Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 04:55 PM JST

PDB ID	:	26IS / pdb_000026is
EMDB ID	:	EMD-80687
Title	:	Structure of recombinant RyR2 in complex with Ryanozole in the closed conformation (EGTA dataset)
Authors	:	Otori, Y.; Takeuchi, S.; Ogawa, H.
Deposited on	:	2026-05-01
Resolution	:	2.90 Å(reported)

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

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

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

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

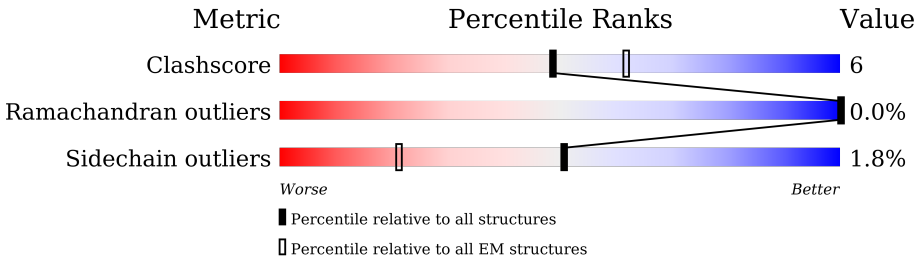
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

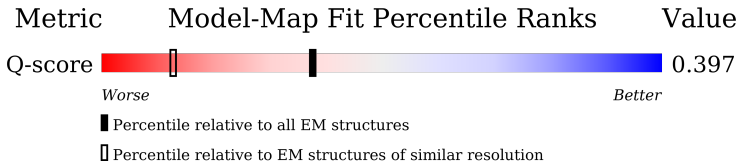
1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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.





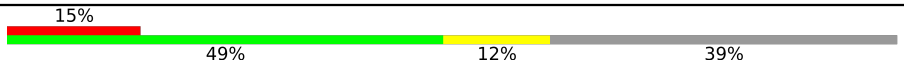
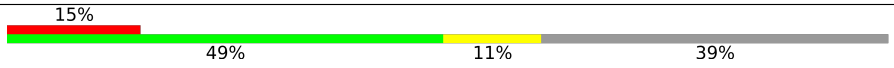
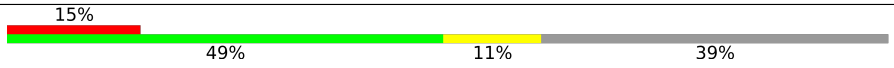
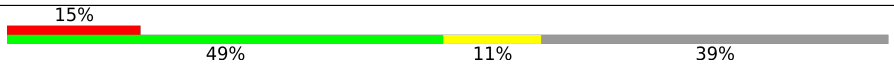
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	22% 59% 11% 30%
1	B	4966	22% 59% 11% 30%
1	C	4966	22% 60% 10% 30%
1	D	4966	22% 59% 11% 30%

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Mol	Chain	Length	Quality of chain
2	G	176	
2	H	176	
2	I	176	
2	J	176	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 228476 atoms, of which 113472 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	3494	Total	C	H	N	O	S	0	0
			55441	17769	27535	4747	5200	190		
1	B	3494	Total	C	H	N	O	S	0	0
			55441	17769	27535	4747	5200	190		
1	C	3494	Total	C	H	N	O	S	0	0
			55441	17769	27535	4747	5200	190		
1	D	3494	Total	C	H	N	O	S	0	0
			55441	17769	27535	4747	5200	190		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	107	Total	C	H	N	O	S	0	0
			1640	516	821	144	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1640	516	821	144	155	4		
2	I	107	Total	C	H	N	O	S	0	0
			1640	516	821	144	155	4		
2	J	107	Total	C	H	N	O	S	0	0
			1640	516	821	144	155	4		

There are 276 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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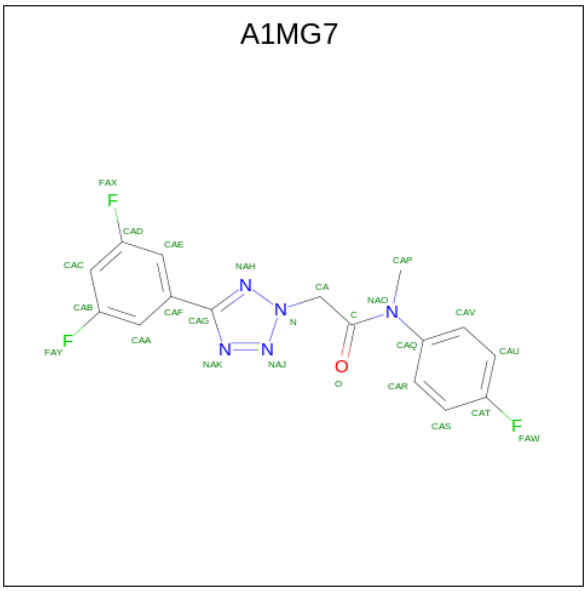
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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	PRO	-	expression tag	UNP P68106
J	-12	GLN	-	expression tag	UNP P68106
J	-11	GLY	-	expression tag	UNP P68106
J	-10	GLN	-	expression tag	UNP P68106
J	-9	ARG	-	expression tag	UNP P68106
J	-8	GLU	-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

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

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

- Molecule 4 is Ryanozole (CCD ID: A1MG7) (formula: $C_{16}H_{12}F_3N_5O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
4	B	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
4	C	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
4	D	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	

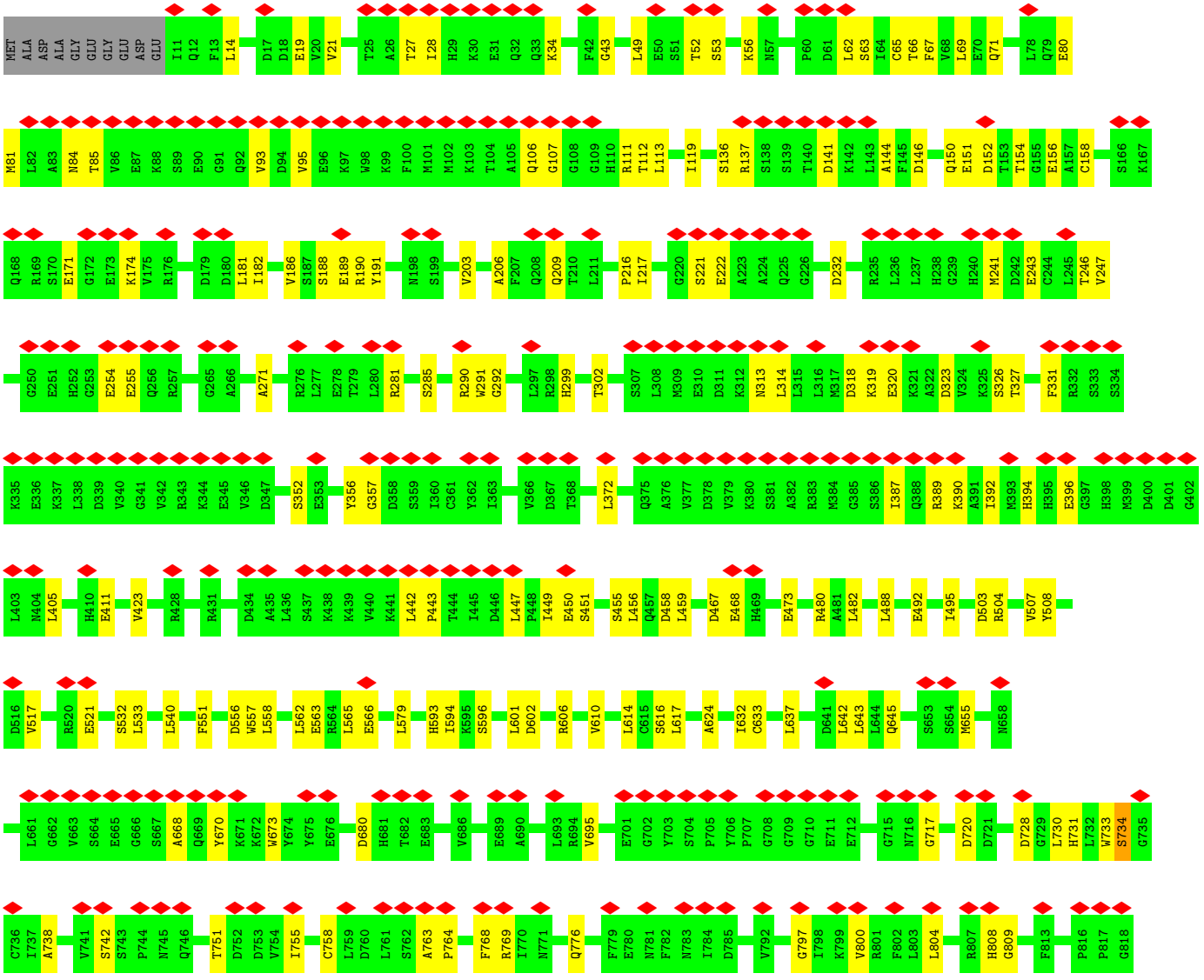
3 Residue-property plots (i)

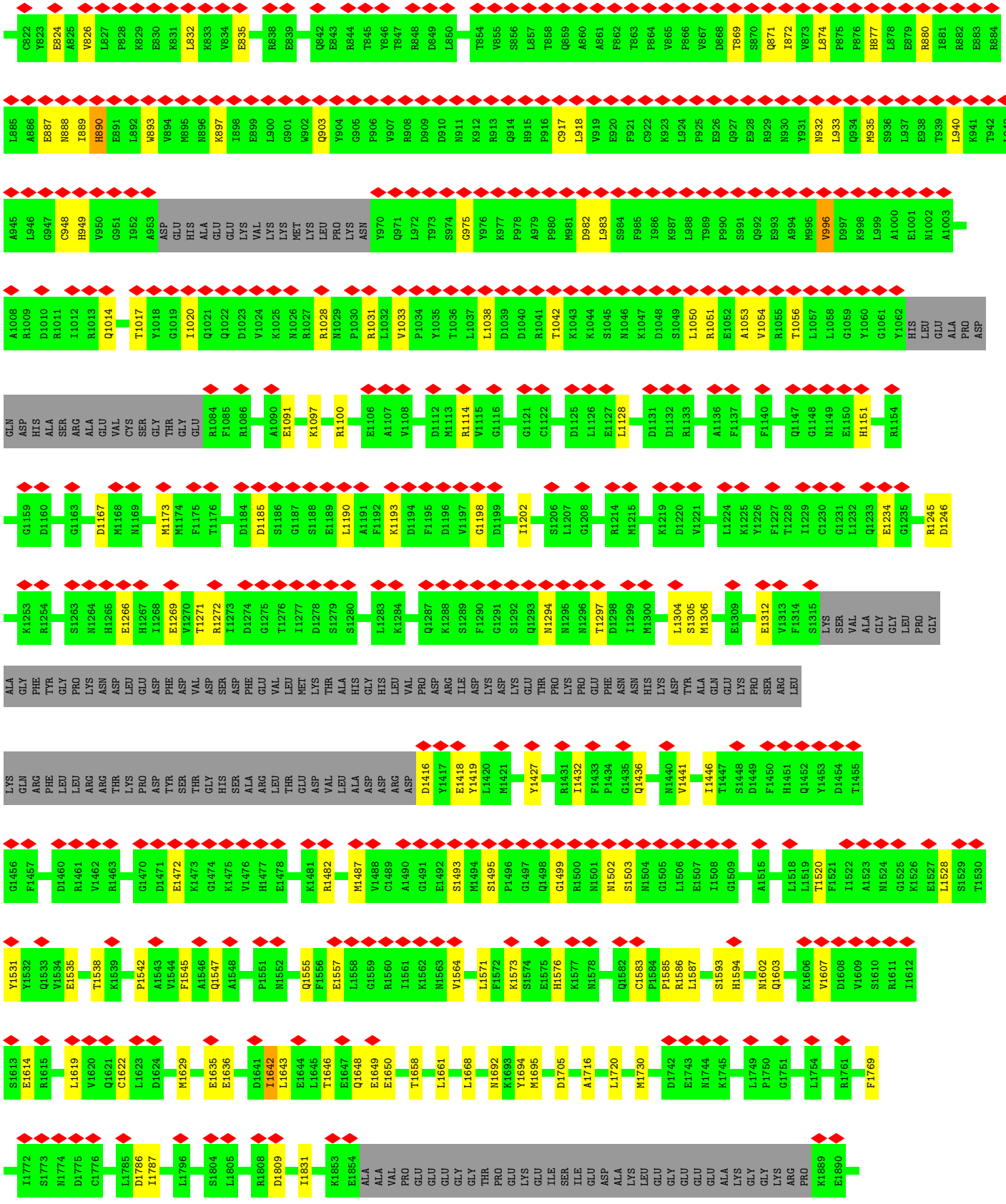
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

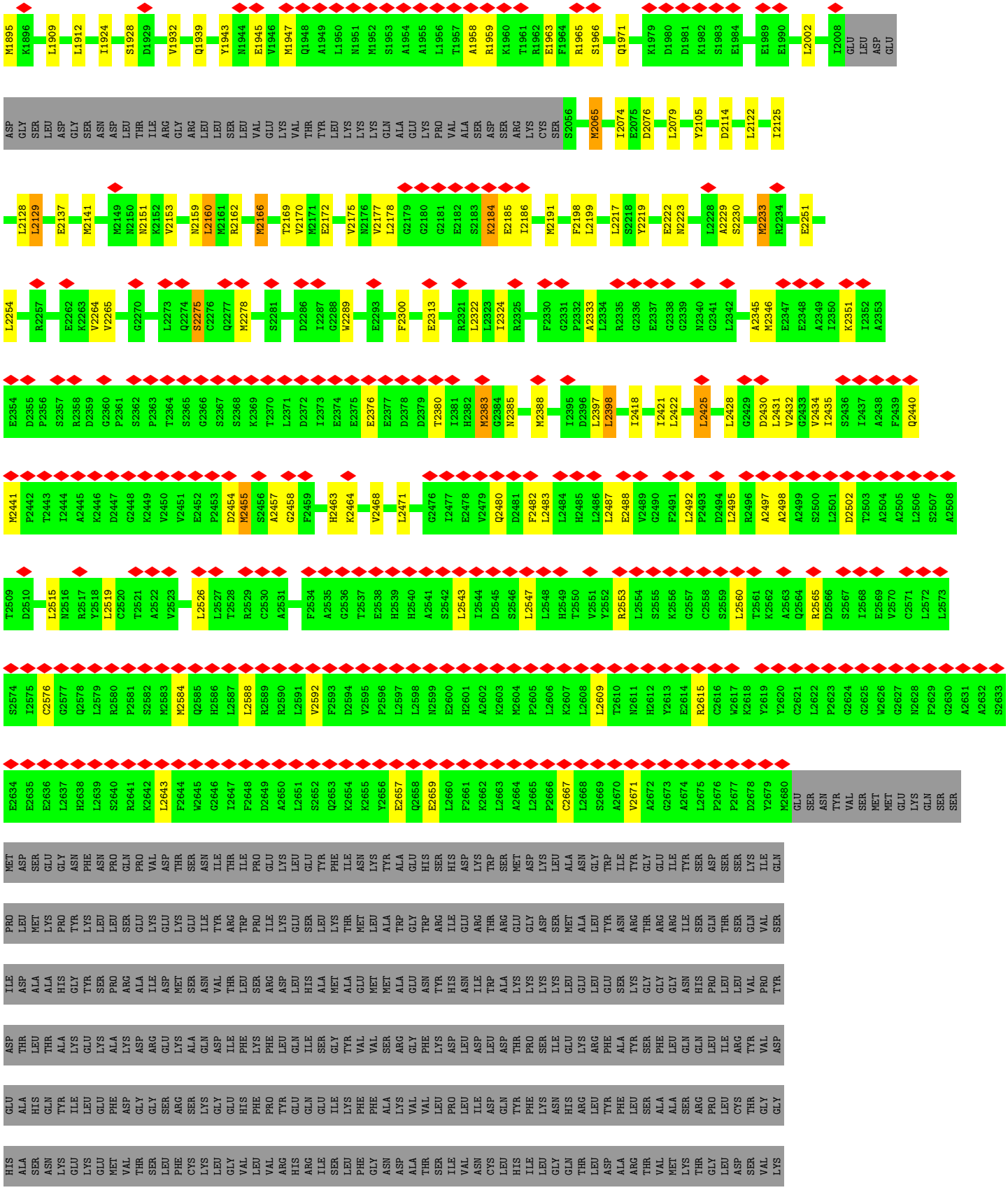
- Molecule 1: Ryanodine receptor 2

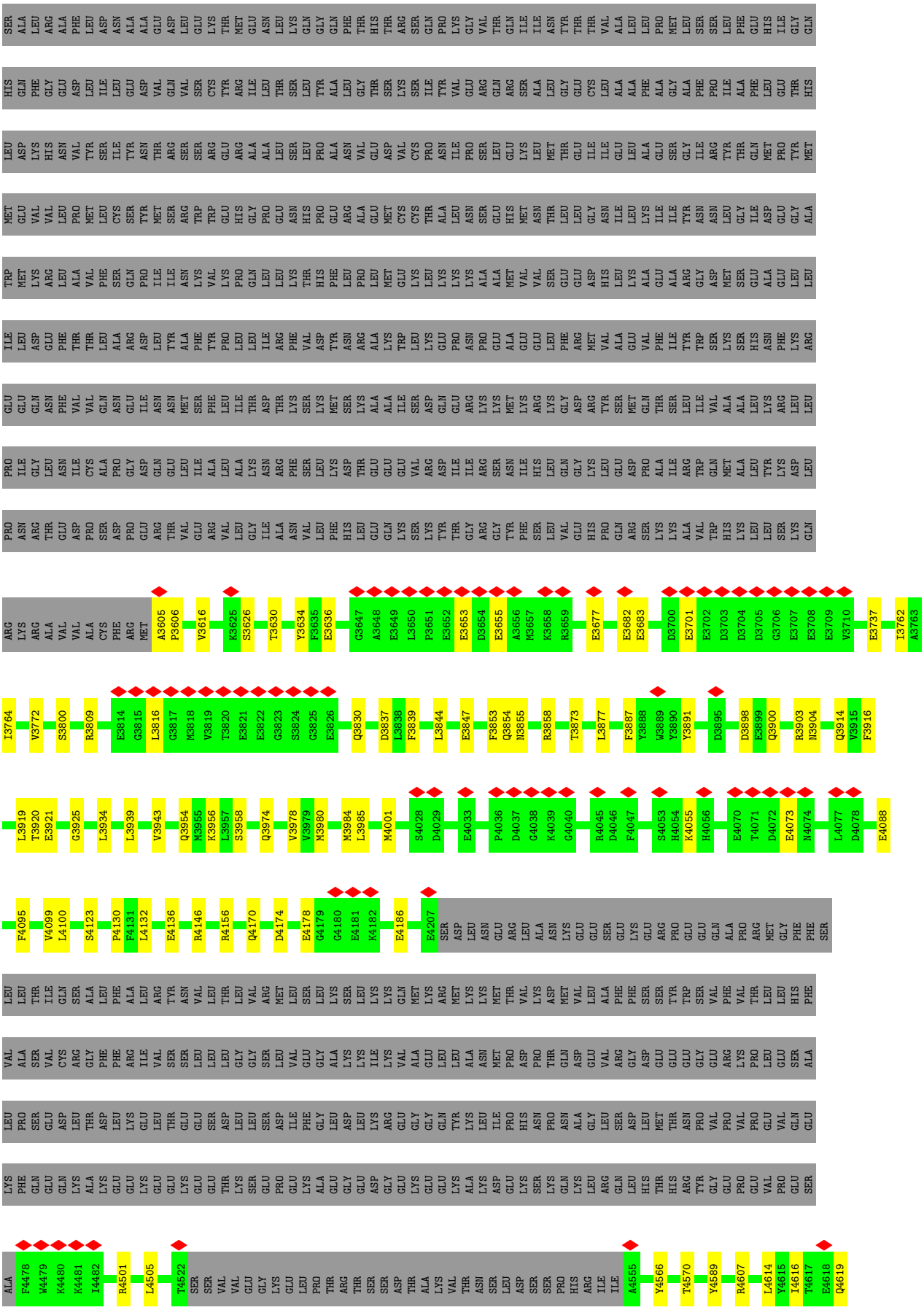
Chain A:

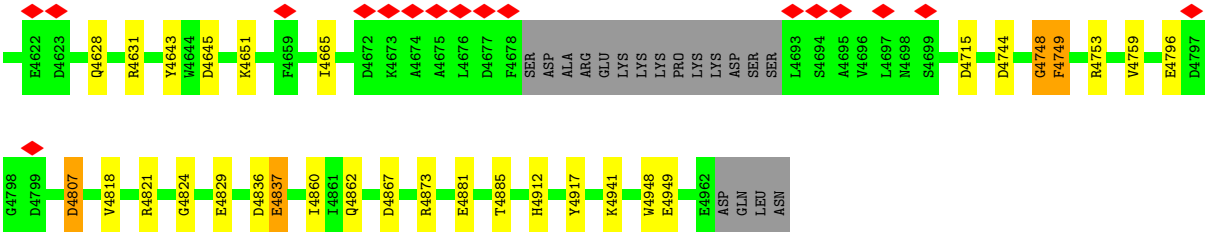





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L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944
A945 L946 G947 C948 H949 V950 G951 I952 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 N1002 A1003
A1008 R1009 D1010 R1011 I1012 R1013 Q1014 T1017 Y1018 G1019 I1020 Q1021 Q1022 D1023 V1024 K1025 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 HIS LEU GLU ALA PRO ASP
GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 A1090 E1091 K1097 R1100 E1106 A1107 V1108 D1112 M1113 R1114 V1115 G1116 G1121 C1122 D1125 L1126 E1127 L1128 D1131 D1132 R1133 A1136 F1137 F1140 Q1147 G1148 N1149 E1150 H1151 R1154
G1159 D1160 G1163 D1167 M1168 N1169 M1173 M1174 F1175 T1176 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1197 G1198 D1199 I1202 S1206 L1207 G1208 R1214 M1215 K1219 D1220 V1221 L1224 K1225 Y1226 F1227 T1228 I1229 C1230 G1231 L1232 Q1233 E1234 G1235 R1245 D1246
K1253 R1254 S1263 N1264 H1265 E1266 H1267 I1268 E1269 Y1270 T1271 R1272 I1273 D1274 G1275 T1276 I1277 D1278 S1279 S1280 L1283 K1284 Q1287 K1288 S1289 F1290 G1291 S1292 Q1293 N1294 N1295 N1296 T1297 D1298 I1299 M1300 L1304 S1305 M1306 E1309 E1312 V1313 F1314 S1315 LYS SER VAL ALA GLY GLY LEU PRO GLY
ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU
LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1417 E1418 Y1419 L1420 M1421 Y1427 R1431 I1432 F1433 P1434 G1435 Q1436 N1440 V1441 I1446 T1447 S1448 D1449 F1450 H1451 Q1452 Y1453 D1454 T1455
G1456 F1457 D1460 R1461 V1462 R1463 G1470 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 K1481 R1482 M1487 V1488 C1489 A1490 G1491 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 S1503 N1504 G1505 L1506 E1507 I1508 G1509 A1515 L1518 L1519 T1520 F1521 I1522 A1523 N1524 G1525 K1526 E1527 L1528 S1529 T1530
Y1531 Y1532 Q1533 V1534 E1535 T1538 K1539 P1542 A1543 V1544 F1545 A1546 Q1547 A1548 P1551 N1552 Q1555 F1556 E1557 L1558 G1559 R1560 I1561 K1562 N1563 V1564 L1571 F1572 K1573 S1574 E1575 H1576 K1577 N1578 Q1582 C1583 P1584 P1585 R1586 L1587 S1593 H1594 N1602 Q1603 K1606 V1607 D1608 V1609 S1610 R1611 I1612
S1613 E1614 R1615 L1619 V1620 Q1621 C1622 L1623 D1624 M1629 E1635 E1636 D1641 I1642 L1643 E1644 L1645 T1646 E1647 Q1648 E1649 E1650 T1658 L1661 L1668 N1692 K1693 Y1694 M1695 D1705 A1716 L1720 M1730 D1742 E1743 N1744 K1745 L1749 P1750 G1751 L1754 R1761 F1769
I1772 S1773 N1774 D1775 C1776 L1785 D1786 I1787 L1796 S1804 L1805 R1808 D1809 I1831 K1853 E1854 ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 E1890


M1895 K1896 L1909 L1912 I1924 S1928 D1929 V1932 Q1939 Y1943 N1944 E1945 V1946 M1947 Q1948 A1949 L1950 N1951 M1962 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961 R1962 E1963 F1964 R1965 S1966 Q1971 K1979 D1980 D1981 K1982 S1983 E1984 E1989 E1990 L2002 I2008 GLU LEU ASP GLU
ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 M2065 I2074 E2075 D2076 L2079 Y2105 D2114 L2122 I2125
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E2354 D2355 P2356 S2357 R2358 D2359 G2360 P2361 S2362 P2363 T2364 S2365 G2366 S2367 S2368 K2369 T2370 L2371 D2372 I2373 E2374 E2375 E2376 E2377 D2378 D2379 T2380 I2381 H2382 M2383 G2384 N2385 M2388 I2395 D2396 L2397 L2398 I2418 I2421 L2422 L2425 L2428 G2429 D2430 L2431 V2432 G2433 V2434 I2435 S2436 I2437 A2438 F2439 Q2440
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T2509 D2510 L2515 W2516 R2517 Y2518 L2519 C2520 T2521 A2522 V2523 L2526 L2527 T2528 R2529 C2530 A2531 F2534 A2535 G2536 T2537 E2538 H2539 H2540 A2541 S2542 L2543 I2544 D2545 S2546 L2547 L2548 H2549 T2550 V2551 Y2552 R2553 L2554 S2555 K2556 G2557 C2558 S2559 L2560 T2561 K2562 A2563 Q2564 R2565 D2566 S2567 I2568 E2569 V2570 C2571 L2572 L2573
S2574 I2575 C2576 G2577 Q2578 L2579 R2580 P2581 S2582 M2583 M2584 Q2585 H2586 L2587 L2588 R2589 R2590 L2591 V2592 F2593 D2594 V2595 P2596 L2597 L2598 N2599 E2600 H2601 A2602 K2603 M2604 P2605 L2606 K2607 L2608 L2609 T2610 N2611 H2612 Y2613 E2614 R2615 C2616 W2617 K2618 Y2619 Y2620 C2621 L2622 P2623 G2624 G2625 W2626 G2627 N2628 F2629 G2630 A2631 A2632 S2633
E2634 E2635 E2636 L2637 H2638 L2639 S2640 R2641 K2642 L2643 F2644 W2645 G2646 I2647 F2648 D2649 A2650 L2651 S2652 Q2653 K2654 K2655 Y2656 E2657 Q2658 E2659 L2660 F2661 K2662 L2663 A2664 L2665 P2666 C2667 L2668 S2669 A2670 V2671 A2672 G2673 A2674 L2675 P2676 P2677 D2678 Y2679 M2680 GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER
MET ASP SER GLU GLY ASN PHE ASN PRO GLN PRO VAL ASP THR SER ASN ILE THR ILE PRO GLU LYS LEU GLU TYR PHE ILE ASN LYS TYR ALA GLU HIS SER HIS ASP LYS LEU ALA ASN GLY TRP ILE TYR GLY GLU ILE TYR SER ASP SER SER LYS ILE GLN
PRO LEU MET LYS PRO TYR LYS LEU LEU SER GLU LYS GLU ILE TYR ARG TRP PRO ILE LYS GLU SER LEU LYS THR MET LEU ALA TRP GLY GLY TRP ARG ILE GLU ARG THR ARG GLU GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER
ILE ASP ALA ALA HIS GLY TYR SER PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG ASP LEU HIS ALA MET ALA GLU MET MET ALA GLU ASN TYR HIS ASN ILE TRP ALA LYS LYS LYS LEU GLU LEU GLU SER LYS GLY GLY ASN HIS PRO LEU LEU VAL PRO TYR
ASP THR LEU THR ALA LYS GLU LYS ALA LYS ASP ARG GLU LYS ALA GLN ASP ILE PHE LYS PHE LEU GLN ILE SER GLY TYR VAL VAL SER ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP
GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU CYS THR GLY GLY
HIS ALA SER ASN LYS GLU LYS GLU MET VAL THR SER LEU PHE CYS LYS LEU GLY VAL LEU VAL ARG HIS ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE LEU GLY GLN THR LEU ASP ALA ARG THR VAL MET LYS THR GLY LEU ASP SER VAL LYS

