRO:HG2	1:C:1265:HIS:HB2	1.66	0.76
1:A:76:ARG:NH2	1:B:3889:TRP:O	2.18	0.76
1:B:1743:GLU:OE1	1:B:1744:ASN:N	2.18	0.75
2:H:69:LEU:HA	2:H:104:LEU:HD22	1.67	0.75
1:B:162:ILE:HD11	1:B:181:LEU:HD22	1.69	0.75
2:J:69:LEU:HA	2:J:104:LEU:HD22	1.67	0.74
1:A:162:ILE:HD11	1:A:181:LEU:HD22	1.69	0.74
1:A:4824:GLY:O	1:B:4821:ARG:NH1	2.20	0.74
1:D:486:GLN:HB3	1:D:544:ASN:HD21	1.52	0.74
1:A:486:GLN:HB3	1:A:544:ASN:HD21	1.52	0.74
1:C:162:ILE:HD11	1:C:181:LEU:HD22	1.69	0.74
1:A:1681:VAL:HG23	1:A:1682:ASP:H	1.53	0.73
1:B:1681:VAL:HG23	1:B:1682:ASP:H	1.53	0.73
1:B:3934:LEU:HD12	1:B:3939:LEU:HD22	1.70	0.73
1:D:3934:LEU:HD12	1:D:3939:LEU:HD22	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:GLN:HB3	1:C:544:ASN:HD21	1.52	0.73
1:B:76:ARG:HH12	1:C:3889:TRP:HE3	1.37	0.73
1:C:3934:LEU:HD12	1:C:3939:LEU:HD22	1.71	0.73
1:D:162:ILE:HD11	1:D:181:LEU:HD22	1.69	0.73
1:A:3934:LEU:HD12	1:A:3939:LEU:HD22	1.70	0.72
1:A:4046:ASP:HA	1:A:4049:LYS:HG2	1.72	0.72
1:B:486:GLN:HB3	1:B:544:ASN:HD21	1.52	0.72
1:B:4046:ASP:HA	1:B:4049:LYS:HG2	1.72	0.72
1:A:1741:PRO:HB3	1:A:1746:LYS:HE3	1.72	0.72
1:C:1681:VAL:HG23	1:C:1682:ASP:H	1.53	0.72
1:D:1681:VAL:HG23	1:D:1682:ASP:H	1.53	0.72
1:A:1286:THR:HG1	1:A:1583:CYS:HG	1.35	0.72
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.72	0.72
1:A:76:ARG:NH1	1:B:3889:TRP:HB3	2.03	0.72
1:D:1741:PRO:HB3	1:D:1746:LYS:HE3	1.71	0.72
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.72	0.72
1:D:4046:ASP:HA	1:D:4049:LYS:HG2	1.72	0.72
1:C:4046:ASP:HA	1:C:4049:LYS:HG2	1.72	0.71
1:A:1177:LEU:HB2	1:A:1182:LEU:HD11	1.72	0.71
1:B:1177:LEU:HB2	1:B:1182:LEU:HD11	1.72	0.71
1:A:3889:TRP:O	1:D:76:ARG:NH2	2.24	0.70
1:A:4863:GLY:HA2	1:B:4866:ILE:HG12	1.72	0.70
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.72	0.70
1:B:1741:PRO:HB3	1:B:1746:LYS:HE3	1.71	0.70
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.72	0.70
1:C:1741:PRO:HB3	1:C:1746:LYS:HE3	1.71	0.70
1:D:1286:THR:HG1	1:D:1583:CYS:HG	1.38	0.70
1:B:1791:LYS:O	1:B:1795:MET:HG3	1.92	0.70
1:C:1177:LEU:HB2	1:C:1182:LEU:HD11	1.72	0.70
1:D:1177:LEU:HB2	1:D:1182:LEU:HD11	1.72	0.69
1:A:4867:ASP:OD1	1:B:4873:ARG:NH1	2.25	0.69
1:C:1791:LYS:O	1:C:1795:MET:HG3	1.92	0.69
1:C:2258:GLU:HG2	1:C:2261:LEU:HB2	1.74	0.69
1:D:4480:LYS:H	1:D:4480:LYS:HD2	1.57	0.69
1:A:1791:LYS:O	1:A:1795:MET:HG3	1.92	0.69
1:A:973:THR:OG1	1:A:976:TYR:O	2.10	0.69
1:A:4480:LYS:H	1:A:4480:LYS:HD2	1.58	0.69
1:B:4480:LYS:HD2	1:B:4480:LYS:H	1.58	0.69
1:A:3889:TRP:HE3	1:D:76:ARG:NH1	1.91	0.69
1:B:1573:LYS:HE2	1:B:1584:PRO:HG2	1.75	0.69
1:A:2258:GLU:HG2	1:A:2261:LEU:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HH12	1:B:3889:TRP:HE3	1.41	0.68
1:A:1573:LYS:HE2	1:A:1584:PRO:HG2	1.75	0.68
1:D:660:PHE:HB3	1:D:787:LEU:HD23	1.76	0.68
1:D:1791:LYS:O	1:D:1795:MET:HG3	1.92	0.68
1:D:2275:SER:OG	1:D:2287:ILE:O	2.12	0.68
1:D:2258:GLU:HG2	1:D:2261:LEU:HB2	1.74	0.68
1:B:844:ARG:HE	1:B:845:THR:H	1.40	0.68
1:B:189:GLU:OE1	1:C:2417:ARG:HD3	1.93	0.68
1:A:660:PHE:HB3	1:A:787:LEU:HD23	1.76	0.68
1:C:373:THR:HG22	1:C:397:GLY:HA2	1.76	0.68
1:D:1573:LYS:HE2	1:D:1584:PRO:HG2	1.75	0.68
1:A:844:ARG:HE	1:A:845:THR:H	1.40	0.67
1:B:2258:GLU:HG2	1:B:2261:LEU:HB2	1.74	0.67
1:C:76:ARG:HH12	1:D:3889:TRP:HE3	1.42	0.67
1:C:660:PHE:HB3	1:C:787:LEU:HD23	1.76	0.67
1:B:76:ARG:NH1	1:C:3889:TRP:HE3	1.92	0.67
1:C:1190:LEU:HD22	1:C:1193:LYS:HE3	1.76	0.67
1:C:4480:LYS:H	1:C:4480:LYS:HD2	1.57	0.67
1:D:1190:LEU:HD22	1:D:1193:LYS:HE3	1.76	0.67
1:A:2275:SER:OG	1:A:2287:ILE:O	2.12	0.67
1:C:844:ARG:HE	1:C:845:THR:H	1.40	0.67
1:C:1573:LYS:HE2	1:C:1584:PRO:HG2	1.75	0.67
1:A:1932:VAL:HG21	1:A:3616:VAL:HA	1.76	0.67
1:B:373:THR:HG22	1:B:397:GLY:HA2	1.76	0.67
1:D:373:THR:HG22	1:D:397:GLY:HA2	1.76	0.67
1:B:660:PHE:HB3	1:B:787:LEU:HD23	1.76	0.66
1:B:2275:SER:OG	1:B:2287:ILE:O	2.12	0.66
1:D:973:THR:OG1	1:D:976:TYR:O	2.10	0.66
1:A:373:THR:HG22	1:A:397:GLY:HA2	1.76	0.66
1:D:844:ARG:HE	1:D:845:THR:H	1.40	0.66
1:D:1932:VAL:HG21	1:D:3616:VAL:HA	1.76	0.66
1:A:2107:ILE:HG13	1:A:2108:ASN:H	1.60	0.66
1:B:76:ARG:NH2	1:C:3889:TRP:O	2.28	0.66
1:C:1286:THR:HG1	1:C:1583:CYS:HG	1.42	0.66
1:C:2275:SER:OG	1:C:2287:ILE:O	2.12	0.66
2:H:22:THR:HG22	2:H:108:GLU:HB3	1.78	0.66
1:A:1610:SER:HB3	1:A:1619:LEU:HB3	1.78	0.66
2:G:22:THR:HG22	2:G:108:GLU:HB3	1.78	0.66
1:C:2000:GLU:O	1:C:2004:THR:HG22	1.95	0.66
1:A:1190:LEU:HD22	1:A:1193:LYS:HE3	1.76	0.66
1:B:973:THR:OG1	1:B:976:TYR:O	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1359:ILE:HG13	1:C:1360:ASP:H	1.61	0.66
1:D:2107:ILE:HG13	1:D:2108:ASN:H	1.60	0.66
1:B:1190:LEU:HD22	1:B:1193:LYS:HE3	1.76	0.65
1:D:2092:ASP:OD1	1:D:2093:GLY:N	2.30	0.65
1:A:2000:GLU:O	1:A:2004:THR:HG22	1.95	0.65
1:C:844:ARG:O	1:C:848:ARG:NH2	2.29	0.65
1:D:3639:LEU:HD23	1:D:3693:ILE:HG21	1.79	0.65
1:B:1932:VAL:HG21	1:B:3616:VAL:HA	1.76	0.65
1:B:1989:GLU:HA	1:B:1992:ARG:HD3	1.79	0.65
1:C:1345:VAL:HG21	1:C:1374:LYS:HE2	1.78	0.65
1:C:1610:SER:HB3	1:C:1619:LEU:HB3	1.78	0.65
1:C:3639:LEU:HD23	1:C:3693:ILE:HG21	1.79	0.65
1:D:1610:SER:HB3	1:D:1619:LEU:HB3	1.78	0.65
1:B:1610:SER:HB3	1:B:1619:LEU:HB3	1.78	0.65
1:B:3639:LEU:HD23	1:B:3693:ILE:HG21	1.79	0.65
1:C:290:ARG:HH12	1:C:343:ARG:HG2	1.61	0.65
1:D:844:ARG:O	1:D:848:ARG:NH2	2.29	0.65
1:A:838:ARG:H	1:A:841:LYS:HZ1	1.44	0.65
1:D:290:ARG:HH12	1:D:343:ARG:HG2	1.61	0.65
1:D:1345:VAL:HG21	1:D:1374:LYS:HE2	1.78	0.65
1:B:1359:ILE:HG13	1:B:1360:ASP:H	1.61	0.65
1:B:2000:GLU:O	1:B:2004:THR:HG22	1.95	0.65
1:B:2092:ASP:OD1	1:B:2093:GLY:N	2.30	0.65
1:B:2107:ILE:HG13	1:B:2108:ASN:H	1.60	0.65
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.30	0.65
1:C:1932:VAL:HG21	1:C:3616:VAL:HA	1.76	0.65
1:D:620:CYS:SG	1:D:621:HIS:N	2.70	0.65
1:D:2784:TRP:HE3	1:D:2842:MET:HE2	1.62	0.65
1:A:620:CYS:SG	1:A:621:HIS:N	2.70	0.65
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.30	0.65
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.30	0.65
1:B:2316:ALA:O	1:B:2320:VAL:HG23	1.97	0.65
1:C:2092:ASP:OD1	1:C:2093:GLY:N	2.30	0.65
2:I:22:THR:HG22	2:I:108:GLU:HB3	1.78	0.65
1:D:2000:GLU:O	1:D:2004:THR:HG22	1.95	0.65
1:A:3639:LEU:HD23	1:A:3693:ILE:HG21	1.79	0.65
1:C:544:ASN:ND2	1:C:547:ASN:OD1	2.30	0.65
1:D:3831:ASP:HB3	1:D:3834:PHE:HB3	1.78	0.65
1:A:844:ARG:O	1:A:848:ARG:NH2	2.29	0.64
1:A:2316:ALA:O	1:A:2320:VAL:HG23	1.97	0.64
1:B:191:TYR:HE2	1:C:2325:ARG:CZ	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1999:HIS:CG	1:B:3627:TRP:HE1	2.16	0.64
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.30	0.64
1:D:2316:ALA:O	1:D:2320:VAL:HG23	1.97	0.64
1:A:2092:ASP:OD1	1:A:2093:GLY:N	2.30	0.64
1:B:544:ASN:ND2	1:B:547:ASN:OD1	2.30	0.64
1:A:290:ARG:HH12	1:A:343:ARG:HG2	1.61	0.64
1:A:674:TYR:HD2	1:A:758:CYS:HG	1.44	0.64
1:A:1989:GLU:HA	1:A:1992:ARG:HD3	1.79	0.64
1:A:1999:HIS:CG	1:A:3627:TRP:HE1	2.16	0.64
1:C:1999:HIS:CG	1:C:3627:TRP:HE1	2.16	0.64
1:C:2107:ILE:HG13	1:C:2108:ASN:H	1.60	0.64
1:B:357:GLY:O	1:B:404:ASN:ND2	2.28	0.64
1:B:844:ARG:O	1:B:848:ARG:NH2	2.29	0.64
1:C:620:CYS:SG	1:C:621:HIS:N	2.70	0.64
1:C:1989:GLU:HA	1:C:1992:ARG:HD3	1.79	0.64
1:D:1999:HIS:CG	1:D:3627:TRP:HE1	2.16	0.64
1:A:3831:ASP:HB3	1:A:3834:PHE:HB3	1.78	0.64
1:B:290:ARG:HH12	1:B:343:ARG:HG2	1.61	0.64
1:B:4942:MET:HE2	1:B:4950:PHE:HB3	1.80	0.64
1:B:1345:VAL:HG21	1:B:1374:LYS:HE2	1.78	0.64
1:B:2784:TRP:HE3	1:B:2842:MET:HE2	1.63	0.64
1:C:76:ARG:NH2	1:D:3889:TRP:O	2.31	0.64
1:A:544:ASN:ND2	1:A:547:ASN:OD1	2.30	0.64
1:A:1359:ILE:HG13	1:A:1360:ASP:H	1.61	0.64
1:A:4821:ARG:NH1	1:D:4824:GLY:O	2.30	0.64
1:B:4570:THR:HA	1:B:4573:ILE:HG12	1.79	0.64
1:D:544:ASN:ND2	1:D:547:ASN:OD1	2.30	0.64
1:D:1359:ILE:HG13	1:D:1360:ASP:H	1.61	0.64
2:J:22:THR:HG22	2:J:108:GLU:HB3	1.78	0.64
1:B:3845:LEU:HB3	1:B:3853:PHE:CE2	2.30	0.63
1:C:3831:ASP:HB3	1:C:3834:PHE:HB3	1.78	0.63
1:C:4570:THR:HA	1:C:4573:ILE:HG12	1.79	0.63
1:A:4570:THR:HA	1:A:4573:ILE:HG12	1.79	0.63
1:B:620:CYS:SG	1:B:621:HIS:N	2.70	0.63
1:D:419:ILE:HG21	1:D:492:GLU:HG3	1.80	0.63
1:D:1009:ARG:O	1:D:1013:ARG:NH1	2.32	0.63
1:D:1989:GLU:HA	1:D:1992:ARG:HD3	1.79	0.63
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.80	0.63
1:C:1009:ARG:O	1:C:1013:ARG:NH1	2.32	0.63
1:C:2316:ALA:O	1:C:2320:VAL:HG23	1.97	0.63
1:A:1345:VAL:HG21	1:A:1374:LYS:HE2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ILE:HG21	1:B:492:GLU:HG3	1.80	0.63
1:B:3831:ASP:HB3	1:B:3834:PHE:HB3	1.78	0.63
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.80	0.63
1:C:973:THR:OG1	1:C:976:TYR:O	2.10	0.63
1:D:4570:THR:HA	1:D:4573:ILE:HG12	1.79	0.63
1:A:4632:LEU:HB2	1:A:4703:LYS:HE2	1.81	0.63
1:D:1102:TYR:HB2	1:D:1165:MET:HG2	1.81	0.63
1:A:182:ILE:HD11	1:A:191:TYR:CE1	2.34	0.62
1:C:4632:LEU:HB2	1:C:4703:LYS:HE2	1.82	0.62
1:D:182:ILE:HD11	1:D:191:TYR:CE1	2.34	0.62
1:D:4568:GLU:HG2	1:D:4569:PRO:HD3	1.81	0.62
1:B:2838:ALA:O	1:B:2841:GLU:HG3	2.00	0.62
1:C:880:ARG:HG3	1:C:881:ILE:HD12	1.81	0.62
1:A:1102:TYR:HB2	1:A:1165:MET:HG2	1.81	0.62
1:B:2067:ARG:O	1:B:2071:GLU:HG2	1.99	0.62
1:C:419:ILE:HG21	1:C:492:GLU:HG3	1.80	0.62
1:C:2067:ARG:O	1:C:2071:GLU:HG2	2.00	0.62
1:D:305:TYR:HE1	1:D:319:LYS:HG2	1.65	0.62
1:D:880:ARG:HG3	1:D:881:ILE:HD12	1.81	0.62
1:A:419:ILE:HG21	1:A:492:GLU:HG3	1.80	0.62
1:A:4568:GLU:HG2	1:A:4569:PRO:HD3	1.81	0.62
1:B:182:ILE:HD11	1:B:191:TYR:CE1	2.34	0.62
1:B:2232:ALA:HB3	1:B:2233:MET:HE2	1.80	0.62
1:D:355:LYS:HE3	1:D:356:TYR:H	1.65	0.62
1:D:1359:ILE:HG12	1:D:1363:LYS:HD2	1.82	0.62
1:D:4632:LEU:HB2	1:D:4703:LYS:HE2	1.81	0.62
1:A:490:GLN:HB2	1:A:547:ASN:HD21	1.65	0.62
1:B:1009:ARG:O	1:B:1013:ARG:NH1	2.31	0.62
1:D:2838:ALA:O	1:D:2841:GLU:HG3	2.00	0.62
1:A:3993:THR:HA	1:A:3996:LYS:HE2	1.81	0.62
1:C:182:ILE:HD11	1:C:191:TYR:CE1	2.34	0.62
1:A:1359:ILE:HG12	1:A:1363:LYS:HD2	1.82	0.62
1:A:3754:VAL:HA	1:A:3757:THR:HG22	1.82	0.62
1:B:908:ARG:HG2	1:B:916:PRO:HG3	1.82	0.62
1:B:4632:LEU:HB2	1:B:4703:LYS:HE2	1.81	0.62
1:C:908:ARG:HG2	1:C:916:PRO:HG3	1.82	0.62
1:C:1359:ILE:HG12	1:C:1363:LYS:HD2	1.82	0.62
1:C:3845:LEU:HB3	1:C:3853:PHE:CE2	2.30	0.62
1:D:1383:ARG:HH11	1:D:1385:LYS:HB2	1.64	0.62
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.81	0.62
1:C:2784:TRP:HE3	1:C:2842:MET:HE2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:SER:HB2	1:D:190:ARG:HH11	1.65	0.62
1:D:3754:VAL:HA	1:D:3757:THR:HG22	1.82	0.62
1:A:1383:ARG:HH11	1:A:1385:LYS:HB2	1.64	0.62
1:B:1359:ILE:HG12	1:B:1363:LYS:HD2	1.82	0.62
1:D:908:ARG:HG2	1:D:916:PRO:HG3	1.82	0.62
1:A:908:ARG:HG2	1:A:916:PRO:HG3	1.82	0.61
1:A:1009:ARG:O	1:A:1013:ARG:NH1	2.31	0.61
1:B:490:GLN:OE1	1:B:547:ASN:ND2	2.33	0.61
1:B:2348:GLU:O	1:B:2352:ILE:HG12	2.00	0.61
1:C:2838:ALA:O	1:C:2841:GLU:HG3	2.00	0.61
1:C:2348:GLU:O	1:C:2352:ILE:HG12	2.00	0.61
1:C:4942:MET:HE2	1:C:4950:PHE:HB3	1.81	0.61
1:A:305:TYR:HE1	1:A:319:LYS:HG2	1.65	0.61
1:A:355:LYS:HE3	1:A:356:TYR:H	1.65	0.61
1:C:305:TYR:HE1	1:C:319:LYS:HG2	1.65	0.61
1:C:1383:ARG:HH11	1:C:1385:LYS:HB2	1.64	0.61
1:C:3754:VAL:HA	1:C:3757:THR:HG22	1.82	0.61
1:D:3845:LEU:HB3	1:D:3853:PHE:CE2	2.30	0.61
1:A:2348:GLU:O	1:A:2352:ILE:HG12	2.00	0.61
1:B:880:ARG:HG3	1:B:881:ILE:HD12	1.81	0.61
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.33	0.61
1:B:3754:VAL:HA	1:B:3757:THR:HG22	1.82	0.61
1:C:355:LYS:HE3	1:C:356:TYR:H	1.65	0.61
1:C:3993:THR:HA	1:C:3996:LYS:HE2	1.81	0.61
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.80	0.61
1:A:3845:LEU:HB3	1:A:3853:PHE:CE2	2.30	0.61
1:B:490:GLN:HB2	1:B:547:ASN:HD21	1.65	0.61
1:C:674:TYR:HD2	1:C:758:CYS:HG	1.47	0.61
1:A:490:GLN:OE1	1:A:547:ASN:ND2	2.33	0.61
1:B:188:SER:HB2	1:B:190:ARG:HH11	1.65	0.61
1:B:3993:THR:HA	1:B:3996:LYS:HE2	1.81	0.61
1:B:4568:GLU:HG2	1:B:4569:PRO:HD3	1.81	0.61
1:C:188:SER:HB2	1:C:190:ARG:HH11	1.65	0.61
1:C:2159:ASN:OD1	1:C:2162:ARG:NH2	2.33	0.61
1:D:3993:THR:HA	1:D:3996:LYS:HE2	1.81	0.61
2:J:26:HIS:NE2	2:J:41:ARG:HG2	2.16	0.61
1:A:2838:ALA:O	1:A:2841:GLU:HG3	2.00	0.61
1:B:4949:GLU:OE1	1:B:4949:GLU:N	2.29	0.61
1:A:2067:ARG:O	1:A:2071:GLU:HG2	2.00	0.61
1:B:1383:ARG:HH11	1:B:1385:LYS:HB2	1.64	0.61
1:D:2335:ARG:HE	1:D:2336:GLY:N	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2233:MET:N	1:A:2233:MET:HE2	2.16	0.61
1:B:305:TYR:HE1	1:B:319:LYS:HG2	1.65	0.61
1:C:377:VAL:HG21	1:C:390:LYS:HG2	1.83	0.61
1:C:1102:TYR:HB2	1:C:1165:MET:HG2	1.81	0.61
1:D:490:GLN:OE1	1:D:547:ASN:ND2	2.33	0.61
1:B:355:LYS:HE3	1:B:356:TYR:H	1.65	0.61
1:B:377:VAL:HG21	1:B:390:LYS:HG2	1.83	0.61
1:C:2335:ARG:HE	1:C:2335:ARG:C	2.04	0.61
2:I:26:HIS:NE2	2:I:41:ARG:HG2	2.16	0.61
1:A:377:VAL:HG21	1:A:390:LYS:HG2	1.83	0.60
1:D:490:GLN:HB2	1:D:547:ASN:HD21	1.65	0.60
1:D:2067:ARG:O	1:D:2071:GLU:HG2	2.00	0.60
1:D:4305:PHE:HA	1:D:4308:VAL:HG22	1.83	0.60
1:A:188:SER:HB2	1:A:190:ARG:HH11	1.65	0.60
1:A:880:ARG:HG3	1:A:881:ILE:HD12	1.81	0.60
1:B:1102:TYR:HB2	1:B:1165:MET:HG2	1.81	0.60
1:B:2335:ARG:HE	1:B:2335:ARG:C	2.04	0.60
1:D:2335:ARG:HE	1:D:2335:ARG:C	2.04	0.60
1:A:2335:ARG:C	1:A:2335:ARG:HE	2.04	0.60
2:G:22:THR:HB	2:G:50:ARG:HG2	1.84	0.60
1:B:1225:LYS:HB3	1:B:1226:TYR:CD2	2.36	0.60
1:D:357:GLY:O	1:D:404:ASN:ND2	2.28	0.60
1:D:377:VAL:HG21	1:D:390:LYS:HG2	1.83	0.60
1:D:1383:ARG:NH1	1:D:1385:LYS:O	2.34	0.60
1:D:2348:GLU:O	1:D:2352:ILE:HG12	2.00	0.60
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.33	0.60
1:A:2335:ARG:HE	1:A:2336:GLY:N	1.99	0.60
1:A:4305:PHE:HA	1:A:4308:VAL:HG22	1.83	0.60
2:H:22:THR:HB	2:H:50:ARG:HG2	1.83	0.60
1:C:1383:ARG:NH1	1:C:1385:LYS:O	2.34	0.60
1:C:3659:ARG:HG3	1:C:3660:VAL:H	1.66	0.60
1:D:2159:ASN:OD1	1:D:2162:ARG:NH2	2.33	0.60
1:B:2335:ARG:HE	1:B:2336:GLY:N	1.99	0.60
1:C:4568:GLU:HG2	1:C:4569:PRO:HD3	1.81	0.60
1:D:760:ASP:HB3	1:D:764:PRO:HG2	1.83	0.60
1:B:1383:ARG:NH1	1:B:1385:LYS:O	2.34	0.60
1:C:1769:PHE:O	2:I:83:TYR:OH	2.11	0.60
2:J:22:THR:HB	2:J:50:ARG:HG2	1.83	0.60
1:A:4949:GLU:OE1	1:A:4949:GLU:N	2.29	0.60
2:G:26:HIS:NE2	2:G:41:ARG:HG2	2.16	0.60
1:B:2838:ALA:O	1:B:2842:MET:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1788:LEU:O	1:D:1792:THR:OG1	2.20	0.60
1:D:2838:ALA:O	1:D:2842:MET:HG3	2.01	0.60
1:B:2108:ASN:HD21	1:B:2111:SER:HB3	1.67	0.60
1:C:490:GLN:OE1	1:C:547:ASN:ND2	2.33	0.60
1:C:587:ASN:OD1	1:C:2132:ARG:NH1	2.35	0.60
1:A:747:HIS:CG	1:A:750:ARG:HH12	2.20	0.60
1:B:3659:ARG:HG3	1:B:3660:VAL:H	1.66	0.60
1:B:3891:TYR:O	1:B:3956:LYS:NZ	2.26	0.60
1:C:2838:ALA:O	1:C:2842:MET:HG3	2.01	0.60
1:A:1233:GLN:HG2	1:B:3493:UNK:HA	1.83	0.60
1:A:2838:ALA:O	1:A:2842:MET:HG3	2.01	0.60
2:H:26:HIS:NE2	2:H:41:ARG:HG2	2.16	0.60
1:C:4196:ILE:HG23	1:C:4922:MET:HE2	1.83	0.60
1:D:587:ASN:OD1	1:D:2132:ARG:NH1	2.35	0.60
1:D:1223:THR:O	1:D:1225:LYS:HD3	2.02	0.60
1:A:1225:LYS:HB3	1:A:1226:TYR:CD2	2.36	0.59
1:B:587:ASN:OD1	1:B:2132:ARG:NH1	2.35	0.59
1:C:2335:ARG:HE	1:C:2336:GLY:N	1.99	0.59
1:A:1383:ARG:NH1	1:A:1385:LYS:O	2.34	0.59
1:C:2108:ASN:HD21	1:C:2111:SER:HB3	1.67	0.59
1:D:3659:ARG:HG3	1:D:3660:VAL:H	1.66	0.59
1:A:76:ARG:O	1:A:79:GLN:HG2	2.03	0.59
1:A:1223:THR:O	1:A:1225:LYS:HD3	2.02	0.59
1:A:1788:LEU:O	1:A:1792:THR:OG1	2.20	0.59
1:B:760:ASP:HB3	1:B:764:PRO:HG2	1.83	0.59
1:C:1225:LYS:HB3	1:C:1226:TYR:CD2	2.36	0.59
1:C:409:GLN:N	1:C:412:GLU:OE2	2.35	0.59
1:A:875:PRO:O	1:A:882:ARG:NH2	2.35	0.59
1:A:2220:LEU:HD11	1:A:2242:ALA:HB2	1.84	0.59
1:A:3998:MET:O	1:A:4001:MET:HG3	2.03	0.59
1:B:4305:PHE:HA	1:B:4308:VAL:HG22	1.83	0.59
1:C:760:ASP:HB3	1:C:764:PRO:HG2	1.83	0.59
1:D:1225:LYS:HB3	1:D:1226:TYR:CD2	2.36	0.59
1:D:1286:THR:OG1	1:D:1583:CYS:SG	2.58	0.59
1:A:2081:ARG:HG3	1:A:3686:LEU:HD22	1.85	0.59
1:A:4842:ARG:NH1	1:A:4846:ASP:OD2	2.36	0.59
1:B:1788:LEU:O	1:B:1792:THR:OG1	2.20	0.59
1:C:76:ARG:O	1:C:79:GLN:HG2	2.03	0.59
2:I:22:THR:HB	2:I:50:ARG:HG2	1.84	0.59
1:D:747:HIS:CG	1:D:750:ARG:HH12	2.20	0.59
1:D:4942:MET:HE2	1:D:4950:PHE:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ARG:HG2	1:A:728:ASP:HB3	1.84	0.59
1:A:3659:ARG:HG3	1:A:3660:VAL:H	1.66	0.59
1:B:1223:THR:O	1:B:1225:LYS:HD3	2.02	0.59
1:B:3998:MET:O	1:B:4001:MET:HG3	2.03	0.59
1:C:490:GLN:HB2	1:C:547:ASN:HD21	1.65	0.59
1:C:875:PRO:O	1:C:882:ARG:NH2	2.35	0.59
1:C:4001:MET:HA	1:C:4004:GLU:HG2	1.85	0.59
1:D:838:ARG:H	1:D:841:LYS:HZ1	1.48	0.59
1:D:3998:MET:O	1:D:4001:MET:HG3	2.03	0.59
1:C:3891:TYR:O	1:C:3956:LYS:NZ	2.26	0.59
1:B:1286:THR:HG1	1:B:1583:CYS:HG	1.46	0.59
1:B:2081:ARG:HG3	1:B:3686:LEU:HD22	1.85	0.59
1:B:4001:MET:HA	1:B:4004:GLU:HG2	1.85	0.59
1:C:1223:THR:O	1:C:1225:LYS:HD3	2.02	0.59
1:A:587:ASN:OD1	1:A:2132:ARG:NH1	2.35	0.59
1:B:2220:LEU:HD11	1:B:2242:ALA:HB2	1.84	0.59
1:B:4842:ARG:NH1	1:B:4846:ASP:OD2	2.36	0.59
1:C:1788:LEU:O	1:C:1792:THR:OG1	2.20	0.59
1:C:3998:MET:O	1:C:4001:MET:HG3	2.03	0.59
1:C:4305:PHE:HA	1:C:4308:VAL:HG22	1.84	0.59
1:D:933:LEU:O	1:D:937:LEU:HG	2.03	0.59
1:D:2108:ASN:HD21	1:D:2111:SER:HB3	1.67	0.59
1:D:4842:ARG:NH1	1:D:4846:ASP:OD2	2.36	0.59
1:B:3810:GLN:NE2	1:B:3826:GLU:OE1	2.35	0.58
1:D:3810:GLN:NE2	1:D:3826:GLU:OE1	2.35	0.58
1:A:20:VAL:HB	1:A:214:VAL:HG13	1.85	0.58
1:A:2108:ASN:HD21	1:A:2111:SER:HB3	1.67	0.58
1:B:933:LEU:O	1:B:937:LEU:HG	2.03	0.58
1:C:20:VAL:HB	1:C:214:VAL:HG13	1.86	0.58
1:D:76:ARG:O	1:D:79:GLN:HG2	2.03	0.58
1:D:2220:LEU:HD11	1:D:2242:ALA:HB2	1.84	0.58
1:A:76:ARG:NH1	1:B:3889:TRP:HE3	2.01	0.58
1:A:760:ASP:HB3	1:A:764:PRO:HG2	1.83	0.58
1:B:76:ARG:O	1:B:79:GLN:HG2	2.03	0.58
1:B:747:HIS:CG	1:B:750:ARG:HH12	2.20	0.58
1:C:747:HIS:CG	1:C:750:ARG:HH12	2.20	0.58
1:C:2716:LEU:O	1:C:2720:ILE:HG12	2.04	0.58
1:D:694:ARG:HG2	1:D:728:ASP:HB3	1.84	0.58
1:A:436:LEU:HD21	1:A:517:VAL:HG12	1.86	0.58
1:A:2716:LEU:O	1:A:2720:ILE:HG12	2.04	0.58
1:B:2716:LEU:O	1:B:2720:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4842:ARG:NH1	1:C:4846:ASP:OD2	2.36	0.58
1:A:933:LEU:O	1:A:937:LEU:HG	2.03	0.58
1:B:235:ARG:NH1	1:B:268:SER:O	2.37	0.58
1:B:694:ARG:HG2	1:B:728:ASP:HB3	1.84	0.58
1:C:235:ARG:NH1	1:C:268:SER:O	2.37	0.58
1:C:694:ARG:HG2	1:C:728:ASP:HB3	1.84	0.58
1:D:20:VAL:HB	1:D:214:VAL:HG13	1.85	0.58
1:D:2716:LEU:O	1:D:2720:ILE:HG12	2.04	0.58
1:C:750:ARG:HH21	2:I:10:PRO:HD3	1.69	0.58
1:D:674:TYR:HD2	1:D:758:CYS:HG	1.52	0.58
1:D:2081:ARG:HG3	1:D:3686:LEU:HD22	1.85	0.58
1:B:409:GLN:N	1:B:412:GLU:OE2	2.35	0.58
1:C:2220:LEU:HD11	1:C:2242:ALA:HB2	1.84	0.58
1:D:875:PRO:O	1:D:882:ARG:NH2	2.35	0.58
1:A:235:ARG:NH1	1:A:268:SER:O	2.37	0.58
1:A:1245:ARG:NH1	1:A:1809:ASP:O	2.33	0.58
1:C:2112:VAL:O	1:C:2116:ILE:HG13	2.04	0.58
1:C:2848:HIS:CE1	1:C:2876:LEU:HD21	2.39	0.58
1:B:20:VAL:HB	1:B:214:VAL:HG13	1.85	0.58
1:D:4949:GLU:OE1	1:D:4949:GLU:N	2.29	0.58
1:A:357:GLY:O	1:A:404:ASN:ND2	2.28	0.57
1:A:363:ILE:HG22	1:A:372:LEU:HD23	1.86	0.57
1:A:409:GLN:N	1:A:412:GLU:OE2	2.35	0.57
1:B:436:LEU:HD21	1:B:517:VAL:HG12	1.86	0.57
1:B:674:TYR:HD2	1:B:758:CYS:HG	1.52	0.57
1:B:875:PRO:O	1:B:882:ARG:NH2	2.35	0.57
1:B:2112:VAL:O	1:B:2116:ILE:HG13	2.04	0.57
1:B:2228:LEU:HD22	1:B:2296:ARG:HG3	1.86	0.57
1:C:363:ILE:HG22	1:C:372:LEU:HD23	1.86	0.57
1:D:4001:MET:HA	1:D:4004:GLU:HG2	1.85	0.57
1:C:933:LEU:O	1:C:937:LEU:HG	2.03	0.57
1:C:2081:ARG:HG3	1:C:3686:LEU:HD22	1.85	0.57
1:C:2228:LEU:HD22	1:C:2296:ARG:HG3	1.86	0.57
1:C:3810:GLN:NE2	1:C:3826:GLU:OE1	2.35	0.57
1:C:4649:LYS:NZ	1:C:4669:LEU:O	2.37	0.57
1:D:235:ARG:NH1	1:D:268:SER:O	2.37	0.57
1:A:4001:MET:HA	1:A:4004:GLU:HG2	1.85	0.57
1:B:2848:HIS:CE1	1:B:2876:LEU:HD21	2.39	0.57
1:C:838:ARG:H	1:C:841:LYS:HZ1	1.52	0.57
1:D:363:ILE:HG22	1:D:372:LEU:HD23	1.86	0.57
1:D:2233:MET:N	1:D:2233:MET:HE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:83:TYR:HB3	2:J:87:GLY:HA2	1.86	0.57
1:D:2848:HIS:CE1	1:D:2876:LEU:HD21	2.39	0.57
1:A:2784:TRP:HE3	1:A:2842:MET:HE2	1.69	0.57
1:B:929:ARG:HA	1:B:932:ASN:HD21	1.70	0.57
1:A:4649:LYS:NZ	1:A:4669:LEU:O	2.37	0.57
1:A:4660:TYR:HB3	1:A:4664:ARG:HH12	1.70	0.57
1:C:140:THR:O	1:D:2337:GLU:HG3	2.04	0.57
2:I:83:TYR:HB3	2:I:87:GLY:HA2	1.86	0.57
1:A:896:ASN:OD1	1:A:897:LYS:N	2.38	0.57
1:A:2848:HIS:CE1	1:A:2876:LEU:HD21	2.39	0.57
1:D:436:LEU:HD21	1:D:517:VAL:HG12	1.86	0.57
1:A:227:TYR:CD2	1:A:352:SER:HB3	2.40	0.57
1:C:1286:THR:OG1	1:C:1583:CYS:SG	2.58	0.57
1:C:2763:SER:H	1:C:2766:GLU:HB2	1.70	0.57
1:A:2228:LEU:HD22	1:A:2296:ARG:HG3	1.86	0.57
1:B:363:ILE:HG22	1:B:372:LEU:HD23	1.86	0.57
1:B:672:LYS:HB3	1:B:819:TYR:HA	1.87	0.57
1:B:4196:ILE:HG23	1:B:4922:MET:HE2	1.87	0.57
1:D:227:TYR:CD2	1:D:352:SER:HB3	2.40	0.57
1:D:4660:TYR:HB3	1:D:4664:ARG:HH12	1.70	0.57
1:A:4196:ILE:HG23	1:A:4922:MET:HE2	1.86	0.56
1:B:4649:LYS:NZ	1:B:4669:LEU:O	2.37	0.56
1:D:2228:LEU:HD22	1:D:2296:ARG:HG3	1.86	0.56
1:A:1829:LEU:HB3	1:A:1834:ILE:HD11	1.87	0.56
1:C:436:LEU:HD21	1:C:517:VAL:HG12	1.86	0.56
1:A:1048:ASP:HA	1:A:1051:ARG:HD2	1.87	0.56
1:A:2112:VAL:O	1:A:2116:ILE:HG13	2.04	0.56
1:B:1829:LEU:HB3	1:B:1834:ILE:HD11	1.87	0.56
1:B:4660:TYR:HB3	1:B:4664:ARG:HH12	1.70	0.56
1:C:227:TYR:CD2	1:C:352:SER:HB3	2.40	0.56
1:C:896:ASN:OD1	1:C:897:LYS:N	2.38	0.56
1:C:1829:LEU:HB3	1:C:1834:ILE:HD11	1.87	0.56
1:C:2232:ALA:HB3	1:C:2233:MET:HE2	1.86	0.56
1:D:59:PRO:HD3	1:D:322:ALA:HB3	1.87	0.56
1:D:896:ASN:OD1	1:D:897:LYS:N	2.38	0.56
1:D:1684:PRO:HD3	2:J:42:ASP:HB3	1.87	0.56
1:D:4649:LYS:NZ	1:D:4669:LEU:O	2.37	0.56
1:B:227:TYR:CD2	1:B:352:SER:HB3	2.40	0.56
1:B:4778:TYR:O	1:B:4782:VAL:HG12	2.06	0.56
2:H:83:TYR:HB3	2:H:87:GLY:HA2	1.86	0.56
1:D:929:ARG:HA	1:D:932:ASN:HD21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2112:VAL:O	1:D:2116:ILE:HG13	2.04	0.56
1:A:672:LYS:HB3	1:A:819:TYR:HA	1.87	0.56
2:G:83:TYR:HB3	2:G:87:GLY:HA2	1.86	0.56
1:B:2763:SER:H	1:B:2766:GLU:HB2	1.70	0.56
1:A:59:PRO:HD3	1:A:322:ALA:HB3	1.87	0.56
1:A:677:LEU:HD23	1:A:755:ILE:HD11	1.87	0.56
1:A:4567:MET:HA	1:A:4570:THR:HG22	1.88	0.56
1:B:1048:ASP:HA	1:B:1051:ARG:HD2	1.87	0.56
1:B:2335:ARG:HH21	1:B:2336:GLY:HA2	1.71	0.56
1:B:2488:GLU:HA	1:B:2492:LEU:HD12	1.88	0.56
1:C:672:LYS:HB3	1:C:819:TYR:HA	1.87	0.56
1:C:2488:GLU:HA	1:C:2492:LEU:HD12	1.88	0.56
1:D:4196:ILE:HG23	1:D:4922:MET:HE2	1.87	0.56
1:A:2488:GLU:HA	1:A:2492:LEU:HD12	1.88	0.56
1:A:4942:MET:HE2	1:A:4950:PHE:HB3	1.88	0.56
1:B:36:CYS:SG	1:B:37:LEU:N	2.79	0.56
1:C:36:CYS:SG	1:C:37:LEU:N	2.79	0.56
1:C:357:GLY:O	1:C:404:ASN:ND2	2.28	0.56
1:C:1048:ASP:HA	1:C:1051:ARG:HD2	1.87	0.56
1:D:36:CYS:SG	1:D:37:LEU:N	2.79	0.56
1:B:896:ASN:OD1	1:B:897:LYS:N	2.38	0.56
1:B:4567:MET:HA	1:B:4570:THR:HG22	1.88	0.56
1:C:1928:SER:HG	1:C:3619:PHE:HD2	1.54	0.56
1:D:1048:ASP:HA	1:D:1051:ARG:HD2	1.87	0.56
1:D:2335:ARG:HH21	1:D:2336:GLY:HA2	1.71	0.56
1:A:36:CYS:SG	1:A:37:LEU:N	2.79	0.56
1:A:929:ARG:HA	1:A:932:ASN:HD21	1.70	0.56
1:C:433:LEU:HD11	1:C:504:ARG:HD3	1.88	0.56
1:C:677:LEU:HD23	1:C:755:ILE:HD11	1.87	0.56
1:C:4660:TYR:HB3	1:C:4664:ARG:HH12	1.70	0.56
1:A:3810:GLN:NE2	1:A:3826:GLU:OE1	2.35	0.56
1:B:677:LEU:HD23	1:B:755:ILE:HD11	1.87	0.56
1:B:4784:ALA:HA	1:B:4788:PHE:HD2	1.71	0.56
1:C:4778:TYR:O	1:C:4782:VAL:HG12	2.06	0.56
1:C:4808:MET:HG2	1:D:4516:LEU:HA	1.87	0.55
1:A:2763:SER:H	1:A:2766:GLU:HB2	1.70	0.55
1:B:433:LEU:HD11	1:B:504:ARG:HD3	1.88	0.55
1:A:991:SER:O	1:A:995:MET:HG2	2.06	0.55
1:A:3891:TYR:O	1:A:3956:LYS:NZ	2.26	0.55
1:A:4784:ALA:HA	1:A:4788:PHE:HD2	1.71	0.55
1:B:59:PRO:HD3	1:B:322:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:929:ARG:HA	1:C:932:ASN:HD21	1.70	0.55
1:D:1829:LEU:HB3	1:D:1834:ILE:HD11	1.87	0.55
1:D:2488:GLU:HA	1:D:2492:LEU:HD12	1.88	0.55
1:D:2763:SER:H	1:D:2766:GLU:HB2	1.70	0.55
1:A:799:LYS:HG2	1:A:1621:GLN:HE22	1.72	0.55
1:A:1152:TYR:HE2	1:A:1191:ALA:HA	1.71	0.55
1:B:3728:ALA:HA	1:B:3731:HIS:ND1	2.22	0.55
1:C:59:PRO:HD3	1:C:322:ALA:HB3	1.87	0.55
1:D:409:GLN:N	1:D:412:GLU:OE2	2.35	0.55
1:D:991:SER:O	1:D:995:MET:HG2	2.06	0.55
1:A:2335:ARG:HH21	1:A:2336:GLY:HA2	1.71	0.55
1:A:4881:GLU:O	1:A:4885:THR:HG23	2.07	0.55
1:C:76:ARG:NH1	1:D:3889:TRP:HB3	2.22	0.55
1:C:76:ARG:NH1	1:D:3889:TRP:HE3	2.04	0.55
2:I:22:THR:HA	2:I:50:ARG:HA	1.89	0.55
1:D:672:LYS:HB3	1:D:819:TYR:HA	1.87	0.55
1:D:4567:MET:HA	1:D:4570:THR:HG22	1.88	0.55
1:A:1795:MET:HA	1:A:1798:GLU:OE2	2.07	0.55
1:B:1152:TYR:HE2	1:B:1191:ALA:HA	1.71	0.55
1:B:1972:ILE:HD12	1:B:1975:LEU:HD11	1.89	0.55
1:C:2107:ILE:HG13	1:C:2108:ASN:N	2.22	0.55
1:C:4948:TRP:HD1	1:C:4950:PHE:CE1	2.24	0.55
2:J:50:ARG:N	2:J:55:GLU:OE2	2.40	0.55
1:C:1972:ILE:HD12	1:C:1975:LEU:HD11	1.89	0.55
1:C:2335:ARG:HH21	1:C:2336:GLY:HA2	1.71	0.55
1:D:799:LYS:HG2	1:D:1621:GLN:HE22	1.72	0.55
1:D:2107:ILE:HG13	1:D:2108:ASN:N	2.21	0.55
1:D:3728:ALA:HA	1:D:3731:HIS:ND1	2.22	0.55
1:A:1928:SER:HG	1:A:3619:PHE:HD2	1.55	0.55
1:A:4948:TRP:HD1	1:A:4950:PHE:CE1	2.24	0.55
1:B:168:GLN:HG3	1:B:169:ARG:HG3	1.89	0.55
1:B:2342:LEU:HB3	1:B:2434:VAL:HG21	1.89	0.55
1:B:4948:TRP:HD1	1:B:4950:PHE:CE1	2.24	0.55
1:C:991:SER:O	1:C:995:MET:HG2	2.06	0.55
1:D:747:HIS:HE1	1:D:770:ILE:HD11	1.72	0.55
1:D:1928:SER:HG	1:D:3619:PHE:HD2	1.55	0.55
2:J:22:THR:HA	2:J:50:ARG:HA	1.88	0.55
1:A:433:LEU:HD11	1:A:504:ARG:HD3	1.88	0.55
1:A:747:HIS:HE1	1:A:770:ILE:HD11	1.72	0.55
2:I:50:ARG:N	2:I:55:GLU:OE2	2.40	0.55
1:D:4948:TRP:HD1	1:D:4950:PHE:CE1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3728:ALA:HA	1:A:3731:HIS:ND1	2.22	0.54
1:B:1795:MET:HA	1:B:1798:GLU:OE2	2.07	0.54
1:B:2254:LEU:O	1:B:3809:ARG:HD3	2.08	0.54
1:C:3728:ALA:HA	1:C:3731:HIS:ND1	2.22	0.54
1:C:4784:ALA:HA	1:C:4788:PHE:HD2	1.71	0.54
1:D:2232:ALA:HB3	1:D:2233:MET:HE2	1.89	0.54
1:A:168:GLN:HG3	1:A:169:ARG:HG3	1.89	0.54
1:A:2287:ILE:HD12	1:A:2383:MET:HE2	1.89	0.54
1:A:4778:TYR:O	1:A:4782:VAL:HG12	2.06	0.54
1:B:991:SER:O	1:B:995:MET:HG2	2.06	0.54
1:B:4496:ASN:O	1:B:4500:MET:HG2	2.07	0.54
1:C:27:THR:HG22	1:C:32:GLN:HG3	1.89	0.54
1:D:433:LEU:HD11	1:D:504:ARG:HD3	1.88	0.54
1:D:4784:ALA:HA	1:D:4788:PHE:HD2	1.71	0.54
1:C:1811:VAL:HB	1:C:1818:LEU:HD13	1.90	0.54
1:D:1253:LYS:HD2	1:D:1596:LEU:HB3	1.90	0.54
1:D:4881:GLU:O	1:D:4885:THR:HG23	2.07	0.54
1:A:1934:LYS:HE3	1:A:1991:ILE:HG22	1.90	0.54
2:G:50:ARG:N	2:G:55:GLU:OE2	2.40	0.54
1:B:838:ARG:H	1:B:841:LYS:HZ1	1.54	0.54
1:B:2107:ILE:HG13	1:B:2108:ASN:N	2.21	0.54
1:C:1266:GLU:O	1:C:1267:HIS:ND1	2.41	0.54
1:C:4567:MET:HA	1:C:4570:THR:HG22	1.88	0.54
1:D:2061:ILE:O	1:D:2065:MET:HG2	2.08	0.54
1:A:2254:LEU:O	1:A:3809:ARG:HD3	2.08	0.54
1:A:3889:TRP:HB3	1:D:76:ARG:NH1	2.22	0.54
1:B:27:THR:HG22	1:B:32:GLN:HG3	1.89	0.54
1:B:699:SER:OG	1:B:700:THR:N	2.41	0.54
1:B:1266:GLU:O	1:B:1267:HIS:ND1	2.41	0.54
1:B:1934:LYS:HE3	1:B:1991:ILE:HG22	1.90	0.54
1:B:4881:GLU:O	1:B:4885:THR:HG23	2.07	0.54
1:C:168:GLN:HG3	1:C:169:ARG:HG3	1.89	0.54
1:C:799:LYS:HG2	1:C:1621:GLN:HE22	1.72	0.54
1:D:677:LEU:HD23	1:D:755:ILE:HD11	1.87	0.54
1:D:718:VAL:HG23	1:D:724:SER:HB2	1.90	0.54
1:D:2348:GLU:HA	1:D:2351:LYS:HD3	1.90	0.54
1:D:4895:ASP:OD1	1:D:4896:TYR:N	2.41	0.54
1:A:732:LEU:HB3	1:A:779:PHE:CZ	2.43	0.54
1:A:1972:ILE:HD12	1:A:1975:LEU:HD11	1.89	0.54
1:B:1811:VAL:HB	1:B:1818:LEU:HD13	1.89	0.54
2:H:24:VAL:HG12	2:H:105:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:SER:OG	1:C:700:THR:N	2.41	0.54
1:C:747:HIS:HE1	1:C:770:ILE:HD11	1.72	0.54
1:C:1152:TYR:HE2	1:C:1191:ALA:HA	1.71	0.54
1:C:2342:LEU:HB3	1:C:2434:VAL:HG21	1.89	0.54
2:I:24:VAL:HG12	2:I:105:LEU:HD13	1.90	0.54
1:A:2061:ILE:O	1:A:2065:MET:HG2	2.08	0.54
1:A:2342:LEU:HB3	1:A:2434:VAL:HG21	1.89	0.54