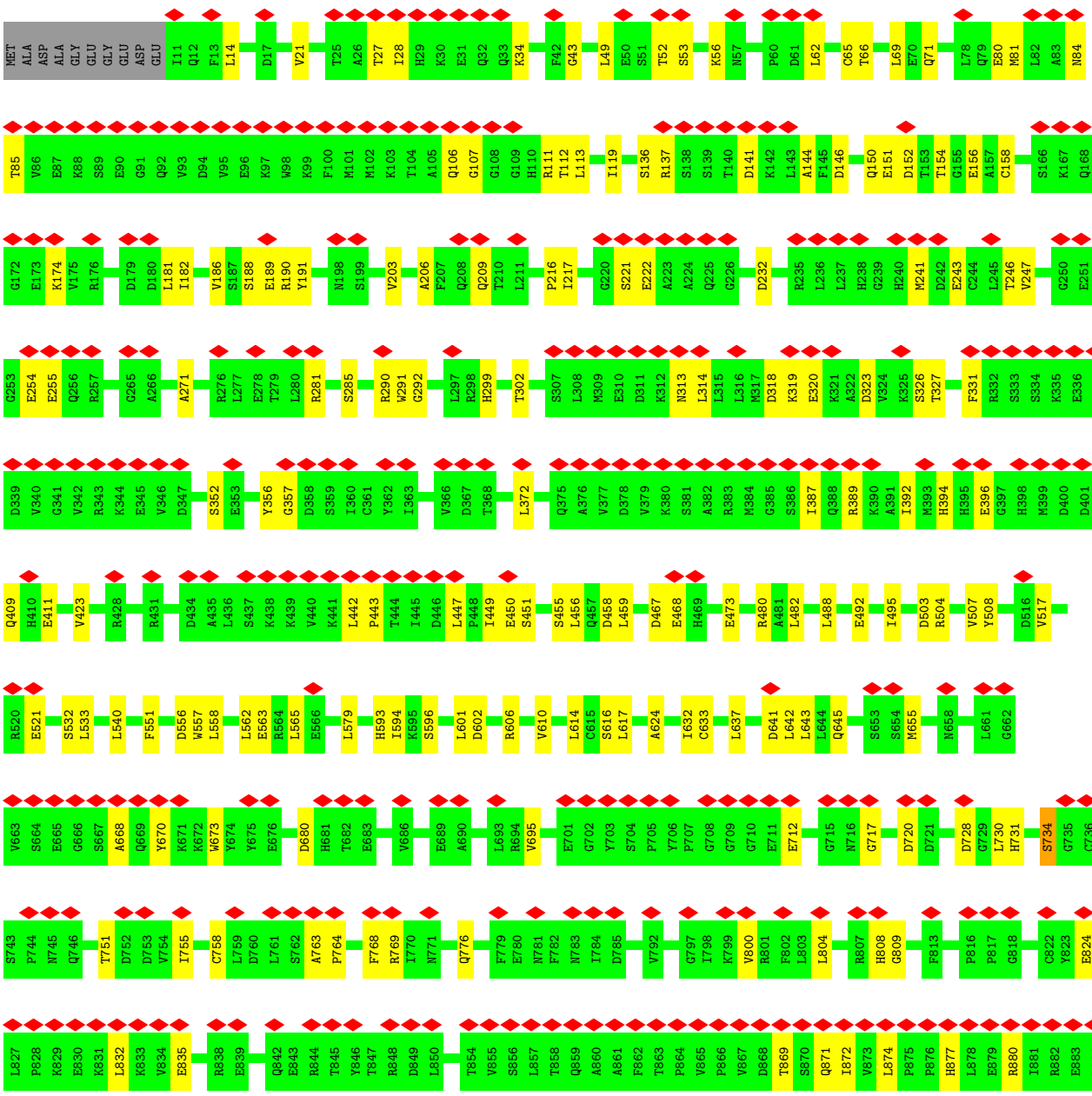


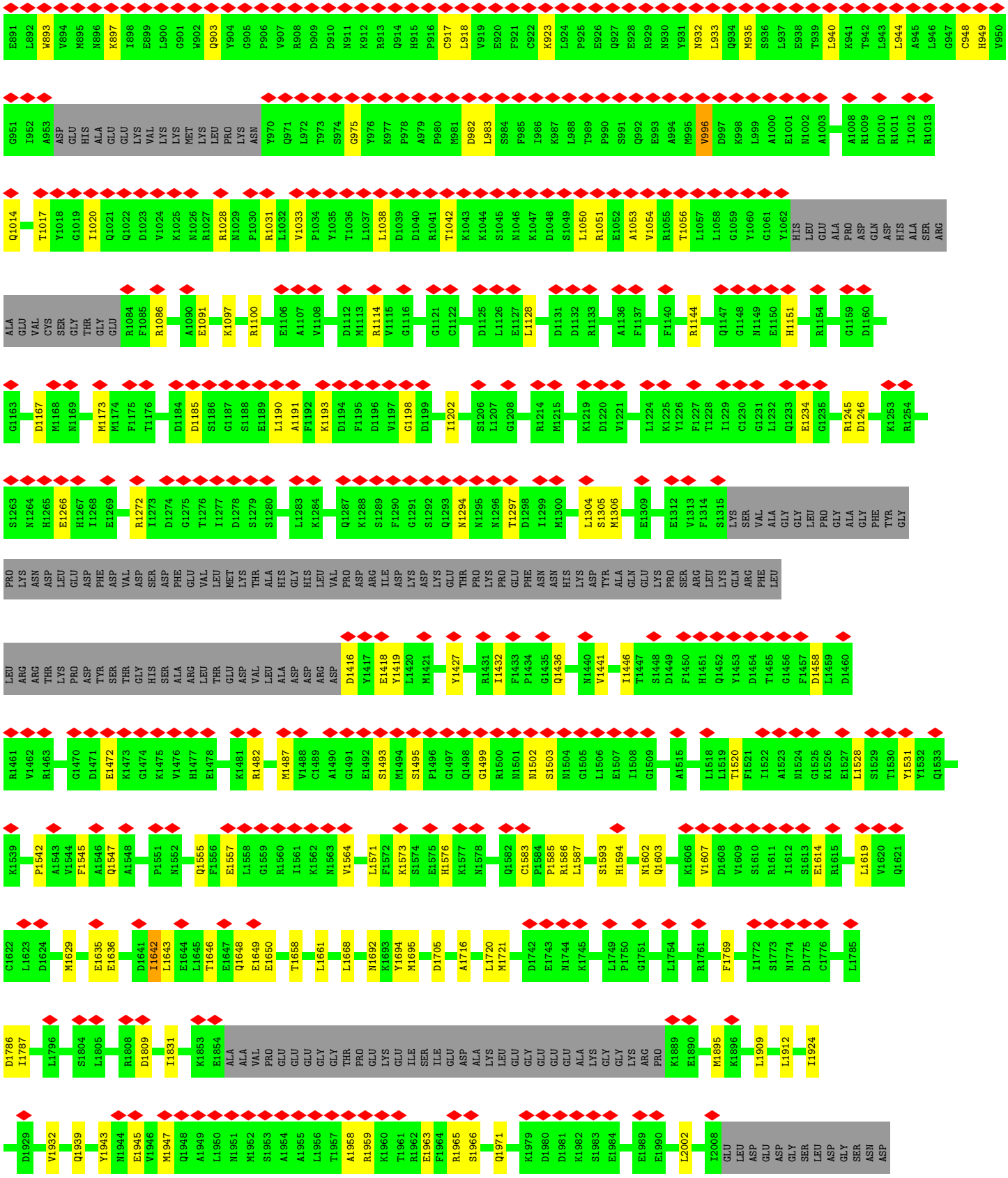


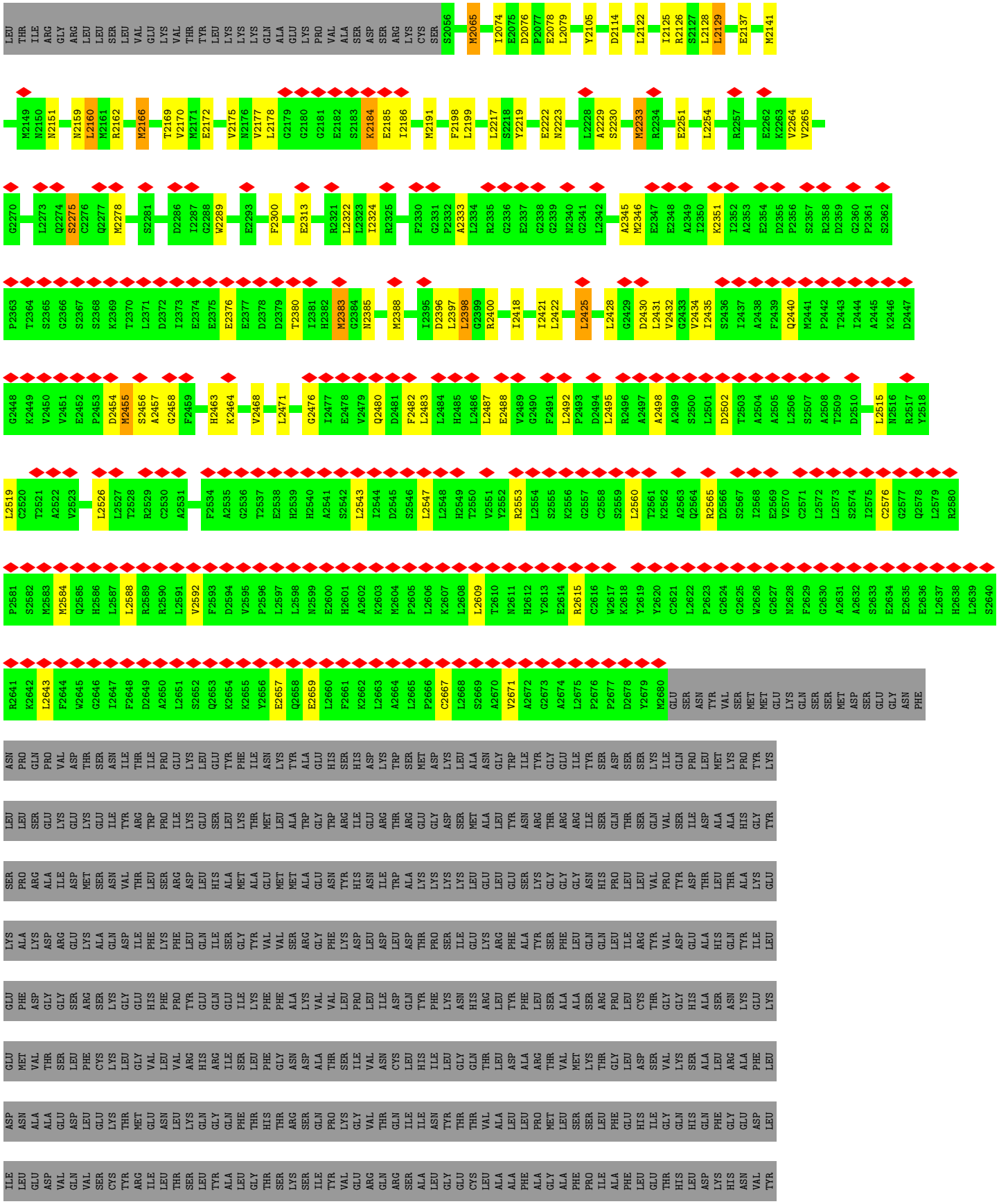
• Molecule 1: Ryanodine receptor 2

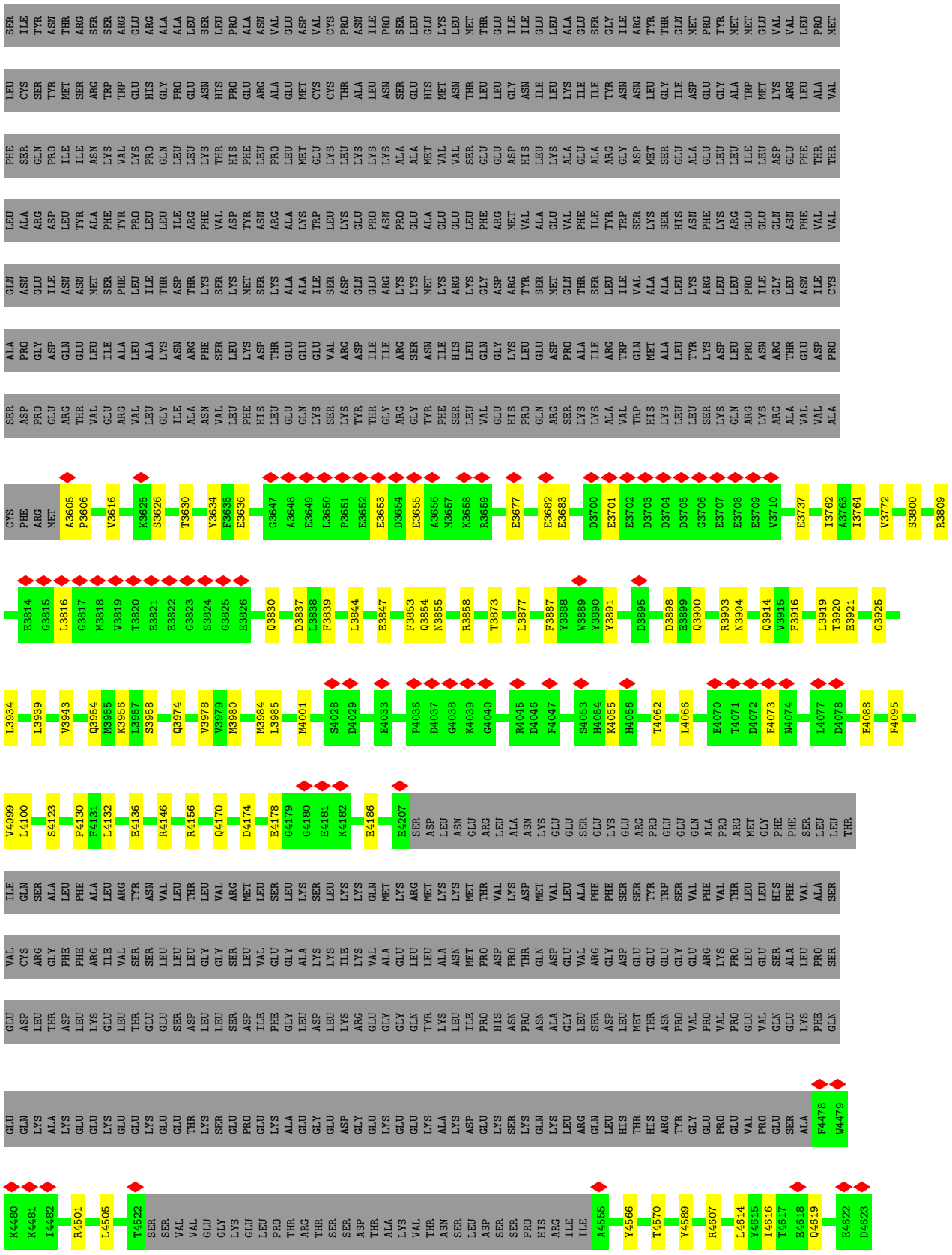
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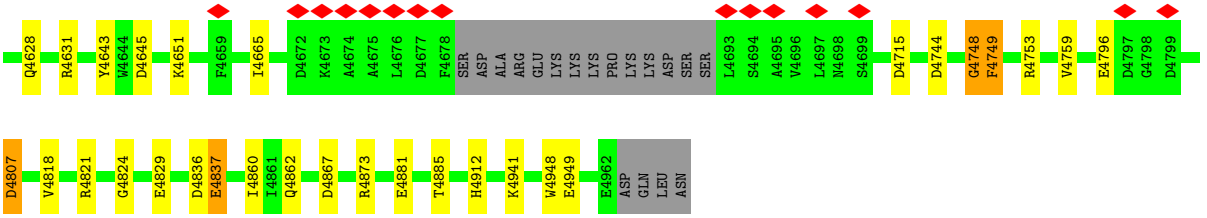





E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950
G951 I952 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 N1002 A1003 A1008 R1009 D1010 R1011 I1012 R1013
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ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 A1090 E1091 K1097 R1100 E1106 A1107 V1108 D1112 M1113 R1114 V1115 G1116 G1121 C1122 D1125 L1126 E1127 L1128 D1131 D1132 R1133 A1136 F1137 F1140 R1144 Q1147 G1148 N1149 E1150 H1151 R1154 G1159 D1160
G1163 D1167 M1168 N1169 M1173 M1174 F1175 T1176 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1197 G1198 D1199 I1202 S1206 L1207 G1208 R1214 M1215 K1219 D1220 V1221 L1224 K1225 Y1226 F1227 T1228 I1229 C1230 G1231 L1232 Q1233 E1234 G1235 R1245 D1246 K1253 R1254
S1263 N1264 H1265 E1266 H1267 I1268 E1269 R1272 I1273 D1274 G1275 T1276 I1277 D1278 S1279 S1280 L1283 K1284 Q1287 K1288 S1289 F1290 G1291 S1292 Q1293 N1294 N1295 N1296 T1297 D1298 I1299 M1300 L1304 S1305 M1306 E1309 E1312 V1313 F1314 S1315 LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY
PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU
LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1417 E1418 Y1419 L1420 M1421 Y1427 R1431 I1432 F1433 P1434 G1435 Q1436 N1440 V1441 I1446 T1447 S1448 D1449 F1450 H1451 Q1452 Y1453 D1454 T1455 G1456 F1457 D1458 L1459 D1460
R1461 V1462 R1463 G1470 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 K1481 R1482 M1487 V1488 C1489 A1490 G1491 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 S1503 N1504 G1505 L1506 E1507 I1508 G1509 A1515 L1518 L1519 T1520 F1521 I1522 A1523 N1524 G1525 K1526 E1527 L1528 S1529 T1530 Y1531 Q1532 Q1533
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C1622 L1623 D1624 M1629 E1635 E1636 D1641 I1642 L1643 E1644 L1645 T1646 E1647 Q1648 E1649 E1650 T1658 L1661 L1668 N1692 K1693 Y1694 M1695 D1705 A1716 L1720 M1721 D1742 E1743 N1744 K1745 L1749 P1750 G1751 L1754 R1761 F1769 I1772 S1773 N1774 D1775 C1776 L1785
D1786 I1787 L1796 S1804 L1805 R1808 D1809 I1831 K1853 E1854 ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 E1890 M1895 K1896 L1909 L1912 I1924
D1929 V1932 Q1939 Y1943 N1944 E1945 V1946 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961 R1962 E1963 F1964 R1965 S1966 Q1971 K1979 D1980 D1981 K1982 S1983 E1984 E1989 E1990 L2002 I2008 GLU LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP


LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 M2065 I2074 E2075 D2076 P2077 E2078 L2079 Y2105 D2114 L2122 I2125 R2126 S2127 L2128 L2129 E2137 M2141
M2149 N2150 N2151 N2159 L2160 M2161 R2162 M2166 T2169 V2170 M2171 E2172 V2175 N2176 V2177 L2178 G2179 G2180 G2181 E2182 S2183 K2184 E2185 I2186 M2191 F2198 L2199 L2217 S2218 Y2219 E2222 N2223 L2228 A2229 S2230 M2233 R2234 E2251 L2254 R2257 E2262 K2263 V2264 V2265
G2270 L2273 Q2274 S2275 C2276 Q2277 M2278 S2281 D2286 I2287 G2288 W2289 E2293 F2300 E2313 I2321 L2322 L2323 I2324 R2325 F2330 G2331 P2332 A2333 L2334 R2335 G2336 E2337 G2338 G2339 N2340 G2341 L2342 A2345 M2346 E2347 E2348 A2349 I2350 K2351 I2352 A2353 E2354 D2355 P2356 S2357 R2358 D2359 G2360 P2361 S2362
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G2448 K2449 V2450 V2451 E2452 P2453 D2454 M2455 S2456 A2457 G2458 F2459 H2463 K2464 V2468 L2471 G2476 I2477 E2478 V2479 Q2480 D2481 F2482 L2483 L2484 H2485 L2486 L2487 E2488 V2489 G2490 F2491 L2492 P2493 D2494 L2495 R2496 A2497 A2498 A2499 S2500 L2501 D2502 T2503 A2504 A2505 L2506 S2507 A2508 T2509 D2510 L2515 N2516 R2517 Y2518
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ASN PRO GLN PRO VAL ASP THR SER ASN ILE THR ILE PRO GLU LYS LEU GLU GLU TYR PHE ILE ASN LYS TYR ALA GLU HIS SER HIS ASP LYS TRP SER MET ASP LYS LEU ALA ASN GLY TRP ILE TYR SER ASP SER SER LYS ILE GLN PRO LEU MET LYS PRO TYR LYS
LEU LEU SER GLU LYS GLU LYS GLU ILE TYR ARG TRP PRO ILE LYS GLU SER LEU LYS THR MET LEU ALA TRP GLY TRP ARG ILE GLU ARG THR ARG GLU GLY GLY ASP SER MET ALA ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY TYR
SER PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG ASP LEU HIS ALA MET ALA GLU MET MET ALA GLU ASN TYR HIS ASN ILE TRP ALA LYS LYS LYS LEU GLU GLU LEU GLU SER ALA LYS GLY GLY ASN HIS PRO LEU LEU VAL PRO TYR ASP THR LEU ALA LYS GLU
LYS ALA LYS ASP ARG GLU LYS ALA GLN ASP ILE ILE PHE PHE LYS PHE LEU GLN ILE SER GLY TYR TYR VAL VAL SER ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU
GLU PHE ASP GLY GLY SER LYS GLY GLU HIS PHE PRO PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU LEU CYS THR GLY GLY GLY HIS ALA SER ASN LYS GLU LYS
GLU MET VAL THR SER LEU PHE CYS LYS LEU GLY VAL LEU VAL ARG HIS ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER THR VAL ASN CYS LEU LEU HIS ILE LEU GLY GLN THR THR LEU ASP ALA ARG THR VAL MET LYS THR GLY LEU ASP SER VAL LYS SER ALA LEU ARG ALA PHE LEU
ASP ASN ALA ALA GLU ASP LEU GLU LYS GLN GLY GLN PHE THR HIS THR ARG SER GLN PRO LYS GLY VAL THR GLN ARG ILE ILE ASN TYR THR THR VAL ALA LEU LEU PRO MET LEU SER SER LEU PHE GLU HIS GLN GLN HIS PHE GLY ASP LEU
ILE LEU GLU ASP VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU HIS LEU ASP LYS HIS ASN VAL TYR

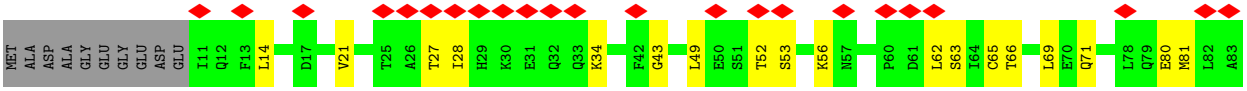


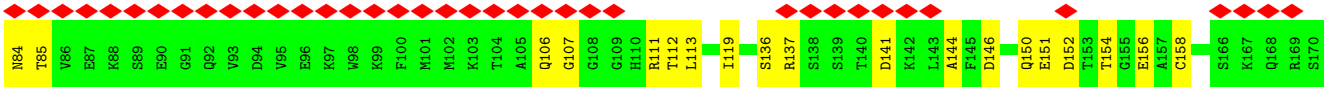


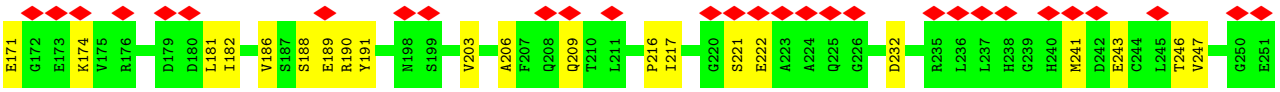
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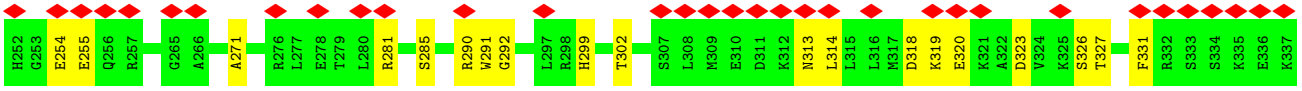
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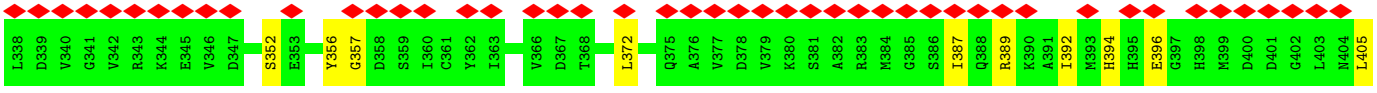