1:B:747:HIS:HE1	1:B:770:ILE:HD11	1.72	0.54
1:B:2061:ILE:O	1:B:2065:MET:HG2	2.08	0.54
1:B:4948:TRP:HD1	1:B:4950:PHE:HE1	1.55	0.54
1:C:1567:LEU:HD22	1:C:1581:PRO:HB3	1.90	0.54
1:D:1225:LYS:HB3	1:D:1226:TYR:HD2	1.73	0.54
1:A:2107:ILE:HG13	1:A:2108:ASN:N	2.21	0.54
1:A:4928:ASP:O	1:A:4932:HIS:NE2	2.41	0.54
2:G:22:THR:HA	2:G:50:ARG:HA	1.89	0.54
1:C:1225:LYS:HB3	1:C:1226:TYR:HD2	1.73	0.54
1:C:4895:ASP:OD1	1:C:4896:TYR:N	2.41	0.54
1:C:4928:ASP:O	1:C:4932:HIS:NE2	2.41	0.54
1:D:2254:LEU:O	1:D:3809:ARG:HD3	2.08	0.54
1:D:4778:TYR:O	1:D:4782:VAL:HG12	2.06	0.54
1:D:4928:ASP:O	1:D:4932:HIS:NE2	2.41	0.54
1:A:2335:ARG:NH2	1:A:2336:GLY:HA2	2.23	0.54
1:A:4873:ARG:NH1	1:D:4867:ASP:OD1	2.41	0.54
1:B:1286:THR:OG1	1:B:1583:CYS:SG	2.58	0.54
1:C:1253:LYS:HD2	1:C:1596:LEU:HB3	1.90	0.54
1:C:4881:GLU:O	1:C:4885:THR:HG23	2.07	0.54
1:D:168:GLN:HG3	1:D:169:ARG:HG3	1.89	0.54
1:D:732:LEU:HB3	1:D:779:PHE:CZ	2.43	0.54
1:D:1152:TYR:HE2	1:D:1191:ALA:HA	1.71	0.54
1:D:1266:GLU:O	1:D:1267:HIS:ND1	2.41	0.54
1:D:2287:ILE:HD12	1:D:2383:MET:HE2	1.89	0.54
1:D:3920:THR:O	1:D:3924:GLN:HB2	2.08	0.54
2:J:24:VAL:HG12	2:J:105:LEU:HD13	1.90	0.54
1:A:2348:GLU:HA	1:A:2351:LYS:HD3	1.90	0.54
2:G:24:VAL:HG12	2:G:105:LEU:HD13	1.90	0.54
1:B:189:GLU:OE2	1:C:2417:ARG:NH1	2.40	0.54
1:B:711:GLU:HA	1:B:711:GLU:OE2	2.08	0.54
1:C:1795:MET:HA	1:C:1798:GLU:OE2	2.07	0.54
1:D:1795:MET:HA	1:D:1798:GLU:OE2	2.07	0.54
1:D:4496:ASN:O	1:D:4500:MET:HG2	2.07	0.54
1:A:1266:GLU:O	1:A:1267:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1898:PRO:O	1:A:1902:LYS:HG2	2.08	0.53
1:A:4496:ASN:O	1:A:4500:MET:HG2	2.07	0.53
1:C:115:TYR:CZ	1:C:175:VAL:HG22	2.44	0.53
1:C:1683:GLU:HB3	2:I:42:ASP:HB3	1.90	0.53
1:C:4496:ASN:O	1:C:4500:MET:HG2	2.07	0.53
1:D:1972:ILE:HD12	1:D:1975:LEU:HD11	1.89	0.53
1:D:4948:TRP:HD1	1:D:4950:PHE:HE1	1.55	0.53
1:A:1567:LEU:HD22	1:A:1581:PRO:HB3	1.90	0.53
1:B:799:LYS:HG2	1:B:1621:GLN:HE22	1.72	0.53
1:B:1567:LEU:HD22	1:B:1581:PRO:HB3	1.90	0.53
1:B:1898:PRO:O	1:B:1902:LYS:HG2	2.08	0.53
1:B:4895:ASP:OD1	1:B:4896:TYR:N	2.41	0.53
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.91	0.53
1:C:2254:LEU:O	1:C:3809:ARG:HD3	2.08	0.53
1:C:2287:ILE:HD12	1:C:2383:MET:HE2	1.89	0.53
1:C:2335:ARG:NH2	1:C:2336:GLY:HA2	2.23	0.53
1:C:4949:GLU:OE1	1:C:4949:GLU:N	2.29	0.53
1:D:557:TRP:HE1	1:D:561:ARG:HH21	1.56	0.53
2:J:14:ARG:HG2	2:J:15:THR:HG23	1.91	0.53
1:A:2233:MET:HE2	1:A:2233:MET:H	1.73	0.53
1:A:3920:THR:O	1:A:3924:GLN:HB2	2.08	0.53
1:A:4895:ASP:OD1	1:A:4896:TYR:N	2.41	0.53
1:B:718:VAL:HG23	1:B:724:SER:HB2	1.90	0.53
1:B:2287:ILE:HD12	1:B:2383:MET:HE2	1.89	0.53
1:B:4928:ASP:O	1:B:4932:HIS:NE2	2.41	0.53
2:H:14:ARG:HG2	2:H:15:THR:HG23	1.90	0.53
1:C:732:LEU:HB3	1:C:779:PHE:CZ	2.43	0.53
1:D:115:TYR:CZ	1:D:175:VAL:HG22	2.43	0.53
1:D:1567:LEU:HD22	1:D:1581:PRO:HB3	1.90	0.53
1:D:1811:VAL:HB	1:D:1818:LEU:HD13	1.90	0.53
1:D:2342:LEU:HB3	1:D:2434:VAL:HG21	1.89	0.53
1:A:115:TYR:CZ	1:A:175:VAL:HG22	2.44	0.53
1:A:711:GLU:HA	1:A:711:GLU:OE2	2.08	0.53
2:H:50:ARG:N	2:H:55:GLU:OE2	2.40	0.53
1:C:711:GLU:HA	1:C:711:GLU:OE2	2.08	0.53
1:C:1934:LYS:HE3	1:C:1991:ILE:HG22	1.90	0.53
1:C:2061:ILE:O	1:C:2065:MET:HG2	2.08	0.53
1:C:2348:GLU:HA	1:C:2351:LYS:HD3	1.90	0.53
1:C:3920:THR:O	1:C:3924:GLN:HB2	2.08	0.53
1:D:1232:LEU:HB3	1:D:1233:GLN:NE2	2.24	0.53
1:A:1225:LYS:HB3	1:A:1226:TYR:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:LEU:HB3	1:A:1233:GLN:NE2	2.24	0.53
1:B:2335:ARG:NH2	1:B:2336:GLY:HA2	2.23	0.53
1:C:1898:PRO:O	1:C:1902:LYS:HG2	2.08	0.53
2:I:14:ARG:HG2	2:I:15:THR:HG23	1.91	0.53
1:D:699:SER:OG	1:D:700:THR:N	2.41	0.53
1:D:1898:PRO:O	1:D:1902:LYS:HG2	2.08	0.53
1:B:732:LEU:HB3	1:B:779:PHE:CZ	2.43	0.53
1:B:1253:LYS:HB3	1:B:1598:SER:HB2	1.91	0.53
1:B:3920:THR:O	1:B:3924:GLN:HB2	2.08	0.53
1:C:1253:LYS:HB3	1:C:1598:SER:HB2	1.91	0.53
1:C:2233:MET:HE2	1:C:2233:MET:N	2.24	0.53
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.12	0.53
1:A:281:ARG:O	1:A:285:SER:OG	2.27	0.53
1:A:557:TRP:HE1	1:A:561:ARG:HH21	1.56	0.53
1:A:4948:TRP:HD1	1:A:4950:PHE:HE1	1.55	0.53
2:G:14:ARG:HG2	2:G:15:THR:HG23	1.90	0.53
1:B:1747:HIS:O	1:B:1747:HIS:ND1	2.39	0.53
1:C:182:ILE:HD11	1:C:191:TYR:HE1	1.74	0.53
1:D:1934:LYS:HE3	1:D:1991:ILE:HG22	1.90	0.53
1:D:2720:ILE:HD11	1:D:2778:LEU:HD22	1.91	0.53
1:A:1811:VAL:HB	1:A:1818:LEU:HD13	1.89	0.53
1:A:3729:ARG:O	1:A:3733:ARG:NH1	2.42	0.53
1:B:115:TYR:CZ	1:B:175:VAL:HG22	2.43	0.53
1:B:755:ILE:HG22	1:B:770:ILE:HD12	1.91	0.53
1:B:1253:LYS:HD2	1:B:1596:LEU:HB3	1.89	0.53
1:B:2348:GLU:HA	1:B:2351:LYS:HD3	1.90	0.53
2:H:22:THR:HA	2:H:50:ARG:HA	1.89	0.53
1:C:718:VAL:HG23	1:C:724:SER:HB2	1.90	0.53
1:C:1294:ASN:ND2	1:C:1296:ASN:OD1	2.38	0.53
1:C:1770:VAL:O	2:I:57:ILE:HG23	2.08	0.53
1:D:943:LEU:HD11	1:D:948:CYS:HB3	1.91	0.53
1:A:677:LEU:HD22	1:A:695:VAL:HG21	1.91	0.53
1:A:1253:LYS:HB3	1:A:1598:SER:HB2	1.91	0.53
1:A:1253:LYS:HD2	1:A:1596:LEU:HB3	1.89	0.53
1:A:2406:HIS:HA	1:A:2409:HIS:HB3	1.91	0.53
1:B:557:TRP:HE1	1:B:561:ARG:HH21	1.56	0.53
1:C:943:LEU:HD11	1:C:948:CYS:HB3	1.91	0.53
1:C:2101:LEU:O	1:C:2104:THR:HG22	2.09	0.53
1:D:27:THR:HG22	1:D:32:GLN:HG3	1.89	0.53
1:B:182:ILE:HD11	1:B:191:TYR:HE1	1.74	0.53
1:B:1397:UNK:HA	1:B:1412:UNK:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4009:VAL:HA	1:B:4012:ILE:HG12	1.91	0.53
1:C:755:ILE:HG22	1:C:770:ILE:HD12	1.91	0.53
1:C:2406:HIS:HA	1:C:2409:HIS:HB3	1.91	0.53
1:D:711:GLU:HA	1:D:711:GLU:OE2	2.08	0.53
1:D:727:PHE:HB2	1:D:768:PHE:CE1	2.44	0.53
1:D:1397:UNK:HA	1:D:1412:UNK:HA	1.91	0.53
1:D:3957:LEU:HB2	1:D:3967:LEU:HD13	1.91	0.53
1:A:27:THR:HG22	1:A:32:GLN:HG3	1.89	0.52
1:A:727:PHE:HB2	1:A:768:PHE:CE1	2.44	0.52
1:B:676:GLU:HB2	1:B:803:LEU:HB2	1.91	0.52
1:B:1734:THR:HA	1:B:1756:THR:HG21	1.91	0.52
1:C:1680:HIS:NE2	2:I:90:GLY:O	2.42	0.52
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.91	0.52
1:D:2406:HIS:HA	1:D:2409:HIS:HB3	1.91	0.52
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.12	0.52
1:A:718:VAL:HG23	1:A:724:SER:HB2	1.90	0.52
1:A:1734:THR:HA	1:A:1756:THR:HG21	1.91	0.52
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.91	0.52
1:B:2080:VAL:HG13	1:B:3669:LEU:HD22	1.92	0.52
1:B:2254:LEU:HD22	1:B:3809:ARG:HG3	1.92	0.52
1:C:4081:GLU:O	1:C:4085:ARG:HG2	2.10	0.52
1:C:4948:TRP:HD1	1:C:4950:PHE:HE1	1.55	0.52
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.91	0.52
1:D:2335:ARG:NH2	1:D:2336:GLY:HA2	2.23	0.52
1:D:4081:GLU:O	1:D:4085:ARG:HG2	2.10	0.52
1:C:191:TYR:N	1:C:206:ALA:O	2.35	0.52
1:D:2080:VAL:HG13	1:D:3669:LEU:HD22	1.92	0.52
1:A:1397:UNK:HA	1:A:1412:UNK:HA	1.91	0.52
1:B:113:LEU:HD21	1:B:162:ILE:HD13	1.91	0.52
1:B:1219:LYS:HE3	1:B:1240:ALA:O	2.10	0.52
1:B:2406:HIS:HA	1:B:2409:HIS:HB3	1.91	0.52
1:C:557:TRP:HE1	1:C:561:ARG:HH21	1.56	0.52
1:C:677:LEU:HD22	1:C:695:VAL:HG21	1.91	0.52
1:C:1397:UNK:HA	1:C:1412:UNK:HA	1.91	0.52
1:D:4042:ILE:HG21	1:D:4047:PHE:HB2	1.92	0.52
1:A:699:SER:OG	1:A:700:THR:N	2.41	0.52
1:A:3957:LEU:HB2	1:A:3967:LEU:HD13	1.91	0.52
1:A:4009:VAL:HA	1:A:4012:ILE:HG12	1.91	0.52
1:B:727:PHE:HB2	1:B:768:PHE:CE1	2.44	0.52
1:B:1232:LEU:HB3	1:B:1233:GLN:NE2	2.24	0.52
1:B:1925:VAL:HG22	1:B:3620:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LEU:HD21	1:C:162:ILE:HD13	1.91	0.52
1:C:1734:THR:HA	1:C:1756:THR:HG21	1.92	0.52
1:B:2313:GLU:OE1	1:B:3812:LYS:NZ	2.40	0.52
1:C:1925:VAL:HG22	1:C:3620:LEU:HD11	1.92	0.52
1:D:1219:LYS:HE3	1:D:1240:ALA:O	2.10	0.52
1:D:1734:THR:HA	1:D:1756:THR:HG21	1.91	0.52
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.91	0.52
1:A:1969:GLN:HA	1:A:1969:GLN:OE1	2.10	0.52
1:A:2101:LEU:O	1:A:2104:THR:HG22	2.09	0.52
1:B:1969:GLN:OE1	1:B:1969:GLN:HA	2.10	0.52
1:C:281:ARG:O	1:C:285:SER:OG	2.27	0.52
1:C:2254:LEU:HD22	1:C:3809:ARG:HG3	1.92	0.52
1:C:2720:ILE:HD11	1:C:2778:LEU:HD22	1.91	0.52
1:D:1253:LYS:HB3	1:D:1598:SER:HB2	1.91	0.52
1:A:2080:VAL:HG13	1:A:3669:LEU:HD22	1.92	0.52
1:B:1928:SER:HG	1:B:3619:PHE:HD2	1.58	0.52
1:B:2101:LEU:O	1:B:2104:THR:HG22	2.09	0.52
1:C:2080:VAL:HG13	1:C:3669:LEU:HD22	1.92	0.52
1:C:3729:ARG:O	1:C:3733:ARG:NH1	2.42	0.52
1:C:4042:ILE:HG21	1:C:4047:PHE:HB2	1.92	0.52
1:D:677:LEU:HD22	1:D:695:VAL:HG21	1.91	0.52
1:D:1294:ASN:ND2	1:D:1296:ASN:OD1	2.38	0.52
1:D:1925:VAL:HG22	1:D:3620:LEU:HD11	1.92	0.52
1:D:2101:LEU:O	1:D:2104:THR:HG22	2.09	0.52
1:A:1962:ARG:O	1:A:1966:SER:OG	2.28	0.52
1:A:2713:PRO:HG2	1:A:2716:LEU:HD12	1.91	0.52
1:B:669:GLN:HB3	1:B:673:TRP:HZ2	1.75	0.52
1:C:727:PHE:HB2	1:C:768:PHE:CE1	2.44	0.52
1:C:1962:ARG:O	1:C:1966:SER:OG	2.28	0.52
1:C:3957:LEU:HB2	1:C:3967:LEU:HD13	1.91	0.52
1:C:4009:VAL:HA	1:C:4012:ILE:HG12	1.91	0.52
1:D:113:LEU:HD21	1:D:162:ILE:HD13	1.91	0.52
1:D:386:SER:HB3	1:D:388:GLN:HE22	1.75	0.52
1:D:3729:ARG:O	1:D:3733:ARG:NH1	2.42	0.52
1:D:3891:TYR:O	1:D:3956:LYS:NZ	2.26	0.52
1:A:1294:ASN:ND2	1:A:1296:ASN:OD1	2.38	0.52
1:A:2254:LEU:HD22	1:A:3809:ARG:HG3	1.92	0.52
1:B:1962:ARG:O	1:B:1966:SER:OG	2.28	0.52
1:B:2720:ILE:HD11	1:B:2778:LEU:HD22	1.91	0.52
1:B:3729:ARG:O	1:B:3733:ARG:NH1	2.42	0.52
1:C:1219:LYS:HE3	1:C:1240:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2713:PRO:HG2	1:C:2716:LEU:HD12	1.91	0.52
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.91	0.51
1:A:4081:GLU:O	1:A:4085:ARG:HG2	2.10	0.51
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.12	0.51
1:C:669:GLN:HB3	1:C:673:TRP:HZ2	1.75	0.51
1:D:1969:GLN:HA	1:D:1969:GLN:OE1	2.10	0.51
1:D:2713:PRO:HG2	1:D:2716:LEU:HD12	1.91	0.51
1:A:113:LEU:HD21	1:A:162:ILE:HD13	1.91	0.51
1:A:386:SER:HB3	1:A:388:GLN:HE22	1.75	0.51
1:A:644:LEU:HD13	1:A:1631:LEU:HD23	1.93	0.51
1:A:1219:LYS:HE3	1:A:1240:ALA:O	2.10	0.51
1:B:943:LEU:HD11	1:B:948:CYS:HB3	1.91	0.51
1:B:1294:ASN:ND2	1:B:1296:ASN:OD1	2.38	0.51
1:B:2713:PRO:HG2	1:B:2716:LEU:HD12	1.91	0.51
1:B:4118:LEU:O	1:B:4122:GLU:HG2	2.11	0.51
1:D:755:ILE:HG22	1:D:770:ILE:HD12	1.91	0.51
1:A:755:ILE:HG22	1:A:770:ILE:HD12	1.91	0.51
1:A:943:LEU:HD11	1:A:948:CYS:HB3	1.91	0.51
1:A:4103:ASN:OD1	1:A:4107:HIS:ND1	2.38	0.51
1:A:4863:GLY:CA	1:B:4866:ILE:HG12	2.40	0.51
1:B:1972:ILE:HA	1:B:1975:LEU:HG	1.92	0.51
1:B:3957:LEU:HB2	1:B:3967:LEU:HD13	1.91	0.51
1:C:587:ASN:HA	1:C:2132:ARG:HH12	1.76	0.51
1:C:4118:LEU:O	1:C:4122:GLU:HG2	2.11	0.51
1:D:587:ASN:HA	1:D:2132:ARG:HH12	1.76	0.51
1:D:4118:LEU:O	1:D:4122:GLU:HG2	2.11	0.51
1:A:587:ASN:HA	1:A:2132:ARG:HH12	1.76	0.51
1:A:1925:VAL:HG22	1:A:3620:LEU:HD11	1.92	0.51
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.12	0.51
1:B:587:ASN:HA	1:B:2132:ARG:HH12	1.76	0.51
1:B:644:LEU:HD13	1:B:1631:LEU:HD23	1.93	0.51
1:C:386:SER:HB3	1:C:388:GLN:HE22	1.75	0.51
1:C:4115:GLN:O	1:C:4119:GLU:HG2	2.11	0.51
1:C:4867:ASP:OD1	1:D:4873:ARG:NH1	2.44	0.51
1:D:474:ASP:O	1:D:478:ARG:HG2	2.11	0.51
1:D:763:ALA:HB3	1:D:764:PRO:HD3	1.92	0.51
1:A:766:ILE:HG22	1:A:768:PHE:CE2	2.46	0.51
1:A:2313:GLU:OE1	1:A:3812:LYS:NZ	2.40	0.51
1:B:763:ALA:HB3	1:B:764:PRO:HD3	1.92	0.51
1:B:4042:ILE:HG21	1:B:4047:PHE:HB2	1.92	0.51
1:C:644:LEU:HD13	1:C:1631:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4103:ASN:OD1	1:C:4107:HIS:ND1	2.38	0.51
1:D:644:LEU:HD13	1:D:1631:LEU:HD23	1.93	0.51
1:D:1986:PRO:HB2	1:D:1988:PRO:HD2	1.93	0.51
1:A:669:GLN:HB3	1:A:673:TRP:HZ2	1.75	0.51
1:B:677:LEU:HD22	1:B:695:VAL:HG21	1.91	0.51
1:B:1052:GLU:HA	1:B:1055:ARG:HB2	1.92	0.51
1:B:1789:LYS:HB2	1:B:1835:PHE:CE1	2.46	0.51
1:B:1986:PRO:HB2	1:B:1988:PRO:HD2	1.93	0.51
1:C:1052:GLU:HA	1:C:1055:ARG:HB2	1.92	0.51
1:D:669:GLN:HB3	1:D:673:TRP:HZ2	1.75	0.51
1:A:1253:LYS:NZ	1:A:1597:TRP:O	2.44	0.51
1:A:1999:HIS:O	1:A:2003:MET:HG2	2.11	0.51
1:A:4118:LEU:O	1:A:4122:GLU:HG2	2.11	0.51
1:B:4081:GLU:O	1:B:4085:ARG:HG2	2.10	0.51
1:C:763:ALA:HB3	1:C:764:PRO:HD3	1.92	0.51
1:C:1704:TYR:O	1:C:1708:ILE:HG12	2.10	0.51
1:C:1986:PRO:HB2	1:C:1988:PRO:HD2	1.93	0.51
1:D:182:ILE:HD11	1:D:191:TYR:HE1	1.74	0.51
1:D:281:ARG:O	1:D:285:SER:OG	2.27	0.51
1:D:4115:GLN:O	1:D:4119:GLU:HG2	2.11	0.51
1:A:4042:ILE:HG21	1:A:4047:PHE:HB2	1.92	0.51
1:B:191:TYR:N	1:B:206:ALA:O	2.35	0.51
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.91	0.51
1:D:486:GLN:CB	1:D:544:ASN:HD21	2.24	0.51
1:D:2254:LEU:HD22	1:D:3809:ARG:HG3	1.91	0.51
1:A:228:LEU:HD22	1:A:289:ILE:HB	1.93	0.51
1:A:442:LEU:HG	1:A:444:THR:HG22	1.93	0.51
1:A:497:LEU:O	1:A:500:GLU:HG2	2.11	0.51
1:A:3801:VAL:HG13	1:A:3883:SER:HB2	1.93	0.51
1:A:4115:GLN:O	1:A:4119:GLU:HG2	2.11	0.51
1:B:228:LEU:HD22	1:B:289:ILE:HB	1.93	0.51
1:B:766:ILE:HG22	1:B:768:PHE:CE2	2.46	0.51
1:B:1704:TYR:O	1:B:1708:ILE:HG12	2.10	0.51
1:B:3801:VAL:HG13	1:B:3883:SER:HB2	1.93	0.51
2:I:28:THR:HA	2:I:39:SER:HA	1.93	0.51
1:D:1789:LYS:HB2	1:D:1835:PHE:CE1	2.46	0.51
1:A:1704:TYR:O	1:A:1708:ILE:HG12	2.10	0.50
1:B:386:SER:HB3	1:B:388:GLN:HE22	1.75	0.50
1:B:497:LEU:O	1:B:500:GLU:HG2	2.11	0.50
1:B:1225:LYS:HB3	1:B:1226:TYR:HD2	1.73	0.50
1:B:1999:HIS:O	1:B:2003:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:LEU:HD22	1:C:289:ILE:HB	1.93	0.50
1:C:474:ASP:O	1:C:478:ARG:HG2	2.11	0.50
1:C:1665:VAL:HG23	1:C:1677:LEU:HD11	1.93	0.50
1:C:1789:LYS:HB2	1:C:1835:PHE:CE1	2.46	0.50
1:C:1969:GLN:OE1	1:C:1969:GLN:HA	2.10	0.50
1:C:1999:HIS:O	1:C:2003:MET:HG2	2.11	0.50
1:D:497:LEU:O	1:D:500:GLU:HG2	2.11	0.50
1:D:766:ILE:HG22	1:D:768:PHE:CE2	2.46	0.50
1:D:1999:HIS:O	1:D:2003:MET:HG2	2.11	0.50
1:D:3801:VAL:HG13	1:D:3883:SER:HB2	1.93	0.50
1:D:4009:VAL:HA	1:D:4012:ILE:HG12	1.91	0.50
1:A:1789:LYS:HB2	1:A:1835:PHE:HE1	1.76	0.50
1:A:2720:ILE:HD11	1:A:2778:LEU:HD22	1.91	0.50
1:B:1253:LYS:NZ	1:B:1597:TRP:O	2.44	0.50
1:C:1253:LYS:NZ	1:C:1597:TRP:O	2.44	0.50
1:D:890:HIS:O	1:D:894:VAL:HG23	2.11	0.50
1:D:1704:TYR:O	1:D:1708:ILE:HG12	2.10	0.50
1:D:1749:LEU:HD13	1:D:1844:LEU:HD12	1.93	0.50
1:B:474:ASP:O	1:B:478:ARG:HG2	2.11	0.50
1:B:1665:VAL:HG23	1:B:1677:LEU:HD11	1.93	0.50
1:B:4851:PHE:O	1:B:4856:ILE:HG12	2.12	0.50
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.93	0.50
1:C:497:LEU:O	1:C:500:GLU:HG2	2.11	0.50
1:C:890:HIS:O	1:C:894:VAL:HG23	2.11	0.50
1:C:1245:ARG:NH1	1:C:1809:ASP:O	2.33	0.50
1:C:1972:ILE:HA	1:C:1975:LEU:HG	1.92	0.50
1:A:1789:LYS:HB2	1:A:1835:PHE:CE1	2.46	0.50
1:C:442:LEU:HG	1:C:444:THR:HG22	1.93	0.50
1:C:4851:PHE:O	1:C:4856:ILE:HG12	2.12	0.50
1:D:1303:ARG:N	1:D:1590:GLN:O	2.35	0.50
1:D:1629:MET:HG3	1:D:1642:ILE:HB	1.94	0.50
2:J:28:THR:HA	2:J:39:SER:HA	1.93	0.50
1:A:182:ILE:HD11	1:A:191:TYR:HE1	1.74	0.50
1:A:1986:PRO:HB2	1:A:1988:PRO:HD2	1.93	0.50
1:B:2086:LEU:O	1:B:2090:GLN:HG2	2.12	0.50
1:C:766:ILE:HG22	1:C:768:PHE:CE2	2.46	0.50
1:D:191:TYR:N	1:D:206:ALA:O	2.35	0.50
1:D:1962:ARG:O	1:D:1966:SER:OG	2.28	0.50
1:A:474:ASP:O	1:A:478:ARG:HG2	2.11	0.50
1:A:2232:ALA:HB3	1:A:2233:MET:HE2	1.92	0.50
1:B:837:SER:H	1:B:841:LYS:HZ2	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1938:ASN:ND2	1:B:1988:PRO:HB3	2.27	0.50
1:B:4115:GLN:O	1:B:4119:GLU:HG2	2.11	0.50
1:B:4283:PHE:HB2	1:B:4513:PHE:CE1	2.47	0.50
1:D:1665:VAL:HG23	1:D:1677:LEU:HD11	1.93	0.50
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.92	0.50
1:A:1665:VAL:HG23	1:A:1677:LEU:HD11	1.93	0.50
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.93	0.50
1:B:4772:LEU:HD13	1:C:4752:LEU:HD21	1.94	0.50
1:D:228:LEU:HD22	1:D:289:ILE:HB	1.93	0.50
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.77	0.50
1:D:1245:ARG:NH1	1:D:1809:ASP:O	2.33	0.50
1:D:1972:ILE:HA	1:D:1975:LEU:HG	1.92	0.50
1:A:1052:GLU:HA	1:A:1055:ARG:HB2	1.92	0.50
1:A:1972:ILE:HA	1:A:1975:LEU:HG	1.92	0.50
1:A:2271:CYS:SG	1:A:2294:GLY:N	2.85	0.50
1:B:634:ASP:HA	2:H:90:GLY:HA2	1.94	0.50
2:H:28:THR:HA	2:H:39:SER:HA	1.93	0.50
2:I:88:HIS:H	2:I:92:ILE:HB	1.77	0.50
1:D:2086:LEU:O	1:D:2090:GLN:HG2	2.12	0.50
1:A:1629:MET:HG3	1:A:1642:ILE:HB	1.94	0.50
1:A:4851:PHE:O	1:A:4856:ILE:HG12	2.12	0.50
2:G:88:HIS:H	2:G:92:ILE:HB	1.77	0.50
1:B:1789:LYS:HB2	1:B:1835:PHE:HE1	1.76	0.50
1:C:1226:TYR:CD2	1:C:1226:TYR:N	2.80	0.50
1:C:1789:LYS:HB2	1:C:1835:PHE:HE1	1.76	0.50
1:C:2258:GLU:N	1:C:2259:PRO:HD2	2.27	0.50
1:D:654:SER:HB2	1:D:837:SER:HB2	1.94	0.50
1:D:674:TYR:N	1:D:820:ALA:O	2.45	0.50
1:D:1789:LYS:HB2	1:D:1835:PHE:HE1	1.76	0.50
2:J:11:GLY:HA3	2:J:71:GLN:HB2	1.94	0.50
1:A:747:HIS:CE1	1:A:770:ILE:HD11	2.47	0.49
1:A:4283:PHE:HB2	1:A:4513:PHE:CE1	2.47	0.49
1:B:1245:ARG:NH1	1:B:1809:ASP:O	2.33	0.49
1:B:2258:GLU:N	1:B:2259:PRO:HD2	2.27	0.49
1:C:1749:LEU:HD13	1:C:1844:LEU:HD12	1.93	0.49
1:C:2086:LEU:O	1:C:2090:GLN:HG2	2.12	0.49
1:C:4283:PHE:HB2	1:C:4513:PHE:CE1	2.47	0.49
1:D:2233:MET:HE2	1:D:2233:MET:H	1.77	0.49
1:D:4851:PHE:O	1:D:4856:ILE:HG12	2.12	0.49
1:A:3636:GLU:HG3	1:A:3693:ILE:HG23	1.94	0.49
1:B:176:ARG:N	1:B:179:ASP:OD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:TYR:N	1:B:820:ALA:O	2.45	0.49
1:C:674:TYR:N	1:C:820:ALA:O	2.45	0.49
1:C:1938:ASN:ND2	1:C:1988:PRO:HB3	2.27	0.49
1:D:442:LEU:HG	1:D:444:THR:HG22	1.93	0.49
1:D:1052:GLU:HA	1:D:1055:ARG:HB2	1.92	0.49
1:D:1253:LYS:NZ	1:D:1597:TRP:O	2.44	0.49
1:D:2258:GLU:N	1:D:2259:PRO:HD2	2.27	0.49
1:D:2271:CYS:SG	1:D:2294:GLY:N	2.85	0.49
1:A:4668:LEU:HD12	1:A:4669:LEU:HD12	1.95	0.49
1:B:890:HIS:O	1:B:894:VAL:HG23	2.11	0.49
1:B:1682:ASP:HB2	1:B:1685:GLN:HG2	1.94	0.49
2:H:88:HIS:H	2:H:92:ILE:HB	1.77	0.49
1:C:1165:MET:HB3	1:C:1236:TYR:CE2	2.47	0.49
1:C:1629:MET:HG3	1:C:1642:ILE:HB	1.94	0.49
1:C:2231:PRO:HD3	1:C:2381:ILE:HD11	1.95	0.49
1:C:2271:CYS:SG	1:C:2294:GLY:N	2.85	0.49
1:C:3801:VAL:HG13	1:C:3883:SER:HB2	1.93	0.49
2:I:11:GLY:HA3	2:I:71:GLN:HB2	1.94	0.49
1:D:1226:TYR:CD2	1:D:1226:TYR:N	2.80	0.49
1:D:4044:LYS:HB2	1:D:4075:GLU:HG2	1.95	0.49
1:D:4283:PHE:HB2	1:D:4513:PHE:CE1	2.47	0.49
1:A:2258:GLU:N	1:A:2259:PRO:HD2	2.27	0.49
1:A:4029:ASP:OD2	1:A:4054:HIS:NE2	2.43	0.49
2:H:62:GLU:O	2:H:66:GLN:HG3	2.12	0.49
2:J:24:VAL:HG22	2:J:48:LYS:HG2	1.93	0.49
2:J:62:GLU:O	2:J:66:GLN:HG3	2.12	0.49
1:B:125:TYR:OH	1:B:417:ARG:HB3	2.13	0.49
1:B:654:SER:HB2	1:B:837:SER:HB2	1.94	0.49
1:B:747:HIS:CE1	1:B:770:ILE:HD11	2.47	0.49
1:C:799:LYS:HG2	1:C:1621:GLN:NE2	2.28	0.49
1:D:1114:ARG:HB2	1:D:1128:LEU:HD23	1.95	0.49
1:D:2313:GLU:OE1	1:D:3812:LYS:NZ	2.40	0.49
1:D:4668:LEU:HD12	1:D:4669:LEU:HD12	1.95	0.49
1:A:76:ARG:HH12	1:B:3889:TRP:HB3	1.74	0.49
1:A:1165:MET:HB3	1:A:1236:TYR:CE2	2.47	0.49
1:A:1226:TYR:CD2	1:A:1226:TYR:N	2.80	0.49
1:A:1749:LEU:HD13	1:A:1844:LEU:HD12	1.93	0.49
1:A:2086:LEU:O	1:A:2090:GLN:HG2	2.12	0.49
1:A:3961:SER:OG	1:A:3962:SER:N	2.45	0.49
1:B:442:LEU:HG	1:B:444:THR:HG22	1.93	0.49
1:B:799:LYS:HG2	1:B:1621:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1629:MET:HG3	1:B:1642:ILE:HB	1.94	0.49
2:H:11:GLY:HA3	2:H:71:GLN:HB2	1.94	0.49
1:C:1303:ARG:N	1:C:1590:GLN:O	2.35	0.49
1:C:1747:HIS:O	1:C:1747:HIS:ND1	2.39	0.49
1:C:2262:GLU:O	1:C:2266:ARG:HG3	2.13	0.49
2:I:24:VAL:HG22	2:I:48:LYS:HG2	1.93	0.49
1:D:323:ASP:O	1:D:327:THR:OG1	2.26	0.49
1:D:2262:GLU:O	1:D:2266:ARG:HG3	2.13	0.49
2:J:88:HIS:H	2:J:92:ILE:HB	1.77	0.49
1:A:313:ASN:ND2	1:A:391:ALA:O	2.46	0.49
1:B:647:ARG:HE	2:H:36:LYS:HE2	1.77	0.49
1:B:1114:ARG:HB2	1:B:1128:LEU:HD23	1.95	0.49
1:B:2171:MET:O	1:B:2175:VAL:HG23	2.13	0.49
1:B:2231:PRO:HD3	1:B:2381:ILE:HD11	1.95	0.49
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.77	0.49
1:C:1114:ARG:HB2	1:C:1128:LEU:HD23	1.95	0.49
1:C:1362:ASP:N	1:C:1362:ASP:OD1	2.46	0.49
2:I:62:GLU:O	2:I:66:GLN:HG3	2.12	0.49
1:D:125:TYR:OH	1:D:417:ARG:HB3	2.13	0.49
1:D:1165:MET:HB3	1:D:1236:TYR:CE2	2.47	0.49
1:D:1362:ASP:OD1	1:D:1362:ASP:N	2.46	0.49
1:A:674:TYR:N	1:A:820:ALA:O	2.45	0.49
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.77	0.49
1:A:1114:ARG:HB2	1:A:1128:LEU:HD23	1.95	0.49
1:A:1683:GLU:HB3	2:G:42:ASP:HB3	1.95	0.49
2:G:11:GLY:HA3	2:G:71:GLN:HB2	1.94	0.49
1:C:747:HIS:CE1	1:C:770:ILE:HD11	2.47	0.49
1:D:3636:GLU:HG3	1:D:3693:ILE:HG23	1.94	0.49
1:A:654:SER:HB2	1:A:837:SER:HB2	1.94	0.49
1:A:1166:VAL:HG22	1:A:1173:MET:SD	2.53	0.49
2:G:28:THR:HA	2:G:39:SER:HA	1.93	0.49
1:B:1165:MET:HB3	1:B:1236:TYR:CE2	2.47	0.49
1:B:1226:TYR:CD2	1:B:1226:TYR:N	2.80	0.49
1:B:2271:CYS:SG	1:B:2294:GLY:N	2.85	0.49
1:B:4103:ASN:OD1	1:B:4107:HIS:ND1	2.38	0.49
1:C:191:TYR:HE2	1:D:2325:ARG:CZ	2.26	0.49
1:C:1359:ILE:HG13	1:C:1360:ASP:N	2.28	0.49
1:C:3961:SER:OG	1:C:3962:SER:N	2.45	0.49
1:C:4044:LYS:HB2	1:C:4075:GLU:HG2	1.94	0.49
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.46	0.49
1:A:2171:MET:O	1:A:2175:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4044:LYS:HB2	1:A:4075:GLU:HG2	1.94	0.49
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.77	0.49
1:B:1166:VAL:HG22	1:B:1173:MET:SD	2.53	0.49
1:C:313:ASN:ND2	1:C:391:ALA:O	2.46	0.49
1:C:654:SER:HB2	1:C:837:SER:HB2	1.94	0.49
1:C:1968:PRO:HA	1:C:1971:GLN:HB3	1.95	0.49
1:D:313:ASN:ND2	1:D:391:ALA:O	2.46	0.49
1:D:799:LYS:HG2	1:D:1621:GLN:NE2	2.28	0.49
2:J:17:PRO:HG2	2:J:64:ALA:O	2.13	0.49
1:A:890:HIS:O	1:A:894:VAL:HG23	2.11	0.48
1:A:3965:GLU:O	1:A:3969:GLU:HG2	2.13	0.48
2:G:62:GLU:O	2:G:66:GLN:HG3	2.12	0.48
1:B:313:ASN:ND2	1:B:391:ALA:O	2.46	0.48
1:B:844:ARG:HE	1:B:845:THR:HG22	1.78	0.48
1:B:1358:ARG:NH2	1:B:1359:ILE:O	2.46	0.48
1:B:1359:ILE:HG13	1:B:1360:ASP:N	2.28	0.48
1:B:2196:CYS:HB2	1:B:2236:SER:HB3	1.95	0.48
1:B:3965:GLU:O	1:B:3969:GLU:HG2	2.13	0.48
2:H:17:PRO:HG2	2:H:64:ALA:O	2.13	0.48
1:C:2487:LEU:HA	1:C:2491:PHE:HB2	1.94	0.48
1:C:4913:ASN:HB3	1:C:4916:ASN:HB2	1.95	0.48
1:B:296:ARG:HH21	1:B:324:VAL:HG12	1.78	0.48
1:B:2262:GLU:O	1:B:2266:ARG:HG3	2.13	0.48
1:B:4668:LEU:HD12	1:B:4669:LEU:HD12	1.95	0.48
1:C:1682:ASP:HB2	1:C:1685:GLN:HG2	1.94	0.48
1:C:2170:VAL:HG21	1:C:2198:PHE:CD2	2.48	0.48
1:C:4668:LEU:HD12	1:C:4669:LEU:HD12	1.95	0.48
1:D:446:ASP:OD1	1:D:446:ASP:N	2.45	0.48
1:D:1358:ARG:NH2	1:D:1359:ILE:O	2.46	0.48
1:A:125:TYR:OH	1:A:417:ARG:HB3	2.13	0.48
1:A:296:ARG:HH21	1:A:324:VAL:HG12	1.78	0.48
1:A:2262:GLU:O	1:A:2266:ARG:HG3	2.13	0.48
1:B:1749:LEU:HD13	1:B:1844:LEU:HD12	1.93	0.48
1:C:125:TYR:OH	1:C:417:ARG:HB3	2.13	0.48
1:C:1166:VAL:HG22	1:C:1173:MET:SD	2.53	0.48
1:C:2197:ARG:HB3	1:C:2236:SER:OG	2.14	0.48
1:C:4024:ASP:OD1	1:C:4025:LEU:N	2.47	0.48
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.46	0.48
1:D:747:HIS:CE1	1:D:770:ILE:HD11	2.47	0.48
1:D:2231:PRO:HD3	1:D:2381:ILE:HD11	1.95	0.48
1:A:191:TYR:N	1:A:206:ALA:O	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2170:VAL:HG21	1:A:2198:PHE:CD2	2.48	0.48
1:C:176:ARG:N	1:C:179:ASP:OD2	2.42	0.48
1:C:1358:ARG:NH2	1:C:1359:ILE:O	2.46	0.48
1:C:2196:CYS:HB2	1:C:2236:SER:HB3	1.96	0.48
1:D:1682:ASP:HB2	1:D:1685:GLN:HG2	1.94	0.48
1:A:2197:ARG:HB3	1:A:2236:SER:OG	2.14	0.48
1:A:2487:LEU:HA	1:A:2491:PHE:HB2	1.94	0.48
2:G:17:PRO:HG2	2:G:64:ALA:O	2.13	0.48
1:B:4661:GLY:H	1:B:4664:ARG:NH1	2.12	0.48
1:C:2171:MET:O	1:C:2175:VAL:HG23	2.13	0.48
1:C:3636:GLU:HG3	1:C:3693:ILE:HG23	1.94	0.48
1:C:3965:GLU:O	1:C:3969:GLU:HG2	2.13	0.48
2:I:17:PRO:HG2	2:I:64:ALA:O	2.13	0.48
1:D:231:GLY:O	1:D:276:ARG:NH1	2.47	0.48
1:D:3961:SER:OG	1:D:3962:SER:N	2.45	0.48
1:D:4661:GLY:H	1:D:4664:ARG:NH1	2.12	0.48
1:D:4913:ASN:HB3	1:D:4916:ASN:HB2	1.95	0.48
1:A:844:ARG:HE	1:A:845:THR:HG22	1.78	0.48
1:A:1966:SER:OG	1:A:1966:SER:O	2.32	0.48
1:A:2196:CYS:HB2	1:A:2236:SER:HB3	1.96	0.48
1:B:3636:GLU:HG3	1:B:3693:ILE:HG23	1.94	0.48
1:B:4044:LYS:HB2	1:B:4075:GLU:HG2	1.94	0.48
2:H:18:LYS:HB2	2:H:18:LYS:NZ	2.29	0.48
1:C:759:LEU:HD13	1:C:766:ILE:HG12	1.95	0.48
1:D:394:HIS:ND1	1:D:395:HIS:N	2.62	0.48
1:D:2191:MET:HE2	1:D:2191:MET:O	2.14	0.48
1:D:2197:ARG:HB3	1:D:2236:SER:OG	2.13	0.48
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.46	0.48
1:A:4024:ASP:OD1	1:A:4025:LEU:N	2.47	0.48
1:B:231:GLY:O	1:B:276:ARG:NH1	2.47	0.48
1:B:2170:VAL:HG21	1:B:2198:PHE:CD2	2.48	0.48
1:B:2191:MET:HE2	1:B:2191:MET:O	2.13	0.48
1:D:844:ARG:HE	1:D:845:THR:HG22	1.78	0.48
1:D:1166:VAL:HG22	1:D:1173:MET:SD	2.53	0.48
1:D:1359:ILE:HG13	1:D:1360:ASP:N	2.28	0.48
1:D:1931:PHE:CE2	1:D:1995:LEU:HB2	2.49	0.48
1:A:140:THR:O	1:B:2337:GLU:HG3	2.12	0.48
1:A:169:ARG:HH12	1:A:176:ARG:HE	1.62	0.48
1:A:231:GLY:O	1:A:276:ARG:NH1	2.47	0.48
1:A:799:LYS:HG2	1:A:1621:GLN:NE2	2.28	0.48
1:A:3688:MET:SD	1:A:3752:PRO:HB2	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4304:PHE:O	1:A:4308:VAL:HG13	2.14	0.48
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.46	0.48
1:B:486:GLN:HB3	1:B:544:ASN:ND2	2.26	0.48
1:B:2197:ARG:HB3	1:B:2236:SER:OG	2.14	0.48
1:B:2487:LEU:HA	1:B:2491:PHE:HB2	1.94	0.48
1:C:231:GLY:O	1:C:276:ARG:NH1	2.47	0.48
1:C:631:LEU:O	1:C:635:ASN:HB2	2.14	0.48
1:D:2257:ARG:HB3	1:D:2259:PRO:HD2	1.96	0.48
1:D:4304:PHE:O	1:D:4308:VAL:HG13	2.14	0.48
1:A:1682:ASP:HB2	1:A:1685:GLN:HG2	1.94	0.48
2:G:18:LYS:HB2	2:G:18:LYS:NZ	2.29	0.48
1:B:1677:LEU:HA	1:B:1680:HIS:HB2	1.96	0.48
1:C:1226:TYR:HD2	1:C:1226:TYR:N	2.12	0.48
1:C:1931:PHE:CE2	1:C:1995:LEU:HB2	2.49	0.48
1:C:3919:LEU:HD22	1:C:3934:LEU:HD11	1.96	0.48
2:J:18:LYS:HB2	2:J:18:LYS:NZ	2.29	0.48
1:A:1359:ILE:HG13	1:A:1360:ASP:N	2.28	0.48
1:A:1931:PHE:CE2	1:A:1995:LEU:HB2	2.49	0.48
1:A:2191:MET:HE2	1:A:2191:MET:O	2.14	0.48
1:A:2231:PRO:HD3	1:A:2381:ILE:HD11	1.95	0.48
1:B:3961:SER:OG	1:B:3962:SER:N	2.45	0.48
1:D:2170:VAL:HG21	1:D:2198:PHE:CD2	2.48	0.48
1:A:851:LEU:HB3	1:A:1212:VAL:HG12	1.96	0.47
1:A:875:PRO:HD2	1:A:882:ARG:HH12	1.79	0.47
1:A:1968:PRO:HA	1:A:1971:GLN:HB3	1.95	0.47
1:B:394:HIS:ND1	1:B:395:HIS:N	2.62	0.47
1:B:875:PRO:HD2	1:B:882:ARG:HH12	1.79	0.47
1:B:4913:ASN:HB3	1:B:4916:ASN:HB2	1.95	0.47
1:C:323:ASP:O	1:C:327:THR:OG1	2.26	0.47
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.46	0.47
2:I:3:VAL:HG11	2:I:59:GLY:HA2	1.96	0.47
1:D:1677:LEU:HA	1:D:1680:HIS:HB2	1.96	0.47
1:D:2487:LEU:HA	1:D:2491:PHE:HB2	1.94	0.47
1:D:3613:HIS:HA	1:D:3616:VAL:HG12	1.96	0.47
1:A:394:HIS:ND1	1:A:395:HIS:N	2.62	0.47
1:A:1156:TRP:HB3	1:A:1177:LEU:HD11	1.95	0.47
1:A:1257:GLN:HA	1:A:1384:LEU:HD22	1.95	0.47
1:A:4661:GLY:H	1:A:4664:ARG:NH1	2.12	0.47
1:B:631:LEU:O	1:B:635:ASN:HB2	2.14	0.47
1:B:759:LEU:HD13	1:B:766:ILE:HG12	1.95	0.47
1:B:1362:ASP:N	1:B:1362:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4298:ALA:HA	1:B:4301:CYS:SG	2.55	0.47
1:C:296:ARG:HH21	1:C:324:VAL:HG12	1.78	0.47
1:C:851:LEU:HB3	1:C:1212:VAL:HG12	1.96	0.47
1:C:1677:LEU:HA	1:C:1680:HIS:HB2	1.96	0.47
1:C:2191:MET:HE2	1:C:2191:MET:O	2.14	0.47
1:D:169:ARG:HH12	1:D:176:ARG:HE	1.62	0.47
1:D:801:ARG:HA	1:D:1618:TRP:O	2.14	0.47
1:D:1968:PRO:HA	1:D:1971:GLN:HB3	1.95	0.47
1:D:3919:LEU:HD22	1:D:3934:LEU:HD11	1.96	0.47
1:D:4024:ASP:OD1	1:D:4025:LEU:N	2.47	0.47
1:A:631:LEU:O	1:A:635:ASN:HB2	2.14	0.47
1:A:801:ARG:HA	1:A:1618:TRP:O	2.14	0.47
1:A:1358:ARG:NH2	1:A:1359:ILE:O	2.46	0.47
1:A:1677:LEU:HA	1:A:1680:HIS:HB2	1.96	0.47
1:A:4044:LYS:O	1:A:4045:ARG:NH1	2.48	0.47
1:B:851:LEU:HB3	1:B:1212:VAL:HG12	1.96	0.47
1:B:3688:MET:SD	1:B:3752:PRO:HB2	2.54	0.47
1:B:4304:PHE:O	1:B:4308:VAL:HG13	2.14	0.47
1:C:837:SER:H	1:C:841:LYS:HZ2	1.61	0.47
1:D:4298:ALA:HA	1:D:4301:CYS:SG	2.55	0.47
1:A:4298:ALA:HA	1:A:4301:CYS:SG	2.55	0.47
1:B:1226:TYR:HD2	1:B:1226:TYR:N	2.12	0.47
1:B:1257:GLN:HA	1:B:1384:LEU:HD22	1.95	0.47
1:B:2132:ARG:HG2	1:B:2133:MET:H	1.80	0.47
1:B:2278:MET:O	1:B:2282:LYS:HG2	2.15	0.47
1:B:3919:LEU:HD22	1:B:3934:LEU:HD11	1.96	0.47
1:B:4024:ASP:OD1	1:B:4025:LEU:N	2.47	0.47
2:H:3:VAL:HG11	2:H:59:GLY:HA2	1.96	0.47
1:C:1156:TRP:HB3	1:C:1177:LEU:HD11	1.95	0.47
1:C:4298:ALA:HA	1:C:4301:CYS:SG	2.55	0.47
1:D:227:TYR:HD2	1:D:352:SER:HB3	1.80	0.47
1:D:486:GLN:HB3	1:D:544:ASN:ND2	2.26	0.47
1:D:631:LEU:O	1:D:635:ASN:HB2	2.14	0.47
1:D:1156:TRP:HB3	1:D:1177:LEU:HD11	1.95	0.47
1:D:1226:TYR:HD2	1:D:1226:TYR:N	2.12	0.47
1:D:1960:LYS:HD3	1:D:1960:LYS:HA	1.60	0.47
1:D:2196:CYS:HB2	1:D:2236:SER:HB3	1.96	0.47
1:A:589:ILE:HG13	1:A:617:LEU:HD21	1.97	0.47
1:A:2405:MET:HG3	1:A:2405:MET:O	2.14	0.47
1:A:2716:LEU:HD22	1:A:2778:LEU:HD21	1.97	0.47
1:A:4177:ASN:HD21	1:A:4875:GLN:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4913:ASN:HB3	1:A:4916:ASN:HB2	1.95	0.47
1:B:1156:TRP:HB3	1:B:1177:LEU:HD11	1.95	0.47
1:B:1968:PRO:HA	1:B:1971:GLN:HB3	1.95	0.47
1:C:2132:ARG:HG2	1:C:2133:MET:H	1.80	0.47
1:D:2765:LYS:O	1:D:2769:ILE:HG23	2.15	0.47
1:D:3688:MET:SD	1:D:3752:PRO:HB2	2.54	0.47
1:D:3965:GLU:O	1:D:3969:GLU:HG2	2.13	0.47
1:A:759:LEU:HD13	1:A:766:ILE:HG12	1.95	0.47
1:A:2257:ARG:HB3	1:A:2259:PRO:HD2	1.96	0.47
1:A:2278:MET:O	1:A:2282:LYS:HG2	2.14	0.47
1:A:3613:HIS:HA	1:A:3616:VAL:HG12	1.96	0.47
1:B:281:ARG:O	1:B:285:SER:OG	2.27	0.47
1:B:2257:ARG:HB3	1:B:2259:PRO:HD2	1.96	0.47
1:B:2716:LEU:HD22	1:B:2778:LEU:HD21	1.97	0.47
1:B:4177:ASN:HD21	1:B:4875:GLN:HB3	1.79	0.47
1:C:270:HIS:CD2	1:C:491:GLU:HG3	2.49	0.47
1:C:766:ILE:HG22	1:C:768:PHE:HE2	1.80	0.47
1:C:844:ARG:HE	1:C:845:THR:HG22	1.78	0.47
1:C:4661:GLY:H	1:C:4664:ARG:NH1	2.12	0.47
1:D:759:LEU:HD13	1:D:766:ILE:HG12	1.95	0.47
1:D:3940:TRP:HA	1:D:3943:VAL:HG22	1.97	0.47
1:D:4792:TYR:HH	1:D:4815:HIS:HE2	1.61	0.47
1:A:270:HIS:CD2	1:A:491:GLU:HG3	2.49	0.47
1:A:1226:TYR:HD2	1:A:1226:TYR:N	2.12	0.47
1:A:3919:LEU:HD22	1:A:3934:LEU:HD11	1.96	0.47
1:B:270:HIS:CD2	1:B:491:GLU:HG3	2.49	0.47
1:B:589:ILE:HG13	1:B:617:LEU:HD21	1.97	0.47
1:B:747:HIS:HB2	1:B:750:ARG:HH22	1.80	0.47
1:B:874:LEU:HD11	1:B:941:LYS:HD3	1.97	0.47
1:B:1931:PHE:CE2	1:B:1995:LEU:HB2	2.49	0.47
1:B:2765:LYS:O	1:B:2769:ILE:HG23	2.15	0.47
1:B:4029:ASP:OD2	1:B:4054:HIS:NE2	2.43	0.47
1:B:4044:LYS:O	1:B:4045:ARG:NH1	2.48	0.47
1:C:169:ARG:HH12	1:C:176:ARG:HE	1.62	0.47
1:C:839:GLU:HG2	1:C:840:TYR:CD1	2.50	0.47
1:C:875:PRO:HD2	1:C:882:ARG:HH12	1.79	0.47
1:C:2257:ARG:HB3	1:C:2259:PRO:HD2	1.96	0.47
1:C:2716:LEU:HD22	1:C:2778:LEU:HD21	1.97	0.47
1:C:4304:PHE:O	1:C:4308:VAL:HG13	2.14	0.47
1:D:296:ARG:HH21	1:D:324:VAL:HG12	1.78	0.47
1:D:2171:MET:O	1:D:2175:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2385:ASN:HD22	1:D:2457:ALA:C	2.18	0.47
1:D:4029:ASP:OD2	1:D:4054:HIS:NE2	2.43	0.47
1:B:721:ASP:OD1	1:B:721:ASP:N	2.48	0.47
1:B:4045:ARG:CZ	1:B:4045:ARG:HA	2.45	0.47
1:C:394:HIS:ND1	1:C:395:HIS:N	2.62	0.47
1:C:486:GLN:HB3	1:C:544:ASN:ND2	2.26	0.47
1:C:1966:SER:OG	1:C:1966:SER:O	2.32	0.47
1:C:4044:LYS:O	1:C:4045:ARG:NH1	2.48	0.47
1:D:874:LEU:HD11	1:D:941:LYS:HD3	1.97	0.47
1:D:1683:GLU:HB3	2:J:42:ASP:HB3	1.96	0.47
1:D:2405:MET:O	1:D:2405:MET:HG3	2.14	0.47
1:D:2716:LEU:HD22	1:D:2778:LEU:HD21	1.97	0.47
2:G:38:ASP:OD1	2:G:39:SER:N	2.48	0.47
1:B:336:GLU:HG3	1:B:338:LEU:HD22	1.97	0.47
1:B:801:ARG:HA	1:B:1618:TRP:O	2.14	0.47
1:B:2261:LEU:O	1:B:2265:VAL:HG23	2.15	0.47
1:C:227:TYR:HD2	1:C:352:SER:HB3	1.79	0.47
1:C:589:ILE:HG13	1:C:617:LEU:HD21	1.97	0.47
1:C:801:ARG:HA	1:C:1618:TRP:O	2.14	0.47
1:C:1173:MET:HB3	1:C:1191:ALA:HB3	1.97	0.47
2:I:18:LYS:NZ	2:I:18:LYS:HB2	2.29	0.47
1:D:851:LEU:HB3	1:D:1212:VAL:HG12	1.96	0.47
1:A:850:LEU:HD23	1:A:1213:GLY:O	2.15	0.47
1:B:169:ARG:HH12	1:B:176:ARG:HE	1.62	0.47
1:B:1173:MET:HB3	1:B:1191:ALA:HB3	1.97	0.47
1:B:1173:MET:HB2	1:B:1192:PHE:H	1.80	0.47
1:C:2278:MET:O	1:C:2282:LYS:HG2	2.14	0.47
1:D:270:HIS:CD2	1:D:491:GLU:HG3	2.49	0.47
1:D:721:ASP:N	1:D:721:ASP:OD1	2.48	0.47
1:D:2261:LEU:O	1:D:2265:VAL:HG23	2.15	0.47
1:D:3822:GLU:HB3	1:D:3826:GLU:HA	1.98	0.47
1:D:4029:ASP:OD1	1:D:4029:ASP:N	2.48	0.47
1:B:1966:SER:OG	1:B:1966:SER:O	2.32	0.46
1:B:4750:LYS:HA	1:B:4753:ARG:HG2	1.97	0.46
1:C:721:ASP:OD1	1:C:721:ASP:N	2.48	0.46
1:C:750:ARG:NH2	2:I:10:PRO:HD3	2.29	0.46
1:C:4045:ARG:HA	1:C:4045:ARG:CZ	2.45	0.46
1:D:839:GLU:HG2	1:D:840:TYR:CD1	2.50	0.46
1:D:1747:HIS:O	1:D:1747:HIS:ND1	2.39	0.46
2:J:3:VAL:HG11	2:J:59:GLY:HA2	1.96	0.46
1:A:2132:ARG:HG2	1:A:2133:MET:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2385:ASN:HD22	1:A:2457:ALA:C	2.18	0.46
1:A:4045:ARG:CZ	1:A:4045:ARG:HA	2.45	0.46
1:A:4606:ALA:HB1	1:A:4648:VAL:HG21	1.97	0.46
1:A:4909:LEU:O	1:A:4913:ASN:ND2	2.49	0.46
1:B:766:ILE:HG22	1:B:768:PHE:HE2	1.80	0.46
1:B:2405:MET:HG3	1:B:2405:MET:O	2.14	0.46
1:C:336:GLU:HG3	1:C:338:LEU:HD22	1.97	0.46
1:C:747:HIS:HB2	1:C:750:ARG:HH22	1.80	0.46
1:C:2405:MET:HG3	1:C:2405:MET:O	2.14	0.46
1:C:4177:ASN:HD21	1:C:4875:GLN:HB3	1.79	0.46
1:D:723:PHE:HE2	1:D:1385:LYS:HE2	1.79	0.46
1:D:1256:PRO:HG2	1:D:1592:LEU:HD21	1.97	0.46
1:D:4177:ASN:HD21	1:D:4875:GLN:HB3	1.79	0.46
1:A:176:ARG:N	1:A:179:ASP:OD2	2.42	0.46
1:A:1008:ALA:O	1:A:1012:ILE:HG23	2.15	0.46
2:G:3:VAL:HG11	2:G:59:GLY:HA2	1.96	0.46
1:B:2240:ASP:OD1	1:B:2296:ARG:NH2	2.49	0.46
1:B:4941:LYS:HE3	1:B:4941:LYS:HB3	1.75	0.46
1:C:1173:MET:HB2	1:C:1192:PHE:H	1.80	0.46
1:C:1257:GLN:HA	1:C:1384:LEU:HD22	1.95	0.46
1:C:2240:ASP:OD1	1:C:2296:ARG:NH2	2.49	0.46
1:C:2765:LYS:O	1:C:2769:ILE:HG23	2.15	0.46
1:C:3822:GLU:HB3	1:C:3826:GLU:HA	1.98	0.46
1:D:875:PRO:HD2	1:D:882:ARG:HH12	1.79	0.46
1:D:1257:GLN:HA	1:D:1384:LEU:HD22	1.95	0.46
1:D:4750:LYS:HA	1:D:4753:ARG:HG2	1.97	0.46
1:A:336:GLU:HG3	1:A:338:LEU:HD22	1.97	0.46
1:A:747:HIS:HB2	1:A:750:ARG:HH22	1.80	0.46
1:A:1684:PRO:HD3	2:G:42:ASP:HB3	1.96	0.46
1:A:2765:LYS:O	1:A:2769:ILE:HG23	2.15	0.46
1:A:4866:ILE:HG12	1:D:4863:GLY:HA2	1.98	0.46
1:B:839:GLU:HG2	1:B:840:TYR:CD1	2.50	0.46
1:B:1008:ALA:O	1:B:1012:ILE:HG23	2.15	0.46
1:B:2238:PRO:HA	1:B:2241:VAL:HG12	1.98	0.46
1:B:3762:ILE:HD12	1:B:3840:ARG:HG3	1.98	0.46
1:B:4785:PHE:HA	1:B:4789:ARG:HH21	1.81	0.46
1:C:723:PHE:HE2	1:C:1385:LYS:HE2	1.80	0.46
1:C:1256:PRO:HG2	1:C:1592:LEU:HD21	1.97	0.46
1:C:2385:ASN:HD22	1:C:2457:ALA:C	2.18	0.46
1:D:336:GLU:HG3	1:D:338:LEU:HD22	1.98	0.46
1:D:850:LEU:HD23	1:D:1213:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4044:LYS:O	1:D:4045:ARG:NH1	2.48	0.46
1:A:227:TYR:HD2	1:A:352:SER:HB3	1.80	0.46
1:A:1747:HIS:O	1:A:1747:HIS:ND1	2.39	0.46
1:A:2839:MET:HB3	1:A:2892:PHE:CZ	2.51	0.46
1:B:323:ASP:O	1:B:327:THR:OG1	2.26	0.46
1:B:2271:CYS:SG	1:B:2293:GLU:HB2	2.56	0.46
1:B:2839:MET:HB3	1:B:2892:PHE:CZ	2.51	0.46
1:B:3719:GLU:HA	1:B:3722:LYS:HG2	1.98	0.46
1:B:3822:GLU:HB3	1:B:3826:GLU:HA	1.98	0.46
1:C:2118:LEU:HB2	1:C:2151:ASN:HD21	1.80	0.46
1:C:2261:LEU:O	1:C:2265:VAL:HG23	2.15	0.46
1:C:3613:HIS:HA	1:C:3616:VAL:HG12	1.96	0.46
1:C:3688:MET:SD	1:C:3752:PRO:HB2	2.54	0.46
1:C:3940:TRP:HA	1:C:3943:VAL:HG22	1.97	0.46
1:D:713:TRP:HE1	1:D:1604:PHE:HD1	1.64	0.46
1:A:486:GLN:HB3	1:A:544:ASN:ND2	2.26	0.46
1:A:2240:ASP:OD1	1:A:2296:ARG:NH2	2.49	0.46
1:A:3762:ILE:HD12	1:A:3840:ARG:HG3	1.98	0.46
1:A:4762:ASN:O	1:A:4764:LYS:N	2.49	0.46
1:B:3613:HIS:HA	1:B:3616:VAL:HG12	1.96	0.46
1:B:4606:ALA:HB1	1:B:4648:VAL:HG21	1.97	0.46
1:C:850:LEU:HD23	1:C:1213:GLY:O	2.15	0.46
1:C:874:LEU:HD11	1:C:941:LYS:HD3	1.97	0.46
1:C:4648:VAL:O	1:C:4652:VAL:HG12	2.16	0.46
1:C:4941:LYS:HE3	1:C:4941:LYS:HB3	1.75	0.46
1:D:589:ILE:HG13	1:D:617:LEU:HD21	1.97	0.46
1:D:1900:PRO:O	1:D:1904:GLN:HG2	2.16	0.46
1:D:2132:ARG:HG2	1:D:2133:MET:H	1.80	0.46
1:D:2853:LYS:HA	1:D:2856:LYS:HG2	1.98	0.46
1:A:884:ARG:HB3	1:A:1060:TYR:HE2	1.81	0.46
1:A:1357:ASP:OD1	1:A:1358:ARG:N	2.44	0.46
1:A:2065:MET:SD	1:A:2086:LEU:HD23	2.56	0.46
1:A:2853:LYS:HA	1:A:2856:LYS:HG2	1.98	0.46
1:B:380:LYS:HD2	1:B:380:LYS:HA	1.75	0.46
1:B:644:LEU:HD11	1:B:1651:LEU:HD22	1.98	0.46
1:C:713:TRP:HE1	1:C:1604:PHE:HD1	1.64	0.46
1:C:1900:PRO:O	1:C:1904:GLN:HG2	2.16	0.46
2:I:38:ASP:OD1	2:I:39:SER:N	2.48	0.46
1:D:238:HIS:HB2	1:D:241:MET:HB2	1.98	0.46
1:D:2088:HIS:HB2	1:D:3690:TYR:CE1	2.51	0.46
1:D:2240:ASP:OD1	1:D:2296:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2278:MET:O	1:D:2282:LYS:HG2	2.15	0.46
1:D:3762:ILE:HD12	1:D:3840:ARG:HG3	1.98	0.46
1:D:4606:ALA:HB1	1:D:4648:VAL:HG21	1.97	0.46
1:D:4909:LEU:O	1:D:4913:ASN:ND2	2.49	0.46
1:A:238:HIS:HB2	1:A:241:MET:HB2	1.98	0.46
1:A:446:ASP:OD1	1:A:446:ASP:N	2.45	0.46
1:A:766:ILE:HG22	1:A:768:PHE:HE2	1.80	0.46
1:A:839:GLU:HG2	1:A:840:TYR:CD1	2.50	0.46
1:A:1219:LYS:HE2	1:A:1219:LYS:HA	1.98	0.46
1:B:343:ARG:HH21	1:B:345:GLU:H	1.64	0.46
1:B:486:GLN:CB	1:B:544:ASN:HD21	2.24	0.46
1:B:2118:LEU:HB2	1:B:2151:ASN:HD21	1.80	0.46
1:B:4648:VAL:O	1:B:4652:VAL:HG12	2.16	0.46
1:C:169:ARG:HH22	1:C:176:ARG:HH21	1.64	0.46
1:C:4060:SER:O	1:C:4063:GLU:HG2	2.16	0.46
1:D:4045:ARG:CZ	1:D:4045:ARG:HA	2.45	0.46
1:D:4060:SER:O	1:D:4063:GLU:HG2	2.16	0.46
1:A:343:ARG:HH21	1:A:345:GLU:H	1.64	0.46
1:B:2385:ASN:HD22	1:B:2457:ALA:C	2.18	0.46
1:B:3940:TRP:HA	1:B:3943:VAL:HG22	1.97	0.46
1:C:644:LEU:HD11	1:C:1651:LEU:HD22	1.98	0.46
1:C:3748:GLY:HA2	1:C:3795:LEU:HG	1.98	0.46
1:D:1008:ALA:O	1:D:1012:ILE:HG23	2.15	0.46
1:D:2454:ASP:OD1	1:D:2454:ASP:N	2.49	0.46
1:A:1679:SER:HB2	2:G:37:PHE:O	2.16	0.46
1:A:1900:PRO:O	1:A:1904:GLN:HG2	2.16	0.46
1:A:3748:GLY:HA2	1:A:3795:LEU:HG	1.98	0.46
1:A:3822:GLU:HB3	1:A:3826:GLU:HA	1.98	0.46
1:A:4785:PHE:HA	1:A:4789:ARG:HH21	1.81	0.46
1:B:2853:LYS:HA	1:B:2856:LYS:HG2	1.98	0.46
1:B:3898:ASP:OD1	1:B:3898:ASP:N	2.49	0.46
1:B:4762:ASN:O	1:B:4764:LYS:N	2.49	0.46
1:B:4909:LEU:O	1:B:4913:ASN:ND2	2.49	0.46
1:C:1357:ASP:OD1	1:C:1358:ARG:N	2.44	0.46
1:C:3762:ILE:HD12	1:C:3840:ARG:HG3	1.97	0.46
1:C:4785:PHE:HA	1:C:4789:ARG:HH21	1.81	0.46
1:C:4808:MET:CG	1:D:4516:LEU:HA	2.46	0.46
1:D:1092:LYS:HG2	1:D:1120:PRO:HB3	1.98	0.46
1:D:1641:ASP:OD1	1:D:1642:ILE:N	2.49	0.46
1:D:1679:SER:HB3	1:D:1769:PHE:CE2	2.51	0.46
1:D:2065:MET:SD	1:D:2086:LEU:HD23	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2271:CYS:SG	1:D:2293:GLU:HB2	2.56	0.46
1:D:3719:GLU:HA	1:D:3722:LYS:HG2	1.98	0.46
1:D:3796:MET:HG2	1:D:3838:LEU:HD21	1.98	0.46
1:D:4762:ASN:O	1:D:4764:LYS:N	2.49	0.46
1:A:323:ASP:O	1:A:327:THR:OG1	2.26	0.45
1:A:874:LEU:HD11	1:A:941:LYS:HD3	1.97	0.45
1:A:1092:LYS:HG2	1:A:1120:PRO:HB3	1.98	0.45
1:A:2088:HIS:HB2	1:A:3690:TYR:CE1	2.51	0.45
1:B:227:TYR:HD2	1:B:352:SER:HB3	1.79	0.45
1:B:850:LEU:HD23	1:B:1213:GLY:O	2.15	0.45
1:B:1147:GLN:O	1:B:1147:GLN:HG2	2.17	0.45
1:B:4060:SER:O	1:B:4063:GLU:HG2	2.16	0.45
1:C:884:ARG:HB3	1:C:1060:TYR:HE2	1.81	0.45
1:C:2853:LYS:HA	1:C:2856:LYS:HG2	1.98	0.45
1:C:4606:ALA:HB1	1:C:4648:VAL:HG21	1.97	0.45
1:D:118:ALA:HA	1:D:161:THR:HA	1.98	0.45
1:D:343:ARG:HH21	1:D:345:GLU:H	1.64	0.45
1:D:884:ARG:HB3	1:D:1060:TYR:HE2	1.81	0.45
1:D:1173:MET:HB3	1:D:1191:ALA:HB3	1.97	0.45
1:A:2220:LEU:CD1	1:A:2242:ALA:HB2	2.46	0.45
1:A:3719:GLU:HA	1:A:3722:LYS:HG2	1.98	0.45
1:B:697:TRP:HB2	1:B:766:ILE:HD13	1.98	0.45
1:B:713:TRP:HE1	1:B:1604:PHE:HD1	1.64	0.45
1:B:723:PHE:HE2	1:B:1385:LYS:HE2	1.80	0.45
1:B:1776:CYS:SG	1:B:1778:GLN:HB3	2.57	0.45
1:B:4500:MET:HE2	1:B:4500:MET:HB2	1.72	0.45
1:C:1641:ASP:OD1	1:C:1642:ILE:N	2.50	0.45
1:C:1679:SER:HB3	1:C:1769:PHE:CE2	2.51	0.45
1:C:2065:MET:SD	1:C:2086:LEU:HD23	2.56	0.45
1:D:747:HIS:HB2	1:D:750:ARG:HH22	1.80	0.45
1:D:1681:VAL:HB	1:D:1685:GLN:NE2	2.31	0.45
1:D:2118:LEU:HB2	1:D:2151:ASN:HD21	1.80	0.45
1:D:2839:MET:HB3	1:D:2892:PHE:CZ	2.51	0.45
1:D:4583:PHE:O	1:D:4586:ILE:HG22	2.17	0.45
2:J:38:ASP:OD1	2:J:39:SER:N	2.48	0.45
1:A:783:ASN:ND2	1:A:1393:UNK:O	2.42	0.45
1:A:1147:GLN:O	1:A:1147:GLN:HG2	2.17	0.45
1:A:2238:PRO:HA	1:A:2241:VAL:HG12	1.98	0.45
1:A:2454:ASP:N	1:A:2454:ASP:OD1	2.49	0.45
1:A:2722:LYS:O	1:A:2726:HIS:ND1	2.50	0.45
1:A:4060:SER:O	1:A:4063:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4750:LYS:HA	1:A:4753:ARG:HG2	1.97	0.45
1:B:267:VAL:HA	1:B:270:HIS:ND1	2.32	0.45
1:B:552:SER:O	1:B:555:LEU:HD12	2.16	0.45
1:B:2722:LYS:O	1:B:2726:HIS:ND1	2.50	0.45
1:B:4029:ASP:OD1	1:B:4029:ASP:N	2.48	0.45
1:C:343:ARG:HH21	1:C:345:GLU:H	1.64	0.45
1:C:1008:ALA:O	1:C:1012:ILE:HG23	2.15	0.45
1:C:1092:LYS:HG2	1:C:1120:PRO:HB3	1.98	0.45
1:C:1681:VAL:HB	1:C:1685:GLN:NE2	2.31	0.45
1:C:1776:CYS:SG	1:C:1778:GLN:HB3	2.57	0.45
1:C:2454:ASP:N	1:C:2454:ASP:OD1	2.49	0.45
1:C:4750:LYS:HA	1:C:4753:ARG:HG2	1.97	0.45
1:C:4909:LEU:O	1:C:4913:ASN:ND2	2.49	0.45
1:D:267:VAL:HA	1:D:270:HIS:ND1	2.32	0.45
1:D:839:GLU:HG2	1:D:840:TYR:H	1.82	0.45
1:D:2722:LYS:O	1:D:2726:HIS:ND1	2.50	0.45
1:D:3795:LEU:HD22	1:D:3834:PHE:HZ	1.82	0.45
1:A:891:GLU:HB2	1:A:978:PRO:HB3	1.98	0.45
1:A:1173:MET:HB3	1:A:1191:ALA:HB3	1.97	0.45
1:A:1641:ASP:OD1	1:A:1642:ILE:N	2.49	0.45
1:A:1681:VAL:HB	1:A:1685:GLN:NE2	2.31	0.45
1:A:2118:LEU:HB2	1:A:2151:ASN:HD21	1.80	0.45
1:A:2261:LEU:O	1:A:2265:VAL:HG23	2.15	0.45
1:A:3940:TRP:HA	1:A:3943:VAL:HG22	1.97	0.45
1:B:169:ARG:HH22	1:B:176:ARG:HH21	1.64	0.45
1:B:839:GLU:HG2	1:B:840:TYR:H	1.82	0.45
1:B:4026:THR:O	1:B:4031:PHE:HB3	2.16	0.45
1:C:723:PHE:CE2	1:C:1385:LYS:HE2	2.52	0.45
1:C:1147:GLN:HG2	1:C:1147:GLN:O	2.16	0.45
1:C:1219:LYS:HE2	1:C:1219:LYS:HA	1.98	0.45
1:C:2088:HIS:HB2	1:C:3690:TYR:CE1	2.51	0.45
1:C:2722:LYS:O	1:C:2726:HIS:ND1	2.50	0.45
1:C:2839:MET:HB3	1:C:2892:PHE:CZ	2.51	0.45
1:C:3719:GLU:HA	1:C:3722:LYS:HG2	1.98	0.45
1:D:328:ALA:HB3	1:D:366:VAL:HG11	1.99	0.45
1:D:837:SER:H	1:D:841:LYS:HZ2	1.64	0.45
1:D:4026:THR:O	1:D:4031:PHE:HB3	2.17	0.45
1:D:4785:PHE:HA	1:D:4789:ARG:HH21	1.81	0.45
1:A:723:PHE:HE2	1:A:1385:LYS:HE2	1.79	0.45
1:A:1909:LEU:HB2	1:A:2086:LEU:HD21	1.98	0.45
1:A:2271:CYS:SG	1:A:2293:GLU:HB2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3796:MET:HG2	1:A:3838:LEU:HD21	1.98	0.45
1:A:4176:VAL:HG11	1:A:4879:VAL:HA	1.99	0.45
1:B:328:ALA:HB3	1:B:366:VAL:HG11	1.99	0.45
1:B:1304:LEU:HG	1:B:1340:ASP:HB2	1.98	0.45
1:B:2088:HIS:HB2	1:B:3690:TYR:CE1	2.51	0.45
1:B:3795:LEU:HD22	1:B:3834:PHE:HZ	1.82	0.45
1:B:3919:LEU:O	1:B:3923:ILE:HG12	2.17	0.45
1:C:267:VAL:HA	1:C:270:HIS:ND1	2.32	0.45
1:C:3795:LEU:HD22	1:C:3834:PHE:HZ	1.82	0.45
1:C:3796:MET:HG2	1:C:3838:LEU:HD21	1.98	0.45
1:C:3898:ASP:N	1:C:3898:ASP:OD1	2.49	0.45
1:D:1173:MET:HB2	1:D:1192:PHE:H	1.80	0.45
1:D:3898:ASP:OD1	1:D:3898:ASP:N	2.49	0.45
1:A:267:VAL:HA	1:A:270:HIS:ND1	2.32	0.45
1:A:328:ALA:HB3	1:A:366:VAL:HG11	1.99	0.45
1:A:552:SER:O	1:A:555:LEU:HD12	2.16	0.45
1:A:1256:PRO:HG2	1:A:1592:LEU:HD21	1.97	0.45
1:A:2330:PHE:CD2	1:A:2335:ARG:HG3	2.52	0.45
1:B:723:PHE:CE2	1:B:1385:LYS:HE2	2.52	0.45
1:B:837:SER:N	1:B:841:LYS:HZ2	2.15	0.45
1:B:891:GLU:HB2	1:B:978:PRO:HB3	1.98	0.45
1:B:1219:LYS:HE2	1:B:1219:LYS:HA	1.98	0.45
1:B:1358:ARG:HG3	1:B:1567:LEU:HD23	1.99	0.45
1:B:2330:PHE:CD2	1:B:2335:ARG:HG3	2.52	0.45
1:B:2454:ASP:OD1	1:B:2454:ASP:N	2.49	0.45
1:B:3804:LEU:HD21	1:B:3887:PHE:HA	1.99	0.45
1:C:238:HIS:HB2	1:C:241:MET:HB2	1.98	0.45
1:C:2330:PHE:CD2	1:C:2335:ARG:HG3	2.52	0.45
1:C:2383:MET:O	1:C:2387:ILE:HG13	2.17	0.45
1:D:176:ARG:N	1:D:179:ASP:OD2	2.42	0.45
1:A:644:LEU:HD11	1:A:1651:LEU:HD22	1.98	0.45
1:A:839:GLU:HG2	1:A:840:TYR:H	1.82	0.45
1:A:1102:TYR:HA	1:A:1164:CYS:O	2.17	0.45
1:A:1304:LEU:HG	1:A:1340:ASP:HB2	1.99	0.45
1:A:3720:LYS:HB2	1:A:3720:LYS:HE3	1.77	0.45
1:A:3919:LEU:O	1:A:3923:ILE:HG12	2.17	0.45
1:A:4583:PHE:O	1:A:4586:ILE:HG22	2.16	0.45
1:B:1303:ARG:N	1:B:1590:GLN:O	2.35	0.45
1:B:1641:ASP:OD1	1:B:1642:ILE:N	2.50	0.45
1:B:1900:PRO:O	1:B:1904:GLN:HG2	2.16	0.45
1:B:2383:MET:O	1:B:2387:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3796:MET:HG2	1:B:3838:LEU:HD21	1.98	0.45
1:B:4931:GLU:N	1:B:4931:GLU:OE2	2.49	0.45
1:C:2271:CYS:SG	1:C:2293:GLU:HB2	2.56	0.45
1:C:4029:ASP:OD1	1:C:4029:ASP:N	2.48	0.45
1:C:4931:GLU:N	1:C:4931:GLU:OE2	2.49	0.45
1:D:644:LEU:HD11	1:D:1651:LEU:HD22	1.98	0.45
1:D:1219:LYS:NZ	1:D:1243:THR:H	2.15	0.45
1:A:723:PHE:CE2	1:A:1385:LYS:HE2	2.52	0.45
1:A:1776:CYS:SG	1:A:1778:GLN:HB3	2.57	0.45
1:A:4072:ASP:O	1:A:4073:GLU:HG3	2.17	0.45
1:A:4648:VAL:O	1:A:4652:VAL:HG12	2.16	0.45
2:G:22:THR:CB	2:G:50:ARG:HG2	2.46	0.45
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.99	0.45
1:B:1092:LYS:HG2	1:B:1120:PRO:HB3	1.98	0.45
1:B:1256:PRO:HG2	1:B:1592:LEU:HD21	1.97	0.45
1:B:1681:VAL:HB	1:B:1685:GLN:NE2	2.32	0.45
1:B:2077:PRO:HA	1:B:2080:VAL:HG12	1.99	0.45
1:B:2233:MET:HE2	1:B:2233:MET:N	2.32	0.45
1:B:3748:GLY:HA2	1:B:3795:LEU:HG	1.98	0.45
1:C:3919:LEU:O	1:C:3923:ILE:HG12	2.17	0.45
1:D:1102:TYR:HA	1:D:1164:CYS:O	2.17	0.45
1:D:2220:LEU:CD1	1:D:2242:ALA:HB2	2.46	0.45
1:D:2238:PRO:HA	1:D:2241:VAL:HG12	1.98	0.45
1:D:2383:MET:O	1:D:2387:ILE:HG13	2.17	0.45
1:A:118:ALA:HA	1:A:161:THR:HA	1.98	0.45
1:A:1303:ARG:N	1:A:1590:GLN:O	2.35	0.45
1:A:1384:LEU:C	1:A:1385:LYS:HD2	2.37	0.45
1:A:1679:SER:HB3	1:A:1769:PHE:CE2	2.51	0.45
1:A:2383:MET:O	1:A:2387:ILE:HG13	2.17	0.45
1:B:238:HIS:HB2	1:B:241:MET:HB2	1.98	0.45
1:B:2065:MET:SD	1:B:2086:LEU:HD23	2.56	0.45
1:C:59:PRO:HB3	1:C:296:ARG:NH1	2.32	0.45
1:C:839:GLU:HG2	1:C:840:TYR:H	1.82	0.45
1:C:1832:MET:HB3	1:C:1832:MET:HE2	1.79	0.45
1:C:4026:THR:O	1:C:4031:PHE:HB3	2.16	0.45
1:C:4029:ASP:OD2	1:C:4054:HIS:NE2	2.43	0.45
1:C:4762:ASN:O	1:C:4764:LYS:N	2.49	0.45
1:D:552:SER:O	1:D:555:LEU:HD12	2.16	0.45
1:D:697:TRP:HB2	1:D:766:ILE:HD13	1.98	0.45
1:D:1219:LYS:HE2	1:D:1219:LYS:HA	1.98	0.45
1:D:4176:VAL:HG11	1:D:4879:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4648:VAL:O	1:D:4652:VAL:HG12	2.16	0.45
1:D:4931:GLU:N	1:D:4931:GLU:OE2	2.49	0.45
2:J:22:THR:CB	2:J:50:ARG:HG2	2.46	0.45
1:A:1358:ARG:HG3	1:A:1567:LEU:HD23	1.99	0.45
1:A:3804:LEU:HD21	1:A:3887:PHE:HA	1.99	0.45
1:C:328:ALA:HB3	1:C:366:VAL:HG11	1.99	0.45
1:C:1709:ASP:HA	1:C:1713:SER:HB3	1.99	0.45
1:C:2238:PRO:HA	1:C:2241:VAL:HG12	1.98	0.45
1:D:1384:LEU:C	1:D:1385:LYS:HD2	2.37	0.45
1:D:1981:ASP:OD1	1:D:1982:LYS:N	2.50	0.45
1:A:721:ASP:N	1:A:721:ASP:OD1	2.48	0.44
1:A:1173:MET:HB2	1:A:1192:PHE:H	1.80	0.44
1:A:1981:ASP:OD1	1:A:1982:LYS:N	2.50	0.44
1:A:4931:GLU:OE2	1:A:4931:GLU:N	2.49	0.44
1:B:59:PRO:HB3	1:B:296:ARG:NH1	2.32	0.44
1:B:884:ARG:HB3	1:B:1060:TYR:HE2	1.81	0.44
1:B:1305:SER:OG	1:B:1588:HIS:O	2.31	0.44
1:B:1909:LEU:HB2	1:B:2086:LEU:HD21	1.98	0.44
1:C:118:ALA:HA	1:C:161:THR:HA	1.98	0.44
1:C:552:SER:O	1:C:555:LEU:HD12	2.16	0.44
1:C:891:GLU:HB2	1:C:978:PRO:HB3	1.98	0.44
1:A:1305:SER:OG	1:A:1588:HIS:O	2.31	0.44
1:A:3795:LEU:HD22	1:A:3834:PHE:HZ	1.82	0.44
1:A:4042:ILE:HD11	1:A:4079:TYR:HD1	1.82	0.44
1:B:337:LYS:NZ	1:B:371:TRP:HE1	2.16	0.44
1:B:676:GLU:OE1	1:B:812:LYS:N	2.45	0.44
1:B:1679:SER:HB3	1:B:1769:PHE:CE2	2.51	0.44
1:B:2083:MET:HB2	1:B:2083:MET:HE3	1.64	0.44
1:B:4072:ASP:O	1:B:4073:GLU:HG3	2.17	0.44
1:C:1384:LEU:C	1:C:1385:LYS:HD2	2.37	0.44
1:C:4583:PHE:O	1:C:4586:ILE:HG22	2.16	0.44
1:D:169:ARG:HH22	1:D:176:ARG:HH21	1.64	0.44
1:D:1147:GLN:O	1:D:1147:GLN:HG2	2.17	0.44
1:D:2330:PHE:CD2	1:D:2335:ARG:HG3	2.52	0.44
1:D:3804:LEU:HD21	1:D:3887:PHE:HA	1.99	0.44
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.99	0.44
1:B:262:TYR:HE1	1:B:391:ALA:HB2	1.82	0.44
1:B:4176:VAL:HG11	1:B:4879:VAL:HA	1.99	0.44
2:H:38:ASP:OD1	2:H:39:SER:N	2.48	0.44
1:C:1153:GLY:HA3	1:C:1182:LEU:HD23	2.00	0.44
1:C:1761:ARG:NE	1:C:1763:ARG:HH12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2077:PRO:HA	1:C:2080:VAL:HG12	1.99	0.44
1:C:2233:MET:HE2	1:C:2233:MET:H	1.81	0.44
1:C:2313:GLU:OE1	1:C:3812:LYS:NZ	2.40	0.44
2:I:22:THR:CB	2:I:50:ARG:HG2	2.46	0.44
1:D:723:PHE:CE2	1:D:1385:LYS:HE2	2.52	0.44
1:D:766:ILE:HG22	1:D:768:PHE:HE2	1.80	0.44
1:D:891:GLU:HB2	1:D:978:PRO:HB3	1.98	0.44
1:D:3919:LEU:O	1:D:3923:ILE:HG12	2.17	0.44
1:A:4026:THR:O	1:A:4031:PHE:HB3	2.17	0.44
1:A:4632:LEU:H	1:A:4632:LEU:HD23	1.82	0.44
1:B:409:GLN:HB2	1:B:412:GLU:OE1	2.18	0.44
1:B:1683:GLU:HB3	2:H:42:ASP:HB3	1.99	0.44
1:B:4789:ARG:NH2	1:B:4805:CYS:SG	2.91	0.44
2:H:26:HIS:CD2	2:H:41:ARG:HG2	2.52	0.44
1:C:262:TYR:HE1	1:C:391:ALA:HB2	1.82	0.44
1:D:1304:LEU:HG	1:D:1340:ASP:HB2	1.98	0.44
1:D:1305:SER:OG	1:D:1588:HIS:O	2.31	0.44
1:A:169:ARG:HH22	1:A:176:ARG:HH21	1.64	0.44
1:A:262:TYR:HE1	1:A:391:ALA:HB2	1.82	0.44
1:A:697:TRP:HB2	1:A:766:ILE:HD13	1.98	0.44
1:A:4941:LYS:HB3	1:A:4941:LYS:HE3	1.75	0.44
1:B:118:ALA:HA	1:B:161:THR:HA	1.98	0.44
1:B:1709:ASP:HA	1:B:1713:SER:HB3	1.99	0.44
1:B:1761:ARG:NE	1:B:1763:ARG:HH12	2.16	0.44
1:B:1981:ASP:OD1	1:B:1982:LYS:N	2.50	0.44
1:B:4632:LEU:HD23	1:B:4632:LEU:H	1.83	0.44
1:C:888:ASN:O	1:C:891:GLU:HG2	2.18	0.44
1:C:1893:LEU:CD1	1:C:2060:LEU:HD21	2.48	0.44
1:C:1987:CYS:N	1:C:1988:PRO:HD2	2.33	0.44
1:C:2220:LEU:CD1	1:C:2242:ALA:HB2	2.46	0.44
1:C:2335:ARG:NE	1:C:2336:GLY:N	2.65	0.44
1:C:4779:LEU:HD21	1:D:4742:LEU:HB2	1.98	0.44
1:D:1966:SER:OG	1:D:1966:SER:O	2.32	0.44
1:A:804:LEU:HB2	1:A:808:HIS:HB2	2.00	0.44
1:A:1153:GLY:HA3	1:A:1182:LEU:HD23	2.00	0.44
1:A:1924:ILE:HA	1:A:1998:PHE:HZ	1.82	0.44
1:A:4500:MET:HB2	1:A:4500:MET:HE2	1.73	0.44
1:B:312:LYS:HE3	1:B:315:LEU:HD12	2.00	0.44
1:B:1814:THR:HG23	1:B:1816:GLU:HG2	2.00	0.44
1:B:4042:ILE:HD11	1:B:4079:TYR:HD1	1.82	0.44
1:C:486:GLN:CB	1:C:544:ASN:HD21	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:TRP:HB2	1:C:766:ILE:HD13	1.98	0.44
1:C:1219:LYS:NZ	1:C:1243:THR:H	2.15	0.44
1:C:1304:LEU:HG	1:C:1340:ASP:HB2	1.98	0.44
1:C:1730:MET:CE	1:C:3616:VAL:HG11	2.48	0.44
1:C:2481:ASP:OD1	1:C:2482:PHE:N	2.51	0.44
1:D:1776:CYS:SG	1:D:1778:GLN:HB3	2.57	0.44
1:A:337:LYS:NZ	1:A:371:TRP:HE1	2.16	0.44
1:A:2763:SER:N	1:A:2766:GLU:HB2	2.33	0.44
1:B:1153:GLY:HA3	1:B:1182:LEU:HD23	2.00	0.44
1:B:1219:LYS:NZ	1:B:1243:THR:H	2.15	0.44
1:B:1384:LEU:C	1:B:1385:LYS:HD2	2.37	0.44
1:B:4583:PHE:O	1:B:4586:ILE:HG22	2.17	0.44
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.99	0.44
1:C:1679:SER:HB2	2:I:37:PHE:O	2.18	0.44
1:C:3663:LEU:O	1:C:3667:ILE:HG12	2.18	0.44
2:I:26:HIS:CD2	2:I:41:ARG:HG2	2.52	0.44
1:D:1970:GLU:HA	1:D:1973:ASN:HB2	2.00	0.44
1:D:4072:ASP:O	1:D:4073:GLU:HG3	2.17	0.44
1:A:1219:LYS:NZ	1:A:1243:THR:H	2.15	0.44
1:B:1893:LEU:CD1	1:B:2060:LEU:HD21	2.48	0.44
1:B:2763:SER:N	1:B:2766:GLU:HB2	2.33	0.44
2:H:22:THR:CB	2:H:50:ARG:HG2	2.46	0.44
1:C:49:LEU:HD21	1:C:203:VAL:HG13	2.00	0.44
1:C:1146:HIS:CE1	1:C:1147:GLN:OE1	2.71	0.44
1:C:1924:ILE:HA	1:C:1998:PHE:HZ	1.82	0.44
1:D:59:PRO:HB3	1:D:296:ARG:NH1	2.32	0.44
1:D:888:ASN:O	1:D:891:GLU:HG2	2.18	0.44
1:D:1146:HIS:HB2	1:D:1192:PHE:HE2	1.83	0.44
1:D:1304:LEU:HD21	1:D:1354:LEU:HD22	2.00	0.44
1:D:1761:ARG:NE	1:D:1763:ARG:HH12	2.16	0.44
1:D:1814:THR:HG23	1:D:1816:GLU:HG2	2.00	0.44
1:D:1909:LEU:HB2	1:D:2086:LEU:HD21	1.98	0.44
1:D:1924:ILE:HA	1:D:1998:PHE:HZ	1.82	0.44
1:D:3748:GLY:HA2	1:D:3795:LEU:HG	1.97	0.44
1:D:4103:ASN:OD1	1:D:4107:HIS:ND1	2.38	0.44
1:D:4789:ARG:NH2	1:D:4805:CYS:SG	2.91	0.44
2:J:26:HIS:CD2	2:J:41:ARG:HG2	2.52	0.44
1:A:59:PRO:HB3	1:A:296:ARG:NH1	2.32	0.44
1:A:894:VAL:HA	1:A:918:LEU:HD22	2.00	0.44
1:A:4807:ASP:HB3	1:A:4810:THR:HB	2.00	0.44
1:B:137:ARG:HG2	1:B:146:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:LEU:HD12	1:B:1088:PHE:CD2	2.53	0.44
1:B:1146:HIS:HB2	1:B:1192:PHE:HE2	1.83	0.44
1:B:1947:MET:HE2	1:B:1947:MET:HA	2.00	0.44
1:B:2873:TYR:HA	1:B:2876:LEU:HD13	2.00	0.44
1:C:228:LEU:HD12	1:C:405:LEU:HD13	2.00	0.44
1:C:337:LYS:NZ	1:C:371:TRP:HE1	2.16	0.44
1:C:783:ASN:ND2	1:C:1393:UNK:O	2.41	0.44
1:D:1146:HIS:CE1	1:D:1147:GLN:OE1	2.71	0.44
1:D:2481:ASP:OD1	1:D:2482:PHE:N	2.51	0.44
1:D:4039:LYS:HB2	1:D:4039:LYS:HE2	1.80	0.44
1:D:4807:ASP:HB3	1:D:4810:THR:HB	2.00	0.44
1:A:312:LYS:HE3	1:A:315:LEU:HD12	2.00	0.43
1:A:486:GLN:CB	1:A:544:ASN:HD21	2.24	0.43
1:A:713:TRP:HE1	1:A:1604:PHE:HD1	1.64	0.43
1:A:850:LEU:HD12	1:A:1088:PHE:CD2	2.53	0.43
1:A:1893:LEU:CD1	1:A:2060:LEU:HD21	2.48	0.43
1:A:2167:HIS:HB3	1:A:2202:PHE:CE2	2.53	0.43
1:A:3699:HIS:HB2	1:A:3723:LEU:HD12	2.00	0.43
1:B:804:LEU:HB2	1:B:808:HIS:HB2	2.00	0.43
1:B:1355:VAL:HB	1:B:1365:THR:OG1	2.18	0.43
1:B:1357:ASP:OD1	1:B:1358:ARG:N	2.44	0.43
1:B:2220:LEU:CD1	1:B:2242:ALA:HB2	2.46	0.43
1:C:694:ARG:NH1	1:C:720:ASP:OD2	2.51	0.43
1:C:1102:TYR:HA	1:C:1164:CYS:O	2.17	0.43
1:C:1909:LEU:HB2	1:C:2086:LEU:HD21	1.98	0.43
1:C:1981:ASP:OD1	1:C:1982:LYS:N	2.50	0.43
1:C:3804:LEU:HD21	1:C:3887:PHE:HA	1.99	0.43
1:C:4072:ASP:O	1:C:4073:GLU:HG3	2.17	0.43
1:C:4789:ARG:NH2	1:C:4805:CYS:SG	2.91	0.43
1:D:694:ARG:NH1	1:D:720:ASP:OD2	2.52	0.43
1:D:1242:ASN:O	1:D:1808:ARG:HG2	2.18	0.43
1:D:1730:MET:CE	1:D:3616:VAL:HG11	2.48	0.43
1:D:2747:SER:O	1:D:2753:GLN:NE2	2.47	0.43
1:D:4042:ILE:HD11	1:D:4079:TYR:HD1	1.82	0.43
1:A:1242:ASN:O	1:A:1808:ARG:HG2	2.18	0.43
1:A:1355:VAL:HB	1:A:1365:THR:OG1	2.18	0.43
1:A:1709:ASP:HA	1:A:1713:SER:HB3	1.99	0.43
1:A:2077:PRO:HA	1:A:2080:VAL:HG12	1.99	0.43
1:A:3829:LEU:HD12	1:A:3829:LEU:HA	1.87	0.43
1:A:4789:ARG:NH2	1:A:4805:CYS:SG	2.91	0.43
1:B:228:LEU:HD12	1:B:405:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4807:ASP:HB3	1:B:4810:THR:HB	2.00	0.43
1:C:850:LEU:HD12	1:C:1088:PHE:CD2	2.53	0.43
1:C:1242:ASN:O	1:C:1808:ARG:HG2	2.18	0.43
1:C:1680:HIS:HE2	2:I:91:VAL:HA	1.83	0.43
1:C:4176:VAL:HG11	1:C:4879:VAL:HA	1.99	0.43
1:D:1153:GLY:HA3	1:D:1182:LEU:HD23	2.00	0.43
1:D:3699:HIS:HB2	1:D:3723:LEU:HD12	2.00	0.43
1:A:888:ASN:O	1:A:891:GLU:HG2	2.18	0.43
1:A:1167:ASP:HB3	1:A:1172:THR:HB	2.00	0.43
1:A:1730:MET:CE	1:A:3616:VAL:HG11	2.48	0.43
1:B:36:CYS:SG	1:B:65:CYS:HB3	2.59	0.43
1:B:49:LEU:HD21	1:B:203:VAL:HG13	2.00	0.43
1:B:888:ASN:O	1:B:891:GLU:HG2	2.18	0.43
1:B:1102:TYR:HA	1:B:1164:CYS:O	2.17	0.43
1:B:1146:HIS:CE1	1:B:1147:GLN:OE1	2.71	0.43
1:B:1167:ASP:HB3	1:B:1172:THR:HB	2.00	0.43
1:B:1970:GLU:HA	1:B:1973:ASN:HB2	2.00	0.43
1:B:3758:LEU:O	1:B:3762:ILE:HG12	2.19	0.43
1:C:409:GLN:HB2	1:C:412:GLU:OE1	2.18	0.43
1:C:838:ARG:H	1:C:841:LYS:NZ	2.15	0.43
1:C:1167:ASP:HB3	1:C:1172:THR:HB	2.00	0.43
1:D:409:GLN:HB2	1:D:412:GLU:OE1	2.18	0.43
1:D:652:VAL:HG12	1:D:714:GLY:O	2.18	0.43
1:D:804:LEU:HB2	1:D:808:HIS:HB2	2.00	0.43
1:D:3663:LEU:O	1:D:3667:ILE:HG12	2.18	0.43
1:D:4195:THR:HA	1:D:4198:GLU:HG2	2.01	0.43
1:A:1113:MET:HG2	1:A:1207:LEU:HD22	2.01	0.43
1:A:1814:THR:HG23	1:A:1816:GLU:HG2	2.00	0.43
1:A:1947:MET:HA	1:A:1947:MET:HE2	2.01	0.43
1:A:2083:MET:HE3	1:A:2083:MET:HB2	1.65	0.43
1:B:446:ASP:OD1	1:B:446:ASP:N	2.45	0.43
1:B:694:ARG:NH1	1:B:720:ASP:OD2	2.51	0.43
1:B:1987:CYS:N	1:B:1988:PRO:HD2	2.33	0.43
1:B:2167:HIS:HB3	1:B:2202:PHE:CE2	2.53	0.43
1:B:4034:TYR:HE2	1:B:4050:ALA:HB2	1.83	0.43
1:C:380:LYS:HA	1:C:380:LYS:HD2	1.75	0.43
1:C:1113:MET:HG2	1:C:1207:LEU:HD22	2.01	0.43
1:C:1355:VAL:HB	1:C:1365:THR:OG1	2.18	0.43
1:C:1814:THR:HG23	1:C:1816:GLU:HG2	2.00	0.43
1:C:4034:TYR:HE2	1:C:4050:ALA:HB2	1.83	0.43
1:D:137:ARG:HG2	1:D:146:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD21	1:A:203:VAL:HG13	2.00	0.43
1:A:409:GLN:HB2	1:A:412:GLU:OE1	2.18	0.43
1:A:677:LEU:HD12	1:A:801:ARG:O	2.19	0.43
1:A:1761:ARG:NE	1:A:1763:ARG:HH12	2.15	0.43
1:B:894:VAL:HA	1:B:918:LEU:HD22	2.00	0.43
1:B:1730:MET:CE	1:B:3616:VAL:HG11	2.48	0.43
1:B:4001:MET:HE3	1:B:4001:MET:HB2	1.90	0.43
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.99	0.43
1:D:850:LEU:HD12	1:D:1088:PHE:CD2	2.53	0.43
1:D:1167:ASP:HB3	1:D:1172:THR:HB	2.00	0.43