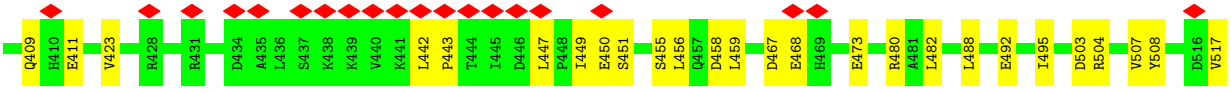


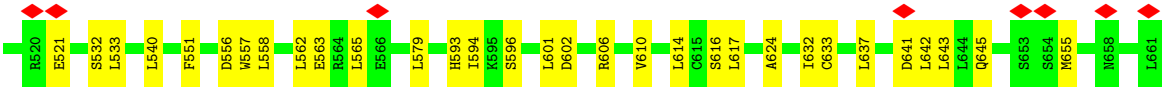


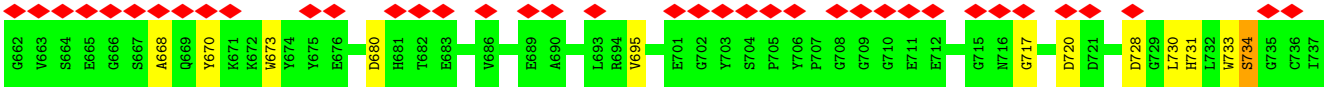


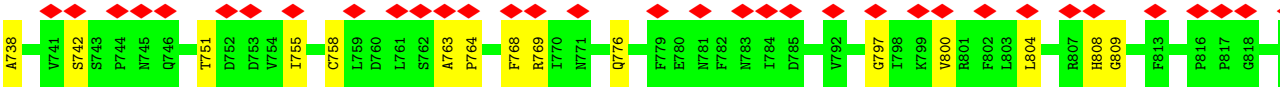


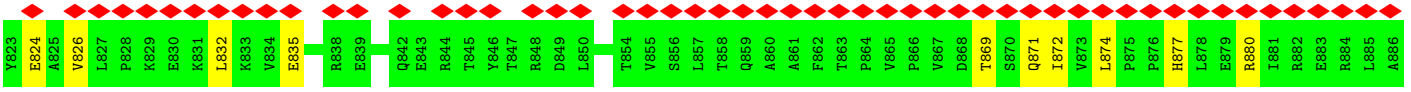


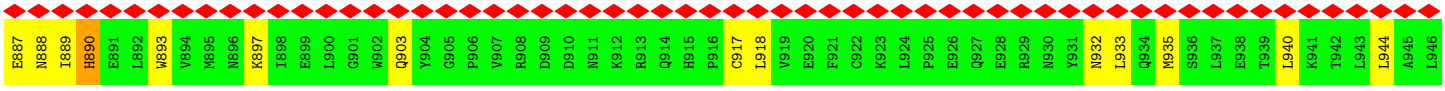


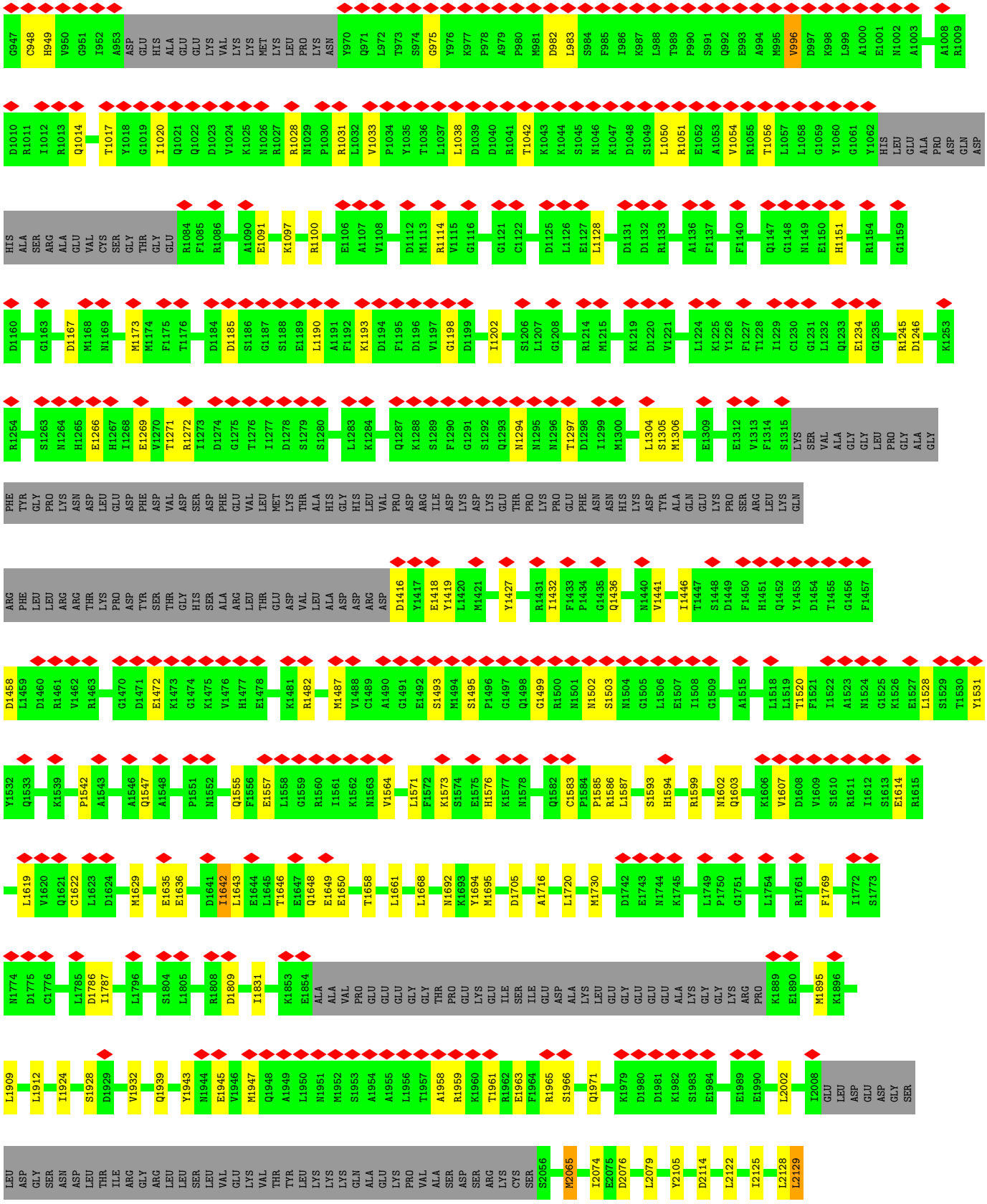


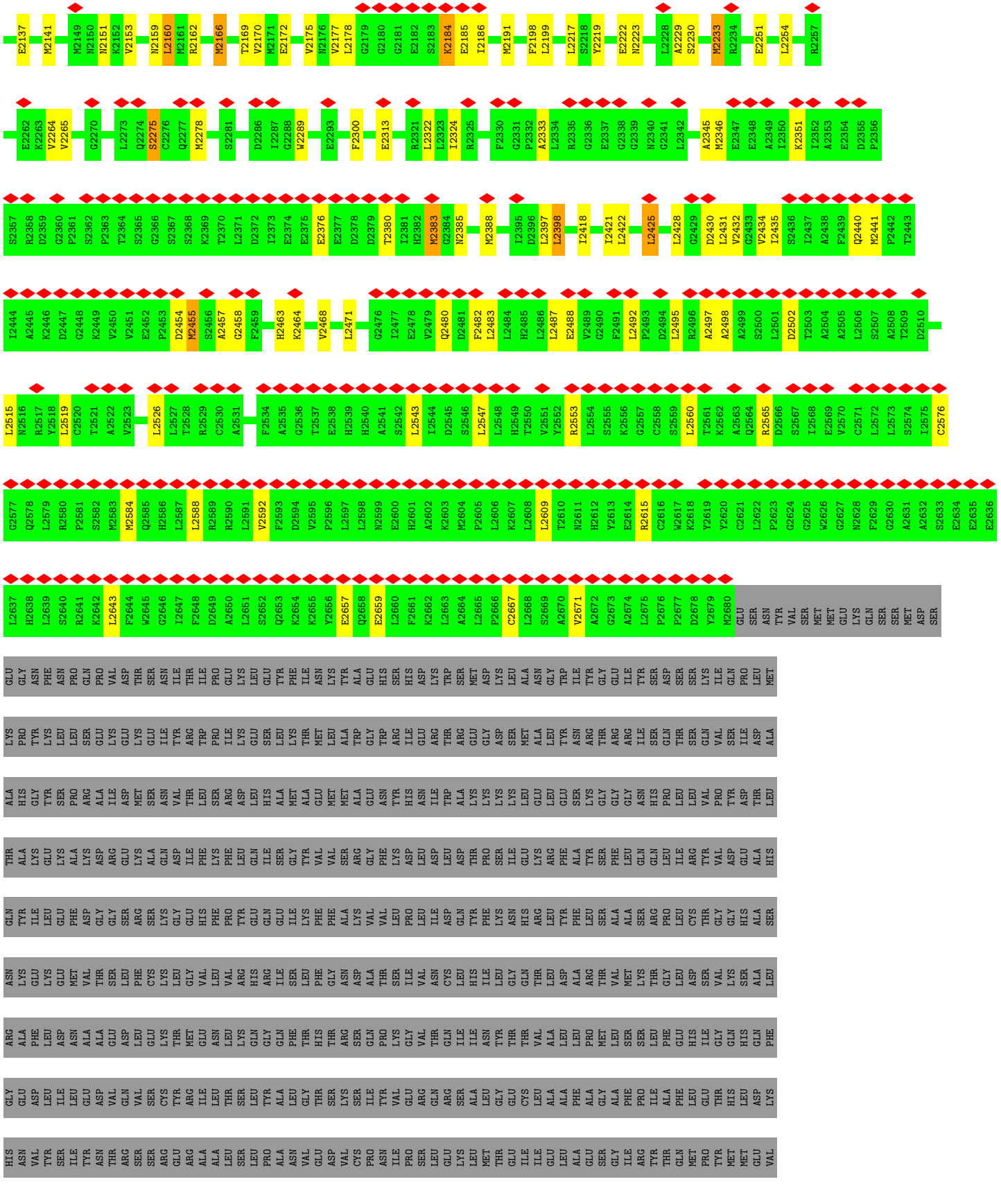


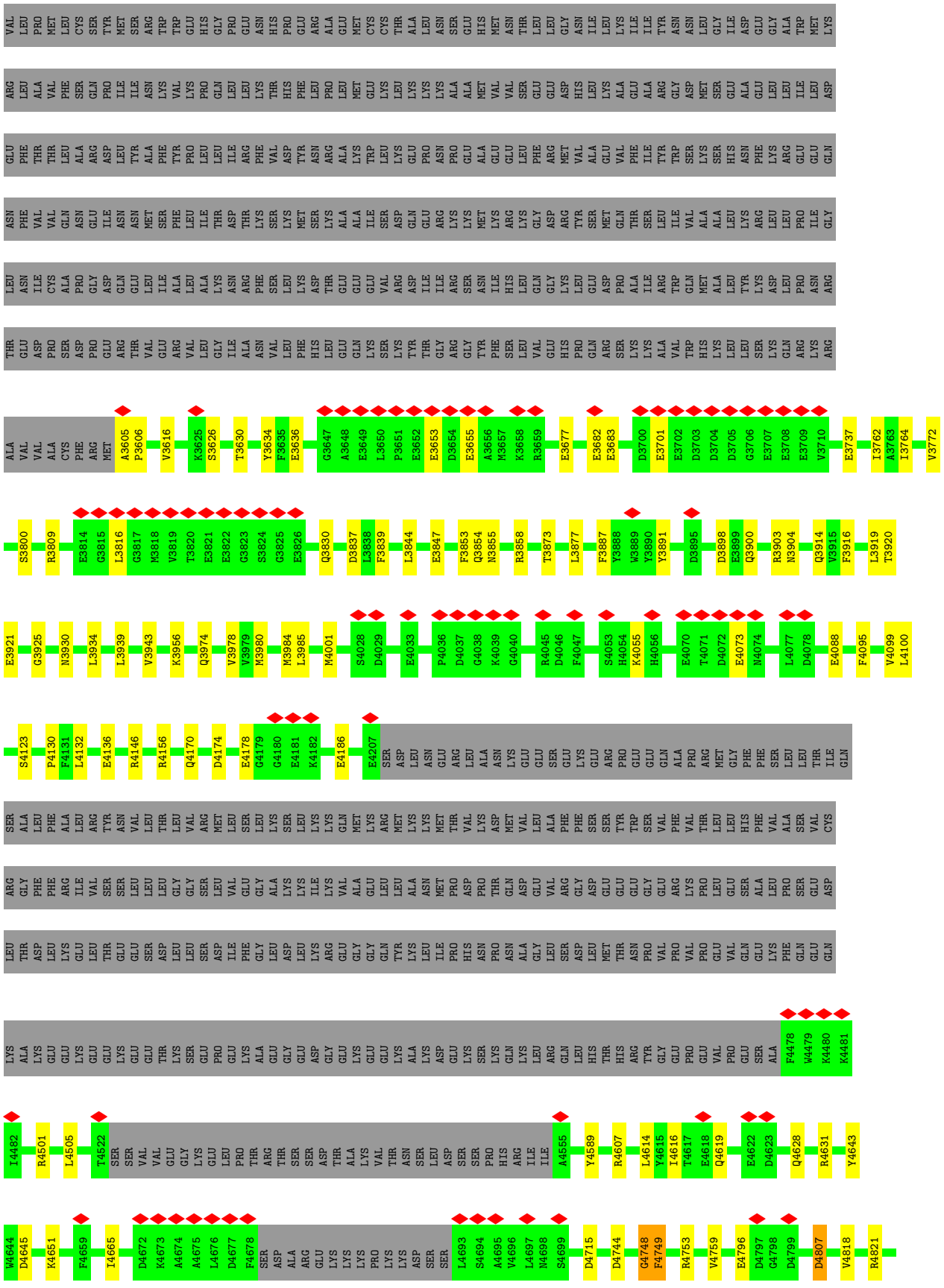







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D1010 R1011 I1012 R1013 Q1014 T1017 Y1018 G1019 I1020 Q1021 Q1022 D1023 V1024 K1025 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062
HIS LEU GLU ALA PRO ASP GLN ASP
HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 A1090 E1091 K1097 R1100 E1106 A1107 V1108 D1112 M1113 R1114 V1115 G1116 G1121 C1122 D1125 L1126 E1127 L1128 D1131 D1132 R1133 A1136 F1137 F1140 Q1147 G1148 N1149 E1150 H1151 R1154 G1159
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LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY
PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN
ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1417 E1418 Y1419 L1420 M1421 Y1427 R1431 I1432 F1433 P1434 G1435 Q1436 N1440 V1441 I1446 T1447 S1448 D1449 F1450 H1451 Q1452 Y1453 D1454 T1455 G1456 F1457
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N1774 D1775 C1776 L1785 D1786 I1787 L1796 S1804 L1805 R1808 D1809 I1831 K1853 E1854 ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 E1890 M1895 K1896
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GLU LEU ASP GLU ASP GLY SER
LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 M2065 I2074 E2075 D2076 L2079 Y2105 D2114 L2122 I2125 L2128 L2129

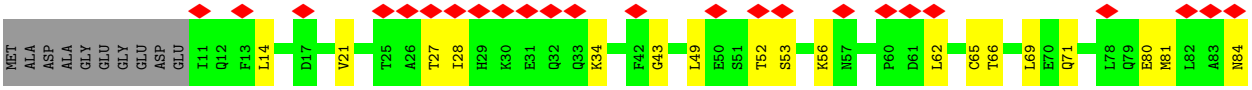

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S2357 R2358 D2359 G2360 P2361 S2362 P2363 T2364 S2365 G2366 S2367 S2368 K2369 T2370 L2371 D2372 I2373 E2374 E2375 E2376 E2377 D2378 D2379 T2380 I2381 H2382 M2383 G2384 N2385 M2388 I2395 D2396 L2397 L2398 I2418 I2421 L2422 L2425 L2428 G2429 D2430 L2431 V2432 G2433 V2434 I2435 S2436 I2437 A2438 F2439 Q2440 M2441 P2442 T2443
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G2577 Q2578 L2579 R2580 P2581 S2582 M2583 M2584 Q2585 H2586 L2587 L2588 R2589 R2590 L2591 V2592 F2593 D2594 V2595 P2596 L2597 L2598 N2599 E2600 H2601 A2602 K2603 M2604 P2605 L2606 K2607 L2608 L2609 T2610 N2611 H2612 Y2613 E2614 R2615 C2616 W2617 K2618 Y2619 Y2620 C2621 L2622 P2623 G2624 G2625 W2626 G2627 P2628 F2629 G2630 A2631 A2632 S2633 E2634 E2635 E2636
L2637 H2638 L2639 S2640 R2641 K2642 L2643 F2644 W2645 G2646 I2647 F2648 D2649 A2650 L2651 S2652 Q2653 K2654 K2655 Y2656 E2657 Q2658 E2659 L2660 F2661 K2662 L2663 A2664 L2665 P2666 C2667 L2668 S2669 A2670 V2671 A2672 G2673 A2674 L2675 P2676 P2677 D2678 Y2679 M2680 GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER
GLU GLY ASN PHE ASN PRO GLN PRO VAL ASP THR SER ASN ILE ILE THR ILE PRO GLU LYS LEU GLU TYR PHE ILE ASN LYS TYR ALA GLU HIS SER HIS ASP LYS TRP SER MET ASP LYS LEU ALA ASN GLY TRP ILE TYR GLY GLU ILE TYR SER ASP SER SER LYS ILE GLN PRO LEU MET
LYS PRO TYR LYS LEU LEU SER GLU LYS GLU ILE TYR ARG TRP PRO ILE LYS GLU SER LEU LYS THR MET LEU ALA TRP GLY TRP ARG ILE GLU ARG THR ARG GLU GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR THR SER GLN VAL SER ILE ASP ALA
ALA HIS GLY TYR SER PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG ASP LEU HIS ALA MET GLU MET MET ALA GLU MET MET ALA GLU GLU ASN TYR HIS ASN ILE TRP ALA LYS LYS LYS LYS LEU GLU LEU GLU SER LYS GLY GLY GLY ASN HIS PRO LEU LEU LEU VAL PRO TYR ASP THR LEU
THR ALA LYS GLU LYS ALA LYS ASP ARG GLU LYS ALA GLN ASP ILE PHE LYS PHE LEU GLN ILE SER GLY TYR VAL VAL SER ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS
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ASN LYS GLU LYS GLU MET VAL THR SER LEU PHE CYS LYS LEU GLY VAL LEU VAL ARG HIS ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE LEU GLY GLN THR LEU ASP ALA ARG THR VAL MET LYS THR GLY LEU ASP SER VAL LYS SER ALA LEU
ARG ALA PHE LEU ASP ASN ALA ALA GLU ASP LEU GLU LYS THR MET GLU ASN LEU LYS THR HIS THR ARG SER GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR THR THR VAL ALA LEU LEU PRO MET LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE
GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER LEU GLU ARG ILE LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS LEU ASP LYS
HIS ASN VAL TYR SER ILE TYR ASN THR ARG SER SER ARG GLU ARG GLU ARG ALA ALA LEU ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU GLU LYS LEU MET THR GLU ILE ILE GLU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO TYR MET THR GLU VAL

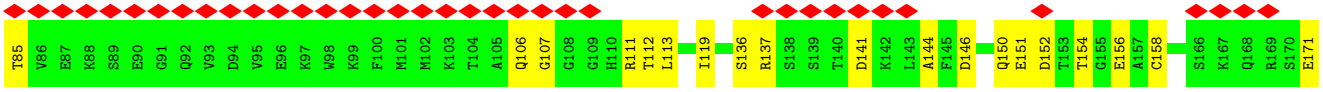


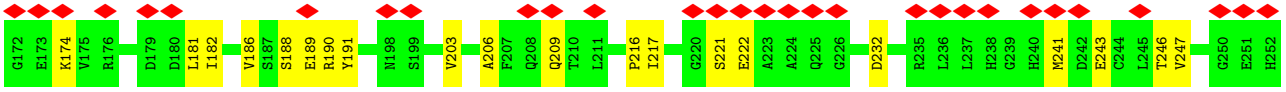


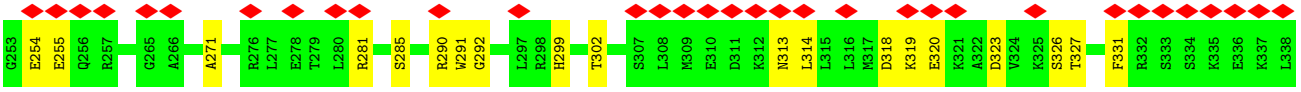
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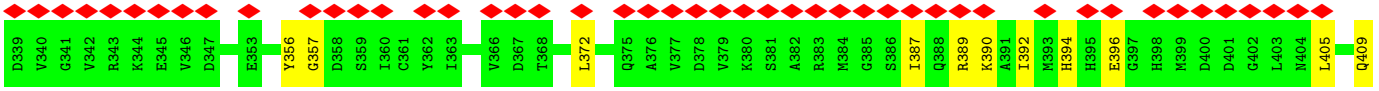


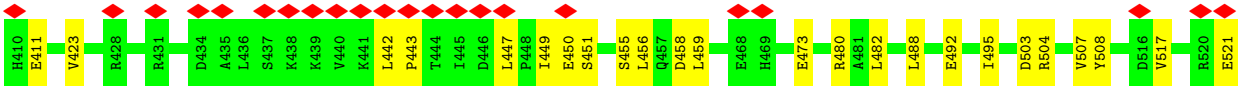


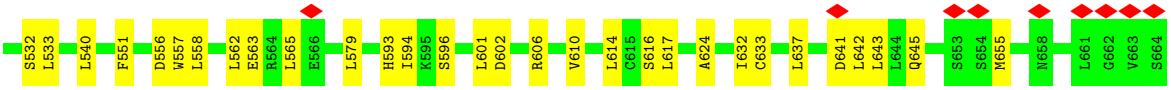


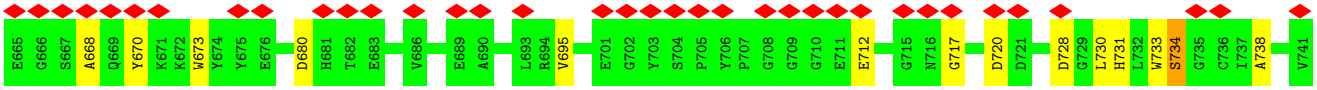


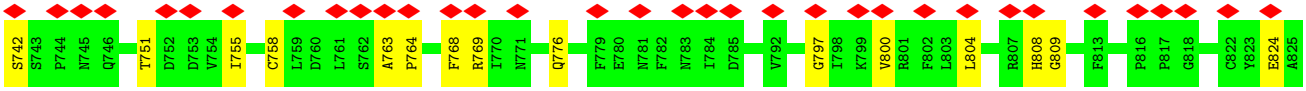


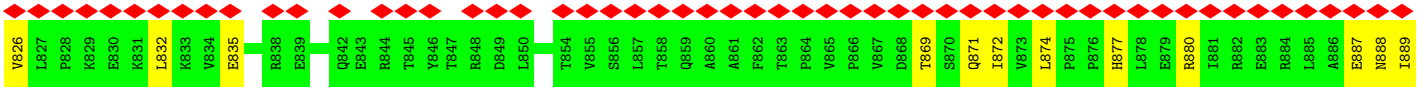


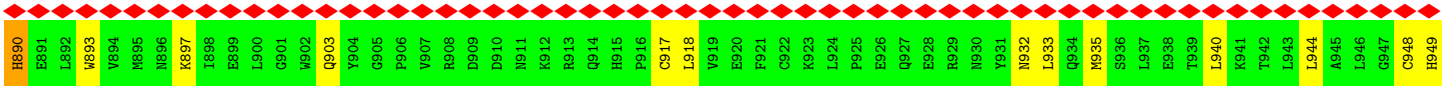


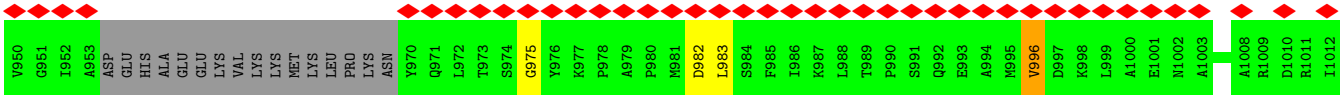


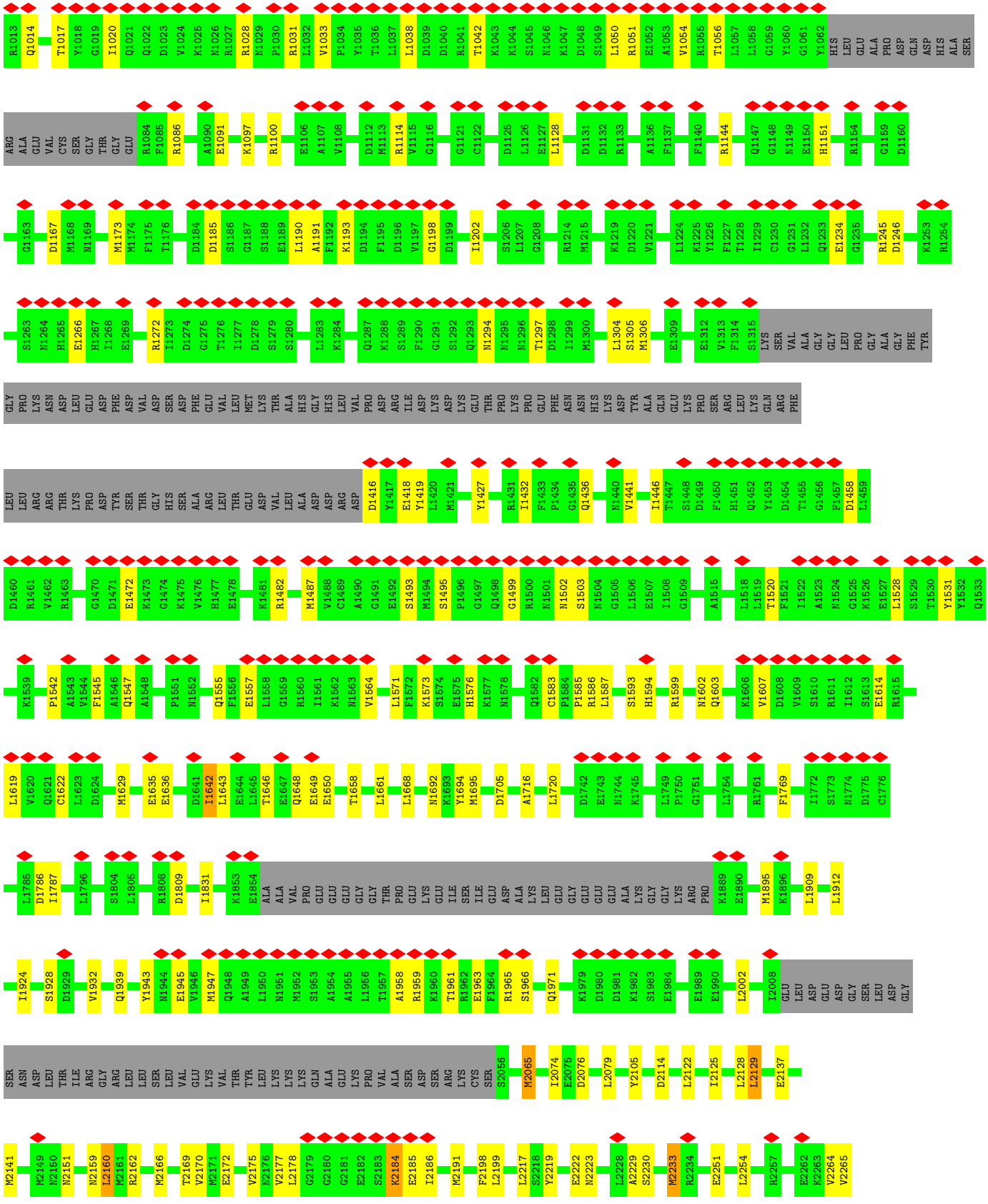


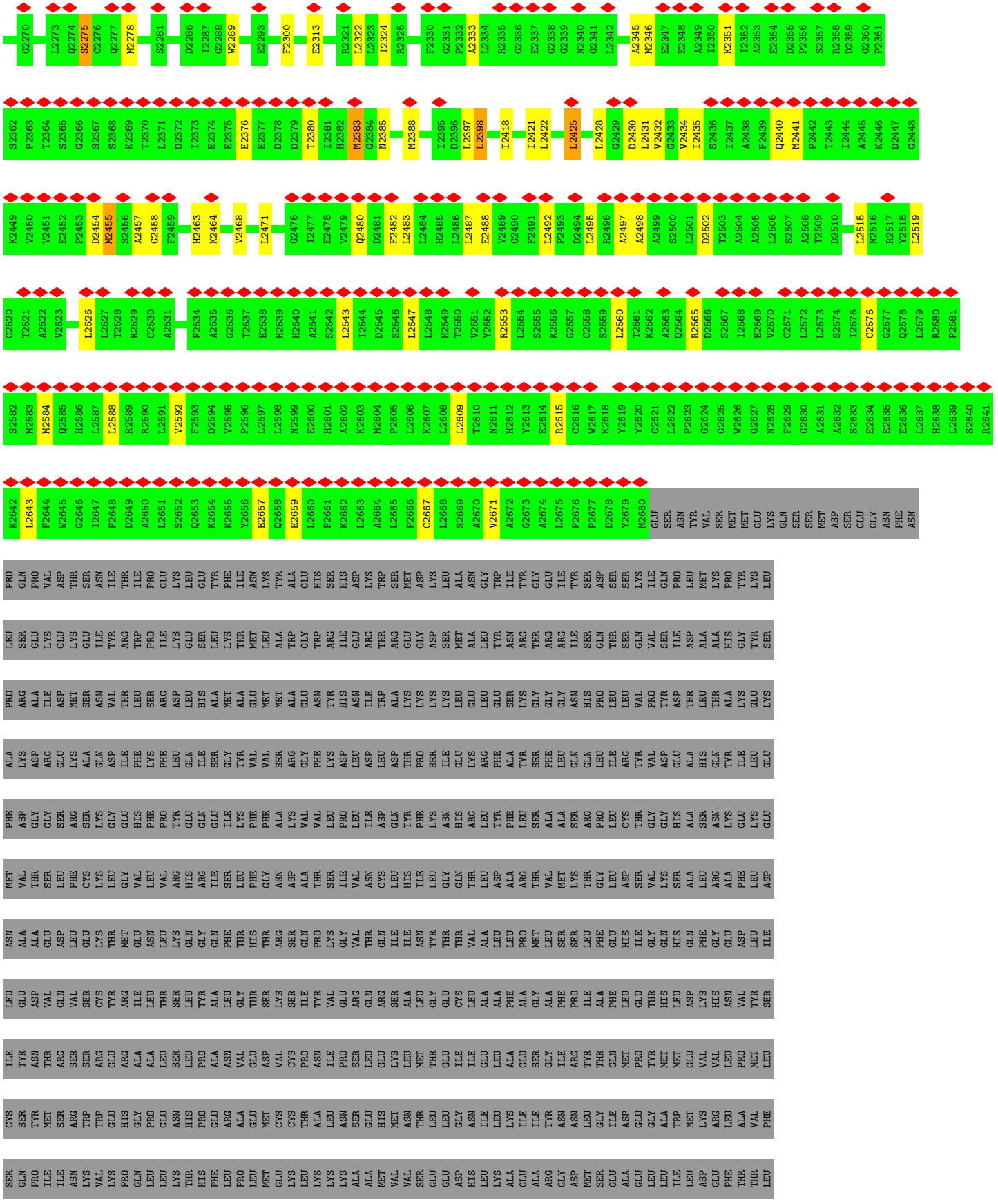


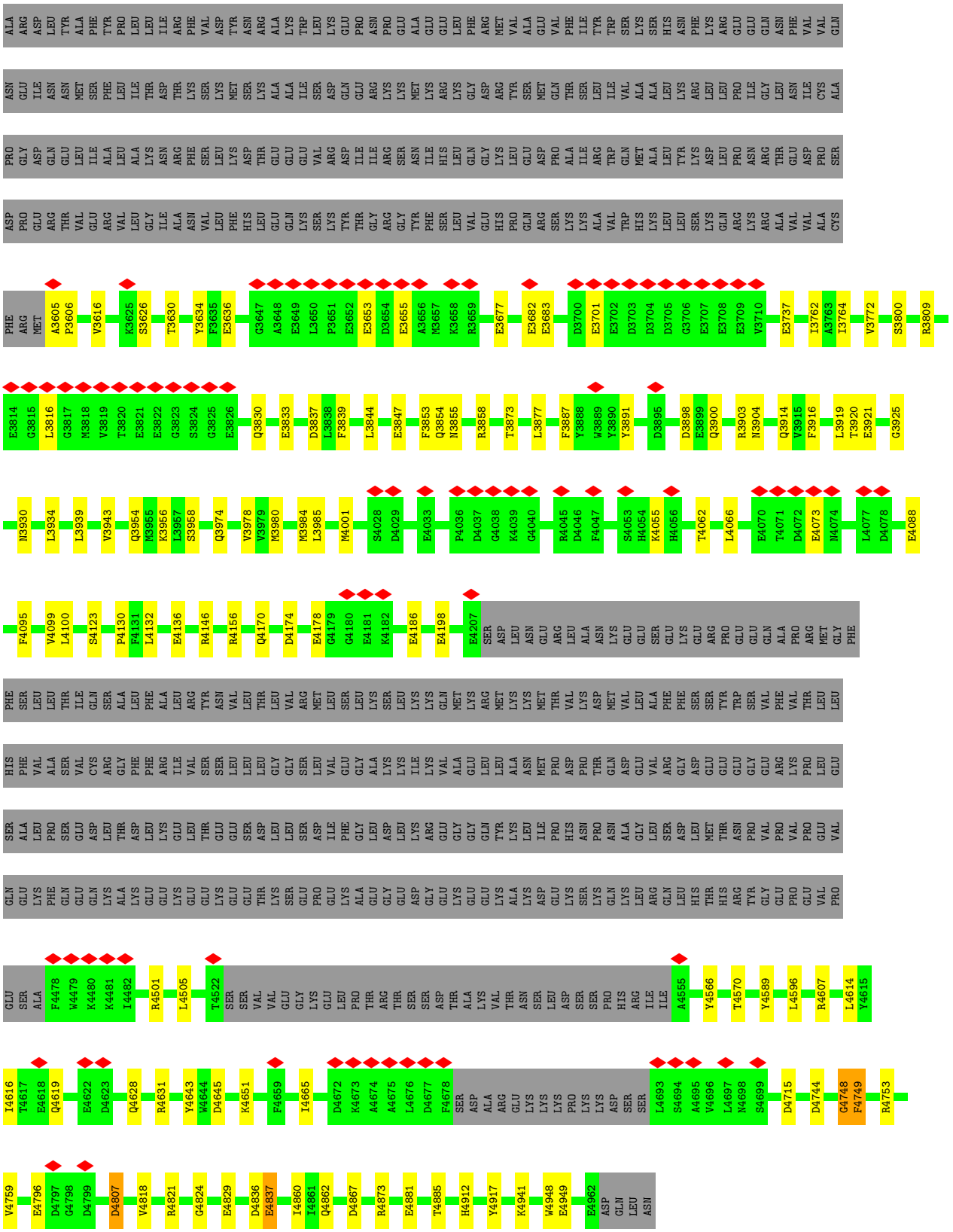






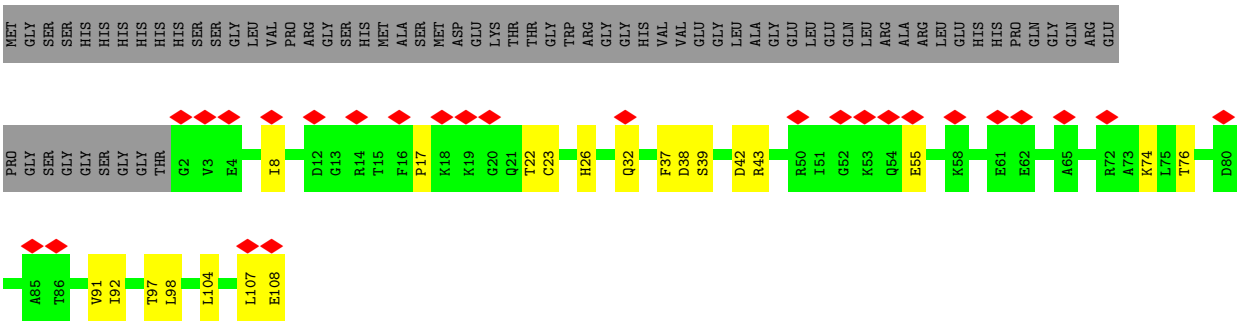



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S2362 P2363 T2364 S2365 G2366 S2367 S2368 K2369 T2370 L2371 D2372 I2373 E2374 E2375 E2376 E2377 D2378 D2379 T2380 I2381 H2382 M2383 G2384 N2385 M2388 T2395 D2396 L2397 L2398 I2418 I2421 L2422 L2425 L2428 G2429 D2430 L2431 V2432 G2433 V2434 I2435 S2436 I2437 A2438 F2439 Q2440 M2441 P2442 T2443 I2444 A2445 K2446 D2447 G2448
K2449 V2450 V2451 E2452 P2453 D2454 M2455 S2456 A2457 G2458 F2459 H2463 K2464 V2468 L2471 G2476 I2477 E2478 V2479 Q2480 D2481 F2482 L2483 L2484 H2485 L2486 L2487 E2488 V2489 G2490 F2491 L2492 P2493 D2494 L2495 R2496 A2497 A2498 A2499 S2500 L2501 D2502 T2503 A2504 A2505 L2506 S2507 A2508 T2509 D2510 L2515 N2516 R2517 Y2518 L2519
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S2582 M2583 M2584 Q2585 H2586 L2587 L2588 R2589 R2590 L2591 V2592 F2593 D2594 V2595 P2596 L2597 L2598 N2599 E2600 H2601 A2602 K2603 M2604 P2605 L2606 K2607 L2608 L2609 T2610 N2611 H2612 Y2613 E2614 R2615 C2616 W2617 K2618 Y2619 Y2620 C2621 L2622 P2623 G2624 G2625 W2626 G2627 N2628 F2629 G2630 A2631 A2632 S2633 E2634 E2635 E2636 L2637 H2638 L2639 S2640 R2641
K2642 L2643 F2644 W2645 G2646 I2647 F2648 D2649 A2650 L2651 S2652 Q2653 K2654 K2655 Y2656 E2657 Q2658 E2659 L2660 F2661 K2662 L2663 A2664 L2665 P2666 C2667 L2668 S2669 A2670 V2671 A2672 G2673 A2674 L2675 P2676 P2677 D2678 Y2679 M2680 GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY ASN PHE ASN
PRO GLN PRO VAL ASP THR SER ASN ILE THR ILE PRO GLU LYS LEU GLU TYR PHE ILE ASN LYS TYR ALA GLU HIS SER HIS ASP LYS TRP SER MET ASP LYS LEU ALA ASN GLY TRP ILE TYR GLY GLU ILE TYR SER ASP SER LYS LEU GLN PRO LEU MET LYS PRO TYR LYS LEU
LEU SER GLU LYS GLU LYS GLU ILE TYR ARG TRP PRO ILE LYS GLU LEU LYS THR MET LEU ALA TRP GLY TRP ARG ILE GLU ARG THR ARG GLU GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY TYR SER
PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG ASP LEU HIS ALA MET ALA GLU MET MET ALA GLU ASN TYR HIS ASN ILE TRP ALA LYS LYS LYS LYS LEU GLU LEU GLU SER LYS GLY GLY ASN HIS PRO LEU LEU VAL PRO TYR ASP THR LEU THR ALA LYS GLU LYS
ALA LYS ASP ARG GLU LYS ALA GLN ASP ILE PHE LYS PHE LEU GLN ILE SER GLY TYR VAL VAL SER ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU
PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE PHE ALA LYS VAL VAL LEU LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU CYS THR GLY GLY GLY HIS ALA SER ASN LYS GLU GLY LYS GLU
MET VAL THR SER LEU PHE CYS LYS LEU GLY VAL LEU VAL ARG HIS ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE LEU GLY GLN THR LEU ASP ALA ARG THR VAL MET LYS THR GLY LEU ASP SER VAL LYS THR GLY LEU ARG ALA PHE LEU ASP
ASN ALA ALA GLU ASP LEU GLU LYS THR MET GLU ASN LEU LYS GLN GLY GLN PHE THR HIS THR ARG SER GLN PRO LYS VAL GLY VAL THR GLN ILE ILE ASN TYR THR THR VAL ALA ALA LEU LEU PRO MET LEU SER SER LEU PHE GLU HIS GLN ILE ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU ILE
LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU ARG GLN ARG SER ALA LEU GLY GLU GLU THR HIS LEU ASP LYS HIS ASN VAL TYR SER LEU SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU GLU THR LEU ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU GLY THR
ILE TYR ASN THR ARG SER SER ARG GLU ARG ALA ALA LEU SER LEU PRO ALA ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU GLU LYS LEU ILE ILE GLU LEU ALA ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO TYR MET MET GLU VAL VAL LEU PRO MET LEU
CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN HIS PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER LEU HIS MET ASN THR LEU LEU GLY ILE LYS LEU LEU ILE TYR ASN ASN LEU TRP GLY ILE ASP GLU GLU GLY ALA TRP LEU ILE LEU LEU ASP GLU PHE THR ALA VAL PHE
SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN GLN LEU LEU LYS THR HIS PHE LEU PRO LEU LYS LYS LYS MET GLU LYS LEU VAL VAL SER GLU GLU ASP HIS LEU LYS ALA GLU LEU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR LEU