1:D:1355:VAL:HB	1:D:1365:THR:OG1	2.18	0.43
1:D:1358:ARG:HG3	1:D:1567:LEU:HD23	1.99	0.43
1:D:1893:LEU:CD1	1:D:2060:LEU:HD21	2.48	0.43
1:D:1987:CYS:N	1:D:1988:PRO:HD2	2.33	0.43
1:D:4500:MET:HE2	1:D:4500:MET:HB2	1.71	0.43
1:A:487:ASN:O	1:A:491:GLU:HG2	2.19	0.43
1:A:652:VAL:HG12	1:A:714:GLY:O	2.18	0.43
1:A:694:ARG:NH1	1:A:720:ASP:OD2	2.51	0.43
1:A:1304:LEU:HD21	1:A:1354:LEU:HD22	2.00	0.43
1:B:169:ARG:HH12	1:B:176:ARG:NE	2.17	0.43
1:B:487:ASN:O	1:B:491:GLU:HG2	2.19	0.43
1:B:541:ILE:HG21	1:B:551:PHE:CZ	2.54	0.43
1:B:2722:LYS:HA	1:B:2722:LYS:HD2	1.77	0.43
1:C:312:LYS:HE3	1:C:315:LEU:HD12	2.00	0.43
1:C:894:VAL:HA	1:C:918:LEU:HD22	2.00	0.43
1:C:2763:SER:N	1:C:2766:GLU:HB2	2.33	0.43
1:C:4632:LEU:HD23	1:C:4632:LEU:H	1.82	0.43
1:D:836:HIS:HB2	1:D:841:LYS:HE3	2.01	0.43
1:D:2197:ARG:HB3	1:D:2236:SER:HG	1.83	0.43
1:D:2233:MET:H	1:D:2233:MET:CE	2.31	0.43
1:D:4632:LEU:HD23	1:D:4632:LEU:H	1.82	0.43
1:A:228:LEU:HD12	1:A:405:LEU:HD13	2.00	0.43
1:A:676:GLU:OE1	1:A:812:LYS:N	2.45	0.43
1:A:1146:HIS:CE1	1:A:1147:GLN:OE1	2.71	0.43
1:A:1970:GLU:HA	1:A:1973:ASN:HB2	2.00	0.43
1:A:3663:LEU:O	1:A:3667:ILE:HG12	2.18	0.43
1:A:4792:TYR:HH	1:A:4815:HIS:HE2	1.63	0.43
2:G:26:HIS:CD2	2:G:41:ARG:HG2	2.52	0.43
1:C:804:LEU:HB2	1:C:808:HIS:HB2	2.00	0.43
1:C:2167:HIS:HB3	1:C:2202:PHE:CE2	2.53	0.43
1:C:3699:HIS:HB2	1:C:3723:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3878:LEU:O	1:C:3882:GLU:HG3	2.18	0.43
1:D:49:LEU:HD21	1:D:203:VAL:HG13	2.00	0.43
1:D:337:LYS:NZ	1:D:371:TRP:HE1	2.16	0.43
1:D:2077:PRO:HA	1:D:2080:VAL:HG12	1.99	0.43
1:A:868:ASP:OD1	1:A:868:ASP:N	2.50	0.43
1:A:1681:VAL:O	1:A:1682:ASP:OD1	2.37	0.43
1:A:3758:LEU:O	1:A:3762:ILE:HG12	2.19	0.43
1:A:3810:GLN:OE1	1:A:3826:GLU:HB3	2.19	0.43
1:A:4846:ASP:HB2	1:B:4817:TYR:HE1	1.83	0.43
1:A:4955:ASP:OD1	1:A:4956:CYS:N	2.52	0.43
1:B:1113:MET:HG2	1:B:1207:LEU:HD22	2.01	0.43
1:B:1242:ASN:O	1:B:1808:ARG:HG2	2.18	0.43
1:B:1924:ILE:HA	1:B:1998:PHE:HZ	1.82	0.43
1:C:169:ARG:HH12	1:C:176:ARG:NE	2.17	0.43
1:D:169:ARG:HH12	1:D:176:ARG:NE	2.17	0.43
1:D:329:PHE:HB3	1:D:363:ILE:HD11	2.01	0.43
1:D:487:ASN:O	1:D:491:GLU:HG2	2.19	0.43
1:D:1113:MET:HG2	1:D:1207:LEU:HD22	2.01	0.43
1:D:1709:ASP:HA	1:D:1713:SER:HB3	1.99	0.43
1:D:2167:HIS:HB3	1:D:2202:PHE:CE2	2.53	0.43
1:D:3878:LEU:O	1:D:3882:GLU:HG3	2.18	0.43
1:A:137:ARG:HG2	1:A:146:ASP:OD2	2.18	0.43
1:A:2481:ASP:OD1	1:A:2482:PHE:N	2.51	0.43
1:A:3878:LEU:O	1:A:3882:GLU:HG3	2.18	0.43
1:B:652:VAL:HG12	1:B:714:GLY:O	2.18	0.43
1:B:807:ARG:O	1:B:1615:ARG:NH2	2.41	0.43
1:B:878:LEU:HA	1:B:881:ILE:HD13	2.01	0.43
1:B:1745:LYS:HE3	1:B:1745:LYS:HB3	1.78	0.43
1:B:2145:LEU:O	1:B:2149:MET:HG2	2.19	0.43
1:B:3699:HIS:HB2	1:B:3723:LEU:HD12	2.00	0.43
1:C:36:CYS:SG	1:C:65:CYS:HB3	2.59	0.43
1:C:137:ARG:HG2	1:C:146:ASP:OD2	2.18	0.43
1:C:677:LEU:HD12	1:C:801:ARG:O	2.19	0.43
1:C:1947:MET:HE2	1:C:1947:MET:HA	2.01	0.43
1:D:677:LEU:HD12	1:D:801:ARG:O	2.19	0.43
1:D:783:ASN:ND2	1:D:1393:UNK:O	2.41	0.43
1:D:2260:ASP:OD1	1:D:2260:ASP:N	2.51	0.43
1:D:2335:ARG:NE	1:D:2336:GLY:N	2.65	0.43
1:D:3758:LEU:O	1:D:3762:ILE:HG12	2.18	0.43
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.84	0.43
1:A:169:ARG:HH12	1:A:176:ARG:NE	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ASN:HA	1:A:935:MET:HE3	2.01	0.43
1:A:1987:CYS:N	1:A:1988:PRO:HD2	2.33	0.43
1:A:2335:ARG:NE	1:A:2336:GLY:N	2.65	0.43
1:A:4034:TYR:HE2	1:A:4050:ALA:HB2	1.83	0.43
1:B:677:LEU:HD12	1:B:801:ARG:O	2.19	0.43
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.84	0.43
1:C:500:GLU:HA	1:C:503:ASP:HB2	2.01	0.43
1:C:652:VAL:HG12	1:C:714:GLY:O	2.18	0.43
1:C:836:HIS:HB2	1:C:841:LYS:HE3	2.01	0.43
1:C:2873:TYR:HA	1:C:2876:LEU:HD13	2.00	0.43
1:C:2876:LEU:HB2	1:C:2881:LYS:HE3	2.01	0.43
1:C:3810:GLN:OE1	1:C:3826:GLU:HB3	2.19	0.43
1:C:3842:LEU:HD23	1:C:3842:LEU:HA	1.89	0.43
1:D:228:LEU:HD12	1:D:405:LEU:HD13	2.00	0.43
1:D:262:TYR:HE1	1:D:391:ALA:HB2	1.82	0.43
1:D:1091:GLU:HB3	1:D:1094:TYR:CD2	2.53	0.43
1:D:1745:LYS:HE3	1:D:1745:LYS:HB3	1.78	0.43
1:D:2145:LEU:O	1:D:2149:MET:HG2	2.19	0.43
1:D:2873:TYR:HA	1:D:2876:LEU:HD13	2.00	0.43
1:D:4924:LEU:HD23	1:D:4924:LEU:HA	1.89	0.43
1:A:36:CYS:SG	1:A:65:CYS:HB3	2.59	0.42
1:A:182:ILE:HD11	1:A:191:TYR:CD1	2.54	0.42
1:A:329:PHE:HB3	1:A:363:ILE:HD11	2.01	0.42
1:A:390:LYS:HA	1:A:390:LYS:HD3	1.87	0.42
1:A:1796:LEU:HD12	1:A:1796:LEU:HA	1.89	0.42
1:A:2145:LEU:O	1:A:2149:MET:HG2	2.19	0.42
1:A:2334:LEU:HD12	1:A:2342:LEU:CD1	2.49	0.42
1:A:3802:LEU:HB2	1:A:3883:SER:OG	2.19	0.42
1:A:3839:PHE:CE1	1:A:3873:THR:HG23	2.54	0.42
1:B:35:LEU:HD23	1:B:51:SER:HA	2.01	0.42
1:B:1091:GLU:HB3	1:B:1094:TYR:CD2	2.53	0.42
1:B:1960:LYS:HD3	1:B:1960:LYS:HA	1.60	0.42
1:B:2260:ASP:OD1	1:B:2260:ASP:N	2.51	0.42
1:B:2481:ASP:OD1	1:B:2482:PHE:N	2.51	0.42
1:B:2747:SER:O	1:B:2753:GLN:NE2	2.47	0.42
1:B:2876:LEU:HB2	1:B:2881:LYS:HE3	2.00	0.42
1:B:3802:LEU:HB2	1:B:3883:SER:OG	2.19	0.42
1:B:3839:PHE:CE1	1:B:3873:THR:HG23	2.54	0.42
1:C:837:SER:N	1:C:841:LYS:HZ2	2.16	0.42
1:C:1091:GLU:HB3	1:C:1094:TYR:CD2	2.53	0.42
1:C:1304:LEU:HD21	1:C:1354:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3829:LEU:HD12	1:C:3829:LEU:HA	1.87	0.42
1:C:4001:MET:HE3	1:C:4001:MET:HB2	1.83	0.42
1:C:4042:ILE:HD11	1:C:4079:TYR:HD1	1.82	0.42
1:C:4807:ASP:HB3	1:C:4810:THR:HB	2.00	0.42
1:D:312:LYS:HE3	1:D:315:LEU:HD12	2.00	0.42
1:D:1085:PHE:HE2	1:D:1087:ILE:HD11	1.84	0.42
1:D:1572:PHE:HZ	1:D:1587:LEU:HD11	1.84	0.42
1:D:1947:MET:HE2	1:D:1947:MET:HA	2.00	0.42
1:A:1085:PHE:HE2	1:A:1087:ILE:HD11	1.84	0.42
1:A:2260:ASP:OD1	1:A:2260:ASP:N	2.51	0.42
1:B:191:TYR:HE2	1:C:2325:ARG:NH2	2.17	0.42
1:B:680:ASP:HB2	1:B:799:LYS:HB2	2.01	0.42
1:B:783:ASN:ND2	1:B:1393:UNK:O	2.41	0.42
1:B:3878:LEU:O	1:B:3882:GLU:HG3	2.18	0.42
1:C:487:ASN:O	1:C:491:GLU:HG2	2.19	0.42
1:C:661:LEU:HD13	1:C:673:TRP:CD1	2.55	0.42
1:C:730:LEU:HD12	2:I:6:GLU:OE1	2.19	0.42
1:C:2233:MET:H	1:C:2233:MET:CE	2.31	0.42
1:C:2334:LEU:HD12	1:C:2342:LEU:CD1	2.50	0.42
1:D:541:ILE:HG21	1:D:551:PHE:CZ	2.54	0.42
1:D:661:LEU:HD13	1:D:673:TRP:CD1	2.55	0.42
1:A:2876:LEU:HB2	1:A:2881:LYS:HE3	2.00	0.42
1:B:548:CYS:HB2	1:B:582:SER:HB3	2.01	0.42
1:B:2335:ARG:NE	1:B:2336:GLY:N	2.65	0.42
1:B:3663:LEU:O	1:B:3667:ILE:HG12	2.18	0.42
1:B:3810:GLN:OE1	1:B:3826:GLU:HB3	2.19	0.42
1:C:1358:ARG:HG3	1:C:1567:LEU:HD23	1.99	0.42
1:C:1786:ASP:O	1:C:1789:LYS:HG2	2.19	0.42
1:C:2145:LEU:O	1:C:2149:MET:HG2	2.19	0.42
1:C:2771:ARG:HH22	1:C:2775:LYS:HD2	1.84	0.42
1:C:3758:LEU:O	1:C:3762:ILE:HG12	2.19	0.42
1:C:3802:LEU:HB2	1:C:3883:SER:OG	2.19	0.42
1:D:680:ASP:HB2	1:D:799:LYS:HB2	2.01	0.42
1:D:838:ARG:H	1:D:841:LYS:NZ	2.15	0.42
1:D:1681:VAL:O	1:D:1682:ASP:OD1	2.37	0.42
1:D:1786:ASP:O	1:D:1789:LYS:HG2	2.19	0.42
1:D:2334:LEU:HD12	1:D:2342:LEU:CD1	2.49	0.42
1:D:4034:TYR:HE2	1:D:4050:ALA:HB2	1.83	0.42
1:A:2873:TYR:HA	1:A:2876:LEU:HD13	2.00	0.42
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.84	0.42
1:C:35:LEU:HD23	1:C:51:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PHE:HB3	1:C:363:ILE:HD11	2.01	0.42
1:C:1146:HIS:HB2	1:C:1192:PHE:HE2	1.83	0.42
1:C:1899:GLU:HB2	1:C:1900:PRO:HD3	2.02	0.42
1:C:3612:ARG:HA	1:C:3612:ARG:HD2	1.86	0.42
1:C:3720:LYS:HE3	1:C:3720:LYS:HB2	1.77	0.42
1:D:441:LYS:HG2	1:D:442:LEU:HD23	2.00	0.42
1:D:894:VAL:HA	1:D:918:LEU:HD22	2.01	0.42
1:D:1152:TYR:CD1	1:D:1152:TYR:C	2.93	0.42
1:D:1899:GLU:HB2	1:D:1900:PRO:HD3	2.02	0.42
1:D:1946:VAL:HG11	1:D:1960:LYS:HE3	2.02	0.42
1:D:2763:SER:N	1:D:2766:GLU:HB2	2.33	0.42
1:A:661:LEU:HD13	1:A:673:TRP:CD1	2.55	0.42
1:A:1146:HIS:HB2	1:A:1192:PHE:HE2	1.83	0.42
1:A:3761:GLY:HA2	1:A:3764:ILE:HG22	2.01	0.42
1:A:3796:MET:HA	1:A:3799:CYS:SG	2.60	0.42
1:A:3898:ASP:OD1	1:A:3898:ASP:N	2.49	0.42
1:B:412:GLU:HB2	1:B:488:LEU:HD21	2.02	0.42
1:B:441:LYS:HG2	1:B:442:LEU:HD23	2.00	0.42
1:B:500:GLU:HA	1:B:503:ASP:HB2	2.01	0.42
1:B:661:LEU:HD13	1:B:673:TRP:CD1	2.55	0.42
1:B:1796:LEU:HD12	1:B:1796:LEU:HA	1.89	0.42
1:B:2233:MET:H	1:B:2233:MET:CE	2.31	0.42
1:B:2732:SER:HA	1:B:2735:LYS:HG3	2.02	0.42
1:C:496:ASN:HA	1:C:499:LEU:HD12	2.02	0.42
1:C:1681:VAL:O	1:C:1682:ASP:OD1	2.37	0.42
1:C:1970:GLU:HA	1:C:1973:ASN:HB2	2.00	0.42
1:C:2722:LYS:HA	1:C:2722:LYS:HD2	1.78	0.42
1:C:3808:GLU:HA	1:C:3811:ASN:HD22	1.85	0.42
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.84	0.42
1:D:35:LEU:HD23	1:D:51:SER:HA	2.01	0.42
1:D:1234:GLU:HG2	1:D:1236:TYR:HD1	1.85	0.42
1:A:541:ILE:HG21	1:A:551:PHE:CZ	2.54	0.42
1:A:1152:TYR:CD1	1:A:1152:TYR:C	2.93	0.42
1:B:624:ALA:HB2	1:B:1668:LEU:HD23	2.02	0.42
1:B:795:SER:OG	1:B:796:ALA:N	2.53	0.42
1:C:1684:PRO:HD3	2:I:42:ASP:HB3	2.00	0.42
1:C:1793:ILE:HD11	1:C:1839:ASP:OD1	2.20	0.42
1:D:36:CYS:SG	1:D:65:CYS:HB3	2.59	0.42
1:D:496:ASN:HA	1:D:499:LEU:HD12	2.02	0.42
1:D:2771:ARG:HH22	1:D:2775:LYS:HD2	1.85	0.42
1:D:3761:GLY:HA2	1:D:3764:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3803:ASP:OD1	1:D:3803:ASP:N	2.53	0.42
1:A:441:LYS:HG2	1:A:442:LEU:HD23	2.00	0.42
1:A:680:ASP:HB2	1:A:799:LYS:HB2	2.01	0.42
1:A:807:ARG:O	1:A:1615:ARG:NH2	2.41	0.42
1:A:1234:GLU:HG2	1:A:1236:TYR:HD1	1.85	0.42
1:A:1835:PHE:O	1:A:1840:LEU:HG	2.20	0.42
1:A:2292:VAL:O	1:A:2296:ARG:HG2	2.20	0.42
1:A:2486:LEU:HG	1:A:2491:PHE:HE2	1.85	0.42
1:A:2732:SER:HA	1:A:2735:LYS:HG3	2.02	0.42
1:A:3802:LEU:HG	1:A:3829:LEU:HD13	2.02	0.42
1:B:836:HIS:HB2	1:B:841:LYS:HE3	2.01	0.42
1:B:838:ARG:H	1:B:841:LYS:NZ	2.15	0.42
1:B:1304:LEU:HD21	1:B:1354:LEU:HD22	2.00	0.42
1:C:1678:CYS:SG	1:C:1679:SER:N	2.93	0.42
1:C:1946:VAL:HG11	1:C:1960:LYS:HE3	2.02	0.42
1:C:2083:MET:HE3	1:C:2083:MET:HB2	1.64	0.42
1:C:2732:SER:HA	1:C:2735:LYS:HG3	2.02	0.42
1:C:4955:ASP:OD1	1:C:4956:CYS:N	2.52	0.42
1:D:500:GLU:HA	1:D:503:ASP:HB2	2.01	0.42
1:D:548:CYS:HB2	1:D:582:SER:HB3	2.01	0.42
1:D:795:SER:OG	1:D:796:ALA:N	2.53	0.42
1:D:868:ASP:OD1	1:D:868:ASP:N	2.50	0.42
1:D:1091:GLU:HB2	1:D:1248:THR:OG1	2.19	0.42
1:D:3612:ARG:HA	1:D:3612:ARG:HD2	1.86	0.42
1:D:3810:GLN:OE1	1:D:3826:GLU:HB3	2.19	0.42
1:A:878:LEU:HA	1:A:881:ILE:HD13	2.01	0.42
1:A:4195:THR:HA	1:A:4198:GLU:HG2	2.01	0.42
1:B:496:ASN:HA	1:B:499:LEU:HD12	2.02	0.42
1:B:1782:GLU:HG2	2:H:45:LYS:NZ	2.35	0.42
1:B:2771:ARG:HH22	1:B:2775:LYS:HD2	1.84	0.42
1:B:3796:MET:HA	1:B:3799:CYS:SG	2.60	0.42
1:C:261:HIS:HB3	1:C:390:LYS:HD3	2.02	0.42
1:C:548:CYS:HB2	1:C:582:SER:HB3	2.01	0.42
1:C:878:LEU:HA	1:C:881:ILE:HD13	2.01	0.42
1:A:496:ASN:HA	1:A:499:LEU:HD12	2.02	0.42
1:A:680:ASP:OD1	1:A:801:ARG:HD3	2.20	0.42
1:A:795:SER:OG	1:A:796:ALA:N	2.53	0.42
1:A:836:HIS:HB2	1:A:841:LYS:HE3	2.01	0.42
1:A:1091:GLU:HB2	1:A:1248:THR:OG1	2.19	0.42
1:A:1572:PHE:HZ	1:A:1587:LEU:HD11	1.84	0.42
1:A:2092:ASP:O	1:A:2094:ILE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ILE:O	1:B:31:GLU:HG2	2.20	0.42
1:B:680:ASP:OD1	1:B:801:ARG:HD3	2.20	0.42
1:B:1085:PHE:HE2	1:B:1087:ILE:HD11	1.84	0.42
1:B:1152:TYR:CD1	1:B:1152:TYR:C	2.93	0.42
1:B:1678:CYS:SG	1:B:1679:SER:N	2.93	0.42
1:B:1786:ASP:O	1:B:1789:LYS:HG2	2.20	0.42
1:B:2334:LEU:HD12	1:B:2342:LEU:CD1	2.50	0.42
1:B:3808:GLU:HA	1:B:3811:ASN:HD22	1.85	0.42
1:B:3925:GLY:O	1:B:3927:CYS:N	2.52	0.42
1:C:986:ILE:O	1:C:1055:ARG:NH1	2.53	0.42
1:C:1091:GLU:HB2	1:C:1248:THR:OG1	2.19	0.42
1:C:1152:TYR:C	1:C:1152:TYR:CD1	2.93	0.42
1:C:2486:LEU:HG	1:C:2491:PHE:HE2	1.84	0.42
1:C:2847:TYR:CD2	1:C:2884:ASP:HB2	2.55	0.42
1:D:182:ILE:HD11	1:D:191:TYR:CD1	2.54	0.42
1:D:837:SER:N	1:D:841:LYS:HZ2	2.18	0.42
1:D:1835:PHE:O	1:D:1840:LEU:HG	2.20	0.42
1:D:2428:LEU:HD21	1:D:2482:PHE:CE2	2.55	0.42
1:D:3796:MET:HA	1:D:3799:CYS:SG	2.60	0.42
1:D:3839:PHE:CE1	1:D:3873:THR:HG23	2.54	0.42
1:A:548:CYS:HB2	1:A:582:SER:HB3	2.01	0.42
1:A:1091:GLU:HB3	1:A:1094:TYR:CD2	2.53	0.42
1:A:1789:LYS:O	1:A:1793:ILE:HG13	2.20	0.42
1:A:2233:MET:H	1:A:2233:MET:CE	2.31	0.42
1:B:1234:GLU:HG2	1:B:1236:TYR:CD1	2.55	0.42
1:B:1681:VAL:O	1:B:1682:ASP:OD1	2.37	0.42
1:B:2486:LEU:HG	1:B:2491:PHE:HE2	1.85	0.42
1:B:3802:LEU:HG	1:B:3829:LEU:HD13	2.02	0.42
1:C:541:ILE:HG21	1:C:551:PHE:CZ	2.54	0.42
1:C:795:SER:OG	1:C:796:ALA:N	2.53	0.42
1:C:1234:GLU:HG2	1:C:1236:TYR:HD1	1.85	0.42
1:C:3761:GLY:HA2	1:C:3764:ILE:HG22	2.01	0.42
1:D:261:HIS:HB3	1:D:390:LYS:HD3	2.02	0.42
1:D:1679:SER:HB2	2:J:37:PHE:O	2.20	0.42
1:A:1946:VAL:HG11	1:A:1960:LYS:HE3	2.02	0.41
1:B:261:HIS:HB3	1:B:390:LYS:HD3	2.02	0.41
1:B:986:ILE:O	1:B:1055:ARG:NH1	2.53	0.41
1:B:1091:GLU:HB2	1:B:1248:THR:OG1	2.19	0.41
1:B:3612:ARG:HD2	1:B:3612:ARG:HA	1.86	0.41
1:B:4195:THR:HA	1:B:4198:GLU:HG2	2.01	0.41
1:C:680:ASP:OD1	1:C:801:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1572:PHE:HZ	1:C:1587:LEU:HD11	1.84	0.41
1:C:4766:LEU:O	1:C:4770:VAL:HG13	2.20	0.41
1:D:30:LYS:HE2	1:D:30:LYS:HB2	1.92	0.41
1:D:680:ASP:OD1	1:D:801:ARG:HD3	2.20	0.41
1:D:1234:GLU:HG2	1:D:1236:TYR:CD1	2.55	0.41
1:D:1678:CYS:SG	1:D:1679:SER:N	2.93	0.41
1:D:1793:ILE:HD11	1:D:1839:ASP:OD1	2.20	0.41
1:D:2876:LEU:HB2	1:D:2881:LYS:HE3	2.01	0.41
1:D:3802:LEU:HG	1:D:3829:LEU:HD13	2.02	0.41
1:D:4607:ARG:NE	1:D:4643:TYR:OH	2.53	0.41
1:A:35:LEU:HD23	1:A:51:SER:HA	2.01	0.41
1:A:412:GLU:HB2	1:A:488:LEU:HD21	2.02	0.41
1:A:634:ASP:HA	2:G:90:GLY:HA2	2.02	0.41
1:A:986:ILE:O	1:A:1055:ARG:NH1	2.53	0.41
1:A:1786:ASP:O	1:A:1789:LYS:HG2	2.19	0.41
1:A:1793:ILE:HD11	1:A:1839:ASP:OD1	2.20	0.41
1:A:2847:TYR:CD2	1:A:2884:ASP:HB2	2.55	0.41
1:B:329:PHE:HB3	1:B:363:ILE:HD11	2.01	0.41
1:B:1793:ILE:HD11	1:B:1839:ASP:OD1	2.20	0.41
1:B:1835:PHE:O	1:B:1840:LEU:HG	2.20	0.41
1:B:1897:LEU:HD22	1:B:1901:VAL:HG11	2.02	0.41
1:B:1910:GLN:HG2	1:B:2086:LEU:HD13	2.02	0.41
1:B:1946:VAL:HG11	1:B:1960:LYS:HE3	2.02	0.41
1:B:4846:ASP:HB2	1:C:4817:TYR:HE1	1.85	0.41
1:C:680:ASP:HB2	1:C:799:LYS:HB2	2.01	0.41
1:C:872:ILE:HD13	1:C:944:LEU:HD22	2.02	0.41
1:C:946:LEU:HD21	1:C:998:LYS:HG2	2.02	0.41
1:D:516:ASP:OD1	1:D:516:ASP:N	2.52	0.41
1:D:587:ASN:HA	1:D:2132:ARG:NH1	2.35	0.41
1:D:624:ALA:HB2	1:D:1668:LEU:HD23	2.02	0.41
1:D:1990:GLU:H	1:D:1990:GLU:HG2	1.62	0.41
1:D:2092:ASP:O	1:D:2094:ILE:N	2.53	0.41
1:D:2847:TYR:CD2	1:D:2884:ASP:HB2	2.55	0.41
1:A:28:ILE:O	1:A:31:GLU:HG2	2.20	0.41
1:A:254:GLU:O	1:A:258:ARG:HG3	2.20	0.41
1:B:254:GLU:O	1:B:258:ARG:HG3	2.21	0.41
1:B:459:LEU:HD23	1:B:459:LEU:HA	1.95	0.41
1:B:516:ASP:N	1:B:516:ASP:OD1	2.52	0.41
1:B:1086:ARG:HB3	1:B:1088:PHE:CE1	2.56	0.41
1:B:2502:ASP:OD1	1:B:2503:THR:N	2.50	0.41
1:C:441:LYS:HG2	1:C:442:LEU:HD23	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1569:ALA:HA	1:C:1572:PHE:CE1	2.56	0.41
1:C:1960:LYS:HD3	1:C:1960:LYS:HA	1.60	0.41
1:C:2243:ALA:O	1:C:2247:MET:HG3	2.20	0.41
1:C:3712:SER:O	1:C:3712:SER:OG	2.38	0.41
1:C:4195:THR:HA	1:C:4198:GLU:HG2	2.01	0.41
1:D:2486:LEU:HG	1:D:2491:PHE:HE2	1.85	0.41
1:D:2732:SER:HA	1:D:2735:LYS:HG3	2.02	0.41
1:A:19:GLU:HG3	1:A:68:VAL:HG22	2.03	0.41
1:A:78:LEU:HD11	1:A:159:TRP:CG	2.56	0.41
1:A:606:ARG:HE	1:A:644:LEU:HG	1.86	0.41
1:A:1234:GLU:HG2	1:A:1236:TYR:CD1	2.55	0.41
1:A:1569:ALA:HA	1:A:1572:PHE:CE1	2.56	0.41
1:A:1678:CYS:SG	1:A:1679:SER:N	2.93	0.41
1:A:1899:GLU:HB2	1:A:1900:PRO:HD3	2.02	0.41
1:B:946:LEU:HD21	1:B:998:LYS:HG2	2.02	0.41
1:B:2428:LEU:HD21	1:B:2482:PHE:CE2	2.55	0.41
1:B:3864:ASN:OD1	1:B:3865:THR:HG23	2.21	0.41
2:H:63:GLY:HA3	2:H:75:LEU:HD21	2.03	0.41
1:C:28:ILE:O	1:C:31:GLU:HG2	2.20	0.41
1:C:182:ILE:HD11	1:C:191:TYR:CD1	2.54	0.41
1:C:1085:PHE:HE2	1:C:1087:ILE:HD11	1.84	0.41
1:C:3925:GLY:O	1:C:3927:CYS:N	2.52	0.41
1:C:4607:ARG:NE	1:C:4643:TYR:OH	2.53	0.41
1:D:28:ILE:O	1:D:31:GLU:HG2	2.20	0.41
1:D:878:LEU:HA	1:D:881:ILE:HD13	2.01	0.41
1:D:1569:ALA:HA	1:D:1572:PHE:CE1	2.56	0.41
1:A:261:HIS:HB3	1:A:390:LYS:HD3	2.02	0.41
1:A:500:GLU:HA	1:A:503:ASP:HB2	2.01	0.41
1:A:1897:LEU:HD22	1:A:1901:VAL:HG11	2.02	0.41
1:A:2428:LEU:HD21	1:A:2482:PHE:CE2	2.55	0.41
1:A:3808:GLU:HA	1:A:3811:ASN:HD22	1.85	0.41
2:G:63:GLY:HA3	2:G:75:LEU:HD21	2.03	0.41
1:B:49:LEU:HD21	1:B:203:VAL:CG1	2.51	0.41
1:B:587:ASN:HA	1:B:2132:ARG:NH1	2.35	0.41
1:B:872:ILE:HD13	1:B:944:LEU:HD22	2.02	0.41
1:B:1234:GLU:HG2	1:B:1236:TYR:HD1	1.85	0.41
1:B:1899:GLU:HB2	1:B:1900:PRO:HD3	2.02	0.41
1:B:1912:LEU:HD23	1:B:1912:LEU:HA	1.88	0.41
1:C:1897:LEU:HD22	1:C:1901:VAL:HG11	2.02	0.41
1:C:2292:VAL:O	1:C:2296:ARG:HG2	2.20	0.41
1:C:3796:MET:HA	1:C:3799:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:63:GLY:HA3	2:I:75:LEU:HD21	2.03	0.41
1:D:49:LEU:HD21	1:D:203:VAL:CG1	2.51	0.41
1:D:1086:ARG:HB3	1:D:1088:PHE:CE1	2.56	0.41
1:D:1310:CYS:SG	1:D:1336:UNK:N	2.94	0.41
1:D:2083:MET:HE3	1:D:2083:MET:HB2	1.63	0.41
1:D:3802:LEU:HB2	1:D:3883:SER:OG	2.19	0.41
1:D:4602:GLU:OE2	1:D:4704:TYR:OH	2.31	0.41
1:A:189:GLU:O	1:B:2325:ARG:NH2	2.53	0.41
1:A:583:PRO:HB3	1:A:620:CYS:SG	2.61	0.41
1:A:670:TYR:HD2	1:A:672:LYS:HB2	1.86	0.41
1:A:837:SER:H	1:A:841:LYS:HZ2	1.69	0.41
1:A:1086:ARG:HB3	1:A:1088:PHE:CE1	2.55	0.41
1:A:1100:ARG:HB3	1:A:1236:TYR:CD2	2.56	0.41
1:A:2771:ARG:HH22	1:A:2775:LYS:HD2	1.84	0.41
1:A:4165:LYS:HE3	1:A:4165:LYS:HB2	1.83	0.41
1:B:19:GLU:HG3	1:B:68:VAL:HG22	2.03	0.41
1:B:2292:VAL:O	1:B:2296:ARG:HG2	2.20	0.41
1:B:2847:TYR:CD2	1:B:2884:ASP:HB2	2.55	0.41
1:C:78:LEU:HD11	1:C:159:TRP:CG	2.56	0.41
1:C:728:ASP:OD1	1:C:728:ASP:N	2.54	0.41
1:C:1234:GLU:HG2	1:C:1236:TYR:CD1	2.55	0.41
1:D:19:GLU:HG3	1:D:68:VAL:HG22	2.03	0.41
1:D:78:LEU:HD11	1:D:159:TRP:CG	2.56	0.41
1:D:2292:VAL:O	1:D:2296:ARG:HG2	2.20	0.41
1:D:2722:LYS:HD2	1:D:2722:LYS:HA	1.78	0.41
1:D:3927:CYS:SG	1:D:3930:ASN:HB2	2.61	0.41
1:A:49:LEU:HD21	1:A:203:VAL:CG1	2.51	0.41
1:A:644:LEU:HD23	1:A:644:LEU:HA	1.96	0.41
1:A:1287:GLN:HB3	1:A:1355:VAL:HG22	2.02	0.41
1:A:1960:LYS:HA	1:A:1960:LYS:HD3	1.60	0.41
1:A:2502:ASP:OD1	1:A:2503:THR:N	2.49	0.41
1:A:4039:LYS:HB2	1:A:4039:LYS:HE2	1.80	0.41
1:A:4515:LEU:HD13	1:A:4736:PHE:HD1	1.86	0.41
1:B:4766:LEU:O	1:B:4770:VAL:HG13	2.20	0.41
2:H:22:THR:CG2	2:H:108:GLU:HB3	2.49	0.41
1:C:1310:CYS:SG	1:C:1336:UNK:N	2.94	0.41
1:C:1902:LYS:HE2	1:C:1902:LYS:HB3	1.92	0.41
1:C:3864:ASN:OD1	1:C:3865:THR:HG23	2.21	0.41
1:D:190:ARG:HB2	1:D:205:ALA:HB1	2.02	0.41
1:D:412:GLU:HB2	1:D:488:LEU:HD21	2.02	0.41
1:D:606:ARG:HE	1:D:644:LEU:HG	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:795:SER:O	1:D:1605:LEU:HD11	2.21	0.41
1:D:1832:MET:HE2	1:D:1832:MET:HB3	1.76	0.41
1:D:1897:LEU:HD22	1:D:1901:VAL:HG11	2.03	0.41
1:D:2502:ASP:OD1	1:D:2503:THR:N	2.49	0.41
1:D:3864:ASN:OD1	1:D:3865:THR:HG23	2.21	0.41
1:A:190:ARG:HB2	1:A:205:ALA:HB1	2.03	0.41
1:A:233:VAL:O	1:A:408:SER:OG	2.37	0.41
1:A:3864:ASN:OD1	1:A:3865:THR:HG23	2.21	0.41
1:A:3878:LEU:HD21	1:A:3938:ARG:NH2	2.36	0.41
1:A:3925:GLY:O	1:A:3927:CYS:N	2.52	0.41
1:A:3927:CYS:SG	1:A:3930:ASN:HB2	2.61	0.41
1:A:4607:ARG:NE	1:A:4643:TYR:OH	2.54	0.41
1:B:76:ARG:NH1	1:C:3889:TRP:HB3	2.36	0.41
1:B:182:ILE:HD11	1:B:191:TYR:CD1	2.54	0.41
1:B:606:ARG:HE	1:B:644:LEU:HG	1.85	0.41
1:B:1569:ALA:HA	1:B:1572:PHE:CE1	2.56	0.41
1:B:3829:LEU:HD12	1:B:3829:LEU:HA	1.87	0.41
1:C:1730:MET:HE2	1:C:3616:VAL:HG11	2.02	0.41
1:C:4039:LYS:HE2	1:C:4039:LYS:HB2	1.80	0.41
1:C:4804:LYS:HE2	1:C:4804:LYS:HB3	1.92	0.41
1:D:390:LYS:HD3	1:D:390:LYS:HA	1.86	0.41
1:D:583:PRO:HB3	1:D:620:CYS:SG	2.61	0.41
1:D:986:ILE:O	1:D:1055:ARG:NH1	2.53	0.41
1:D:1100:ARG:HB3	1:D:1236:TYR:CD2	2.56	0.41
1:D:4034:TYR:CE2	1:D:4050:ALA:HB2	2.56	0.41
1:D:4941:LYS:HE3	1:D:4941:LYS:HB3	1.75	0.41
2:J:50:ARG:HE	2:J:50:ARG:HB3	1.74	0.41
1:A:624:ALA:HB2	1:A:1668:LEU:HD23	2.02	0.41
1:A:946:LEU:HD21	1:A:998:LYS:HG2	2.02	0.41
1:B:583:PRO:HB3	1:B:620:CYS:SG	2.61	0.41
1:B:1110:ALA:HA	1:B:1156:TRP:HE1	1.86	0.41
1:B:1572:PHE:HZ	1:B:1587:LEU:HD11	1.84	0.41
1:B:1789:LYS:O	1:B:1793:ILE:HG13	2.20	0.41
1:B:2243:ALA:O	1:B:2247:MET:HG3	2.20	0.41
1:B:3761:GLY:HA2	1:B:3764:ILE:HG22	2.01	0.41
1:B:3878:LEU:HD21	1:B:3938:ARG:NH2	2.36	0.41
1:B:3927:CYS:SG	1:B:3930:ASN:HB2	2.61	0.41
1:B:4034:TYR:CE2	1:B:4050:ALA:HB2	2.56	0.41
1:B:4955:ASP:OD1	1:B:4956:CYS:N	2.52	0.41
1:C:516:ASP:N	1:C:516:ASP:OD1	2.52	0.41
1:C:583:PRO:HB3	1:C:620:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:ALA:HB2	1:C:1668:LEU:HD23	2.02	0.41
1:C:1086:ARG:HB3	1:C:1088:PHE:CE1	2.56	0.41
1:C:1587:LEU:HD23	1:C:1587:LEU:HA	1.93	0.41
1:C:1682:ASP:OD1	1:C:1685:GLN:NE2	2.54	0.41
1:C:1745:LYS:HE3	1:C:1745:LYS:HB3	1.78	0.41
1:C:1789:LYS:O	1:C:1793:ILE:HG13	2.20	0.41
1:C:1835:PHE:O	1:C:1840:LEU:HG	2.20	0.41
1:C:2092:ASP:O	1:C:2094:ILE:N	2.53	0.41
1:C:2260:ASP:OD1	1:C:2260:ASP:N	2.51	0.41
1:C:2404:GLU:HG3	1:C:2405:MET:N	2.36	0.41
1:C:2850:ILE:HG13	1:C:2851:TRP:N	2.36	0.41
1:C:3802:LEU:HG	1:C:3829:LEU:HD13	2.02	0.41
1:C:3839:PHE:CE1	1:C:3873:THR:HG23	2.54	0.41
1:C:3927:CYS:SG	1:C:3930:ASN:HB2	2.61	0.41
1:D:642:LEU:HG	1:D:643:LEU:HA	2.03	0.41
1:D:2404:GLU:HG3	1:D:2405:MET:N	2.36	0.41
1:D:3888:TYR:CE2	1:D:3889:TRP:CD1	3.09	0.41
1:D:4515:LEU:HD13	1:D:4736:PHE:HD1	1.86	0.41
1:D:4518:TYR:CE1	1:D:4560:LEU:HD12	2.56	0.41
1:D:4636:THR:OG1	1:D:4701:ASP:OD2	2.39	0.41
1:D:4766:LEU:O	1:D:4770:VAL:HG13	2.21	0.41
1:D:4955:ASP:OD1	1:D:4956:CYS:N	2.52	0.41
1:A:872:ILE:HD13	1:A:944:LEU:HD22	2.02	0.41
1:B:42:PHE:CZ	1:B:458:ASP:HB3	2.56	0.41
1:B:727:PHE:HB2	1:B:768:PHE:CD1	2.56	0.41
1:B:4518:TYR:CE1	1:B:4560:LEU:HD12	2.56	0.41
1:C:254:GLU:O	1:C:258:ARG:HG3	2.20	0.41
1:C:3888:TYR:CE2	1:C:3889:TRP:CD1	3.09	0.41
1:D:2130:SER:O	1:D:2130:SER:OG	2.39	0.41
1:D:2243:ALA:O	1:D:2247:MET:HG3	2.20	0.41
1:D:4165:LYS:HE3	1:D:4165:LYS:HB2	1.83	0.41
1:A:42:PHE:CZ	1:A:458:ASP:HB3	2.56	0.40
1:A:449:ILE:HD13	1:A:449:ILE:HA	1.95	0.40
1:A:2243:ALA:O	1:A:2247:MET:HG3	2.20	0.40
1:A:3888:TYR:CE2	1:A:3889:TRP:CD1	3.09	0.40
1:A:4518:TYR:CE1	1:A:4560:LEU:HD12	2.56	0.40
1:A:4584:PHE:HA	1:A:4587:ILE:HG12	2.03	0.40
1:A:4766:LEU:O	1:A:4770:VAL:HG13	2.20	0.40
1:B:262:TYR:CE1	1:B:391:ALA:HB2	2.56	0.40
1:B:1310:CYS:SG	1:B:1336:UNK:N	2.94	0.40
1:B:2404:GLU:HG3	1:B:2405:MET:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4792:TYR:HH	1:B:4815:HIS:HE2	1.66	0.40
1:C:331:PHE:HB3	1:C:361:CYS:HB3	2.04	0.40
1:C:606:ARG:HE	1:C:644:LEU:HG	1.85	0.40
1:C:643:LEU:HD22	1:C:1658:THR:HG23	2.03	0.40
1:C:4515:LEU:HD13	1:C:4736:PHE:HD1	1.86	0.40
1:C:4518:TYR:CE1	1:C:4560:LEU:HD12	2.56	0.40
1:D:262:TYR:CE1	1:D:391:ALA:HB2	2.56	0.40
1:D:643:LEU:HD22	1:D:1658:THR:HG23	2.03	0.40
1:D:1789:LYS:O	1:D:1793:ILE:HG13	2.20	0.40
1:D:3808:GLU:HA	1:D:3811:ASN:HD22	1.85	0.40
1:A:377:VAL:CG2	1:A:390:LYS:HG2	2.50	0.40
1:A:677:LEU:HD11	1:A:800:VAL:CG1	2.51	0.40
1:A:1912:LEU:HD23	1:A:1912:LEU:HA	1.88	0.40
1:A:2325:ARG:CZ	1:D:191:TYR:HE2	2.34	0.40
1:A:4636:THR:OG1	1:A:4701:ASP:OD2	2.39	0.40
1:B:677:LEU:HD11	1:B:800:VAL:CG1	2.51	0.40
1:B:1100:ARG:HB3	1:B:1236:TYR:CD2	2.56	0.40
1:B:1680:HIS:NE2	2:H:91:VAL:HG22	2.37	0.40
1:B:2395:ILE:HD13	1:B:2395:ILE:HA	1.95	0.40
1:C:19:GLU:HG3	1:C:68:VAL:HG22	2.03	0.40
1:C:412:GLU:HB2	1:C:488:LEU:HD21	2.02	0.40
1:C:617:LEU:HA	1:C:617:LEU:HD23	1.88	0.40
1:C:795:SER:O	1:C:1605:LEU:HD11	2.21	0.40
1:C:919:VAL:HG22	1:C:920:GLU:H	1.87	0.40
1:C:1623:LEU:HD23	1:C:1623:LEU:HA	1.93	0.40
1:C:3617:ASN:O	1:C:3621:GLN:HG2	2.22	0.40
1:D:459:LEU:HD23	1:D:459:LEU:HA	1.95	0.40
1:D:670:TYR:HD2	1:D:672:LYS:HB2	1.86	0.40
1:D:1682:ASP:OD1	1:D:1685:GLN:NE2	2.54	0.40
2:J:63:GLY:HA3	2:J:75:LEU:HD21	2.03	0.40
1:A:56:LYS:HA	1:A:324:VAL:HG13	2.03	0.40
1:A:114:LEU:HB2	1:A:117:HIS:CE1	2.56	0.40
1:A:262:TYR:CE1	1:A:391:ALA:HB2	2.56	0.40
1:A:331:PHE:HB3	1:A:361:CYS:HB3	2.04	0.40
1:A:643:LEU:HD22	1:A:1658:THR:HG23	2.03	0.40
1:A:1110:ALA:HA	1:A:1156:TRP:HE1	1.86	0.40
1:A:1310:CYS:SG	1:A:1336:UNK:N	2.94	0.40
1:A:1682:ASP:OD1	1:A:1685:GLN:NE2	2.54	0.40
1:A:3617:ASN:O	1:A:3621:GLN:HG2	2.22	0.40
1:A:3888:TYR:CE1	1:A:3953:MET:HG2	2.56	0.40
2:G:22:THR:CG2	2:G:108:GLU:HB3	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:PHE:HB3	1:B:361:CYS:HB3	2.04	0.40
1:B:377:VAL:CG2	1:B:390:LYS:HG2	2.50	0.40
1:B:642:LEU:HG	1:B:643:LEU:HA	2.03	0.40
1:B:882:ARG:HD2	1:B:937:LEU:HD23	2.04	0.40
1:B:2850:ILE:HG13	1:B:2851:TRP:N	2.36	0.40
1:B:4515:LEU:HD13	1:B:4736:PHE:HD1	1.86	0.40
1:B:4804:LYS:HE2	1:B:4804:LYS:HB3	1.92	0.40
1:C:42:PHE:CZ	1:C:458:ASP:HB3	2.56	0.40
1:C:49:LEU:HD21	1:C:203:VAL:CG1	2.51	0.40
1:C:882:ARG:HD2	1:C:937:LEU:HD23	2.04	0.40
1:C:1677:LEU:O	1:C:1681:VAL:HG22	2.22	0.40
1:C:4034:TYR:CE2	1:C:4050:ALA:HB2	2.56	0.40
2:I:22:THR:CG2	2:I:108:GLU:HB3	2.49	0.40
2:I:50:ARG:HE	2:I:50:ARG:HB3	1.74	0.40
1:D:3878:LEU:HD21	1:D:3938:ARG:NH2	2.36	0.40
1:A:380:LYS:HA	1:A:380:LYS:HD2	1.75	0.40
1:A:882:ARG:HD2	1:A:937:LEU:HD23	2.04	0.40
1:A:2404:GLU:HG3	1:A:2405:MET:N	2.36	0.40
1:A:4034:TYR:CE2	1:A:4050:ALA:HB2	2.56	0.40
1:B:114:LEU:HB2	1:B:117:HIS:CE1	2.56	0.40
1:B:919:VAL:HG22	1:B:920:GLU:H	1.87	0.40
1:B:1175:PHE:O	1:B:1181:ILE:HD12	2.22	0.40
1:B:2479:VAL:HG12	1:B:2482:PHE:H	1.86	0.40
1:B:3888:TYR:CE2	1:B:3889:TRP:CD1	3.09	0.40
1:B:4165:LYS:HE3	1:B:4165:LYS:HB2	1.83	0.40
1:C:587:ASN:HA	1:C:2132:ARG:NH1	2.35	0.40
1:C:642:LEU:HG	1:C:643:LEU:HA	2.03	0.40
1:C:677:LEU:HD11	1:C:800:VAL:CG1	2.51	0.40
1:C:727:PHE:HB2	1:C:768:PHE:CD1	2.56	0.40
1:C:874:LEU:HD21	1:C:937:LEU:HB3	2.04	0.40
1:C:1110:ALA:HA	1:C:1156:TRP:HE1	1.86	0.40
1:C:1265:HIS:ND1	1:C:1268:ILE:HB	2.37	0.40
1:C:3888:TYR:CE1	1:C:3953:MET:HG2	2.56	0.40
1:C:4044:LYS:HE2	1:C:4044:LYS:HB3	1.93	0.40
1:C:4824:GLY:O	1:D:4821:ARG:NH1	2.55	0.40
2:I:79:PRO:O	2:I:84:GLY:N	2.40	0.40
1:D:946:LEU:HD21	1:D:998:LYS:HG2	2.02	0.40
1:D:970:TYR:OH	1:D:978:PRO:O	2.30	0.40
1:D:1910:GLN:HG2	1:D:2086:LEU:HD13	2.02	0.40
1:A:313:ASN:ND2	1:A:392:ILE:HA	2.37	0.40
1:A:1910:GLN:HG2	1:A:2086:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3839:PHE:HE1	1:A:3873:THR:HG23	1.86	0.40
1:B:78:LEU:HD11	1:B:159:TRP:CG	2.56	0.40
1:B:499:LEU:HD22	1:B:557:TRP:CZ3	2.57	0.40
1:B:1287:GLN:HB3	1:B:1355:VAL:HG22	2.02	0.40
1:B:2112:VAL:O	1:B:2115:THR:HG22	2.22	0.40
1:B:3839:PHE:HE1	1:B:3873:THR:HG23	1.86	0.40
1:C:190:ARG:HB2	1:C:205:ALA:HB1	2.03	0.40
1:C:1796:LEU:HD12	1:C:1796:LEU:HA	1.89	0.40
1:C:4786:ASN:HD22	1:C:4786:ASN:N	2.18	0.40
1:D:42:PHE:CZ	1:D:458:ASP:HB3	2.56	0.40
1:D:617:LEU:HA	1:D:617:LEU:HD23	1.88	0.40
1:D:727:PHE:HB2	1:D:768:PHE:CD1	2.56	0.40
1:D:872:ILE:HD13	1:D:944:LEU:HD22	2.02	0.40
1:D:1110:ALA:HA	1:D:1156:TRP:HE1	1.86	0.40
1:D:2112:VAL:O	1:D:2115:THR:HG22	2.22	0.40
1:D:3617:ASN:O	1:D:3621:GLN:HG2	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%)	3044 (94%)	211 (6%)	0	100 100
1	B	3255/4966 (66%)	3044 (94%)	211 (6%)	0	100 100
1	C	3255/4966 (66%)	3044 (94%)	211 (6%)	0	100 100
1	D	3255/4966 (66%)	3044 (94%)	211 (6%)	0	100 100
2	G	105/176 (60%)	100 (95%)	5 (5%)	0	100 100
2	H	105/176 (60%)	100 (95%)	5 (5%)	0	100 100
2	I	105/176 (60%)	100 (95%)	5 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
All	All	13440/20568 (65%)	12576 (94%)	864 (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	2861/3386 (84%)	2801 (98%)	60 (2%)	53	75
1	B	2861/3386 (84%)	2802 (98%)	59 (2%)	53	75
1	C	2861/3386 (84%)	2801 (98%)	60 (2%)	53	75
1	D	2861/3386 (84%)	2801 (98%)	60 (2%)	53	75
2	G	88/140 (63%)	85 (97%)	3 (3%)	37	65
2	H	88/140 (63%)	85 (97%)	3 (3%)	37	65
2	I	88/140 (63%)	85 (97%)	3 (3%)	37	65
2	J	88/140 (63%)	85 (97%)	3 (3%)	37	65
All	All	11796/14104 (84%)	11545 (98%)	251 (2%)	56	75