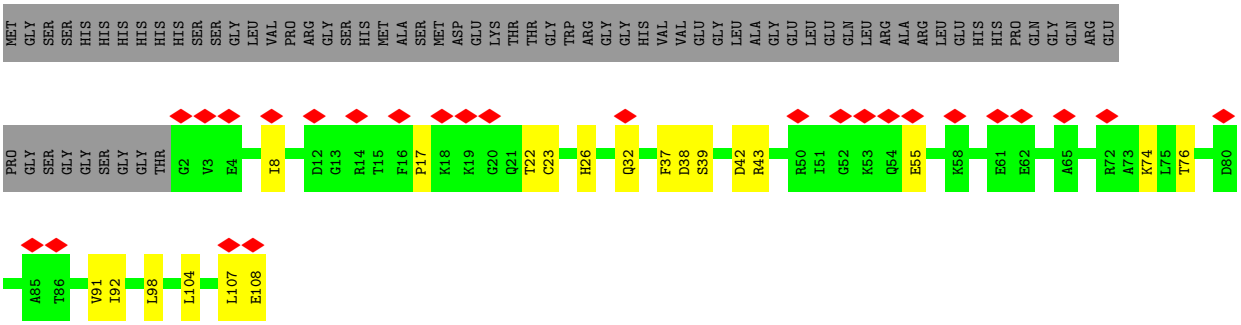
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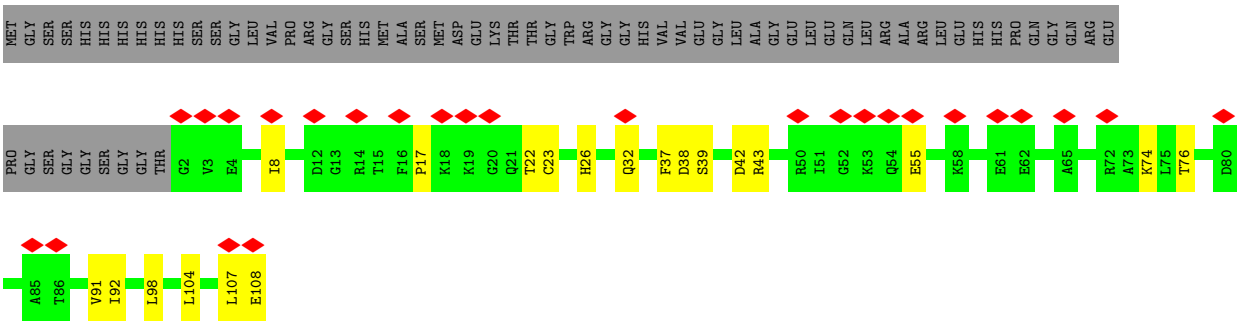
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B





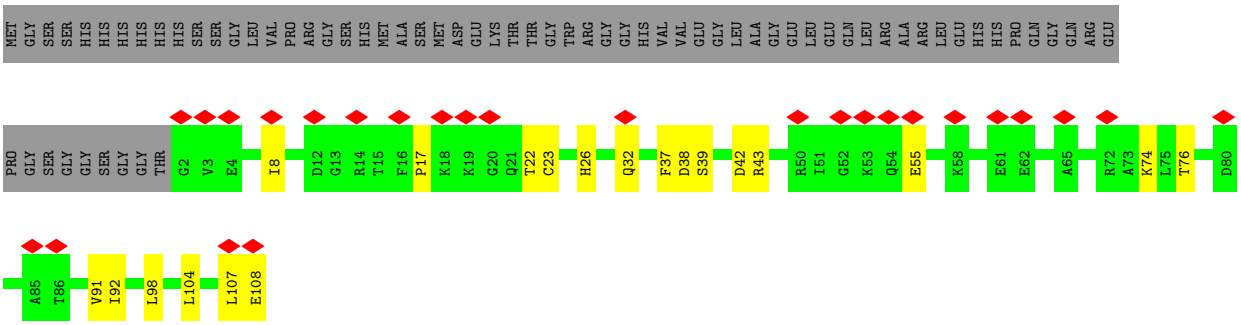
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B





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





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	102955	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	471.04, 471.04, 471.04	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A1MG7

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	0.21	0/28516	0.35	0/38541
1	B	0.21	0/28516	0.35	0/38541
1	C	0.21	0/28516	0.35	0/38541
1	D	0.21	0/28516	0.35	0/38541
2	G	0.17	0/835	0.39	0/1123
2	H	0.17	0/835	0.38	0/1123
2	I	0.17	0/835	0.38	0/1123
2	J	0.17	0/835	0.39	0/1123
All	All	0.21	0/117404	0.35	0/158656

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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3925	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	4748	GLY	Peptide
1	A	4749	PHE	Peptide
1	B	3925	GLY	Peptide
1	B	4748	GLY	Peptide
1	B	4749	PHE	Peptide
1	C	3925	GLY	Peptide
1	C	4748	GLY	Peptide
1	C	4749	PHE	Peptide
1	D	3925	GLY	Peptide
1	D	4748	GLY	Peptide
1	D	4749	PHE	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	27906	27535	27532	327	0
1	B	27906	27535	27532	324	0
1	C	27906	27535	27532	324	0
1	D	27906	27535	27532	327	0
2	G	819	821	821	14	0
2	H	819	821	821	13	0
2	I	819	821	821	13	0
2	J	819	821	821	13	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
4	A	25	12	0	0	0
4	B	25	12	0	0	0
4	C	25	12	0	0	0
4	D	25	12	0	0	0
All	All	115004	113472	113412	1334	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 6.