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
1	A	182	ILE
1	A	203	VAL
1	A	244	CYS
1	A	254	GLU
1	A	497	LEU
1	A	555	LEU
1	A	561	ARG
1	A	625	VAL
1	A	646	THR

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Mol	Chain	Res	Type
1	A	711	GLU
1	A	778	MET
1	A	801	ARG
1	A	1028	ARG
1	A	1133	ARG
1	A	1152	TYR
1	A	1161	VAL
1	A	1190	LEU
1	A	1226	TYR
1	A	1261	VAL
1	A	1300	MET
1	A	1304	LEU
1	A	1682	ASP
1	A	1695	MET
1	A	1721	MET
1	A	1743	GLU
1	A	1792	THR
1	A	1798	GLU
1	A	1905	MET
1	A	1938	ASN
1	A	1969	GLN
1	A	1990	GLU
1	A	2004	THR
1	A	2065	MET
1	A	2113	GLU
1	A	2172	GLU
1	A	2191	MET
1	A	2233	MET
1	A	2274	GLN
1	A	2277	GLN
1	A	2278	MET
1	A	2302	ARG
1	A	2335	ARG
1	A	2405	MET
1	A	2425	LEU
1	A	2454	ASP
1	A	2478	GLU
1	A	2735	LYS
1	A	2771	ARG
1	A	2842	MET
1	A	2893	LYS
1	A	3885	SER