All (1334) 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:C:889:ILE:HG21	1:C:935:MET:HE3	1.67	0.77
1:D:889:ILE:HG21	1:D:935:MET:HE3	1.67	0.77
1:A:889:ILE:HG21	1:A:935:MET:HE3	1.67	0.76
1:D:3800:SER:OG	1:D:3830:GLN:O	2.04	0.76
1:B:889:ILE:HG21	1:B:935:MET:HE3	1.67	0.75
2:G:74:LYS:NZ	2:G:76:THR:OG1	2.19	0.75
2:I:74:LYS:NZ	2:I:76:THR:OG1	2.19	0.75
1:C:80:GLU:OE2	1:C:84:ASN:ND2	2.20	0.74
1:C:3800:SER:OG	1:C:3830:GLN:O	2.04	0.74
1:D:80:GLU:OE2	1:D:84:ASN:ND2	2.20	0.74
1:A:80:GLU:OE2	1:A:84:ASN:ND2	2.20	0.74
1:B:80:GLU:OE2	1:B:84:ASN:ND2	2.20	0.74
1:C:695:VAL:HG11	1:C:755:ILE:HG21	1.69	0.74
1:D:695:VAL:HG11	1:D:755:ILE:HG21	1.69	0.73
1:D:1100:ARG:NH1	1:D:1167:ASP:OD2	2.22	0.73
1:B:323:ASP:O	1:B:327:THR:OG1	2.07	0.73
1:B:695:VAL:HG11	1:B:755:ILE:HG21	1.69	0.73
1:D:323:ASP:O	1:D:327:THR:OG1	2.07	0.72
1:C:1100:ARG:NH1	1:C:1167:ASP:OD2	2.22	0.72
1:C:996:VAL:HG13	1:C:1050:LEU:HD11	1.72	0.72
1:B:1100:ARG:NH1	1:B:1167:ASP:OD2	2.22	0.72
1:A:1100:ARG:NH1	1:A:1167:ASP:OD2	2.22	0.71
1:A:323:ASP:O	1:A:327:THR:OG1	2.07	0.71
1:A:695:VAL:HG11	1:A:755:ILE:HG21	1.69	0.71
1:C:4867:ASP:OD1	1:D:4873:ARG:NH1	2.24	0.71
2:H:74:LYS:NZ	2:H:76:THR:OG1	2.19	0.71
1:A:996:VAL:HG13	1:A:1050:LEU:HD11	1.72	0.71
1:B:996:VAL:HG13	1:B:1050:LEU:HD11	1.72	0.71
1:B:2125:ILE:HG23	1:B:2141:MET:HE1	1.72	0.71
1:B:4867:ASP:OD1	1:C:4873:ARG:NH1	2.23	0.71
2:J:74:LYS:NZ	2:J:76:THR:OG1	2.19	0.71
1:A:3891:TYR:O	1:A:3956:LYS:NZ	2.24	0.71
1:C:3891:TYR:O	1:C:3956:LYS:NZ	2.23	0.71
1:A:4867:ASP:OD1	1:B:4873:ARG:NH1	2.24	0.71
1:C:2114:ASP:OD1	1:C:2151:ASN:ND2	2.24	0.71
1:D:668:ALA:O	1:D:1017:THR:OG1	2.08	0.71
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.64	0.71
1:B:2114:ASP:OD1	1:B:2151:ASN:ND2	2.24	0.71
1:D:2114:ASP:OD1	1:D:2151:ASN:ND2	2.24	0.71
1:A:2114:ASP:OD1	1:A:2151:ASN:ND2	2.24	0.70
1:D:2125:ILE:HG23	1:D:2141:MET:HE1	1.72	0.70
1:D:996:VAL:HG13	1:D:1050:LEU:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:ARG:NH2	1:A:1583:CYS:SG	2.64	0.70
1:B:1272:ARG:NH2	1:B:1583:CYS:SG	2.64	0.70
1:D:3891:TYR:O	1:D:3956:LYS:NZ	2.24	0.70
1:A:4873:ARG:NH1	1:D:4867:ASP:OD1	2.23	0.70
1:B:3891:TYR:O	1:B:3956:LYS:NZ	2.24	0.70
1:C:2125:ILE:HG23	1:C:2141:MET:HE1	1.72	0.70
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.64	0.70
2:G:39:SER:O	2:G:43:ARG:NH1	2.25	0.70
1:A:2125:ILE:HG23	1:A:2141:MET:HE1	1.72	0.70
1:D:3634:TYR:OH	1:D:3701:GLU:OE1	2.09	0.70
1:B:2502:ASP:OD2	1:B:2553:ARG:NH1	2.25	0.69
1:B:3800:SER:OG	1:B:3830:GLN:O	2.04	0.69
1:A:1097:LYS:NZ	1:A:1198:GLY:O	2.26	0.69
2:I:39:SER:O	2:I:43:ARG:NH1	2.25	0.69
1:B:872:ILE:HG23	1:B:944:LEU:HD22	1.74	0.69
1:B:3634:TYR:OH	1:B:3701:GLU:OE1	2.09	0.69
1:B:4645:ASP:OD2	1:B:4651:LYS:NZ	2.25	0.69
1:C:2502:ASP:OD2	1:C:2553:ARG:NH1	2.25	0.69
1:A:3634:TYR:OH	1:A:3701:GLU:OE1	2.09	0.69
1:C:1097:LYS:NZ	1:C:1198:GLY:O	2.25	0.69
1:D:4645:ASP:OD2	1:D:4651:LYS:NZ	2.25	0.69
1:B:3900:GLN:OE1	1:B:3903:ARG:NH2	2.26	0.69
1:C:323:ASP:O	1:C:327:THR:OG1	2.07	0.69
1:C:3634:TYR:OH	1:C:3701:GLU:OE1	2.09	0.69
1:D:1097:LYS:NZ	1:D:1198:GLY:O	2.25	0.69
1:B:1097:LYS:NZ	1:B:1198:GLY:O	2.26	0.69
1:B:3954:GLN:O	1:B:3958:SER:OG	2.10	0.69
1:D:872:ILE:HG23	1:D:944:LEU:HD22	1.74	0.69
2:H:39:SER:O	2:H:43:ARG:NH1	2.25	0.69
2:J:39:SER:O	2:J:43:ARG:NH1	2.25	0.69
1:C:3900:GLN:OE1	1:C:3903:ARG:NH2	2.26	0.69
1:A:2222:GLU:OE1	1:A:2223:ASN:ND2	2.26	0.68
1:A:2502:ASP:OD2	1:A:2553:ARG:NH1	2.25	0.68
1:C:872:ILE:HG23	1:C:944:LEU:HD22	1.74	0.68
1:C:4645:ASP:OD2	1:C:4651:LYS:NZ	2.25	0.68
1:D:3900:GLN:OE1	1:D:3903:ARG:NH2	2.26	0.68
1:A:668:ALA:O	1:A:1017:THR:OG1	2.07	0.68
1:A:3800:SER:OG	1:A:3830:GLN:O	2.04	0.68
1:D:2502:ASP:OD2	1:D:2553:ARG:NH1	2.26	0.68
1:A:872:ILE:HG23	1:A:944:LEU:HD22	1.74	0.68
1:A:3900:GLN:OE1	1:A:3903:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2222:GLU:OE1	1:C:2223:ASN:ND2	2.26	0.68
1:B:2222:GLU:OE1	1:B:2223:ASN:ND2	2.26	0.68
1:D:2222:GLU:OE1	1:D:2223:ASN:ND2	2.26	0.68
1:A:4645:ASP:OD2	1:A:4651:LYS:NZ	2.25	0.67
1:D:2431:LEU:HD22	1:D:2471:LEU:HD23	1.77	0.67
1:B:141:ASP:OD2	1:B:144:ALA:N	2.28	0.67
1:A:141:ASP:OD2	1:A:144:ALA:N	2.28	0.67
1:B:2431:LEU:HD22	1:B:2471:LEU:HD23	1.77	0.67
1:A:2431:LEU:HD22	1:A:2471:LEU:HD23	1.77	0.67
1:C:141:ASP:OD2	1:C:144:ALA:N	2.28	0.66
1:D:141:ASP:OD2	1:D:144:ALA:N	2.28	0.66
1:D:136:SER:OG	1:D:144:ALA:O	2.10	0.66
1:C:2431:LEU:HD22	1:C:2471:LEU:HD23	1.77	0.66
1:A:281:ARG:O	1:A:285:SER:OG	2.14	0.66
1:B:2233:MET:SD	1:B:2233:MET:N	2.70	0.65
1:C:804:LEU:HD13	1:C:832:LEU:HD21	1.79	0.65
1:A:804:LEU:HD13	1:A:832:LEU:HD21	1.79	0.65
1:D:804:LEU:HD13	1:D:832:LEU:HD21	1.79	0.65
1:D:281:ARG:O	1:D:285:SER:OG	2.14	0.65
1:D:320:GLU:N	1:D:320:GLU:OE1	2.30	0.65
1:A:2233:MET:SD	1:A:2233:MET:N	2.70	0.65
1:B:804:LEU:HD13	1:B:832:LEU:HD21	1.79	0.65
1:C:222:GLU:N	1:C:222:GLU:OE1	2.30	0.65
1:C:887:GLU:O	1:C:890:HIS:ND1	2.30	0.65
1:C:320:GLU:OE1	1:C:320:GLU:N	2.30	0.64
1:A:320:GLU:N	1:A:320:GLU:OE1	2.30	0.64
1:C:668:ALA:O	1:C:1017:THR:OG1	2.08	0.64
1:D:2233:MET:SD	1:D:2233:MET:N	2.70	0.64
1:B:668:ALA:O	1:B:1017:THR:OG1	2.08	0.64
1:B:3653:GLU:OE1	1:B:3653:GLU:N	2.31	0.64
1:C:3653:GLU:N	1:C:3653:GLU:OE1	2.31	0.64
1:D:222:GLU:N	1:D:222:GLU:OE1	2.30	0.64
1:A:222:GLU:N	1:A:222:GLU:OE1	2.30	0.64
1:D:3653:GLU:OE1	1:D:3653:GLU:N	2.31	0.64
1:C:2609:LEU:HD13	1:C:2643:LEU:HD21	1.79	0.64
1:A:2383:MET:SD	1:A:2383:MET:N	2.71	0.64
1:B:624:ALA:HB2	1:B:1668:LEU:HD12	1.80	0.64
1:C:2233:MET:N	1:C:2233:MET:SD	2.70	0.64
1:D:887:GLU:O	1:D:890:HIS:ND1	2.30	0.64
1:B:320:GLU:N	1:B:320:GLU:OE1	2.30	0.63
1:B:2455:MET:SD	1:B:2455:MET:N	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2609:LEU:HD13	1:A:2643:LEU:HD21	1.79	0.63
1:A:3653:GLU:N	1:A:3653:GLU:OE1	2.31	0.63
1:B:2383:MET:SD	1:B:2383:MET:N	2.71	0.63
1:C:624:ALA:HB2	1:C:1668:LEU:HD12	1.80	0.63
1:D:2455:MET:SD	1:D:2455:MET:N	2.71	0.63
1:B:222:GLU:OE1	1:B:222:GLU:N	2.30	0.63
1:A:2455:MET:SD	1:A:2455:MET:N	2.71	0.63
1:C:2383:MET:SD	1:C:2383:MET:N	2.71	0.63
1:C:2455:MET:N	1:C:2455:MET:SD	2.71	0.63
1:B:887:GLU:O	1:B:890:HIS:ND1	2.30	0.63
1:C:1963:GLU:O	1:C:1966:SER:OG	2.17	0.63
1:B:313:ASN:HA	1:B:392:ILE:HG22	1.79	0.63
1:B:2609:LEU:HD13	1:B:2643:LEU:HD21	1.79	0.63
1:C:290:ARG:NH1	1:C:291:TRP:O	2.32	0.63
1:C:1246:ASP:OD1	1:C:1694:TYR:OH	2.15	0.63
1:D:473:GLU:N	1:D:473:GLU:OE1	2.32	0.63
1:D:1963:GLU:O	1:D:1966:SER:OG	2.16	0.63
1:B:281:ARG:O	1:B:285:SER:OG	2.14	0.62
1:B:3855:ASN:OD1	1:B:3858:ARG:NH2	2.32	0.62
1:D:313:ASN:HA	1:D:392:ILE:HG22	1.79	0.62
1:A:1246:ASP:OD1	1:A:1694:TYR:OH	2.15	0.62
1:A:1963:GLU:O	1:A:1966:SER:OG	2.17	0.62
1:A:2376:GLU:O	1:A:2380:THR:OG1	2.15	0.62
1:C:473:GLU:N	1:C:473:GLU:OE1	2.32	0.62
1:C:3855:ASN:OD1	1:C:3858:ARG:NH2	2.32	0.62
1:D:2383:MET:SD	1:D:2383:MET:N	2.71	0.62
1:C:1091:GLU:OE2	1:C:1646:THR:OG1	2.08	0.62
1:D:2609:LEU:HD13	1:D:2643:LEU:HD21	1.80	0.62
1:A:473:GLU:N	1:A:473:GLU:OE1	2.32	0.62
1:C:313:ASN:HA	1:C:392:ILE:HG22	1.79	0.62
1:D:290:ARG:NH1	1:D:291:TRP:O	2.32	0.62
1:A:624:ALA:HB2	1:A:1668:LEU:HD12	1.80	0.62
1:A:1234:GLU:N	1:A:1234:GLU:OE1	2.33	0.62
1:B:473:GLU:N	1:B:473:GLU:OE1	2.32	0.62
1:B:1234:GLU:N	1:B:1234:GLU:OE1	2.33	0.62
1:D:3855:ASN:OD1	1:D:3858:ARG:NH2	2.32	0.62
1:C:2376:GLU:O	1:C:2380:THR:OG1	2.15	0.62
1:A:313:ASN:HA	1:A:392:ILE:HG22	1.79	0.62
1:B:290:ARG:NH1	1:B:291:TRP:O	2.32	0.62
1:B:1091:GLU:OE2	1:B:1646:THR:OG1	2.08	0.62
1:D:3919:LEU:HD22	1:D:3934:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:ALA:HB2	1:D:1668:LEU:HD12	1.80	0.61
1:B:4566:TYR:O	1:B:4570:THR:OG1	2.16	0.61
1:C:281:ARG:O	1:C:285:SER:OG	2.14	0.61
1:C:1234:GLU:OE1	1:C:1234:GLU:N	2.33	0.61
1:C:2230:SER:OG	1:C:2233:MET:SD	2.55	0.61
1:D:1234:GLU:N	1:D:1234:GLU:OE1	2.33	0.61
2:J:32:GLN:N	2:J:32:GLN:OE1	2.33	0.61
1:A:3855:ASN:OD1	1:A:3858:ARG:NH2	2.32	0.61
1:A:290:ARG:NH1	1:A:291:TRP:O	2.32	0.61
1:D:221:SER:OG	1:D:222:GLU:OE1	2.19	0.61
2:I:32:GLN:OE1	2:I:32:GLN:N	2.33	0.61
1:A:887:GLU:O	1:A:890:HIS:ND1	2.30	0.61
1:A:3919:LEU:HD22	1:A:3934:LEU:HD11	1.81	0.61
2:I:55:GLU:OE1	2:I:55:GLU:N	2.34	0.61
1:B:3919:LEU:HD22	1:B:3934:LEU:HD11	1.81	0.61
1:B:221:SER:OG	1:B:222:GLU:OE1	2.19	0.61
1:C:3919:LEU:HD22	1:C:3934:LEU:HD11	1.81	0.61
2:H:55:GLU:N	2:H:55:GLU:OE1	2.34	0.61
1:A:643:LEU:O	1:A:645:GLN:NE2	2.34	0.61
2:H:32:GLN:N	2:H:32:GLN:OE1	2.33	0.61
2:G:32:GLN:OE1	2:G:32:GLN:N	2.33	0.60
2:J:55:GLU:N	2:J:55:GLU:OE1	2.34	0.60
1:A:877:HIS:O	1:A:880:ARG:NH1	2.35	0.60
1:C:71:GLN:O	1:C:119:ILE:HD12	2.02	0.60
1:D:877:HIS:O	1:D:880:ARG:NH1	2.35	0.60
1:B:643:LEU:O	1:B:645:GLN:NE2	2.34	0.60
1:C:643:LEU:O	1:C:645:GLN:NE2	2.34	0.60
1:A:221:SER:OG	1:A:222:GLU:OE1	2.19	0.60
1:D:71:GLN:O	1:D:119:ILE:HD12	2.02	0.60
1:B:1014:GLN:N	1:B:1014:GLN:OE1	2.35	0.60
1:A:71:GLN:O	1:A:119:ILE:HD12	2.02	0.60
1:A:1091:GLU:OE2	1:A:1646:THR:OG1	2.08	0.59
1:B:1963:GLU:O	1:B:1966:SER:OG	2.17	0.59
1:D:3737:GLU:OE1	1:D:3737:GLU:N	2.35	0.59
1:D:3764:ILE:HG22	1:D:3772:VAL:HG21	1.84	0.59
1:A:3737:GLU:N	1:A:3737:GLU:OE1	2.35	0.59
1:B:71:GLN:O	1:B:119:ILE:HD12	2.02	0.59
1:C:877:HIS:O	1:C:880:ARG:NH1	2.35	0.59
1:D:1246:ASP:OD1	1:D:1694:TYR:OH	2.15	0.59
1:B:565:LEU:HD11	1:B:1585:PRO:HG3	1.85	0.59
1:C:565:LEU:HD11	1:C:1585:PRO:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3764:ILE:HG22	1:C:3772:VAL:HG21	1.84	0.59
1:D:643:LEU:O	1:D:645:GLN:NE2	2.34	0.59
1:D:4566:TYR:O	1:D:4570:THR:OG1	2.17	0.59
1:B:191:TYR:N	1:B:206:ALA:O	2.36	0.59
1:B:877:HIS:O	1:B:880:ARG:NH1	2.35	0.59
1:C:3737:GLU:N	1:C:3737:GLU:OE1	2.35	0.59
2:G:55:GLU:OE1	2:G:55:GLU:N	2.34	0.59
1:B:3737:GLU:OE1	1:B:3737:GLU:N	2.35	0.59
1:D:292:GLY:N	1:D:331:PHE:O	2.36	0.59
1:D:1635:GLU:OE1	1:D:1635:GLU:N	2.36	0.59
1:C:3916:PHE:O	1:C:3920:THR:HG23	2.03	0.59
1:A:191:TYR:N	1:A:206:ALA:O	2.36	0.58
1:A:292:GLY:N	1:A:331:PHE:O	2.36	0.58
1:C:191:TYR:N	1:C:206:ALA:O	2.36	0.58
1:C:1014:GLN:OE1	1:C:1014:GLN:N	2.35	0.58
1:D:191:TYR:N	1:D:206:ALA:O	2.36	0.58
1:D:565:LEU:HD11	1:D:1585:PRO:HG3	1.85	0.58
1:D:1014:GLN:N	1:D:1014:GLN:OE1	2.35	0.58
1:D:3934:LEU:HD12	1:D:3939:LEU:HD22	1.85	0.58
1:A:62:LEU:O	1:A:66:THR:HG23	2.03	0.58
1:A:3916:PHE:O	1:A:3920:THR:HG23	2.03	0.58
1:C:292:GLY:N	1:C:331:PHE:O	2.36	0.58
1:C:221:SER:OG	1:C:222:GLU:OE1	2.19	0.58
1:D:1692:ASN:OD1	1:D:1695:MET:N	2.36	0.58
1:A:1692:ASN:OD1	1:A:1695:MET:N	2.36	0.58
1:A:3764:ILE:HG22	1:A:3772:VAL:HG21	1.84	0.58
1:B:4073:GLU:N	1:B:4073:GLU:OE1	2.37	0.58
1:C:1692:ASN:OD1	1:C:1695:MET:N	2.36	0.58
1:D:4807:ASP:OD1	1:D:4807:ASP:N	2.37	0.58
1:A:3934:LEU:HD12	1:A:3939:LEU:HD22	1.85	0.58
1:A:3954:GLN:O	1:A:3958:SER:OG	2.10	0.58
1:B:4949:GLU:OE1	1:B:4949:GLU:N	2.37	0.58
1:C:4807:ASP:OD1	1:C:4807:ASP:N	2.37	0.58
1:D:62:LEU:O	1:D:66:THR:HG23	2.03	0.58
1:A:565:LEU:HD11	1:A:1585:PRO:HG3	1.85	0.58
1:A:4807:ASP:OD1	1:A:4807:ASP:N	2.37	0.58
1:D:3916:PHE:O	1:D:3920:THR:HG23	2.03	0.58
1:A:1014:GLN:OE1	1:A:1014:GLN:N	2.35	0.58
1:C:4073:GLU:OE1	1:C:4073:GLU:N	2.37	0.58
1:C:4178:GLU:OE1	1:C:4178:GLU:N	2.37	0.58
1:B:292:GLY:N	1:B:331:PHE:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1692:ASN:OD1	1:B:1695:MET:N	2.36	0.58
1:B:2480:GLN:OE1	1:B:2483:LEU:HD23	2.04	0.58
1:B:3916:PHE:O	1:B:3920:THR:HG23	2.03	0.58
1:C:136:SER:OG	1:C:144:ALA:O	2.11	0.58
1:B:3764:ILE:HG22	1:B:3772:VAL:HG21	1.84	0.58
1:B:3891:TYR:OH	1:B:3898:ASP:OD1	2.22	0.58
1:D:4073:GLU:N	1:D:4073:GLU:OE1	2.37	0.58
1:A:1635:GLU:OE1	1:A:1635:GLU:N	2.36	0.58
1:C:2275:SER:OG	1:C:2289:TRP:N	2.37	0.58
1:C:2480:GLN:OE1	1:C:2483:LEU:HD23	2.04	0.58
1:B:1635:GLU:OE1	1:B:1635:GLU:N	2.36	0.57
1:B:4178:GLU:N	1:B:4178:GLU:OE1	2.37	0.57
1:B:49:LEU:HD21	1:B:203:VAL:HG13	1.86	0.57
1:D:4178:GLU:N	1:D:4178:GLU:OE1	2.37	0.57
1:C:62:LEU:O	1:C:66:THR:HG23	2.03	0.57
1:C:3934:LEU:HD12	1:C:3939:LEU:HD22	1.85	0.57
1:D:2588:LEU:O	1:D:2592:VAL:HG23	2.05	0.57
1:D:4949:GLU:N	1:D:4949:GLU:OE1	2.37	0.57
1:A:4949:GLU:N	1:A:4949:GLU:OE1	2.37	0.57
1:D:2275:SER:OG	1:D:2289:TRP:N	2.37	0.57
1:A:2175:VAL:HG12	1:A:2219:TYR:CZ	2.40	0.57
1:A:2275:SER:OG	1:A:2289:TRP:N	2.37	0.57
1:B:62:LEU:O	1:B:66:THR:HG23	2.03	0.57
1:B:3934:LEU:HD12	1:B:3939:LEU:HD22	1.85	0.57
1:C:49:LEU:HD21	1:C:203:VAL:HG13	1.86	0.57
1:D:2376:GLU:O	1:D:2380:THR:OG1	2.15	0.57
1:A:156:GLU:HB3	1:A:186:VAL:HG23	1.87	0.57
1:A:4178:GLU:N	1:A:4178:GLU:OE1	2.37	0.57
1:C:4796:GLU:N	1:C:4796:GLU:OE1	2.38	0.57
1:D:2175:VAL:HG12	1:D:2219:TYR:CZ	2.40	0.57
1:A:49:LEU:HD21	1:A:203:VAL:HG13	1.86	0.57
1:A:3682:GLU:N	1:A:3682:GLU:OE1	2.38	0.57
1:B:299:HIS:ND1	1:B:302:THR:OG1	2.26	0.57
1:A:3891:TYR:OH	1:A:3898:ASP:OD1	2.22	0.57
1:A:4796:GLU:N	1:A:4796:GLU:OE1	2.38	0.57
1:B:156:GLU:HB3	1:B:186:VAL:HG23	1.87	0.57
1:C:2588:LEU:O	1:C:2592:VAL:HG23	2.05	0.57
1:C:4949:GLU:N	1:C:4949:GLU:OE1	2.37	0.57
1:A:3920:THR:HG22	1:A:3980:MET:HA	1.87	0.56
1:B:1246:ASP:OD1	1:B:1694:TYR:OH	2.15	0.56
1:B:2588:LEU:O	1:B:2592:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4807:ASP:N	1:B:4807:ASP:OD1	2.37	0.56
1:C:897:LYS:NZ	1:C:903:GLN:O	2.38	0.56
1:D:3682:GLU:N	1:D:3682:GLU:OE1	2.38	0.56
1:C:2175:VAL:HG12	1:C:2219:TYR:CZ	2.40	0.56
1:C:3920:THR:HG22	1:C:3980:MET:HA	1.87	0.56
1:D:49:LEU:HD21	1:D:203:VAL:HG13	1.86	0.56
1:D:156:GLU:HB3	1:D:186:VAL:HG23	1.87	0.56
1:B:593:HIS:O	1:B:596:SER:OG	2.22	0.56
1:B:3682:GLU:OE1	1:B:3682:GLU:N	2.38	0.56
1:C:450:GLU:N	1:C:450:GLU:OE1	2.38	0.56
1:D:3920:THR:HG22	1:D:3980:MET:HA	1.87	0.56
1:D:4796:GLU:N	1:D:4796:GLU:OE1	2.38	0.56
1:A:34:LYS:O	1:A:52:THR:OG1	2.18	0.56
1:A:2230:SER:OG	1:A:2233:MET:SD	2.55	0.56
1:A:2480:GLN:OE1	1:A:2483:LEU:HD23	2.04	0.56
1:A:2588:LEU:O	1:A:2592:VAL:HG23	2.05	0.56
1:C:3683:GLU:OE1	1:C:3683:GLU:N	2.39	0.56
1:D:3954:GLN:O	1:D:3958:SER:OG	2.10	0.56
1:A:897:LYS:NZ	1:A:903:GLN:O	2.38	0.56
1:B:2175:VAL:HG12	1:B:2219:TYR:CZ	2.40	0.56
1:B:3683:GLU:N	1:B:3683:GLU:OE1	2.39	0.56
1:B:3920:THR:HG22	1:B:3980:MET:HA	1.87	0.56
1:C:156:GLU:HB3	1:C:186:VAL:HG23	1.87	0.56
1:D:246:THR:OG1	1:D:247:VAL:N	2.39	0.56
1:A:4136:GLU:OE2	1:A:4146:ARG:NH1	2.39	0.56
1:B:246:THR:OG1	1:B:247:VAL:N	2.39	0.56
1:B:897:LYS:NZ	1:B:903:GLN:O	2.38	0.56
1:B:2275:SER:OG	1:B:2289:TRP:N	2.37	0.56
1:D:2480:GLN:OE1	1:D:2483:LEU:HD23	2.04	0.56
1:D:4136:GLU:OE2	1:D:4146:ARG:NH1	2.39	0.56
1:A:136:SER:OG	1:A:144:ALA:O	2.10	0.56
1:B:824:GLU:OE1	1:B:1028:ARG:NH1	2.39	0.56
1:C:824:GLU:OE1	1:C:1028:ARG:NH1	2.39	0.56
1:C:3682:GLU:N	1:C:3682:GLU:OE1	2.38	0.56
1:B:450:GLU:OE1	1:B:450:GLU:N	2.38	0.55
1:C:2159:ASN:OD1	1:C:2162:ARG:NH2	2.39	0.55
1:C:4136:GLU:OE2	1:C:4146:ARG:NH1	2.39	0.55
1:D:450:GLU:OE1	1:D:450:GLU:N	2.37	0.55
1:D:824:GLU:OE1	1:D:1028:ARG:NH1	2.39	0.55
1:D:1091:GLU:OE2	1:D:1646:THR:OG1	2.08	0.55
1:B:606:ARG:NH2	1:B:642:LEU:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ARG:NH2	1:C:642:LEU:O	2.39	0.55
1:A:606:ARG:NH2	1:A:642:LEU:O	2.39	0.55
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.39	0.55
1:B:4136:GLU:OE2	1:B:4146:ARG:NH1	2.39	0.55
1:C:3844:LEU:HD23	1:C:3847:GLU:OE1	2.06	0.55
1:D:606:ARG:NH2	1:D:642:LEU:O	2.39	0.55
1:D:897:LYS:NZ	1:D:903:GLN:O	2.38	0.55
1:A:246:THR:OG1	1:A:247:VAL:N	2.39	0.55
1:A:565:LEU:HD11	1:A:1585:PRO:CG	2.37	0.55
1:A:3683:GLU:OE1	1:A:3683:GLU:N	2.39	0.55
1:D:34:LYS:O	1:D:52:THR:OG1	2.18	0.55
1:A:3844:LEU:HD23	1:A:3847:GLU:OE1	2.07	0.55
1:C:43:GLY:N	1:C:458:ASP:OD2	2.40	0.55
1:C:246:THR:OG1	1:C:247:VAL:N	2.39	0.55
1:C:480:ARG:NH1	1:C:3677:GLU:OE1	2.40	0.55
1:C:551:PHE:CZ	1:C:558:LEU:HD11	2.42	0.55
1:D:480:ARG:NH1	1:D:3677:GLU:OE1	2.40	0.55
1:D:3683:GLU:N	1:D:3683:GLU:OE1	2.39	0.55
1:A:4073:GLU:N	1:A:4073:GLU:OE1	2.37	0.55
1:B:565:LEU:HD11	1:B:1585:PRO:CG	2.37	0.55
1:B:2376:GLU:O	1:B:2380:THR:OG1	2.15	0.55
1:C:3891:TYR:OH	1:C:3898:ASP:OD1	2.22	0.55
1:D:551:PHE:CZ	1:D:558:LEU:HD11	2.42	0.55
1:D:3844:LEU:HD23	1:D:3847:GLU:OE1	2.07	0.55
1:A:450:GLU:N	1:A:450:GLU:OE1	2.38	0.55
1:A:824:GLU:OE1	1:A:1028:ARG:NH1	2.39	0.55
1:A:2313:GLU:OE1	1:A:2313:GLU:N	2.40	0.55
1:D:565:LEU:HD11	1:D:1585:PRO:CG	2.37	0.55
1:B:551:PHE:CZ	1:B:558:LEU:HD11	2.42	0.55
1:D:593:HIS:O	1:D:596:SER:OG	2.22	0.55
1:D:2159:ASN:OD1	1:D:2162:ARG:NH2	2.39	0.55
1:C:2074:ILE:HG23	1:C:2079:LEU:HD23	1.88	0.55
1:D:43:GLY:N	1:D:458:ASP:OD2	2.40	0.54
1:A:43:GLY:N	1:A:458:ASP:OD2	2.40	0.54
1:A:480:ARG:NH1	1:A:3677:GLU:OE1	2.40	0.54
1:A:521:GLU:OE1	1:A:521:GLU:N	2.39	0.54
1:B:3844:LEU:HD23	1:B:3847:GLU:OE1	2.07	0.54
1:B:4796:GLU:OE1	1:B:4796:GLU:N	2.38	0.54
1:C:717:GLY:N	1:C:720:ASP:OD2	2.40	0.54
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.39	0.54
1:B:43:GLY:N	1:B:458:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1635:GLU:N	1:C:1635:GLU:OE1	2.36	0.54
1:D:503:ASP:OD1	1:D:557:TRP:NE1	2.38	0.54
1:D:1932:VAL:HG21	1:D:3616:VAL:HA	1.90	0.54
1:B:717:GLY:N	1:B:720:ASP:OD2	2.40	0.54
1:D:2657:GLU:OE1	1:D:2659:GLU:N	2.41	0.54
1:D:3891:TYR:OH	1:D:3898:ASP:OD1	2.22	0.54
1:A:503:ASP:OD1	1:A:557:TRP:NE1	2.38	0.54
1:A:717:GLY:N	1:A:720:ASP:OD2	2.40	0.54
1:A:2074:ILE:HG23	1:A:2079:LEU:HD23	1.89	0.54
1:B:874:LEU:HD22	1:B:940:LEU:HD13	1.89	0.54
1:B:1472:GLU:N	1:B:1472:GLU:OE1	2.41	0.54
1:B:2657:GLU:OE1	1:B:2659:GLU:N	2.41	0.54
1:C:503:ASP:OD1	1:C:557:TRP:NE1	2.38	0.54
2:H:17:PRO:HA	2:H:107:LEU:HD21	1.89	0.54
1:A:1472:GLU:OE1	1:A:1472:GLU:N	2.41	0.54
1:B:2230:SER:OG	1:B:2233:MET:SD	2.55	0.54
1:B:2351:LYS:NZ	1:B:2351:LYS:O	2.41	0.54
1:A:551:PHE:CZ	1:A:558:LEU:HD11	2.42	0.54
1:C:1306:MET:SD	1:C:1306:MET:N	2.81	0.54
1:C:2351:LYS:NZ	1:C:2351:LYS:O	2.41	0.54
1:C:565:LEU:HD11	1:C:1585:PRO:CG	2.37	0.54
1:C:2657:GLU:OE1	1:C:2659:GLU:N	2.41	0.54
1:D:1245:ARG:NH1	1:D:1809:ASP:O	2.41	0.54
2:I:17:PRO:HA	2:I:107:LEU:HD21	1.89	0.54
1:A:869:THR:HA	1:A:872:ILE:HD13	1.90	0.54
1:A:2657:GLU:OE1	1:A:2659:GLU:N	2.41	0.54
1:B:480:ARG:NH1	1:B:3677:GLU:OE1	2.40	0.54
1:D:1436:GLN:NE2	1:D:1547:GLN:O	2.40	0.54
1:A:755:ILE:HD12	1:A:769:ARG:O	2.08	0.53
1:B:1245:ARG:NH1	1:B:1809:ASP:O	2.41	0.53
1:B:1306:MET:SD	1:B:1306:MET:N	2.81	0.53
1:B:2074:ILE:HG23	1:B:2079:LEU:HD23	1.89	0.53
1:C:874:LEU:HD22	1:C:940:LEU:HD13	1.89	0.53
1:C:1472:GLU:OE1	1:C:1472:GLU:N	2.41	0.53
1:C:1932:VAL:HG21	1:C:3616:VAL:HA	1.90	0.53
1:D:2074:ILE:HG23	1:D:2079:LEU:HD23	1.88	0.53
2:J:17:PRO:HA	2:J:107:LEU:HD21	1.89	0.53
1:D:1306:MET:SD	1:D:1306:MET:N	2.81	0.53
1:D:2076:ASP:OD2	1:D:2079:LEU:N	2.41	0.53
1:A:1436:GLN:NE2	1:A:1547:GLN:O	2.40	0.53
1:A:3626:SER:O	1:A:3630:THR:OG1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:CYS:SG	1:B:949:HIS:N	2.82	0.53
1:D:874:LEU:HD22	1:D:940:LEU:HD13	1.89	0.53
1:D:2122:LEU:HA	1:D:2125:ILE:HD12	1.90	0.53
2:J:38:ASP:OD1	2:J:39:SER:N	2.41	0.53
1:A:874:LEU:HD22	1:A:940:LEU:HD13	1.89	0.53
1:A:1602:ASN:O	1:A:1603:GLN:NE2	2.42	0.53
1:B:243:GLU:OE2	1:B:389:ARG:NH1	2.42	0.53
1:B:755:ILE:HD12	1:B:769:ARG:O	2.08	0.53
1:C:171:GLU:OE1	1:C:171:GLU:N	2.41	0.53
1:D:3762:ILE:HD11	1:D:3837:ASP:O	2.09	0.53
1:A:243:GLU:OE2	1:A:389:ARG:NH1	2.42	0.53
1:A:948:CYS:SG	1:A:949:HIS:N	2.82	0.53
1:A:1306:MET:SD	1:A:1306:MET:N	2.81	0.53
1:B:2122:LEU:HA	1:B:2125:ILE:HD12	1.90	0.53
1:D:171:GLU:N	1:D:171:GLU:OE1	2.41	0.53
1:D:1472:GLU:N	1:D:1472:GLU:OE1	2.41	0.53
1:A:4589:TYR:OH	1:A:4715:ASP:OD2	2.26	0.53
1:C:2313:GLU:N	1:C:2313:GLU:OE1	2.40	0.53
1:D:243:GLU:OE2	1:D:389:ARG:NH1	2.42	0.53
1:D:871:GLN:C	1:D:872:ILE:HD12	2.34	0.53
2:I:92:ILE:HD12	2:I:98:LEU:HD11	1.90	0.53
1:A:2351:LYS:NZ	1:A:2351:LYS:O	2.41	0.53
1:B:254:GLU:OE1	1:B:254:GLU:N	2.42	0.53
1:B:1932:VAL:HG21	1:B:3616:VAL:HA	1.90	0.53
1:C:869:THR:HA	1:C:872:ILE:HD13	1.90	0.53
1:C:4589:TYR:OH	1:C:4715:ASP:OD2	2.26	0.53
1:D:869:THR:HA	1:D:872:ILE:HD13	1.90	0.53
1:B:171:GLU:N	1:B:171:GLU:OE1	2.41	0.53
1:B:503:ASP:OD1	1:B:557:TRP:NE1	2.38	0.53
1:B:869:THR:HA	1:B:872:ILE:HD13	1.90	0.53
1:B:2076:ASP:OD2	1:B:2079:LEU:N	2.41	0.53
1:C:243:GLU:OE2	1:C:389:ARG:NH1	2.42	0.53
1:D:521:GLU:OE1	1:D:521:GLU:N	2.39	0.53
1:D:755:ILE:HD12	1:D:769:ARG:O	2.08	0.53
1:D:2351:LYS:O	1:D:2351:LYS:NZ	2.41	0.53
2:G:92:ILE:HD12	2:G:98:LEU:HD11	1.91	0.53
1:C:34:LYS:O	1:C:52:THR:OG1	2.18	0.53
1:C:1245:ARG:NH1	1:C:1809:ASP:O	2.41	0.53
2:G:17:PRO:HA	2:G:107:LEU:HD21	1.89	0.53
1:A:171:GLU:OE1	1:A:171:GLU:N	2.41	0.52
1:A:2122:LEU:HA	1:A:2125:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:ILE:HD12	1:C:769:ARG:O	2.08	0.52
1:A:871:GLN:C	1:A:872:ILE:HD12	2.34	0.52
1:A:1245:ARG:NH1	1:A:1809:ASP:O	2.41	0.52
1:B:69:LEU:HB3	1:B:119:ILE:HD11	1.92	0.52
1:C:593:HIS:O	1:C:596:SER:OG	2.22	0.52
2:I:38:ASP:OD1	2:I:39:SER:N	2.41	0.52
1:A:2487:LEU:HD21	1:A:2547:LEU:HD22	1.92	0.52
1:B:2129:LEU:HD11	1:B:2172:GLU:CD	2.35	0.52
1:C:734:SER:OG	1:C:1482:ARG:NH1	2.42	0.52
1:C:3762:ILE:HD11	1:C:3837:ASP:O	2.09	0.52
1:D:1602:ASN:O	1:D:1603:GLN:NE2	2.42	0.52
1:A:2398:LEU:CD2	1:A:2422:LEU:HD22	2.39	0.52
1:B:3762:ILE:HD11	1:B:3837:ASP:O	2.09	0.52
1:C:1602:ASN:O	1:C:1603:GLN:NE2	2.42	0.52
1:D:948:CYS:SG	1:D:949:HIS:N	2.82	0.52
2:H:92:ILE:HD12	2:H:98:LEU:HD11	1.90	0.52
1:B:835:GLU:N	1:B:835:GLU:OE1	2.43	0.52
1:C:835:GLU:OE1	1:C:835:GLU:N	2.43	0.52
1:C:2398:LEU:CD2	1:C:2422:LEU:HD22	2.39	0.52
1:D:734:SER:OG	1:D:1482:ARG:NH1	2.42	0.52
1:D:2435:ILE:O	1:D:2464:LYS:NZ	2.39	0.52
2:G:38:ASP:OD1	2:G:39:SER:N	2.42	0.52
1:A:734:SER:OG	1:A:1482:ARG:NH1	2.42	0.52
1:A:2129:LEU:HD11	1:A:2172:GLU:CD	2.35	0.52
1:A:2251:GLU:OE1	1:A:2251:GLU:N	2.41	0.52
1:A:3762:ILE:HD11	1:A:3837:ASP:O	2.09	0.52
1:A:3900:GLN:O	1:A:3904:ASN:ND2	2.43	0.52
1:B:2128:LEU:HD21	1:B:2137:GLU:HB3	1.91	0.52
1:B:2251:GLU:OE1	1:B:2251:GLU:N	2.41	0.52
1:C:69:LEU:HB3	1:C:119:ILE:HD11	1.92	0.52
1:C:152:ASP:OD2	1:C:154:THR:OG1	2.28	0.52
1:C:948:CYS:SG	1:C:949:HIS:N	2.82	0.52
1:D:14:LEU:HB2	1:D:113:LEU:HD21	1.92	0.52
1:A:14:LEU:HB2	1:A:113:LEU:HD21	1.92	0.52
1:B:2398:LEU:CD2	1:B:2422:LEU:HD22	2.39	0.52
1:D:717:GLY:N	1:D:720:ASP:OD2	2.40	0.52
2:J:92:ILE:HD12	2:J:98:LEU:HD11	1.91	0.52
1:A:593:HIS:O	1:A:596:SER:OG	2.22	0.52
1:B:602:ASP:HA	1:B:642:LEU:HD21	1.91	0.52
1:B:1602:ASN:O	1:B:1603:GLN:NE2	2.42	0.52
1:C:602:ASP:HA	1:C:642:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2129:LEU:HD11	1:C:2172:GLU:CD	2.35	0.52
1:D:932:ASN:HA	1:D:935:MET:HE2	1.92	0.52
1:B:734:SER:OG	1:B:1482:ARG:NH1	2.42	0.52
1:B:2487:LEU:HD21	1:B:2547:LEU:HD22	1.92	0.52
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.43	0.52
1:D:835:GLU:N	1:D:835:GLU:OE1	2.43	0.52
1:D:2487:LEU:HD21	1:D:2547:LEU:HD22	1.92	0.52
1:A:69:LEU:HB3	1:A:119:ILE:HD11	1.92	0.52
1:A:2487:LEU:HG	1:A:2543:LEU:HD11	1.92	0.52
1:B:871:GLN:C	1:B:872:ILE:HD12	2.34	0.52
1:B:3900:GLN:O	1:B:3904:ASN:ND2	2.43	0.52
1:D:2128:LEU:HD21	1:D:2137:GLU:HB3	1.91	0.52
1:D:2129:LEU:HD11	1:D:2172:GLU:CD	2.35	0.52
1:D:2398:LEU:CD2	1:D:2422:LEU:HD22	2.39	0.52
1:A:835:GLU:N	1:A:835:GLU:OE1	2.43	0.51
1:A:2128:LEU:HD21	1:A:2137:GLU:HB3	1.91	0.51
1:B:14:LEU:HB2	1:B:113:LEU:HD21	1.92	0.51
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.43	0.51
1:B:2313:GLU:OE1	1:B:2313:GLU:N	2.40	0.51
1:C:14:LEU:HB2	1:C:113:LEU:HD21	1.92	0.51
1:C:871:GLN:C	1:C:872:ILE:HD12	2.34	0.51
1:D:2576:CYS:O	1:D:2615:ARG:NH2	2.43	0.51
2:H:38:ASP:OD1	2:H:39:SER:N	2.41	0.51
1:A:1932:VAL:HG21	1:A:3616:VAL:HA	1.90	0.51
1:B:2184:LYS:NZ	1:B:2185:GLU:O	2.44	0.51
1:B:2388:MET:HE1	1:B:2458:GLY:O	2.11	0.51
1:C:521:GLU:OE1	1:C:521:GLU:N	2.39	0.51
1:C:4088:GLU:N	1:C:4088:GLU:OE1	2.44	0.51
1:D:1033:VAL:HG23	1:D:1038:LEU:HD23	1.92	0.51
1:D:2487:LEU:HG	1:D:2543:LEU:HD11	1.92	0.51
1:D:4088:GLU:N	1:D:4088:GLU:OE1	2.44	0.51
1:B:136:SER:OG	1:B:144:ALA:O	2.10	0.51
1:A:1418:GLU:OE1	1:A:1418:GLU:N	2.44	0.51
1:A:2184:LYS:NZ	1:A:2185:GLU:O	2.44	0.51
1:A:2576:CYS:O	1:A:2615:ARG:NH2	2.43	0.51
1:A:4607:ARG:NH2	1:A:4643:TYR:OH	2.42	0.51
1:B:152:ASP:OD2	1:B:154:THR:OG1	2.28	0.51
1:C:2487:LEU:HG	1:C:2543:LEU:HD11	1.93	0.51
1:D:1418:GLU:N	1:D:1418:GLU:OE1	2.44	0.51
1:D:2609:LEU:CD1	1:D:2643:LEU:HD21	2.41	0.51
1:A:254:GLU:OE1	1:A:254:GLU:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2388:MET:HE1	1:A:2458:GLY:O	2.11	0.51
1:A:4088:GLU:N	1:A:4088:GLU:OE1	2.44	0.51
1:A:4136:GLU:OE1	1:A:4912:HIS:NE2	2.44	0.51
1:B:2254:LEU:O	1:B:3809:ARG:NH1	2.44	0.51
1:B:4088:GLU:N	1:B:4088:GLU:OE1	2.44	0.51
1:C:2122:LEU:HA	1:C:2125:ILE:HD12	1.90	0.51
1:C:2128:LEU:HD21	1:C:2137:GLU:HB3	1.91	0.51
1:C:3900:GLN:O	1:C:3904:ASN:ND2	2.43	0.51
1:C:4836:ASP:OD1	1:C:4837:GLU:N	2.44	0.51
1:D:152:ASP:OD2	1:D:154:THR:OG1	2.28	0.51
1:D:2388:MET:HE1	1:D:2458:GLY:O	2.10	0.51
1:B:1418:GLU:N	1:B:1418:GLU:OE1	2.44	0.51
1:C:1418:GLU:OE1	1:C:1418:GLU:N	2.44	0.51
1:C:1436:GLN:NE2	1:C:1547:GLN:O	2.40	0.51
1:C:2388:MET:HE1	1:C:2458:GLY:O	2.10	0.51
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.43	0.51
1:D:2184:LYS:NZ	1:D:2185:GLU:O	2.44	0.51
1:D:3900:GLN:O	1:D:3904:ASN:ND2	2.43	0.51
1:A:602:ASP:HA	1:A:642:LEU:HD21	1.92	0.51
1:B:2487:LEU:HG	1:B:2543:LEU:HD11	1.92	0.51
1:C:1720:LEU:CD2	1:C:1831:ILE:HD13	2.41	0.51
1:C:2254:LEU:O	1:C:3809:ARG:NH1	2.44	0.51
1:C:2487:LEU:HD21	1:C:2547:LEU:HD22	1.92	0.51
1:C:2609:LEU:CD1	1:C:2643:LEU:HD21	2.41	0.51
1:A:2609:LEU:CD1	1:A:2643:LEU:HD21	2.41	0.51
1:B:2576:CYS:O	1:B:2615:ARG:NH2	2.43	0.51
1:D:69:LEU:HB3	1:D:119:ILE:HD11	1.92	0.51
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.43	0.51
1:B:1720:LEU:CD2	1:B:1831:ILE:HD13	2.41	0.51
1:B:2492:LEU:HA	1:B:2495:LEU:HD12	1.93	0.51
1:B:562:LEU:HD12	1:B:563:GLU:N	2.26	0.51
1:B:1436:GLN:NE2	1:B:1547:GLN:O	2.40	0.51
1:C:932:ASN:HA	1:C:935:MET:HE2	1.92	0.51
1:C:4130:PRO:O	1:C:4156:ARG:NH1	2.44	0.51
1:A:152:ASP:OD2	1:A:154:THR:OG1	2.28	0.50
1:A:1033:VAL:HG23	1:A:1038:LEU:HD23	1.92	0.50
1:A:2254:LEU:O	1:A:3809:ARG:NH1	2.44	0.50
1:A:2492:LEU:HA	1:A:2495:LEU:HD12	1.93	0.50
1:C:562:LEU:HD12	1:C:563:GLU:N	2.26	0.50
1:C:2184:LYS:NZ	1:C:2185:GLU:O	2.44	0.50
1:D:2492:LEU:HA	1:D:2495:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4824:GLY:O	1:B:4821:ARG:NH1	2.43	0.50
1:B:932:ASN:HA	1:B:935:MET:HE2	1.92	0.50
1:B:1033:VAL:HG23	1:B:1038:LEU:HD23	1.92	0.50
1:B:2560:LEU:O	1:B:2565:ARG:NH1	2.44	0.50
1:C:2076:ASP:OD2	1:C:2079:LEU:N	2.41	0.50
1:A:2076:ASP:OD2	1:A:2079:LEU:N	2.41	0.50
1:B:1555:GLN:NE2	1:B:1557:GLU:OE2	2.44	0.50
1:C:1272:ARG:NH1	1:C:1587:LEU:O	2.44	0.50
1:C:2560:LEU:O	1:C:2565:ARG:NH1	2.44	0.50
1:C:2576:CYS:O	1:C:2615:ARG:NH2	2.44	0.50
1:D:4501:ARG:NH2	1:D:4744:ASP:OD1	2.44	0.50
1:D:4836:ASP:OD1	1:D:4837:GLU:N	2.44	0.50
1:A:1555:GLN:NE2	1:A:1557:GLU:OE2	2.44	0.50
1:A:4130:PRO:O	1:A:4156:ARG:NH1	2.44	0.50
1:B:1648:GLN:OE1	1:B:1650:GLU:N	2.45	0.50
1:D:562:LEU:HD12	1:D:563:GLU:N	2.26	0.50
1:D:2251:GLU:OE1	1:D:2251:GLU:N	2.41	0.50
1:B:2609:LEU:CD1	1:B:2643:LEU:HD21	2.41	0.50
1:B:4170:GLN:NE2	1:B:4174:ASP:OD1	2.45	0.50
1:C:254:GLU:OE1	1:C:254:GLU:N	2.42	0.50
1:C:1648:GLN:OE1	1:C:1650:GLU:N	2.45	0.50
1:D:254:GLU:OE1	1:D:254:GLU:N	2.42	0.50
1:D:1720:LEU:CD2	1:D:1831:ILE:HD13	2.41	0.50
1:D:4170:GLN:NE2	1:D:4174:ASP:OD1	2.45	0.50
1:A:562:LEU:HD12	1:A:563:GLU:N	2.26	0.50
1:A:4501:ARG:NH2	1:A:4744:ASP:OD1	2.44	0.50
1:A:4836:ASP:OD1	1:A:4837:GLU:N	2.44	0.50
1:C:1033:VAL:HG23	1:C:1038:LEU:HD23	1.92	0.50
1:C:4170:GLN:NE2	1:C:4174:ASP:OD1	2.45	0.50
1:D:602:ASP:HA	1:D:642:LEU:HD21	1.92	0.50
1:D:4136:GLU:OE1	1:D:4912:HIS:NE2	2.44	0.50
2:H:23:CYS:SG	2:H:104:LEU:HD13	2.52	0.50
1:A:670:TYR:CD1	1:A:1017:THR:HG21	2.47	0.50
1:A:932:ASN:HA	1:A:935:MET:HE2	1.92	0.50
1:B:521:GLU:N	1:B:521:GLU:OE1	2.39	0.50
1:B:4130:PRO:O	1:B:4156:ARG:NH1	2.44	0.50
1:D:1924:ILE:O	1:D:1928:SER:OG	2.26	0.50
1:D:4607:ARG:NH2	1:D:4643:TYR:OH	2.42	0.50
2:G:23:CYS:SG	2:G:104:LEU:HD13	2.52	0.50
1:A:1959:ARG:NE	1:A:1959:ARG:O	2.45	0.50
1:A:2560:LEU:O	1:A:2565:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1959:ARG:O	1:B:1959:ARG:NE	2.45	0.50
1:B:4501:ARG:NH2	1:B:4744:ASP:OD1	2.44	0.50
1:B:4836:ASP:OD1	1:B:4837:GLU:N	2.44	0.50
1:C:1959:ARG:O	1:C:1959:ARG:NE	2.45	0.50
1:C:3626:SER:O	1:C:3630:THR:OG1	2.22	0.50
1:C:4501:ARG:NH2	1:C:4744:ASP:OD1	2.44	0.50
1:D:4130:PRO:O	1:D:4156:ARG:NH1	2.44	0.50
1:B:670:TYR:CD1	1:B:1017:THR:HG21	2.47	0.50
1:B:4824:GLY:O	1:C:4821:ARG:NH1	2.43	0.50
2:I:23:CYS:SG	2:I:104:LEU:HD13	2.52	0.50
1:A:1493:SER:HB2	1:A:1528:LEU:HD11	1.94	0.49
1:C:670:TYR:CD1	1:C:1017:THR:HG21	2.47	0.49
1:C:1493:SER:HB2	1:C:1528:LEU:HD11	1.94	0.49
1:C:4136:GLU:OE1	1:C:4912:HIS:NE2	2.44	0.49
1:D:2560:LEU:O	1:D:2565:ARG:NH1	2.44	0.49
1:A:3974:GLN:O	1:A:3978:VAL:HG23	2.12	0.49
1:A:4170:GLN:NE2	1:A:4174:ASP:OD1	2.45	0.49
1:D:1958:ALA:O	1:D:1965:ARG:NH2	2.45	0.49
1:C:670:TYR:HD1	1:C:1017:THR:HG21	1.78	0.49
1:C:1571:LEU:O	1:C:1573:LYS:NZ	2.45	0.49
1:A:255:GLU:OE1	1:A:255:GLU:N	2.44	0.49
1:A:1720:LEU:CD2	1:A:1831:ILE:HD13	2.41	0.49
1:C:594:ILE:HD11	1:C:632:ILE:HG12	1.95	0.49
1:D:1642:ILE:HD12	1:D:1643:LEU:N	2.27	0.49
1:D:2254:LEU:O	1:D:3809:ARG:NH1	2.44	0.49
1:D:3626:SER:O	1:D:3630:THR:OG1	2.22	0.49
1:D:4589:TYR:OH	1:D:4715:ASP:OD2	2.26	0.49
2:J:23:CYS:SG	2:J:104:LEU:HD13	2.52	0.49
1:C:299:HIS:ND1	1:C:302:THR:OG1	2.26	0.49
1:C:3974:GLN:O	1:C:3978:VAL:HG23	2.12	0.49
1:D:1202:ILE:HD12	1:D:1202:ILE:O	2.13	0.49
1:D:1502:ASN:OD1	1:D:1503:SER:N	2.46	0.49
1:B:1958:ALA:O	1:B:1965:ARG:NH2	2.45	0.49
1:C:1304:LEU:HD12	1:C:1542:PRO:HG2	1.95	0.49
1:C:1502:ASN:OD1	1:C:1503:SER:N	2.46	0.49
1:C:2251:GLU:OE1	1:C:2251:GLU:N	2.41	0.49
1:D:232:ASP:OD2	1:D:356:TYR:OH	2.30	0.49
1:D:670:TYR:CD1	1:D:1017:THR:HG21	2.47	0.49
1:D:1304:LEU:HD12	1:D:1542:PRO:HG2	1.95	0.49
1:D:1648:GLN:OE1	1:D:1650:GLU:N	2.45	0.49
1:A:232:ASP:OD2	1:A:356:TYR:OH	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:HIS:CG	1:A:832:LEU:HD23	2.48	0.49
1:A:4821:ARG:NH1	1:D:4824:GLY:O	2.43	0.49
1:B:1493:SER:HB2	1:B:1528:LEU:HD11	1.94	0.49
1:C:1555:GLN:NE2	1:C:1557:GLU:OE2	2.44	0.49
1:C:1642:ILE:HD12	1:C:1643:LEU:N	2.27	0.49
1:D:1493:SER:HB2	1:D:1528:LEU:HD11	1.94	0.49
2:H:37:PHE:CD2	2:H:92:ILE:HD11	2.48	0.49
1:A:1648:GLN:OE1	1:A:1650:GLU:N	2.45	0.49
1:B:4136:GLU:OE1	1:B:4912:HIS:NE2	2.44	0.49
1:C:1202:ILE:HD12	1:C:1202:ILE:O	2.13	0.49
1:C:2492:LEU:HA	1:C:2495:LEU:HD12	1.93	0.49
1:D:21:VAL:HG22	1:D:217:ILE:HD11	1.95	0.49
1:D:594:ILE:HD11	1:D:632:ILE:HG12	1.95	0.49
1:D:2313:GLU:OE1	1:D:2313:GLU:N	2.40	0.49
2:I:37:PHE:CD2	2:I:92:ILE:HD11	2.48	0.49
1:A:1202:ILE:HD12	1:A:1202:ILE:O	2.13	0.49
1:B:670:TYR:HD1	1:B:1017:THR:HG21	1.78	0.49
1:D:299:HIS:ND1	1:D:302:THR:OG1	2.26	0.49
1:D:888:ASN:OD1	1:D:1056:THR:HG21	2.13	0.49
1:A:670:TYR:HD1	1:A:1017:THR:HG21	1.78	0.49
1:B:808:HIS:CG	1:B:832:LEU:HD23	2.48	0.49
1:C:232:ASP:OD2	1:C:356:TYR:OH	2.30	0.49
1:D:255:GLU:OE1	1:D:255:GLU:N	2.44	0.49
1:D:670:TYR:HD1	1:D:1017:THR:HG21	1.78	0.49
1:D:1266:GLU:OE2	1:D:1294:ASN:ND2	2.46	0.49
1:B:271:ALA:HB2	1:B:488:LEU:HD12	1.95	0.48
1:B:1571:LEU:O	1:B:1573:LYS:NZ	2.46	0.48
1:C:2454:ASP:OD2	1:C:2457:ALA:N	2.46	0.48
1:D:2454:ASP:OD2	1:D:2457:ALA:N	2.46	0.48
2:G:37:PHE:CD2	2:G:92:ILE:HD11	2.48	0.48
1:A:299:HIS:ND1	1:A:302:THR:OG1	2.26	0.48
1:B:888:ASN:OD1	1:B:1056:THR:HG21	2.13	0.48
1:B:1304:LEU:HD12	1:B:1542:PRO:HG2	1.95	0.48
1:C:107:GLY:O	1:C:111:ARG:NH1	2.47	0.48
1:C:2065:MET:SD	1:C:2065:MET:N	2.86	0.48
1:D:1959:ARG:NE	1:D:1959:ARG:O	2.45	0.48
1:A:318:ASP:OD1	1:A:319:LYS:N	2.44	0.48
1:A:888:ASN:OD1	1:A:1056:THR:HG21	2.13	0.48
1:A:2454:ASP:OD2	1:A:2457:ALA:N	2.46	0.48
1:B:1190:LEU:HD21	1:B:1193:LYS:HD3	1.95	0.48
1:B:1202:ILE:HD12	1:B:1202:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:ASN:OD1	1:C:1056:THR:HG21	2.13	0.48
1:C:4824:GLY:O	1:D:4821:ARG:NH1	2.43	0.48
1:D:763:ALA:HB3	1:D:764:PRO:C	2.39	0.48
1:A:1958:ALA:O	1:A:1965:ARG:NH2	2.45	0.48
1:A:4748:GLY:O	1:A:4753:ARG:NH1	2.47	0.48
1:B:34:LYS:O	1:B:52:THR:OG1	2.18	0.48
1:B:3974:GLN:O	1:B:3978:VAL:HG23	2.12	0.48
1:B:4607:ARG:NH2	1:B:4643:TYR:OH	2.42	0.48
1:C:318:ASP:OD1	1:C:319:LYS:N	2.44	0.48
1:C:4748:GLY:O	1:C:4753:ARG:NH1	2.47	0.48
1:D:742:SER:OG	1:D:776:GLN:OE1	2.32	0.48
1:D:2388:MET:HE3	1:D:2463:HIS:NE2	2.28	0.48
1:D:4748:GLY:O	1:D:4753:ARG:NH1	2.47	0.48
1:A:742:SER:OG	1:A:776:GLN:OE1	2.32	0.48
1:A:1571:LEU:O	1:A:1573:LYS:NZ	2.46	0.48
1:A:1642:ILE:HD12	1:A:1643:LEU:N	2.28	0.48
1:B:594:ILE:HD11	1:B:632:ILE:HG12	1.94	0.48
1:B:2454:ASP:OD2	1:B:2457:ALA:N	2.46	0.48
1:A:763:ALA:HB3	1:A:764:PRO:C	2.39	0.48
1:A:893:TRP:CG	1:A:917:CYS:HG	2.32	0.48
1:A:1266:GLU:OE2	1:A:1294:ASN:ND2	2.46	0.48
1:B:255:GLU:OE1	1:B:255:GLU:N	2.44	0.48
1:B:2388:MET:HE3	1:B:2463:HIS:NE2	2.28	0.48
1:C:808:HIS:CG	1:C:832:LEU:HD23	2.48	0.48
1:C:1051:ARG:HA	1:C:1054:VAL:HG22	1.95	0.48
1:C:1958:ALA:O	1:C:1965:ARG:NH2	2.46	0.48
1:C:2435:ILE:O	1:C:2464:LYS:NZ	2.39	0.48
1:B:1502:ASN:OD1	1:B:1503:SER:N	2.46	0.48
1:B:4589:TYR:OH	1:B:4715:ASP:OD2	2.26	0.48
1:C:4607:ARG:NH2	1:C:4643:TYR:OH	2.42	0.48
1:D:271:ALA:HB2	1:D:488:LEU:HD12	1.95	0.48
1:D:808:HIS:CG	1:D:832:LEU:HD23	2.48	0.48
1:D:1051:ARG:HA	1:D:1054:VAL:HG22	1.95	0.48
1:D:2065:MET:SD	1:D:2065:MET:N	2.86	0.48
1:A:21:VAL:HG22	1:A:217:ILE:HD11	1.95	0.48
1:A:2065:MET:N	1:A:2065:MET:SD	2.86	0.48
1:B:318:ASP:OD1	1:B:319:LYS:N	2.44	0.48
1:B:742:SER:OG	1:B:776:GLN:OE1	2.32	0.48
1:B:4748:GLY:O	1:B:4753:ARG:NH1	2.47	0.48
1:C:21:VAL:HG22	1:C:217:ILE:HD11	1.95	0.48
1:C:1416:ASP:OD2	1:C:1419:TYR:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2428:LEU:O	1:C:2432:VAL:HG23	2.14	0.48
1:D:107:GLY:O	1:D:111:ARG:NH1	2.47	0.48
1:D:728:ASP:OD1	1:D:731:HIS:N	2.42	0.48
1:A:594:ILE:HD11	1:A:632:ILE:HG12	1.95	0.48
1:A:1502:ASN:OD1	1:A:1503:SER:N	2.46	0.48
1:B:1495:SER:O	1:B:1499:GLY:N	2.45	0.48
1:C:271:ALA:HB2	1:C:488:LEU:HD12	1.95	0.48
1:C:755:ILE:HD11	1:C:768:PHE:HB3	1.96	0.48
1:B:107:GLY:O	1:B:111:ARG:NH1	2.47	0.48
1:B:1266:GLU:OE2	1:B:1294:ASN:ND2	2.46	0.48
1:B:1642:ILE:HD12	1:B:1643:LEU:N	2.28	0.48
1:C:2388:MET:HE3	1:C:2463:HIS:NE2	2.28	0.48
1:D:755:ILE:HD11	1:D:768:PHE:HB3	1.96	0.48
1:A:1304:LEU:HD12	1:A:1542:PRO:HG2	1.95	0.47
1:D:2128:LEU:HD23	1:D:2128:LEU:O	2.14	0.47
2:J:37:PHE:CD2	2:J:92:ILE:HD11	2.49	0.47
1:D:1190:LEU:HD21	1:D:1193:LYS:HD3	1.95	0.47
1:D:3974:GLN:O	1:D:3978:VAL:HG23	2.12	0.47
1:A:456:LEU:HD23	1:A:532:SER:HB2	1.96	0.47
1:A:755:ILE:HD11	1:A:768:PHE:HB3	1.96	0.47
1:A:2388:MET:HE3	1:A:2463:HIS:NE2	2.28	0.47
1:B:442:LEU:HD12	1:B:443:PRO:HD2	1.96	0.47
1:B:755:ILE:HD11	1:B:768:PHE:HB3	1.96	0.47
1:C:53:SER:O	1:C:56:LYS:NZ	2.45	0.47
1:C:1190:LEU:HD21	1:C:1193:LYS:HD3	1.95	0.47
1:C:1642:ILE:HD12	1:C:1643:LEU:H	1.80	0.47
1:D:1642:ILE:HD12	1:D:1643:LEU:H	1.80	0.47
1:C:893:TRP:CG	1:C:917:CYS:HG	2.33	0.47
1:C:4186:GLU:OE1	1:C:4948:TRP:NE1	2.46	0.47
1:A:1272:ARG:NH1	1:A:1587:LEU:O	2.43	0.47
1:B:21:VAL:HG22	1:B:217:ILE:HD11	1.95	0.47
1:B:763:ALA:HB3	1:B:764:PRO:C	2.39	0.47
1:C:1266:GLU:OE2	1:C:1294:ASN:ND2	2.46	0.47
1:A:107:GLY:O	1:A:111:ARG:NH1	2.47	0.47
1:A:271:ALA:HB2	1:A:488:LEU:HD12	1.95	0.47
1:A:2428:LEU:O	1:A:2432:VAL:HG23	2.14	0.47
1:D:1272:ARG:NH1	1:D:1587:LEU:O	2.44	0.47
1:D:1416:ASP:OD2	1:D:1419:TYR:N	2.44	0.47
1:A:1051:ARG:HA	1:A:1054:VAL:HG22	1.95	0.47
1:A:1495:SER:O	1:A:1499:GLY:N	2.45	0.47
1:B:1416:ASP:OD2	1:B:1419:TYR:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2065:MET:SD	1:B:2065:MET:N	2.86	0.47
1:B:2428:LEU:O	1:B:2432:VAL:HG23	2.14	0.47
1:C:670:TYR:O	1:C:673:TRP:NE1	2.48	0.47
1:C:742:SER:OG	1:C:776:GLN:OE1	2.32	0.47
1:C:763:ALA:HB3	1:C:764:PRO:C	2.39	0.47
1:D:456:LEU:HD23	1:D:532:SER:HB2	1.96	0.47
1:D:2428:LEU:O	1:D:2432:VAL:HG23	2.14	0.47
1:A:4566:TYR:O	1:A:4570:THR:OG1	2.16	0.47
1:B:918:LEU:HD21	1:B:975:GLY:H	1.80	0.47
1:B:1051:ARG:HA	1:B:1054:VAL:HG22	1.95	0.47
1:B:1272:ARG:NH1	1:B:1587:LEU:O	2.43	0.47
1:D:670:TYR:O	1:D:673:TRP:NE1	2.48	0.47
1:A:1924:ILE:O	1:A:1928:SER:OG	2.26	0.47
1:A:2385:ASN:HA	1:A:2388:MET:HE2	1.97	0.47
1:A:4619:GLN:OE1	1:A:4631:ARG:NH2	2.48	0.47
1:A:1190:LEU:HD21	1:A:1193:LYS:HD3	1.96	0.47
1:B:2128:LEU:HD23	1:B:2128:LEU:O	2.15	0.47
1:C:442:LEU:HD12	1:C:443:PRO:HD2	1.96	0.47
1:A:106:GLN:O	1:A:111:ARG:NH2	2.48	0.46
1:A:1416:ASP:OD2	1:A:1419:TYR:N	2.44	0.46
1:B:2385:ASN:HA	1:B:2388:MET:HE2	1.97	0.46
1:C:151:GLU:OE1	1:C:151:GLU:N	2.48	0.46
1:C:2128:LEU:O	1:C:2128:LEU:HD23	2.15	0.46
1:C:49:LEU:CD2	1:C:203:VAL:HG13	2.46	0.46
1:C:81:MET:O	1:C:85:THR:HG22	2.16	0.46
1:D:1786:ASP:OD1	1:D:1787:ILE:N	2.48	0.46
1:A:442:LEU:HD12	1:A:443:PRO:HD2	1.96	0.46
1:A:1642:ILE:HD12	1:A:1643:LEU:H	1.80	0.46
1:A:2128:LEU:O	1:A:2128:LEU:HD23	2.14	0.46
1:A:2264:VAL:HG21	1:A:2300:PHE:HE2	1.81	0.46
1:B:2264:VAL:HG21	1:B:2300:PHE:CE2	2.51	0.46
1:B:2264:VAL:HG21	1:B:2300:PHE:HE2	1.81	0.46
1:C:918:LEU:HD21	1:C:975:GLY:H	1.80	0.46
1:D:918:LEU:HD21	1:D:975:GLY:H	1.80	0.46
1:D:2230:SER:OG	1:D:2233:MET:SD	2.55	0.46
1:D:3636:GLU:OE1	1:D:3636:GLU:N	2.46	0.46
1:C:1786:ASP:OD1	1:C:1787:ILE:N	2.49	0.46
1:D:442:LEU:HD12	1:D:443:PRO:HD2	1.96	0.46
1:D:2264:VAL:HG21	1:D:2300:PHE:CE2	2.51	0.46
1:A:81:MET:O	1:A:85:THR:HG22	2.15	0.46
1:A:2264:VAL:HG21	1:A:2300:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2435:ILE:O	1:B:2464:LYS:NZ	2.39	0.46
1:C:2264:VAL:HG21	1:C:2300:PHE:CE2	2.51	0.46
1:D:81:MET:O	1:D:85:THR:HG22	2.16	0.46
1:D:1939:GLN:NE2	1:D:1971:GLN:OE1	2.49	0.46
1:D:3605:ALA:HB3	1:D:3606:PRO:HD3	1.98	0.46
1:B:1642:ILE:HD12	1:B:1643:LEU:H	1.80	0.46
1:A:49:LEU:CD2	1:A:203:VAL:HG13	2.46	0.46
1:A:670:TYR:O	1:A:673:TRP:NE1	2.48	0.46
1:A:2468:VAL:HG13	1:A:2526:LEU:HD12	1.98	0.46
1:B:456:LEU:HD23	1:B:532:SER:HB2	1.96	0.46
1:B:2487:LEU:CD2	1:B:2547:LEU:HD22	2.46	0.46
1:C:112:THR:HG21	1:C:174:LYS:HE3	1.98	0.46
1:D:1648:GLN:OE1	1:D:1649:GLU:N	2.49	0.46
1:D:2264:VAL:HG21	1:D:2300:PHE:HE2	1.81	0.46
1:A:3636:GLU:OE1	1:A:3636:GLU:N	2.47	0.46
1:C:216:PRO:O	1:C:217:ILE:HD13	2.16	0.46
1:C:3605:ALA:HB3	1:C:3606:PRO:HD3	1.98	0.46
1:C:4619:GLN:OE1	1:C:4631:ARG:NH2	2.48	0.46
1:A:323:ASP:OD1	1:A:326:SER:N	2.45	0.46
1:A:508:TYR:HE1	1:A:517:VAL:HG21	1.81	0.46
1:B:216:PRO:O	1:B:217:ILE:HD13	2.16	0.46
1:C:456:LEU:HD23	1:C:532:SER:HB2	1.97	0.46
1:D:49:LEU:CD2	1:D:203:VAL:HG13	2.46	0.46
1:D:1031:ARG:HH21	1:D:1042:THR:HG21	1.81	0.46
1:D:1924:ILE:HD11	1:D:2002:LEU:HD13	1.98	0.46
1:A:918:LEU:HD21	1:A:975:GLY:H	1.80	0.46
1:A:1031:ARG:HH21	1:A:1042:THR:HG21	1.81	0.46
1:A:1939:GLN:NE2	1:A:1971:GLN:OE1	2.49	0.46
1:B:1939:GLN:NE2	1:B:1971:GLN:OE1	2.49	0.46
1:C:2468:VAL:HG13	1:C:2526:LEU:HD12	1.98	0.46
1:C:2488:GLU:CD	1:C:2543:LEU:HD13	2.41	0.46
1:A:112:THR:HG21	1:A:174:LYS:HE3	1.98	0.45
1:A:1648:GLN:OE1	1:A:1649:GLU:N	2.49	0.45
1:A:1786:ASP:OD1	1:A:1787:ILE:N	2.49	0.45
1:B:1786:ASP:OD1	1:B:1787:ILE:N	2.49	0.45
1:C:1924:ILE:HD11	1:C:2002:LEU:HD13	1.98	0.45
1:C:1939:GLN:NE2	1:C:1971:GLN:OE1	2.49	0.45
1:C:2385:ASN:HA	1:C:2388:MET:HE2	1.97	0.45
1:C:2487:LEU:CD2	1:C:2547:LEU:HD22	2.46	0.45
1:D:318:ASP:OD1	1:D:319:LYS:N	2.44	0.45
1:D:508:TYR:HE1	1:D:517:VAL:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1555:GLN:NE2	1:D:1557:GLU:OE2	2.44	0.45
1:D:2129:LEU:HD12	1:D:2169:THR:HG23	1.98	0.45
1:A:2488:GLU:CD	1:A:2543:LEU:HD13	2.41	0.45
1:B:49:LEU:CD2	1:B:203:VAL:HG13	2.46	0.45
1:B:81:MET:O	1:B:85:THR:HG22	2.15	0.45
1:B:1895:MET:SD	1:B:1895:MET:N	2.89	0.45
1:B:2468:VAL:HG13	1:B:2526:LEU:HD12	1.98	0.45
1:B:2488:GLU:CD	1:B:2543:LEU:HD13	2.41	0.45
1:C:255:GLU:OE1	1:C:255:GLU:N	2.44	0.45
1:C:2264:VAL:HG21	1:C:2300:PHE:HE2	1.81	0.45
1:C:2430:ASP:O	1:C:2434:VAL:HG23	2.17	0.45
1:D:216:PRO:O	1:D:217:ILE:HD13	2.15	0.45
1:D:411:GLU:OE1	1:D:411:GLU:N	2.44	0.45
1:D:1151:HIS:ND1	1:D:1185:ASP:OD1	2.48	0.45
1:A:1730:MET:SD	1:A:1730:MET:N	2.84	0.45
1:A:2191:MET:HE3	1:A:2191:MET:HA	1.98	0.45
1:A:2487:LEU:CD2	1:A:2547:LEU:HD22	2.46	0.45
1:B:2430:ASP:O	1:B:2434:VAL:HG23	2.17	0.45
1:B:3605:ALA:HB3	1:B:3606:PRO:HD3	1.98	0.45
1:B:4619:GLN:OE1	1:B:4631:ARG:NH2	2.48	0.45
1:D:112:THR:HG21	1:D:174:LYS:HE3	1.98	0.45
1:D:151:GLU:OE1	1:D:151:GLU:N	2.48	0.45
1:D:4619:GLN:OE1	1:D:4631:ARG:NH2	2.48	0.45
1:A:3605:ALA:HB3	1:A:3606:PRO:HD3	1.98	0.45
1:C:106:GLN:O	1:C:111:ARG:NH2	2.48	0.45
1:C:323:ASP:OD1	1:C:326:SER:N	2.45	0.45
1:C:3636:GLU:OE1	1:C:3636:GLU:N	2.47	0.45
1:A:2435:ILE:O	1:A:2464:LYS:NZ	2.39	0.45
1:A:4186:GLU:OE1	1:A:4948:TRP:NE1	2.46	0.45
1:C:409:GLN:OE1	1:C:409:GLN:N	2.48	0.45
1:C:1943:TYR:CE2	1:C:1947:MET:HE2	2.52	0.45
1:C:2129:LEU:HD12	1:C:2169:THR:HG23	1.98	0.45
1:D:2385:ASN:HA	1:D:2388:MET:HE2	1.97	0.45
1:D:2468:VAL:HG13	1:D:2526:LEU:HD12	1.98	0.45
1:A:216:PRO:O	1:A:217:ILE:HD13	2.15	0.45
1:A:1924:ILE:HD11	1:A:2002:LEU:HD13	1.98	0.45
1:A:3655:GLU:OE1	1:A:3655:GLU:N	2.50	0.45
1:B:232:ASP:OD2	1:B:356:TYR:OH	2.30	0.45
1:B:323:ASP:OD1	1:B:326:SER:N	2.45	0.45
1:B:1031:ARG:HH21	1:B:1042:THR:HG21	1.81	0.45
1:B:4186:GLU:OE1	1:B:4948:TRP:NE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1648:GLN:OE1	1:C:1649:GLU:N	2.49	0.45
1:C:1924:ILE:O	1:C:1928:SER:OG	2.26	0.45
1:D:495:ILE:HD13	1:D:540:LEU:HD13	1.99	0.45
1:D:4505:LEU:HD22	1:D:4749:PHE:CE2	2.52	0.45
1:A:4818:VAL:HG12	1:A:4829:GLU:HG3	1.98	0.45
1:B:1648:GLN:OE1	1:B:1649:GLU:N	2.49	0.45
1:B:1943:TYR:CE2	1:B:1947:MET:HE2	2.52	0.45
1:D:53:SER:O	1:D:56:LYS:NZ	2.45	0.45
1:D:1571:LEU:O	1:D:1573:LYS:NZ	2.46	0.45
1:A:734:SER:O	1:A:1482:ARG:NH1	2.50	0.45
1:A:2430:ASP:O	1:A:2434:VAL:HG23	2.17	0.45
1:B:112:THR:HG21	1:B:174:LYS:HE3	1.98	0.45
1:B:602:ASP:OD1	1:B:1586:ARG:NH1	2.50	0.45
1:C:495:ILE:HD13	1:C:540:LEU:HD13	1.99	0.45
1:C:508:TYR:HE1	1:C:517:VAL:HG21	1.81	0.45
1:C:602:ASP:OD1	1:C:1586:ARG:NH1	2.50	0.45
1:C:1031:ARG:HH21	1:C:1042:THR:HG21	1.81	0.45
1:C:3655:GLU:N	1:C:3655:GLU:OE1	2.50	0.45
1:D:2487:LEU:CD2	1:D:2547:LEU:HD22	2.46	0.45
1:A:680:ASP:O	1:A:751:THR:HG23	2.17	0.45
1:A:2105:TYR:CB	1:A:2160:LEU:HD23	2.47	0.45
1:B:2667:CYS:O	1:B:2671:VAL:HG23	2.17	0.45
1:C:4818:VAL:HG12	1:C:4829:GLU:HG3	1.98	0.45
1:D:409:GLN:OE1	1:D:409:GLN:N	2.48	0.45
1:D:3655:GLU:OE1	1:D:3655:GLU:N	2.50	0.45
1:D:4818:VAL:HG12	1:D:4829:GLU:HG3	1.98	0.45
1:A:1943:TYR:CE2	1:A:1947:MET:HE2	2.52	0.45
1:B:508:TYR:HE1	1:B:517:VAL:HG21	1.81	0.45
1:B:3626:SER:O	1:B:3630:THR:OG1	2.22	0.45
1:C:579:LEU:HD11	1:C:617:LEU:CD2	2.47	0.45
1:C:601:LEU:HD13	1:C:610:VAL:HG21	1.99	0.45
1:C:1495:SER:O	1:C:1499:GLY:N	2.45	0.45
1:D:680:ASP:O	1:D:751:THR:HG23	2.17	0.45
1:A:2129:LEU:HD12	1:A:2169:THR:HG23	1.98	0.44
1:A:4099:VAL:HG22	1:A:4132:LEU:CD1	2.47	0.44
1:A:4136:GLU:O	1:A:4917:TYR:OH	2.35	0.44
1:B:601:LEU:HD13	1:B:610:VAL:HG21	1.99	0.44
1:B:4505:LEU:HD22	1:B:4749:PHE:CE2	2.52	0.44
1:D:602:ASP:OD1	1:D:1586:ARG:NH1	2.50	0.44
1:D:1943:TYR:CE2	1:D:1947:MET:HE2	2.52	0.44
1:D:2430:ASP:O	1:D:2434:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2488:GLU:CD	1:D:2543:LEU:HD13	2.41	0.44
1:A:53:SER:O	1:A:56:LYS:NZ	2.45	0.44
1:A:601:LEU:HD13	1:A:610:VAL:HG21	1.99	0.44
1:C:680:ASP:O	1:C:751:THR:HG23	2.17	0.44
1:C:2440:GLN:OE1	1:C:2440:GLN:N	2.50	0.44
1:C:2667:CYS:O	1:C:2671:VAL:HG23	2.17	0.44
1:C:3854:GLN:NE2	1:C:3921:GLU:O	2.50	0.44
1:D:579:LEU:HD11	1:D:617:LEU:CD2	2.47	0.44
1:D:2191:MET:HE3	1:D:2191:MET:HA	1.98	0.44
1:A:602:ASP:OD1	1:A:1586:ARG:NH1	2.50	0.44
1:A:809:GLY:N	1:A:1614:GLU:O	2.50	0.44
1:B:579:LEU:HD13	1:B:616:SER:OG	2.18	0.44
1:B:728:ASP:OD1	1:B:731:HIS:N	2.42	0.44
1:B:1924:ILE:HD11	1:B:2002:LEU:HD13	1.98	0.44
1:C:579:LEU:HD13	1:C:616:SER:OG	2.18	0.44
1:C:728:ASP:OD1	1:C:731:HIS:N	2.42	0.44
1:C:1909:LEU:HD23	1:C:1912:LEU:HD12	2.00	0.44
1:C:2324:ILE:HD13	1:C:2425:LEU:HD21	2.00	0.44
1:D:601:LEU:HD13	1:D:610:VAL:HG21	1.99	0.44
2:I:22:THR:N	2:I:108:GLU:OXT	2.50	0.44
1:A:495:ILE:HD13	1:A:540:LEU:HD13	1.99	0.44
1:A:579:LEU:HD13	1:A:616:SER:OG	2.18	0.44
1:A:2324:ILE:HD13	1:A:2425:LEU:HD21	2.00	0.44
1:B:2129:LEU:HD12	1:B:2169:THR:HG23	1.98	0.44
1:B:4818:VAL:HG12	1:B:4829:GLU:HG3	1.98	0.44
1:C:730:LEU:HD11	2:I:8:ILE:HA	2.00	0.44
1:C:1895:MET:SD	1:C:1895:MET:N	2.89	0.44
1:C:4505:LEU:HD22	1:C:4749:PHE:CE2	2.52	0.44
1:D:579:LEU:HD13	1:D:616:SER:OG	2.18	0.44
1:D:730:LEU:HD11	2:J:8:ILE:HA	2.00	0.44
1:D:2105:TYR:CB	1:D:2160:LEU:HD23	2.47	0.44
1:D:2324:ILE:HD13	1:D:2425:LEU:HD21	2.00	0.44
1:A:1769:PHE:CZ	2:G:91:VAL:HG21	2.52	0.44
1:B:271:ALA:HB3	1:B:492:GLU:OE2	2.18	0.44
1:B:4099:VAL:HG22	1:B:4132:LEU:CD1	2.47	0.44
1:C:3839:PHE:CE1	1:C:3873:THR:HG23	2.53	0.44
1:C:4095:PHE:O	1:C:4099:VAL:HG23	2.17	0.44
1:D:4186:GLU:OE1	1:D:4948:TRP:NE1	2.46	0.44
1:A:151:GLU:N	1:A:151:GLU:OE1	2.49	0.44
1:A:271:ALA:HB3	1:A:492:GLU:OE2	2.18	0.44
1:A:579:LEU:HD11	1:A:617:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2428:LEU:HD21	1:A:2482:PHE:CE1	2.53	0.44
1:A:4505:LEU:HD22	1:A:4749:PHE:CE2	2.52	0.44
1:B:2105:TYR:CB	1:B:2160:LEU:HD23	2.47	0.44
1:B:2454:ASP:OD2	1:B:2456:SER:OG	2.30	0.44
1:B:3839:PHE:CE1	1:B:3873:THR:HG23	2.53	0.44
1:B:4095:PHE:O	1:B:4099:VAL:HG23	2.17	0.44
1:D:4095:PHE:O	1:D:4099:VAL:HG23	2.17	0.44
1:A:2667:CYS:O	1:A:2671:VAL:HG23	2.17	0.44
1:B:495:ILE:HD13	1:B:540:LEU:HD13	1.99	0.44
1:B:579:LEU:HD11	1:B:617:LEU:CD2	2.47	0.44
1:B:680:ASP:O	1:B:751:THR:HG23	2.17	0.44
1:B:2324:ILE:HD13	1:B:2425:LEU:HD21	2.00	0.44
1:B:2440:GLN:OE1	1:B:2440:GLN:N	2.51	0.44
1:C:1427:TYR:HB2	1:C:1564:VAL:HG11	2.00	0.44
1:C:2191:MET:HE3	1:C:2191:MET:HA	1.98	0.44
1:C:3914:GLN:O	1:C:3914:GLN:NE2	2.51	0.44
1:D:734:SER:O	1:D:1482:ARG:NH1	2.50	0.44
1:D:1769:PHE:CZ	2:J:91:VAL:HG21	2.52	0.44
1:D:1909:LEU:HD23	1:D:1912:LEU:HD12	2.00	0.44
1:D:2440:GLN:N	1:D:2440:GLN:OE1	2.50	0.44
1:D:2667:CYS:O	1:D:2671:VAL:HG23	2.17	0.44
1:A:730:LEU:HD11	2:G:8:ILE:HA	2.00	0.44
1:B:106:GLN:O	1:B:111:ARG:NH2	2.48	0.44
1:B:641:ASP:OD1	1:B:641:ASP:N	2.51	0.44
1:B:893:TRP:CG	1:B:917:CYS:HG	2.36	0.44
1:B:1520:THR:HG22	1:B:1531:TYR:CD1	2.53	0.44
1:B:2191:MET:HE3	1:B:2191:MET:HA	1.98	0.44
1:B:3914:GLN:O	1:B:3914:GLN:NE2	2.51	0.44
1:C:641:ASP:OD1	1:C:641:ASP:N	2.51	0.44
1:C:1730:MET:SD	1:C:1730:MET:N	2.84	0.44
1:C:2105:TYR:CB	1:C:2160:LEU:HD23	2.47	0.44
1:C:2177:VAL:HG12	1:C:2186:ILE:HD11	2.00	0.44
1:D:106:GLN:O	1:D:111:ARG:NH2	2.48	0.44
1:D:3914:GLN:O	1:D:3914:GLN:NE2	2.51	0.44
1:A:2428:LEU:HD11	1:A:2471:LEU:HD21	2.00	0.44
1:A:3839:PHE:CE1	1:A:3873:THR:HG23	2.53	0.44
1:B:734:SER:O	1:B:1482:ARG:NH1	2.50	0.44
1:B:2428:LEU:HD21	1:B:2482:PHE:CE1	2.53	0.44
1:B:3854:GLN:NE2	1:B:3921:GLU:O	2.50	0.44
1:C:1769:PHE:CZ	2:I:91:VAL:HG21	2.53	0.44
1:C:3985:LEU:HD12	1:C:4100:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1427:TYR:HB2	1:D:1564:VAL:HG11	2.00	0.44
1:D:2428:LEU:HD21	1:D:2482:PHE:CE1	2.53	0.44
1:A:182:ILE:HD12	1:A:209:GLN:OE1	2.18	0.43
1:A:314:LEU:HD11	1:A:372:LEU:HD23	2.00	0.43
1:B:182:ILE:HD12	1:B:209:GLN:OE1	2.18	0.43
1:B:1297:THR:O	1:B:1547:GLN:NE2	2.49	0.43
1:C:137:ARG:N	1:C:146:ASP:OD2	2.51	0.43
1:C:314:LEU:HD11	1:C:372:LEU:HD23	2.00	0.43
1:D:182:ILE:HG23	1:D:209:GLN:OE1	2.18	0.43
1:D:4099:VAL:HG22	1:D:4132:LEU:CD1	2.48	0.43
1:A:137:ARG:N	1:A:146:ASP:OD2	2.51	0.43
1:A:4095:PHE:O	1:A:4099:VAL:HG23	2.17	0.43
1:B:151:GLU:OE1	1:B:151:GLU:N	2.49	0.43
1:B:314:LEU:HD11	1:B:372:LEU:HD23	2.00	0.43
1:B:2177:VAL:HG12	1:B:2186:ILE:HD11	2.00	0.43
1:D:271:ALA:HB3	1:D:492:GLU:OE2	2.18	0.43
1:D:314:LEU:HD11	1:D:372:LEU:HD23	2.00	0.43
1:D:3854:GLN:NE2	1:D:3921:GLU:O	2.50	0.43
1:D:3985:LEU:HD12	1:D:4100:LEU:HD12	2.01	0.43
1:A:3854:GLN:NE2	1:A:3921:GLU:O	2.50	0.43
1:A:3985:LEU:HD12	1:A:4100:LEU:HD12	2.00	0.43
1:C:411:GLU:OE1	1:C:411:GLU:N	2.44	0.43
1:C:734:SER:O	1:C:1482:ARG:NH1	2.50	0.43
1:C:1151:HIS:ND1	1:C:1185:ASP:OD1	2.48	0.43
1:C:2428:LEU:HD21	1:C:2482:PHE:CE1	2.53	0.43
1:D:551:PHE:HZ	1:D:558:LEU:HD11	1.83	0.43
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.50	0.43
1:D:1297:THR:O	1:D:1547:GLN:NE2	2.49	0.43
1:D:3839:PHE:CE1	1:D:3873:THR:HG23	2.53	0.43
1:B:456:LEU:HD23	1:B:532:SER:CB	2.49	0.43
1:B:2229:ALA:HB1	1:B:2278:MET:HE3	2.01	0.43
1:B:3985:LEU:HD12	1:B:4100:LEU:HD12	2.00	0.43
1:C:271:ALA:HB3	1:C:492:GLU:OE2	2.18	0.43
1:C:797:GLY:N	1:C:1622:CYS:O	2.50	0.43
1:C:1520:THR:HG22	1:C:1531:TYR:CD1	2.53	0.43
1:D:137:ARG:N	1:D:146:ASP:OD2	2.51	0.43
1:A:182:ILE:HG23	1:A:209:GLN:OE1	2.18	0.43
1:A:456:LEU:HD23	1:A:532:SER:CB	2.49	0.43
1:B:357:GLY:N	1:B:405:LEU:O	2.52	0.43
1:C:826:VAL:HB	1:C:1020:ILE:HD11	2.01	0.43
1:A:188:SER:O	1:A:190:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:SER:O	1:A:459:LEU:HD23	2.19	0.43
1:A:2177:VAL:HG12	1:A:2186:ILE:HD11	2.00	0.43
1:B:455:SER:O	1:B:459:LEU:HD23	2.19	0.43
1:B:551:PHE:HZ	1:B:558:LEU:HD11	1.83	0.43
1:B:730:LEU:HD11	2:H:8:ILE:HA	2.00	0.43
1:B:826:VAL:HB	1:B:1020:ILE:HD11	2.01	0.43
1:C:455:SER:O	1:C:459:LEU:HD23	2.19	0.43
1:C:643:LEU:HD13	1:C:1658:THR:HG23	2.01	0.43
1:D:643:LEU:HD13	1:D:1658:THR:HG23	2.01	0.43
1:D:826:VAL:HB	1:D:1020:ILE:HD11	2.01	0.43
2:J:22:THR:N	2:J:108:GLU:OXT	2.50	0.43
1:B:182:ILE:HG23	1:B:209:GLN:OE1	2.18	0.43
1:B:504:ARG:O	1:B:507:VAL:HG22	2.19	0.43
1:B:1769:PHE:CZ	2:H:91:VAL:HG21	2.54	0.43
1:D:188:SER:O	1:D:190:ARG:NH1	2.52	0.43
1:D:323:ASP:OD1	1:D:326:SER:N	2.45	0.43
1:D:357:GLY:N	1:D:405:LEU:O	2.52	0.43
1:D:456:LEU:HD23	1:D:532:SER:CB	2.49	0.43
1:A:357:GLY:N	1:A:405:LEU:O	2.52	0.43
1:A:1909:LEU:HD23	1:A:1912:LEU:HD12	2.00	0.43
1:B:1114:ARG:HB2	1:B:1128:LEU:HD23	2.01	0.43
1:D:182:ILE:HD12	1:D:209:GLN:OE1	2.18	0.43
1:D:712:GLU:OE2	1:D:1086:ARG:NH2	2.50	0.43
1:D:1520:THR:HG22	1:D:1531:TYR:CD1	2.53	0.43
1:D:2428:LEU:HD11	1:D:2471:LEU:HD21	2.00	0.43
1:D:4136:GLU:O	1:D:4917:TYR:OH	2.35	0.43
1:A:551:PHE:HZ	1:A:558:LEU:HD11	1.83	0.43
1:A:826:VAL:HB	1:A:1020:ILE:HD11	2.01	0.43
1:A:3914:GLN:O	1:A:3914:GLN:NE2	2.51	0.43
1:B:241:MET:SD	1:B:241:MET:N	2.92	0.43
1:B:411:GLU:OE1	1:B:411:GLU:N	2.44	0.43
1:B:643:LEU:HD13	1:B:1658:THR:HG23	2.01	0.43
1:B:1909:LEU:HD23	1:B:1912:LEU:HD12	2.00	0.43
1:C:504:ARG:O	1:C:507:VAL:HG22	2.19	0.43
1:C:4099:VAL:HG22	1:C:4132:LEU:CD1	2.48	0.43
1:D:504:ARG:O	1:D:507:VAL:HG22	2.19	0.43
1:D:3833:GLU:OE1	1:D:3833:GLU:N	2.49	0.43
2:H:22:THR:N	2:H:108:GLU:OXT	2.50	0.43
1:A:1269:GLU:OE2	1:A:1271:THR:OG1	2.33	0.43
1:B:150:GLN:NE2	1:B:152:ASP:O	2.52	0.43
1:B:670:TYR:O	1:B:673:TRP:NE1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ILE:HD12	1:C:209:GLN:OE1	2.19	0.43
1:D:655:MET:HE3	1:D:1607:VAL:HG11	2.01	0.43
1:D:2229:ALA:HB1	1:D:2278:MET:HE3	2.01	0.43
1:D:3877:LEU:HD22	1:D:3919:LEU:CD1	2.49	0.43
1:A:241:MET:SD	1:A:241:MET:N	2.92	0.42
1:B:137:ARG:N	1:B:146:ASP:OD2	2.51	0.42
1:C:3877:LEU:HD22	1:C:3919:LEU:CD1	2.49	0.42
1:D:2177:VAL:HG12	1:D:2186:ILE:HD11	2.00	0.42
1:A:1427:TYR:HB2	1:A:1564:VAL:HG11	2.00	0.42
1:A:1520:THR:HG22	1:A:1531:TYR:CD1	2.53	0.42
1:C:150:GLN:NE2	1:C:152:ASP:O	2.52	0.42
1:C:241:MET:SD	1:C:241:MET:N	2.92	0.42
1:D:241:MET:SD	1:D:241:MET:N	2.92	0.42
1:A:504:ARG:O	1:A:507:VAL:HG22	2.19	0.42
1:A:3877:LEU:HD22	1:A:3919:LEU:CD1	2.49	0.42
1:A:4759:VAL:CG2	1:D:4860:ILE:HD11	2.49	0.42
1:A:4860:ILE:HD11	1:B:4759:VAL:CG2	2.49	0.42
1:B:1151:HIS:ND1	1:B:1185:ASP:OD1	2.48	0.42
1:B:2428:LEU:HD11	1:B:2471:LEU:HD21	2.00	0.42
1:B:3877:LEU:HD22	1:B:3919:LEU:CD1	2.49	0.42
1:C:182:ILE:HG23	1:C:209:GLN:OE1	2.18	0.42
1:C:188:SER:O	1:C:190:ARG:NH1	2.52	0.42
1:C:357:GLY:N	1:C:405:LEU:O	2.52	0.42
1:C:1716:ALA:HB1	1:C:1831:ILE:HD11	2.02	0.42
1:A:643:LEU:HD13	1:A:1658:THR:HG23	2.01	0.42
1:A:1151:HIS:ND1	1:A:1185:ASP:OD1	2.48	0.42
1:A:1312:GLU:OE2	2:G:97:THR:OG1	2.36	0.42
1:B:712:GLU:OE2	1:B:1086:ARG:NH2	2.50	0.42
1:B:1427:TYR:HB2	1:B:1564:VAL:HG11	2.00	0.42
1:B:4616:ILE:HD12	1:B:4665:ILE:HD13	2.02	0.42
1:B:4628:GLN:OE1	1:B:4631:ARG:NH1	2.53	0.42
1:C:1114:ARG:HB2	1:C:1128:LEU:HD23	2.01	0.42
1:C:2229:ALA:HB1	1:C:2278:MET:HE3	2.01	0.42
1:D:150:GLN:NE2	1:D:152:ASP:O	2.52	0.42
1:D:641:ASP:OD1	1:D:641:ASP:N	2.51	0.42
1:D:1432:ILE:HG12	1:D:1441:VAL:HG11	2.02	0.42
2:H:42:ASP:N	2:H:42:ASP:OD1	2.53	0.42
2:I:42:ASP:OD1	2:I:42:ASP:N	2.53	0.42
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.50	0.42
1:B:3636:GLU:OE1	1:B:3636:GLU:N	2.47	0.42
1:B:3655:GLU:OE1	1:B:3655:GLU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:22:THR:N	2:G:108:GLU:OXT	2.50	0.42
1:A:633:CYS:HA	1:A:637:LEU:HD13	2.02	0.42
1:A:1297:THR:O	1:A:1547:GLN:NE2	2.49	0.42
1:A:2229:ALA:HB1	1:A:2278:MET:HE3	2.01	0.42
1:A:4628:GLN:OE1	1:A:4631:ARG:NH1	2.53	0.42
1:B:1716:ALA:HB1	1:B:1831:ILE:HD11	2.02	0.42
1:B:3943:VAL:HG11	1:B:4001:MET:HE2	2.02	0.42
1:B:4860:ILE:HD11	1:C:4759:VAL:CG2	2.49	0.42
1:C:456:LEU:HD23	1:C:532:SER:CB	2.49	0.42
1:C:1432:ILE:HG12	1:C:1441:VAL:HG11	2.02	0.42
1:C:2428:LEU:HD11	1:C:2471:LEU:HD21	2.00	0.42
1:C:4616:ILE:HD12	1:C:4665:ILE:HD13	2.02	0.42
1:D:1495:SER:O	1:D:1499:GLY:N	2.45	0.42
1:D:1895:MET:SD	1:D:1895:MET:N	2.89	0.42
1:D:2418:ILE:HA	1:D:2421:ILE:HD12	2.01	0.42
1:B:655:MET:HE3	1:B:1607:VAL:HG11	2.01	0.42
1:B:800:VAL:O	1:B:1619:LEU:HD12	2.20	0.42
1:C:1599:ARG:NH2	1:C:1602:ASN:OD1	2.49	0.42
1:C:4860:ILE:HD11	1:D:4759:VAL:CG2	2.49	0.42
1:D:2170:VAL:HG21	1:D:2198:PHE:CD2	2.55	0.42
1:D:3939:LEU:CD2	1:D:3984:MET:HE3	2.50	0.42
2:J:42:ASP:OD1	2:J:42:ASP:N	2.53	0.42
1:B:1432:ILE:HG12	1:B:1441:VAL:HG11	2.02	0.42
1:D:633:CYS:HA	1:D:637:LEU:HD13	2.02	0.42
1:D:800:VAL:O	1:D:1619:LEU:HD12	2.20	0.42
1:A:150:GLN:NE2	1:A:152:ASP:O	2.52	0.42
1:A:447:LEU:O	1:A:449:ILE:N	2.53	0.42
1:A:982:ASP:OD1	1:A:983:LEU:N	2.53	0.42
1:A:2441:MET:HE2	1:A:2497:ALA:HB1	2.02	0.42
1:A:4616:ILE:HD12	1:A:4665:ILE:HD13	2.02	0.42
1:B:394:HIS:ND1	1:B:396:GLU:O	2.48	0.42
1:B:1053:ALA:O	1:B:1056:THR:OG1	2.35	0.42
1:B:2333:ALA:CB	1:B:2345:ALA:HB2	2.50	0.42
1:C:2170:VAL:HG21	1:C:2198:PHE:CD2	2.55	0.42
1:C:3943:VAL:HG11	1:C:4001:MET:HE2	2.02	0.42
1:D:1716:ALA:HB1	1:D:1831:ILE:HD11	2.02	0.42
1:D:2441:MET:HE2	1:D:2497:ALA:HB1	2.02	0.42
1:D:3943:VAL:HG11	1:D:4001:MET:HE2	2.02	0.42
1:A:1432:ILE:HG12	1:A:1441:VAL:HG11	2.02	0.42
1:A:2333:ALA:CB	1:A:2345:ALA:HB2	2.50	0.42
1:B:188:SER:O	1:B:190:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:800:VAL:O	1:C:1619:LEU:HD12	2.20	0.42
1:C:809:GLY:N	1:C:1614:GLU:O	2.49	0.42
1:C:2418:ILE:HA	1:C:2421:ILE:HD12	2.01	0.42
1:D:4628:GLN:OE1	1:D:4631:ARG:NH1	2.53	0.42
1:A:352:SER:O	1:A:352:SER:OG	2.35	0.41
1:A:655:MET:HE3	1:A:1607:VAL:HG11	2.01	0.41
1:A:797:GLY:N	1:A:1622:CYS:O	2.50	0.41
1:A:3939:LEU:CD2	1:A:3984:MET:HE3	2.50	0.41
1:A:3943:VAL:HG11	1:A:4001:MET:HE2	2.02	0.41
1:C:2498:ALA:HB2	1:C:2515:LEU:HD23	2.02	0.41
1:D:455:SER:O	1:D:459:LEU:HD23	2.19	0.41
1:B:809:GLY:N	1:B:1614:GLU:O	2.50	0.41
1:C:633:CYS:HA	1:C:637:LEU:HD13	2.02	0.41
1:C:1269:GLU:OE2	1:C:1271:THR:OG1	2.33	0.41
1:C:1297:THR:O	1:C:1547:GLN:NE2	2.49	0.41
1:C:3939:LEU:CD2	1:C:3984:MET:HE3	2.50	0.41
1:C:4628:GLN:OE1	1:C:4631:ARG:NH1	2.53	0.41
1:D:2498:ALA:HB2	1:D:2515:LEU:HD23	2.02	0.41
1:D:4616:ILE:HD12	1:D:4665:ILE:HD13	2.02	0.41
1:A:1716:ALA:HB1	1:A:1831:ILE:HD11	2.02	0.41
1:A:2440:GLN:OE1	1:A:2440:GLN:N	2.51	0.41
1:B:2178:LEU:HA	1:B:2186:ILE:HD13	2.03	0.41
1:B:2471:LEU:O	1:B:2476:GLY:N	2.50	0.41
1:C:655:MET:HE3	1:C:1607:VAL:HG11	2.01	0.41
1:C:982:ASP:OD1	1:C:983:LEU:N	2.53	0.41
1:C:2431:LEU:CD2	1:C:2471:LEU:HD23	2.49	0.41
1:D:982:ASP:OD1	1:D:983:LEU:N	2.53	0.41
1:A:2166:MET:O	1:A:2170:VAL:HG23	2.21	0.41
1:B:53:SER:O	1:B:56:LYS:NZ	2.45	0.41
1:B:409:GLN:OE1	1:B:409:GLN:N	2.48	0.41
1:B:3939:LEU:CD2	1:B:3984:MET:HE3	2.50	0.41
1:C:63:SER:O	1:C:66:THR:OG1	2.34	0.41
1:C:556:ASP:OD1	1:C:557:TRP:N	2.53	0.41
1:C:594:ILE:HD11	1:C:632:ILE:CG1	2.51	0.41
1:C:2178:LEU:HA	1:C:2186:ILE:HD13	2.03	0.41
1:D:1446:ILE:HG23	1:D:1487:MET:HE1	2.02	0.41
1:A:800:VAL:O	1:A:1619:LEU:HD12	2.20	0.41
1:A:1114:ARG:HB2	1:A:1128:LEU:HD23	2.01	0.41
1:B:2166:MET:O	1:B:2170:VAL:HG23	2.21	0.41
1:B:2170:VAL:HG21	1:B:2198:PHE:CD2	2.55	0.41
1:C:551:PHE:HZ	1:C:558:LEU:HD11	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4881:GLU:O	1:C:4885:THR:HG22	2.21	0.41
1:D:447:LEU:O	1:D:449:ILE:N	2.53	0.41
1:D:1114:ARG:HB2	1:D:1128:LEU:HD23	2.01	0.41
1:D:4099:VAL:HG22	1:D:4132:LEU:HD13	2.03	0.41
1:A:2170:VAL:HG21	1:A:2198:PHE:CD2	2.55	0.41
1:A:2418:ILE:HA	1:A:2421:ILE:HD12	2.01	0.41
1:B:982:ASP:OD1	1:B:983:LEU:N	2.53	0.41
1:C:2333:ALA:CB	1:C:2345:ALA:HB2	2.50	0.41
1:D:113:LEU:HD23	1:D:113:LEU:H	1.86	0.41
1:D:390:LYS:HZ3	1:D:392:ILE:HG23	1.86	0.41
1:D:893:TRP:CG	1:D:917:CYS:HG	2.38	0.41
1:D:1599:ARG:NH2	1:D:1602:ASN:OD1	2.49	0.41
1:D:4881:GLU:O	1:D:4885:THR:HG22	2.21	0.41
1:A:63:SER:O	1:A:66:THR:OG1	2.34	0.41
1:A:390:LYS:HZ3	1:A:392:ILE:HG23	1.85	0.41
1:A:394:HIS:ND1	1:A:396:GLU:O	2.48	0.41
1:B:352:SER:O	1:B:352:SER:OG	2.35	0.41
1:B:1446:ILE:HG21	1:B:1545:PHE:HZ	1.85	0.41
1:B:2418:ILE:HA	1:B:2421:ILE:HD12	2.01	0.41
1:C:456:LEU:HD21	1:C:533:LEU:HG	2.03	0.41
1:C:2170:VAL:HG21	1:C:2198:PHE:CE2	2.56	0.41
1:D:456:LEU:HD21	1:D:533:LEU:HG	2.03	0.41
1:D:733:TRP:CE2	1:D:738:ALA:HB2	2.56	0.41
1:D:2333:ALA:CB	1:D:2345:ALA:HB2	2.50	0.41
1:D:3930:ASN:O	1:D:3934:LEU:HD23	2.21	0.41
1:A:467:ASP:OD1	1:A:468:GLU:N	2.54	0.41
1:A:556:ASP:OD1	1:A:557:TRP:N	2.53	0.41
1:A:579:LEU:HD11	1:A:617:LEU:HG	2.03	0.41
1:A:2346:MET:HG2	1:A:2434:VAL:HG22	2.03	0.41
1:A:4099:VAL:HG22	1:A:4132:LEU:HD13	2.03	0.41
1:B:467:ASP:OD1	1:B:468:GLU:N	2.54	0.41
1:B:556:ASP:OD1	1:B:557:TRP:N	2.53	0.41
1:B:2170:VAL:HG21	1:B:2198:PHE:CE2	2.56	0.41
1:B:2431:LEU:CD2	1:B:2471:LEU:HD23	2.49	0.41
1:C:21:VAL:CG2	1:C:217:ILE:HD11	2.51	0.41
1:A:456:LEU:HD21	1:A:533:LEU:HG	2.03	0.41
1:A:1895:MET:SD	1:A:1895:MET:N	2.89	0.41
1:A:2151:ASN:OD1	1:A:2153:VAL:N	2.54	0.41
1:A:2170:VAL:HG21	1:A:2198:PHE:CE2	2.56	0.41
1:B:456:LEU:HD21	1:B:533:LEU:HG	2.03	0.41
1:B:1446:ILE:HG23	1:B:1487:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2078:GLU:OE1	1:B:2078:GLU:N	2.49	0.41
1:B:4881:GLU:O	1:B:4885:THR:HG22	2.21	0.41
1:C:394:HIS:ND1	1:C:396:GLU:O	2.49	0.41
1:C:733:TRP:CE2	1:C:738:ALA:HB2	2.56	0.41
1:C:1446:ILE:HG23	1:C:1487:MET:HE1	2.02	0.41
1:C:2151:ASN:OD1	1:C:2153:VAL:N	2.54	0.41
1:D:2170:VAL:HG21	1:D:2198:PHE:CE2	2.56	0.41
1:D:2346:MET:HG2	1:D:2434:VAL:HG22	2.03	0.41
1:A:1446:ILE:HG21	1:A:1545:PHE:HZ	1.85	0.41
1:A:2178:LEU:HA	1:A:2186:ILE:HD13	2.03	0.41
1:B:447:LEU:O	1:B:449:ILE:N	2.53	0.41
1:B:594:ILE:HD11	1:B:632:ILE:CG1	2.50	0.41
1:B:633:CYS:HA	1:B:637:LEU:HD13	2.02	0.41
1:C:579:LEU:HD11	1:C:617:LEU:HG	2.03	0.41
1:C:1294:ASN:ND2	1:C:1294:ASN:O	2.54	0.41
1:C:1947:MET:HE1	1:C:1961:THR:HG22	2.03	0.41
1:D:594:ILE:HD11	1:D:632:ILE:CG1	2.51	0.41
1:D:2178:LEU:HA	1:D:2186:ILE:HD13	2.02	0.41
2:G:42:ASP:N	2:G:42:ASP:OD1	2.53	0.41
1:A:21:VAL:CG2	1:A:217:ILE:HD11	2.51	0.40
1:B:21:VAL:CG2	1:B:217:ILE:HD11	2.51	0.40
1:B:2498:ALA:HB2	1:B:2515:LEU:HD23	2.02	0.40
1:B:4062:THR:O	1:B:4066:LEU:HD23	2.22	0.40
1:B:4099:VAL:HG22	1:B:4132:LEU:HD13	2.03	0.40
1:C:2166:MET:O	1:C:2170:VAL:HG23	2.21	0.40
1:C:2346:MET:HG2	1:C:2434:VAL:HG22	2.03	0.40
1:D:556:ASP:OD1	1:D:557:TRP:N	2.53	0.40
1:D:1294:ASN:ND2	1:D:1294:ASN:O	2.54	0.40
1:D:4062:THR:O	1:D:4066:LEU:HD23	2.21	0.40
1:A:2498:ALA:HB2	1:A:2515:LEU:HD23	2.02	0.40
1:A:4881:GLU:O	1:A:4885:THR:HG22	2.21	0.40
1:B:923:LYS:O	1:B:923:LYS:NZ	2.48	0.40
1:C:352:SER:O	1:C:352:SER:OG	2.35	0.40
1:D:1446:ILE:HG21	1:D:1545:PHE:HZ	1.85	0.40
1:D:4198:GLU:HG3	1:D:4596:LEU:HD22	2.04	0.40
1:A:411:GLU:OE1	1:A:411:GLU:N	2.44	0.40
1:A:1446:ILE:HG23	1:A:1487:MET:HE1	2.02	0.40
1:B:1721:MET:SD	1:B:2126:ARG:NH1	2.94	0.40
1:B:2396:ASP:OD1	1:B:2400:ARG:NE	2.55	0.40
1:C:4136:GLU:O	1:C:4917:TYR:OH	2.35	0.40
1:D:579:LEU:HD11	1:D:617:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:OE2	1:A:67:PHE:N	2.54	0.40
1:A:93:VAL:HG12	1:A:95:VAL:HG23	2.03	0.40
1:A:728:ASP:OD1	1:A:731:HIS:N	2.42	0.40
1:A:733:TRP:CE2	1:A:738:ALA:HB2	2.56	0.40
1:C:447:LEU:O	1:C:449:ILE:N	2.53	0.40
1:C:3839:PHE:HE1	1:C:3873:THR:HG23	1.87	0.40
1:C:3930:ASN:O	1:C:3934:LEU:HD23	2.21	0.40
1:D:797:GLY:N	1:D:1622:CYS:O	2.50	0.40
1:D:1947:MET:HE1	1:D:1961:THR:HG22	2.03	0.40
1:A:508:TYR:CE1	1:A:517:VAL:HG21	2.57	0.40
1:A:566:GLU:OE1	1:A:566:GLU:N	2.48	0.40
1:A:1053:ALA:O	1:A:1056:THR:OG1	2.35	0.40
1:A:1535:GLU:O	1:A:1538:THR:OG1	2.36	0.40
1:B:113:LEU:H	1:B:113:LEU:HD23	1.86	0.40
1:B:2346:MET:HG2	1:B:2434:VAL:HG22	2.03	0.40
1:C:467:ASP:OD1	1:C:468:GLU:N	2.54	0.40
1:C:2441:MET:HE2	1:C:2497:ALA:HB1	2.02	0.40
1:D:21:VAL:CG2	1:D:217:ILE:HD11	2.51	0.40
1:D:394:HIS:ND1	1:D:396:GLU:O	2.48	0.40
1:D:809:GLY:N	1:D:1614:GLU:O	2.50	0.40
1:D:2129:LEU:HD11	1:D:2172:GLU:HG3	2.03	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	3474/4966 (70%)	3376 (97%)	97 (3%)	1 (0%)	100	100
1	B	3474/4966 (70%)	3377 (97%)	96 (3%)	1 (0%)	100	100
1	C	3474/4966 (70%)	3378 (97%)	95 (3%)	1 (0%)	100	100
1	D	3474/4966 (70%)	3379 (97%)	94 (3%)	1 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	105/176 (60%)	101 (96%)	4 (4%)	0	100	100
2	H	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	I	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	J	105/176 (60%)	101 (96%)	4 (4%)	0	100	100
All	All	14316/20568 (70%)	13916 (97%)	396 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2184	LYS
1	B	2184	LYS
1	C	2184	LYS
1	D	2184	LYS