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Mol	Chain	Res	Type
1	A	3889	TRP
1	A	3896	ILE
1	A	3972	ASP
1	A	4001	MET
1	A	4045	ARG
1	A	4782	VAL
1	A	4885	THR
1	A	4949	GLU
2	G	14	ARG
2	G	18	LYS
2	G	69	LEU
1	B	133	LEU
1	B	182	ILE
1	B	203	VAL
1	B	244	CYS
1	B	254	GLU
1	B	497	LEU
1	B	555	LEU
1	B	561	ARG
1	B	625	VAL
1	B	646	THR
1	B	711	GLU
1	B	778	MET
1	B	801	ARG
1	B	1028	ARG
1	B	1133	ARG
1	B	1152	TYR
1	B	1161	VAL
1	B	1190	LEU
1	B	1226	TYR
1	B	1261	VAL
1	B	1300	MET
1	B	1304	LEU
1	B	1682	ASP
1	B	1695	MET
1	B	1721	MET
1	B	1743	GLU
1	B	1792	THR
1	B	1798	GLU
1	B	1905	MET
1	B	1969	GLN
1	B	1990	GLU

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Mol	Chain	Res	Type
1	B	2004	THR
1	B	2065	MET
1	B	2113	GLU
1	B	2172	GLU
1	B	2191	MET
1	B	2233	MET
1	B	2274	GLN
1	B	2277	GLN
1	B	2278	MET
1	B	2302	ARG
1	B	2335	ARG
1	B	2405	MET
1	B	2425	LEU
1	B	2454	ASP
1	B	2478	GLU
1	B	2735	LYS
1	B	2771	ARG
1	B	2842	MET
1	B	2893	LYS
1	B	3885	SER
1	B	3889	TRP
1	B	3896	ILE
1	B	3972	ASP
1	B	4001	MET
1	B	4045	ARG
1	B	4782	VAL
1	B	4885	THR
1	B	4949	GLU
2	H	14	ARG
2	H	18	LYS
2	H	69	LEU
1	C	133	LEU
1	C	182	ILE
1	C	203	VAL
1	C	244	CYS
1	C	254	GLU
1	C	497	LEU
1	C	555	LEU
1	C	561	ARG
1	C	625	VAL
1	C	646	THR
1	C	711	GLU