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	3057/4355 (70%)	3003 (98%)	54 (2%)	51	80
1	B	3057/4355 (70%)	3002 (98%)	55 (2%)	51	80
1	C	3057/4355 (70%)	3002 (98%)	55 (2%)	51	80
1	D	3057/4355 (70%)	3002 (98%)	55 (2%)	51	80
2	G	88/140 (63%)	87 (99%)	1 (1%)	65	88
2	H	88/140 (63%)	87 (99%)	1 (1%)	65	88
2	I	88/140 (63%)	87 (99%)	1 (1%)	65	88
2	J	88/140 (63%)	87 (99%)	1 (1%)	65	88
All	All	12580/17980 (70%)	12357 (98%)	223 (2%)	51	80

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	28	ILE
1	A	65	CYS
1	A	158	CYS
1	A	181	LEU
1	A	189	GLU
1	A	387	ILE
1	A	423	VAL
1	A	451	SER
1	A	482	LEU
1	A	614	LEU
1	A	734	SER
1	A	758	CYS
1	A	890	HIS
1	A	933	LEU
1	A	996	VAL
1	A	1173	MET
1	A	1305	SER
1	A	1576	HIS
1	A	1593	SER
1	A	1594	HIS
1	A	1629	MET
1	A	1636	GLU
1	A	1642	ILE
1	A	1661	LEU
1	A	1705	ASP
1	A	1945	GLU
1	A	2065	MET
1	A	2129	LEU
1	A	2160	LEU
1	A	2166	MET
1	A	2199	LEU
1	A	2217	LEU
1	A	2233	MET
1	A	2265	VAL
1	A	2275	SER
1	A	2322	LEU
1	A	2383	MET
1	A	2397	LEU
1	A	2398	LEU
1	A	2425	LEU
1	A	2455	MET
1	A	2519	LEU

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Mol	Chain	Res	Type
1	A	2584	MET
1	A	3816	LEU
1	A	3853	PHE
1	A	3887	PHE
1	A	4055	LYS
1	A	4123	SER
1	A	4614	LEU
1	A	4807	ASP
1	A	4837	GLU
1	A	4862	GLN
1	A	4941	LYS
1	B	27	THR
1	B	28	ILE
1	B	65	CYS
1	B	158	CYS
1	B	181	LEU
1	B	189	GLU
1	B	387	ILE
1	B	423	VAL
1	B	451	SER
1	B	482	LEU
1	B	614	LEU
1	B	734	SER
1	B	758	CYS
1	B	890	HIS
1	B	933	LEU
1	B	996	VAL
1	B	1173	MET
1	B	1305	SER
1	B	1458	ASP
1	B	1576	HIS
1	B	1593	SER
1	B	1594	HIS
1	B	1629	MET
1	B	1636	GLU
1	B	1642	ILE
1	B	1661	LEU
1	B	1705	ASP
1	B	1945	GLU
1	B	2065	MET
1	B	2129	LEU
1	B	2160	LEU

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Mol	Chain	Res	Type
1	B	2166	MET
1	B	2199	LEU
1	B	2217	LEU
1	B	2233	MET
1	B	2265	VAL
1	B	2275	SER
1	B	2322	LEU
1	B	2383	MET
1	B	2397	LEU
1	B	2398	LEU
1	B	2425	LEU
1	B	2455	MET
1	B	2519	LEU
1	B	2584	MET
1	B	3816	LEU
1	B	3853	PHE
1	B	3887	PHE
1	B	4055	LYS
1	B	4123	SER
1	B	4614	LEU
1	B	4807	ASP
1	B	4837	GLU
1	B	4862	GLN
1	B	4941	LYS
1	C	27	THR
1	C	28	ILE
1	C	65	CYS
1	C	158	CYS
1	C	181	LEU
1	C	189	GLU
1	C	387	ILE
1	C	423	VAL
1	C	451	SER
1	C	482	LEU
1	C	614	LEU
1	C	734	SER
1	C	758	CYS
1	C	890	HIS
1	C	933	LEU
1	C	996	VAL
1	C	1173	MET
1	C	1305	SER

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Mol	Chain	Res	Type
1	C	1458	ASP
1	C	1576	HIS
1	C	1593	SER
1	C	1594	HIS
1	C	1629	MET
1	C	1636	GLU
1	C	1642	ILE
1	C	1661	LEU
1	C	1705	ASP
1	C	1945	GLU
1	C	2065	MET
1	C	2129	LEU
1	C	2160	LEU
1	C	2166	MET
1	C	2199	LEU
1	C	2217	LEU
1	C	2233	MET
1	C	2265	VAL
1	C	2275	SER
1	C	2322	LEU
1	C	2383	MET
1	C	2397	LEU
1	C	2398	LEU
1	C	2425	LEU
1	C	2455	MET
1	C	2519	LEU
1	C	2584	MET
1	C	3816	LEU
1	C	3853	PHE
1	C	3887	PHE
1	C	4055	LYS
1	C	4123	SER
1	C	4614	LEU
1	C	4807	ASP
1	C	4837	GLU
1	C	4862	GLN
1	C	4941	LYS
1	D	27	THR
1	D	28	ILE
1	D	65	CYS
1	D	158	CYS
1	D	181	LEU

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Mol	Chain	Res	Type
1	D	189	GLU
1	D	387	ILE
1	D	423	VAL
1	D	451	SER
1	D	482	LEU
1	D	614	LEU
1	D	734	SER
1	D	758	CYS
1	D	890	HIS
1	D	933	LEU
1	D	996	VAL
1	D	1173	MET
1	D	1305	SER
1	D	1458	ASP
1	D	1576	HIS
1	D	1593	SER
1	D	1594	HIS
1	D	1629	MET
1	D	1636	GLU
1	D	1642	ILE
1	D	1661	LEU
1	D	1705	ASP
1	D	1945	GLU
1	D	2065	MET
1	D	2129	LEU
1	D	2160	LEU
1	D	2166	MET
1	D	2199	LEU
1	D	2217	LEU
1	D	2233	MET
1	D	2265	VAL
1	D	2275	SER
1	D	2322	LEU
1	D	2383	MET
1	D	2397	LEU
1	D	2398	LEU
1	D	2425	LEU
1	D	2455	MET
1	D	2519	LEU
1	D	2584	MET
1	D	3816	LEU
1	D	3853	PHE

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Mol	Chain	Res	Type
1	D	3887	PHE
1	D	4055	LYS
1	D	4123	SER
1	D	4614	LEU
1	D	4807	ASP
1	D	4837	GLU
1	D	4862	GLN
1	D	4941	LYS
2	G	26	HIS
2	H	26	HIS
2	I	26	HIS
2	J	26	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	150	GLN
1	A	375	GLN
1	A	608	HIS
1	A	896	ASN
1	A	1178	ASN
1	A	1293	GLN
1	A	1294	ASN
1	A	1616	GLN
1	A	1632	HIS
1	A	1723	ASN
1	A	1774	ASN
1	A	1778	GLN
1	A	2308	ASN
1	A	2315	ASN
1	A	2317	ASN
1	A	3810	GLN
1	A	3902	GLN
1	A	4698	ASN
1	A	4786	ASN
1	B	57	ASN
1	B	150	GLN
1	B	375	GLN
1	B	608	HIS
1	B	896	ASN
1	B	1178	ASN

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Mol	Chain	Res	Type
1	B	1293	GLN
1	B	1294	ASN
1	B	1616	GLN
1	B	1723	ASN
1	B	1778	GLN
1	B	2308	ASN
1	B	2317	ASN
1	B	3810	GLN
1	B	3902	GLN
1	B	3914	GLN
1	B	3997	GLN
1	B	4698	ASN
1	B	4786	ASN
1	C	57	ASN
1	C	150	GLN
1	C	375	GLN
1	C	608	HIS
1	C	836	HIS
1	C	896	ASN
1	C	1178	ASN
1	C	1293	GLN
1	C	1294	ASN
1	C	1616	GLN
1	C	1723	ASN
1	C	1778	GLN
1	C	2317	ASN
1	C	3810	GLN
1	C	3902	GLN
1	C	3914	GLN
1	C	4698	ASN
1	C	4786	ASN
1	D	57	ASN
1	D	150	GLN
1	D	375	GLN
1	D	608	HIS
1	D	896	ASN
1	D	1178	ASN
1	D	1293	GLN
1	D	1294	ASN
1	D	1616	GLN
1	D	1723	ASN
1	D	1774	ASN