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Mol	Chain	Res	Type
1	C	778	MET
1	C	801	ARG
1	C	1028	ARG
1	C	1133	ARG
1	C	1152	TYR
1	C	1161	VAL
1	C	1190	LEU
1	C	1226	TYR
1	C	1261	VAL
1	C	1300	MET
1	C	1304	LEU
1	C	1682	ASP
1	C	1695	MET
1	C	1721	MET
1	C	1743	GLU
1	C	1792	THR
1	C	1798	GLU
1	C	1905	MET
1	C	1969	GLN
1	C	1990	GLU
1	C	2004	THR
1	C	2065	MET
1	C	2113	GLU
1	C	2172	GLU
1	C	2191	MET
1	C	2233	MET
1	C	2274	GLN
1	C	2277	GLN
1	C	2278	MET
1	C	2302	ARG
1	C	2335	ARG
1	C	2405	MET
1	C	2425	LEU
1	C	2454	ASP
1	C	2478	GLU
1	C	2735	LYS
1	C	2771	ARG
1	C	2842	MET
1	C	2893	LYS
1	C	3885	SER
1	C	3889	TRP
1	C	3896	ILE

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Mol	Chain	Res	Type
1	C	3972	ASP
1	C	4001	MET
1	C	4045	ARG
1	C	4782	VAL
1	C	4786	ASN
1	C	4885	THR
1	C	4949	GLU
2	I	14	ARG
2	I	18	LYS
2	I	69	LEU
1	D	133	LEU
1	D	182	ILE
1	D	203	VAL
1	D	244	CYS
1	D	254	GLU
1	D	497	LEU
1	D	555	LEU
1	D	561	ARG
1	D	625	VAL
1	D	646	THR
1	D	711	GLU
1	D	778	MET
1	D	801	ARG
1	D	1028	ARG
1	D	1133	ARG
1	D	1152	TYR
1	D	1161	VAL
1	D	1190	LEU
1	D	1226	TYR
1	D	1261	VAL
1	D	1300	MET
1	D	1304	LEU
1	D	1682	ASP
1	D	1695	MET
1	D	1721	MET
1	D	1743	GLU
1	D	1792	THR
1	D	1798	GLU
1	D	1905	MET
1	D	1938	ASN
1	D	1969	GLN
1	D	1990	GLU

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Mol	Chain	Res	Type
1	D	2004	THR
1	D	2065	MET
1	D	2113	GLU
1	D	2172	GLU
1	D	2191	MET
1	D	2233	MET
1	D	2274	GLN
1	D	2277	GLN
1	D	2278	MET
1	D	2302	ARG
1	D	2335	ARG
1	D	2405	MET
1	D	2425	LEU
1	D	2454	ASP
1	D	2478	GLU
1	D	2735	LYS
1	D	2771	ARG
1	D	2842	MET
1	D	2893	LYS
1	D	3885	SER
1	D	3889	TRP
1	D	3896	ILE
1	D	3972	ASP
1	D	4001	MET
1	D	4045	ARG
1	D	4782	VAL
1	D	4885	THR
1	D	4949	GLU
2	J	14	ARG
2	J	18	LYS
2	J	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	490	GLN
1	A	544	ASN
1	A	547	ASN
1	A	2090	GLN
1	A	2151	ASN
1	A	2385	ASN
1	A	2480	GLN

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Mol	Chain	Res	Type
1	A	2848	HIS
1	A	4177	ASN
1	B	490	GLN
1	B	544	ASN
1	B	547	ASN
1	B	2090	GLN
1	B	2151	ASN
1	B	2385	ASN
1	B	2480	GLN
1	B	2848	HIS
1	B	4177	ASN
1	C	490	GLN
1	C	544	ASN
1	C	547	ASN
1	C	2090	GLN
1	C	2151	ASN
1	C	2385	ASN
1	C	2480	GLN
1	C	2848	HIS
1	C	4786	ASN
1	D	490	GLN
1	D	544	ASN
1	D	547	ASN
1	D	2090	GLN
1	D	2151	ASN
1	D	2385	ASN
1	D	2480	GLN
1	D	2848	HIS
1	D	4177	ASN

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.

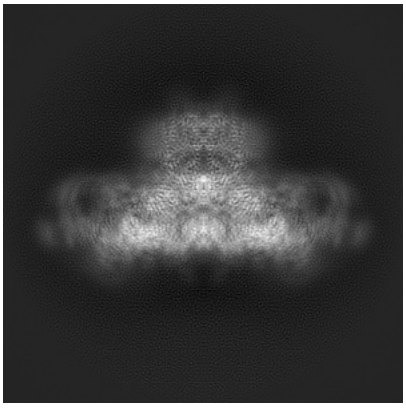
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32036. These allow visual inspection of the internal detail of the map and identification of artifacts.

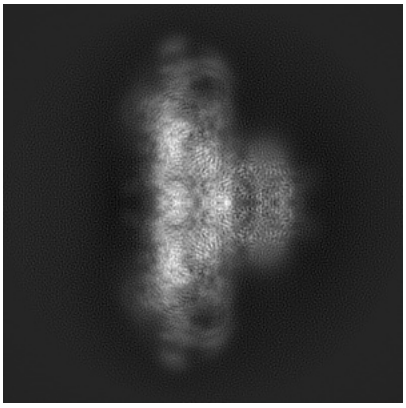
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

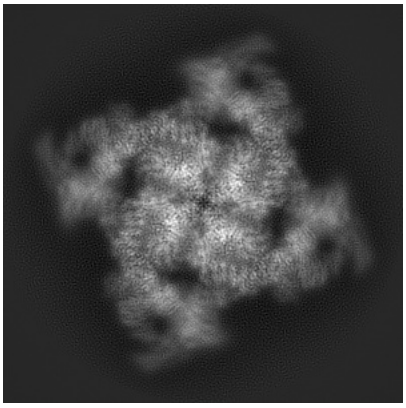
6.1.1 Primary map



X



Y

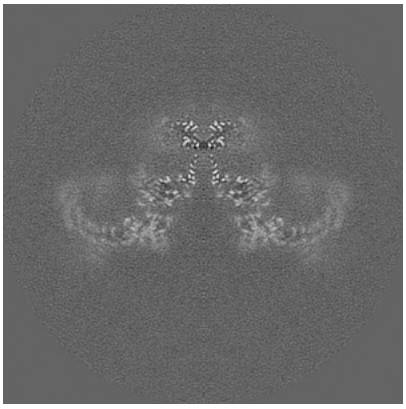


Z

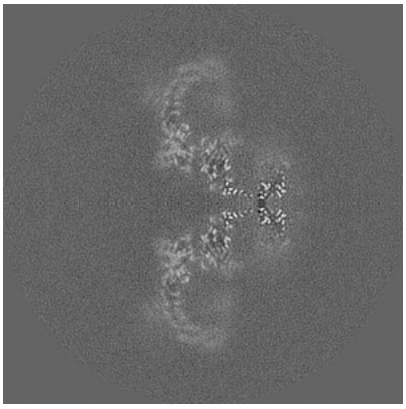
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

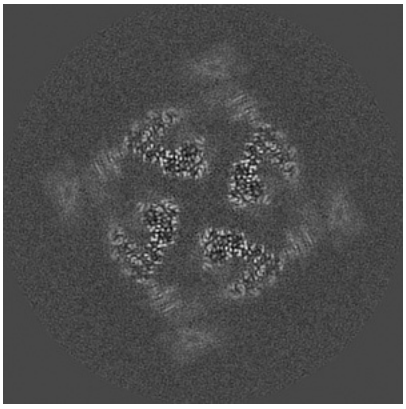
6.2.1 Primary map



X Index: 160



Y Index: 160

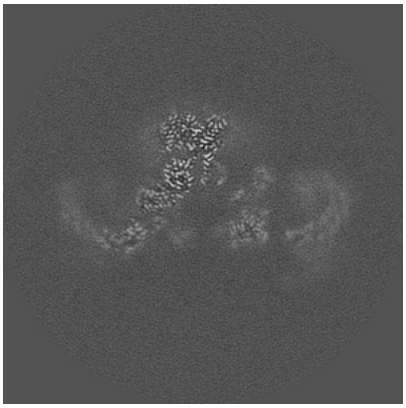


Z Index: 160

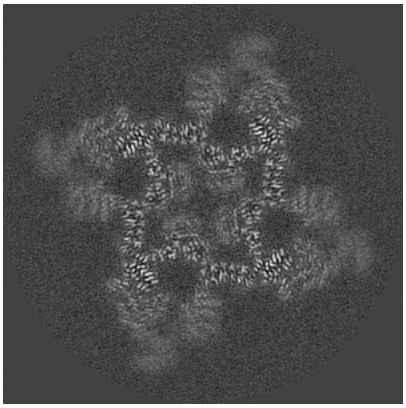
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 167

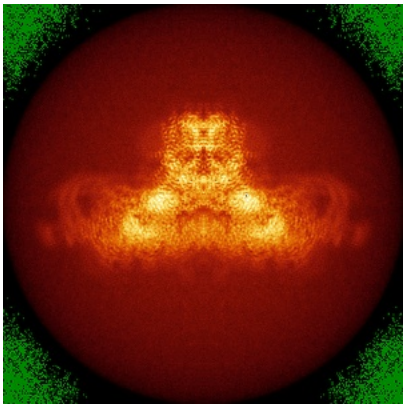
Y Index: 153

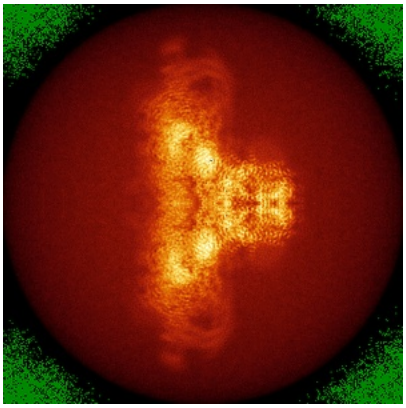

Z Index: 139

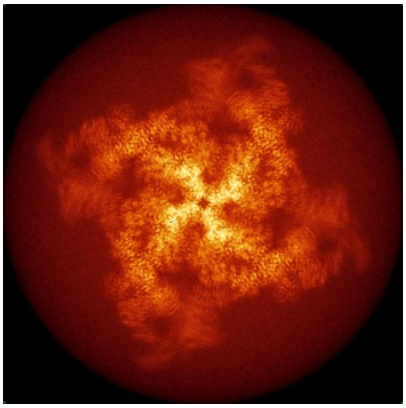
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

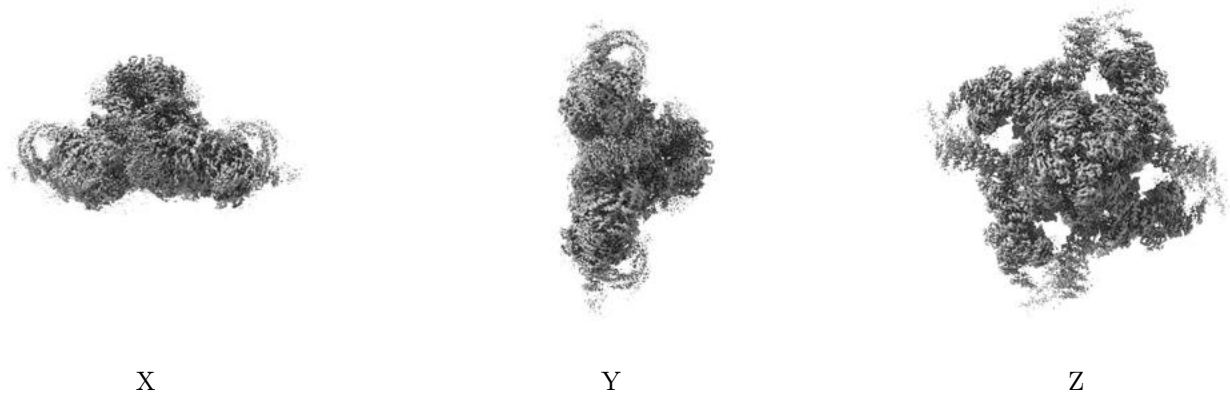

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

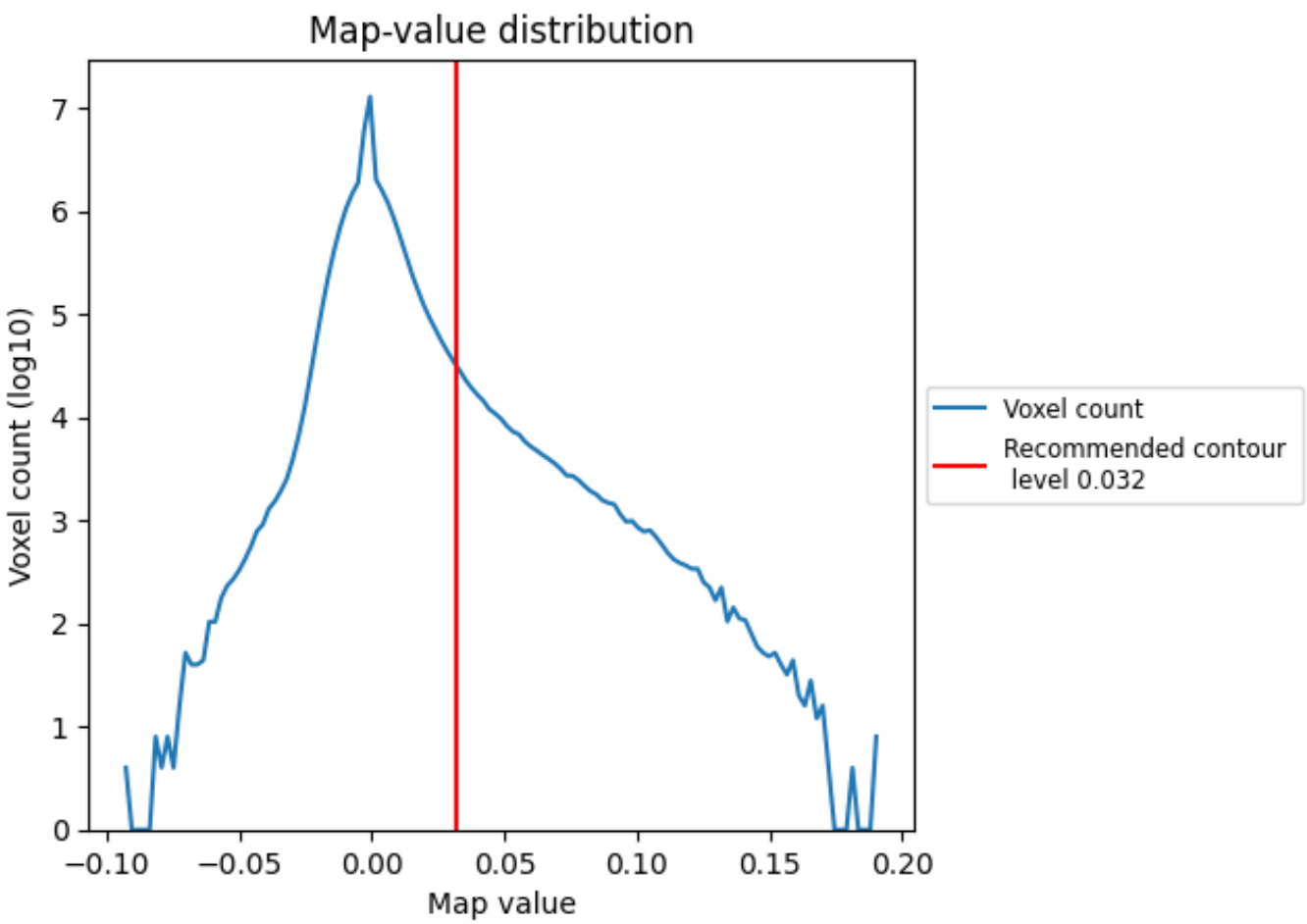
6.6 Mask visualisation (i)

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

7 Map analysis (i)

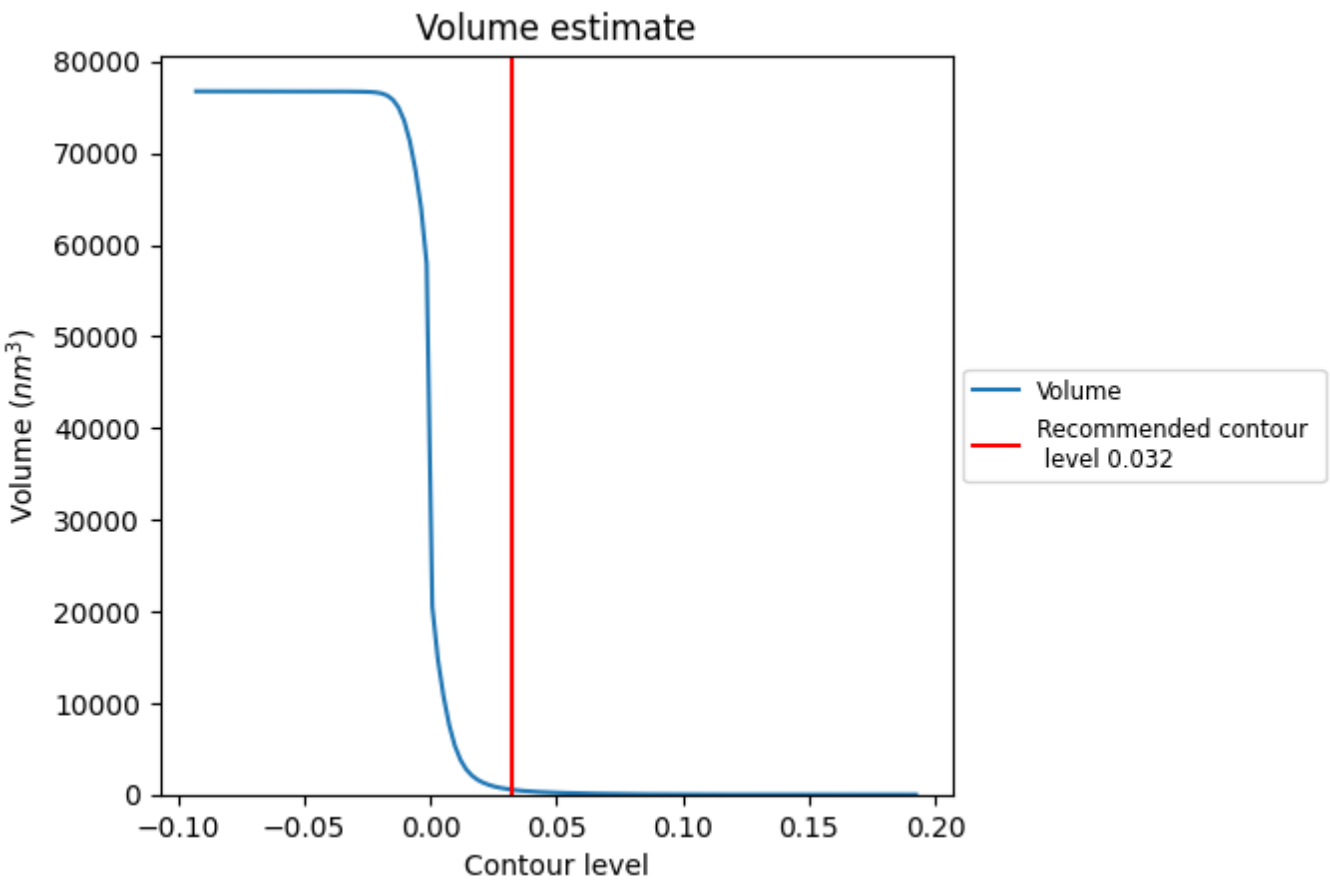
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

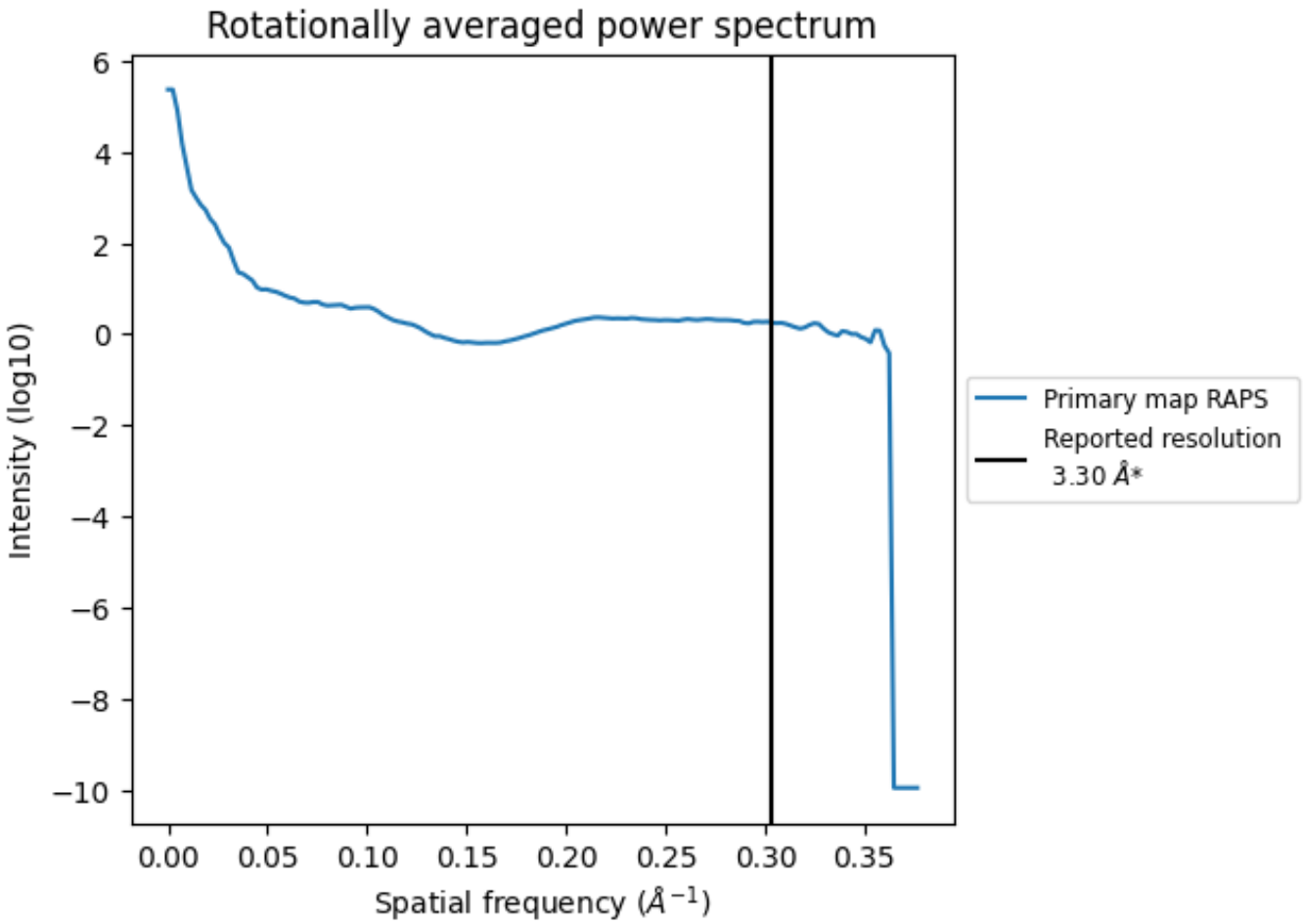
7.2 Volume estimate (i)



The volume at the recommended contour level is 544 nm^3; this corresponds to an approximate mass of 492 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 0.303 Å^{-1}

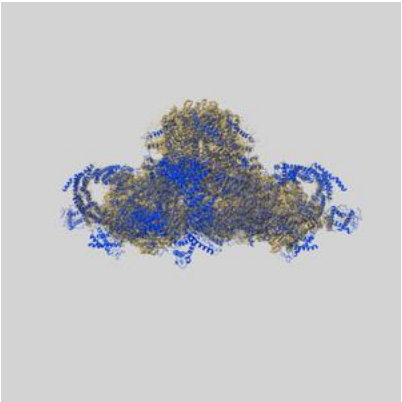
8 Fourier-Shell correlation (i)

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

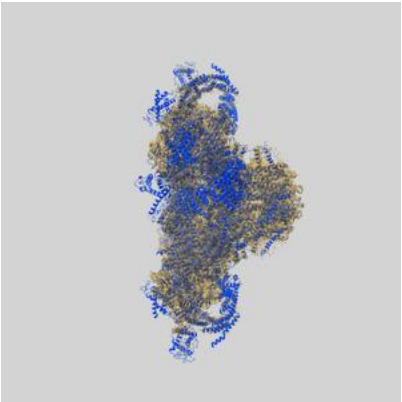
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32036 and PDB model 7VMR. Per-residue inclusion information can be found in section 3 on page 11.

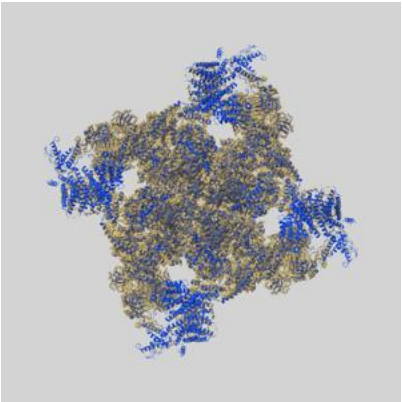
9.1 Map-model overlay (i)



X



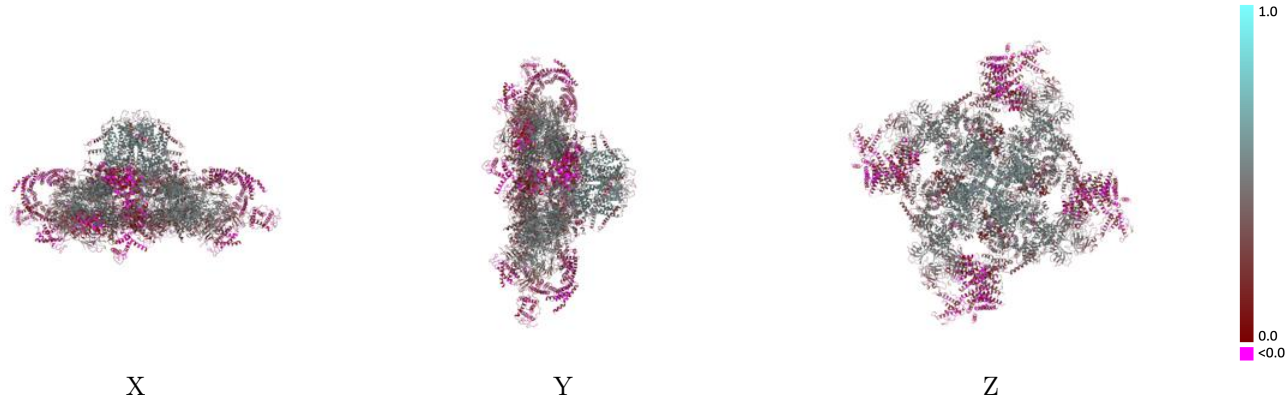
Y



Z

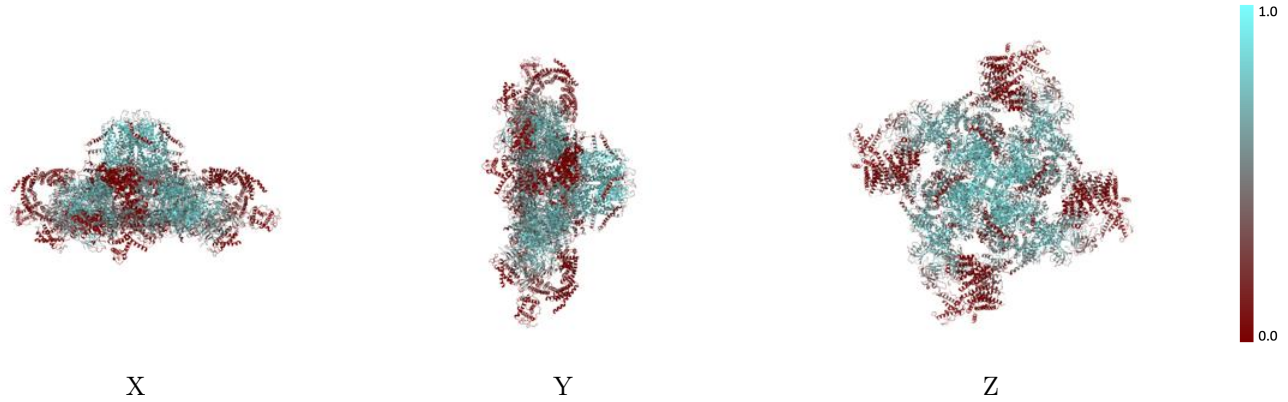
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



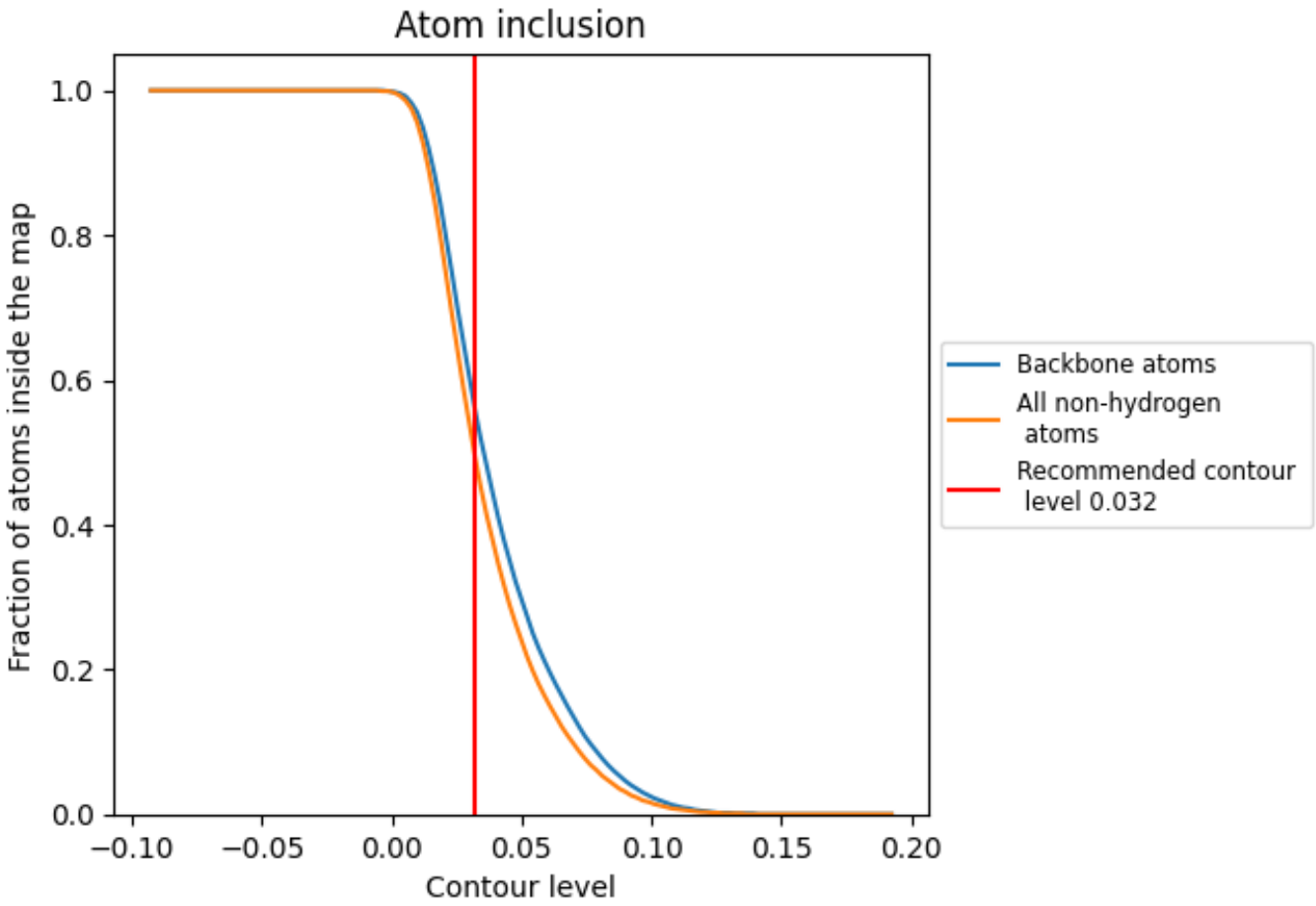
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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 (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4940	0.3620
A	0.4960	0.3640
B	0.4910	0.3580
C	0.4940	0.3580
D	0.4940	0.3600
G	0.5190	0.4230
H	0.5220	0.4280
I	0.5250	0.4320
J	0.5200	0.4280