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Mol	Chain	Res	Type
1	D	1778	GLN
1	D	2317	ASN
1	D	3774	GLN
1	D	3810	GLN
1	D	3881	GLN
1	D	3902	GLN
1	D	4698	ASN
1	D	4786	ASN
2	I	33	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	A1MG7	A	5002	-	27,27,27	1.56	6 (22%)	36,38,38	2.47	11 (30%)
4	A1MG7	D	5002	-	27,27,27	1.57	6 (22%)	36,38,38	2.46	10 (27%)
4	A1MG7	C	5002	-	27,27,27	1.57	6 (22%)	36,38,38	2.46	9 (25%)
4	A1MG7	B	5002	-	27,27,27	1.57	6 (22%)	36,38,38	2.47	10 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1MG7	A	5002	-	-	0/16/16/16	0/3/3/3
4	A1MG7	D	5002	-	-	0/16/16/16	0/3/3/3
4	A1MG7	C	5002	-	-	0/16/16/16	0/3/3/3
4	A1MG7	B	5002	-	-	0/16/16/16	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5002	A1MG7	C-NAO	4.70	1.45	1.35
4	B	5002	A1MG7	C-NAO	4.66	1.45	1.35
4	C	5002	A1MG7	C-NAO	4.65	1.45	1.35
4	A	5002	A1MG7	C-NAO	4.65	1.45	1.35
4	A	5002	A1MG7	N-NAH	2.95	1.37	1.33
4	B	5002	A1MG7	N-NAH	2.94	1.37	1.33
4	D	5002	A1MG7	N-NAH	2.93	1.37	1.33
4	C	5002	A1MG7	N-NAH	2.87	1.37	1.33
4	C	5002	A1MG7	NAK-NAJ	2.86	1.36	1.32
4	D	5002	A1MG7	NAK-NAJ	2.81	1.36	1.32
4	B	5002	A1MG7	N-NAJ	2.81	1.36	1.32
4	C	5002	A1MG7	N-NAJ	2.80	1.36	1.32
4	A	5002	A1MG7	NAK-NAJ	2.79	1.36	1.32
4	B	5002	A1MG7	NAK-NAJ	2.79	1.36	1.32
4	A	5002	A1MG7	N-NAJ	2.75	1.36	1.32
4	D	5002	A1MG7	N-NAJ	2.72	1.36	1.32
4	D	5002	A1MG7	CAF-CAG	2.66	1.51	1.47
4	C	5002	A1MG7	CAF-CAG	2.63	1.51	1.47
4	A	5002	A1MG7	CAF-CAG	2.62	1.51	1.47
4	B	5002	A1MG7	CAF-CAG	2.62	1.51	1.47
4	B	5002	A1MG7	O-C	-2.10	1.18	1.23
4	C	5002	A1MG7	O-C	-2.10	1.18	1.23
4	D	5002	A1MG7	O-C	-2.10	1.18	1.23
4	A	5002	A1MG7	O-C	-2.05	1.18	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	5002	A1MG7	CAG-NAH-N	7.60	107.72	101.70
4	B	5002	A1MG7	CAG-NAH-N	7.53	107.66	101.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5002	A1MG7	CAG-NAH-N	7.49	107.62	101.70
4	D	5002	A1MG7	CAG-NAH-N	7.45	107.60	101.70
4	B	5002	A1MG7	NAH-N-NAJ	-6.74	108.31	114.03
4	A	5002	A1MG7	NAH-N-NAJ	-6.69	108.36	114.03
4	C	5002	A1MG7	NAH-N-NAJ	-6.68	108.36	114.03
4	D	5002	A1MG7	NAH-N-NAJ	-6.64	108.40	114.03
4	A	5002	A1MG7	CA-N-NAJ	6.12	127.34	122.59
4	D	5002	A1MG7	CA-N-NAJ	6.11	127.33	122.59
4	B	5002	A1MG7	CA-N-NAJ	6.10	127.33	122.59
4	C	5002	A1MG7	CA-N-NAJ	6.04	127.28	122.59
4	C	5002	A1MG7	NAH-CAG-NAK	-3.50	108.73	112.00
4	A	5002	A1MG7	NAH-CAG-NAK	-3.47	108.76	112.00
4	B	5002	A1MG7	NAH-CAG-NAK	-3.47	108.76	112.00
4	D	5002	A1MG7	NAH-CAG-NAK	-3.47	108.76	112.00
4	A	5002	A1MG7	CAE-CAD-CAC	-2.87	119.90	123.52
4	B	5002	A1MG7	CAE-CAD-CAC	-2.87	119.90	123.52
4	D	5002	A1MG7	CAE-CAD-CAC	-2.87	119.90	123.52
4	C	5002	A1MG7	CAE-CAD-CAC	-2.85	119.91	123.52
4	D	5002	A1MG7	CAF-CAG-NAK	2.70	127.11	123.96
4	A	5002	A1MG7	CAF-CAG-NAK	2.68	127.08	123.96
4	B	5002	A1MG7	CAF-CAG-NAK	2.68	127.08	123.96
4	C	5002	A1MG7	CAF-CAG-NAK	2.63	127.03	123.96
4	A	5002	A1MG7	CAC-CAB-CAA	-2.63	120.20	123.52
4	B	5002	A1MG7	CAC-CAB-CAA	-2.63	120.20	123.52
4	C	5002	A1MG7	CAC-CAB-CAA	-2.61	120.22	123.52
4	D	5002	A1MG7	CAC-CAB-CAA	-2.61	120.22	123.52
4	A	5002	A1MG7	CAD-CAC-CAB	2.51	120.04	116.13
4	B	5002	A1MG7	CAD-CAC-CAB	2.51	120.04	116.13
4	C	5002	A1MG7	CAD-CAC-CAB	2.51	120.04	116.13
4	D	5002	A1MG7	CAD-CAC-CAB	2.51	120.04	116.13
4	A	5002	A1MG7	CAG-NAK-NAJ	2.12	107.60	105.91
4	B	5002	A1MG7	CAG-NAK-NAJ	2.12	107.60	105.91
4	C	5002	A1MG7	CAG-NAK-NAJ	2.10	107.58	105.91
4	D	5002	A1MG7	CAG-NAK-NAJ	2.08	107.57	105.91
4	D	5002	A1MG7	N-NAJ-NAK	2.05	107.67	105.99
4	B	5002	A1MG7	N-NAJ-NAK	2.04	107.67	105.99
4	A	5002	A1MG7	N-NAJ-NAK	2.03	107.66	105.99
4	A	5002	A1MG7	CAQ-NAO-C	-2.01	120.73	123.77

There are no chirality outliers.

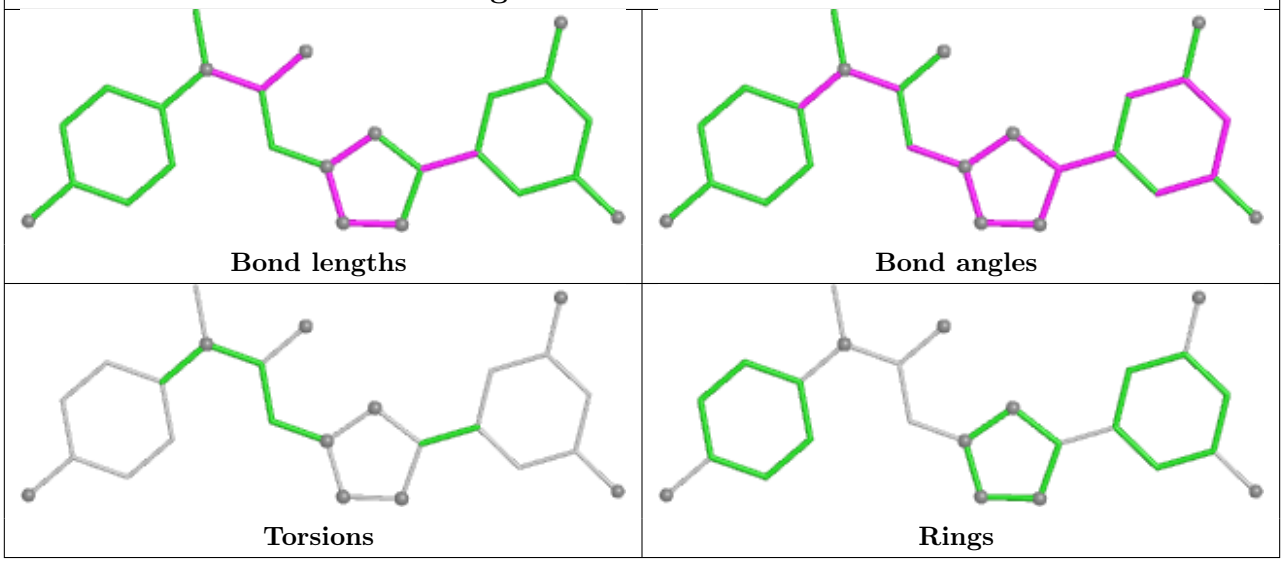
There are no torsion outliers.

There are no ring outliers.

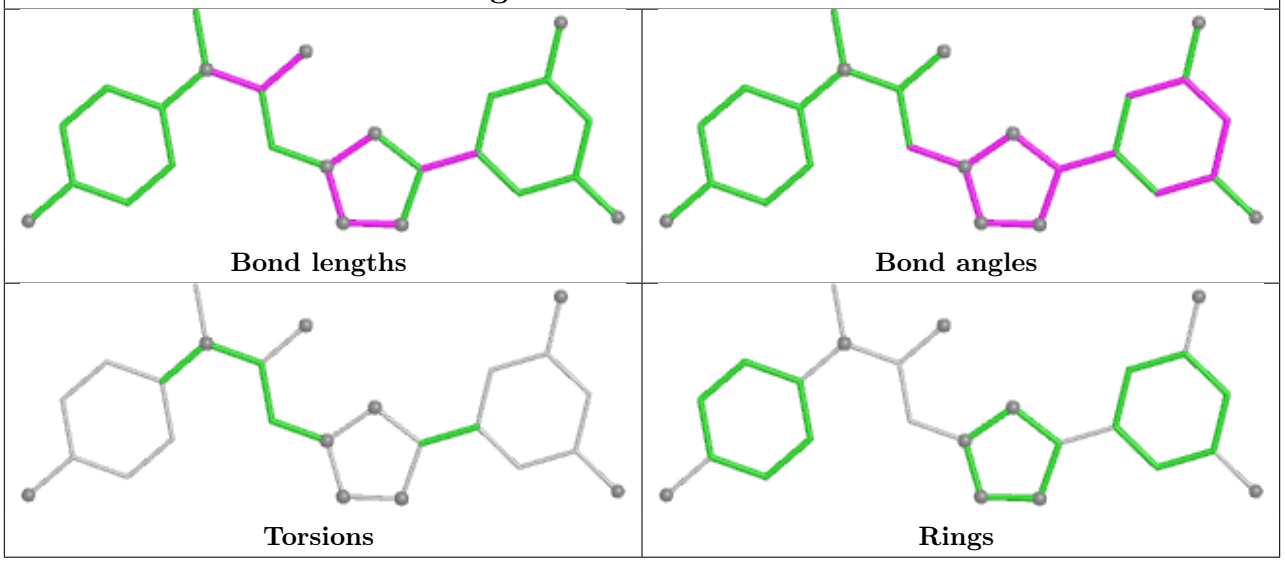
No monomer is involved in short contacts.

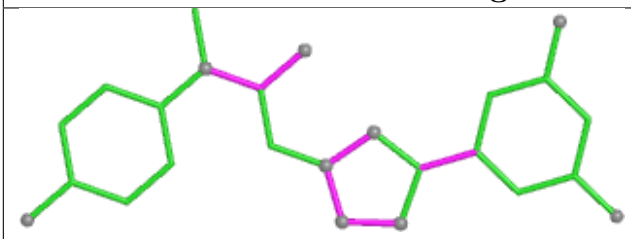
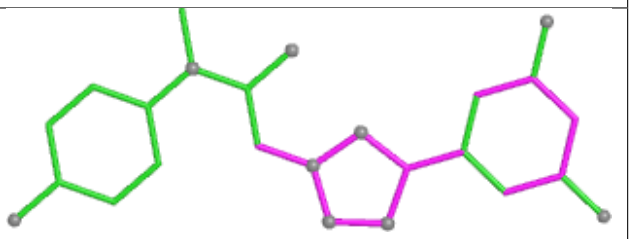
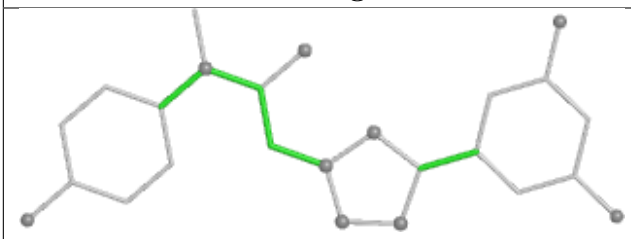
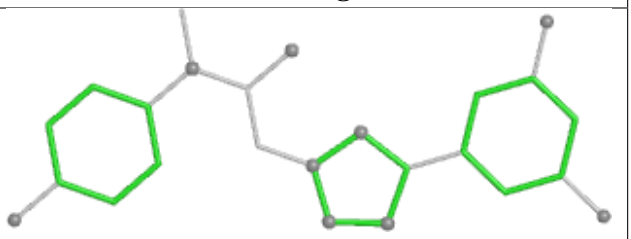
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

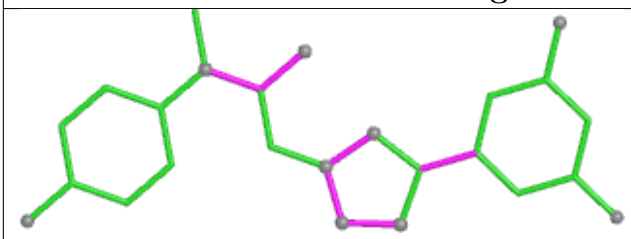
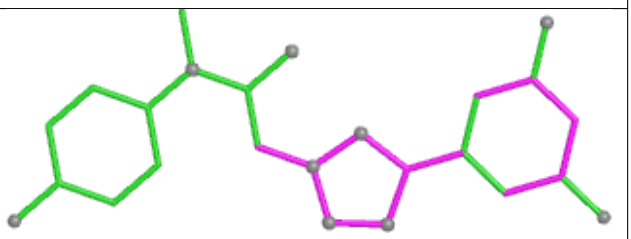
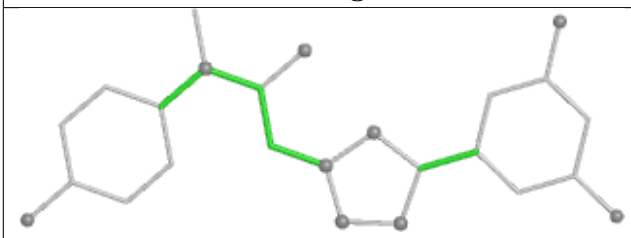
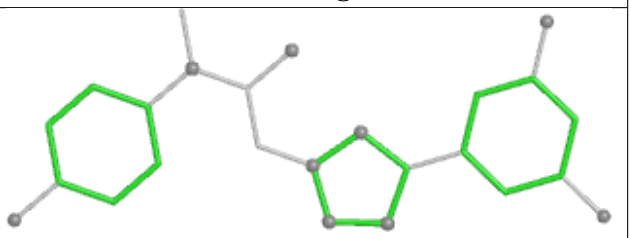
Ligand A1MG7 A 5002



Ligand A1MG7 D 5002



Ligand A1MG7 C 5002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1MG7 B 5002	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

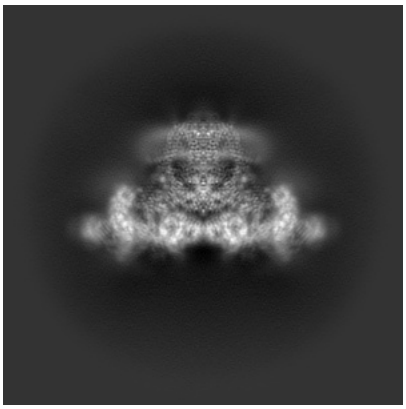
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-80687. These allow visual inspection of the internal detail of the map and identification of artifacts.

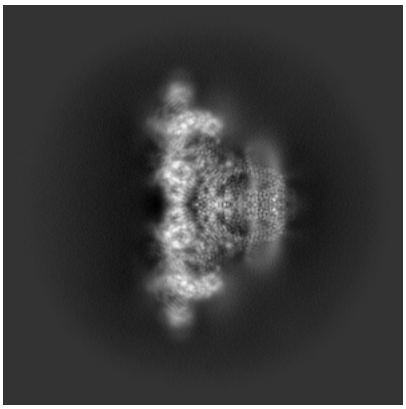
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

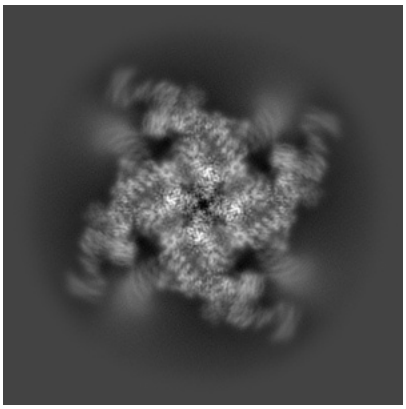
6.1.1 Primary map



X

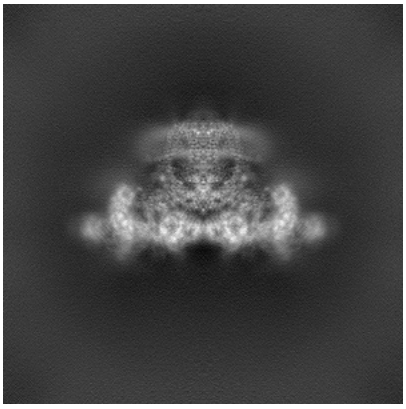


Y

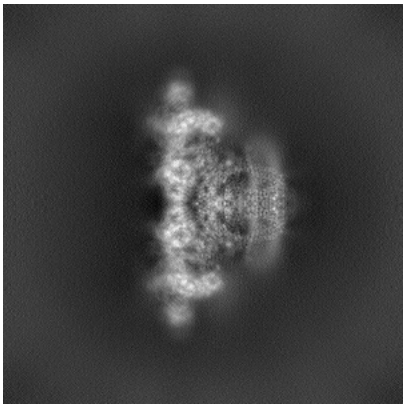


Z

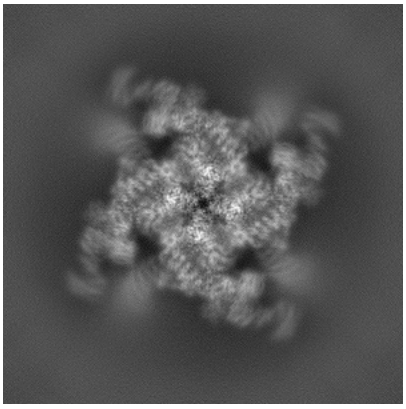
6.1.2 Raw map



X



Y

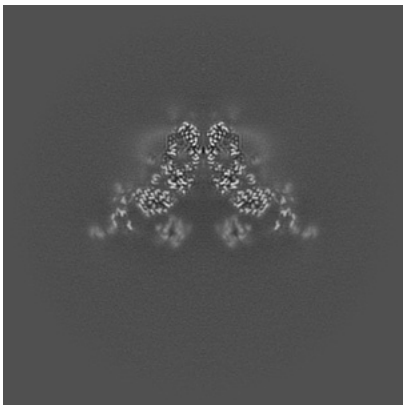


Z

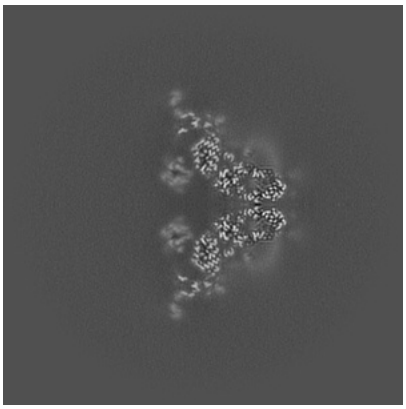
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

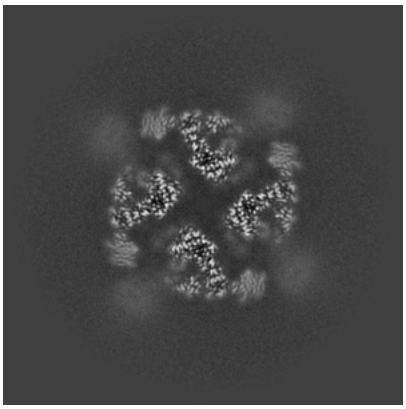
6.2.1 Primary map



X Index: 256

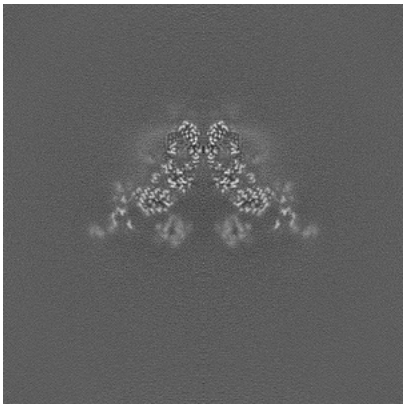


Y Index: 256

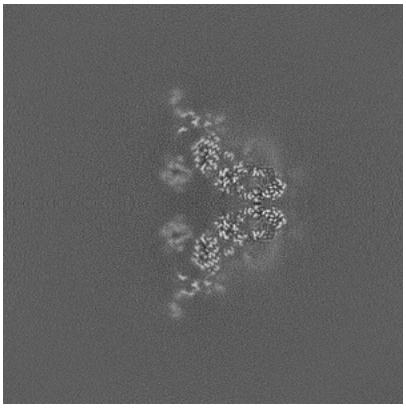


Z Index: 256

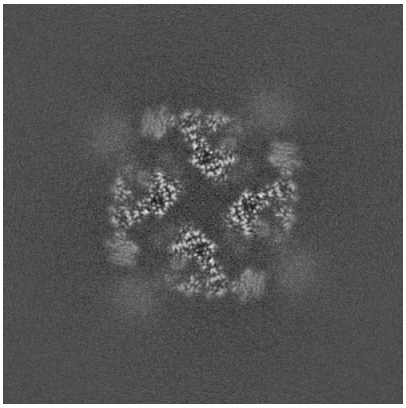
6.2.2 Raw map



X Index: 256



Y Index: 256

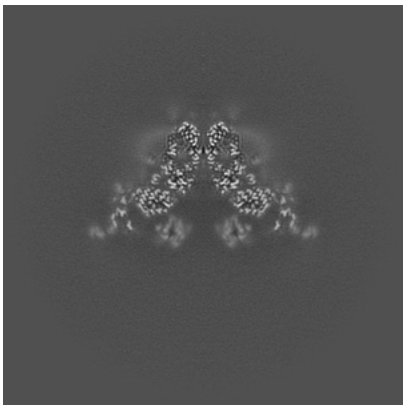


Z Index: 256

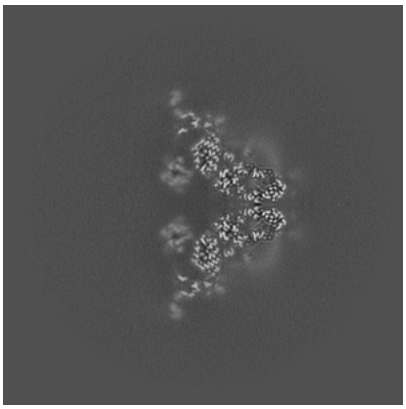
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

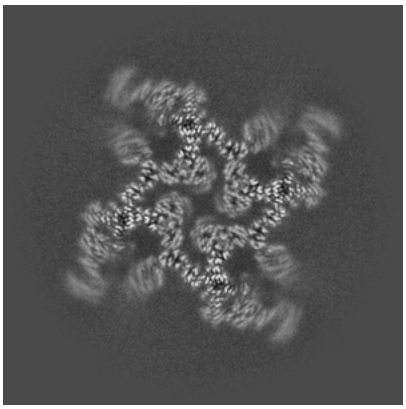
6.3.1 Primary map



X Index: 256

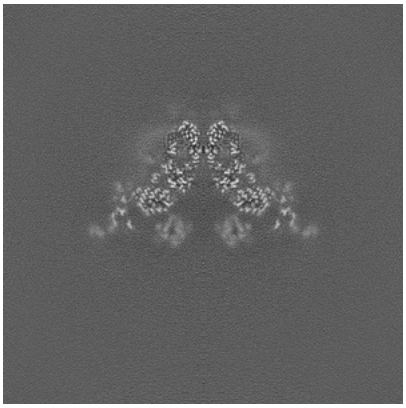


Y Index: 256

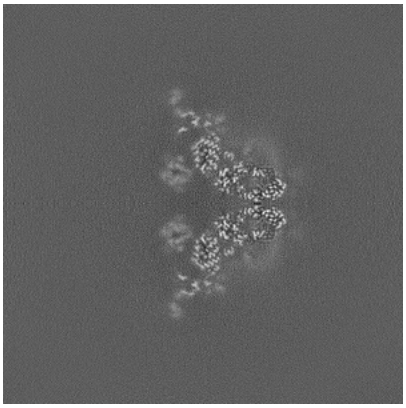


Z Index: 225

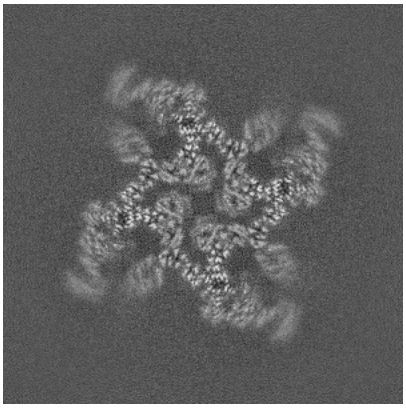
6.3.2 Raw map



X Index: 256



Y Index: 256

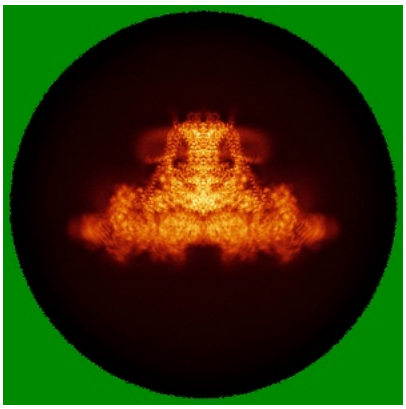


Z Index: 225

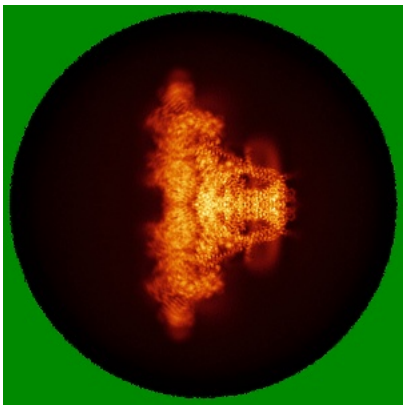
The images above show the largest variance slices of the map in three orthogonal directions.

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

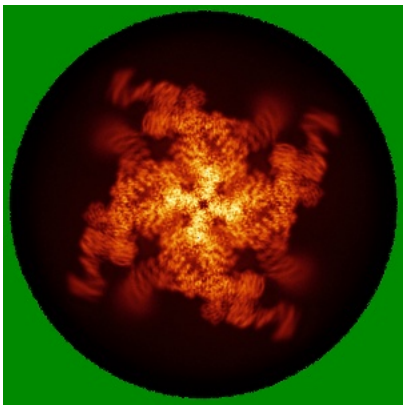
6.4.1 Primary map



X

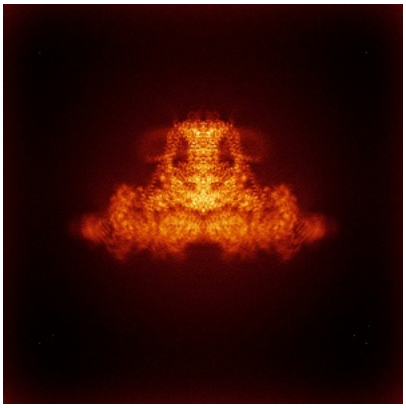


Y

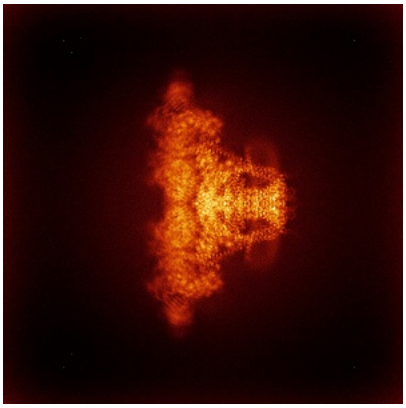


Z

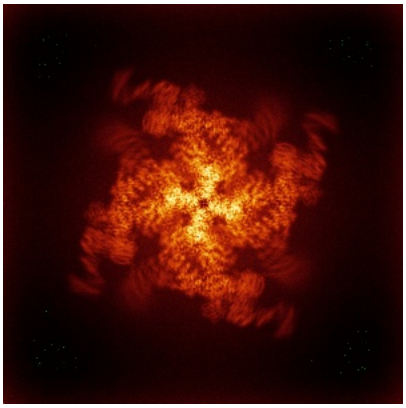
6.4.2 Raw map



X



Y

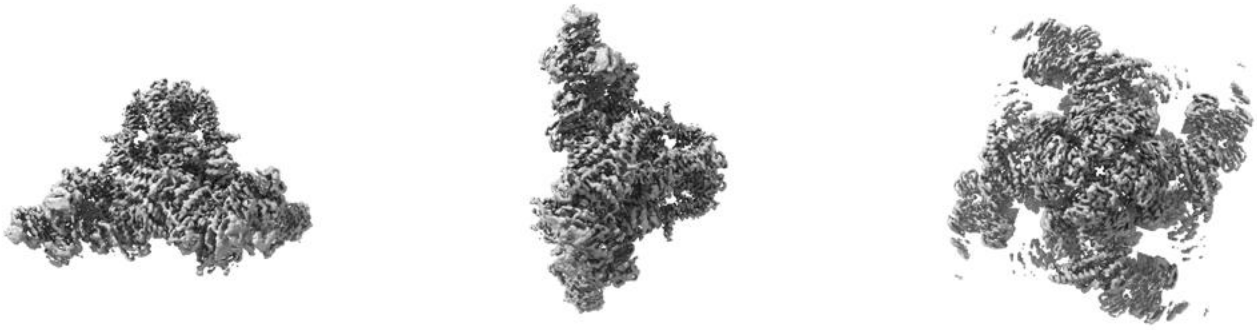


Z

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

6.5 Orthogonal surface views (i)

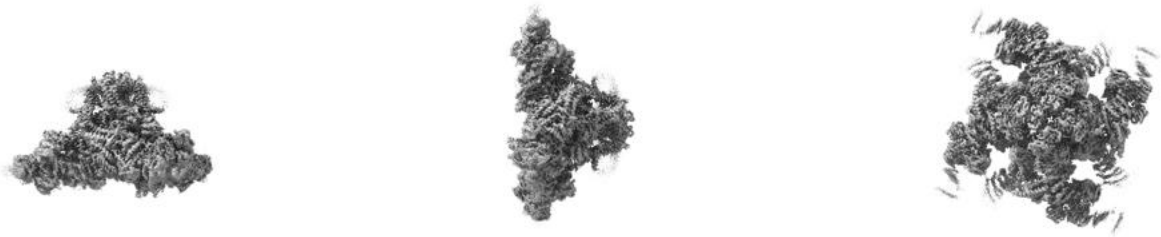
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

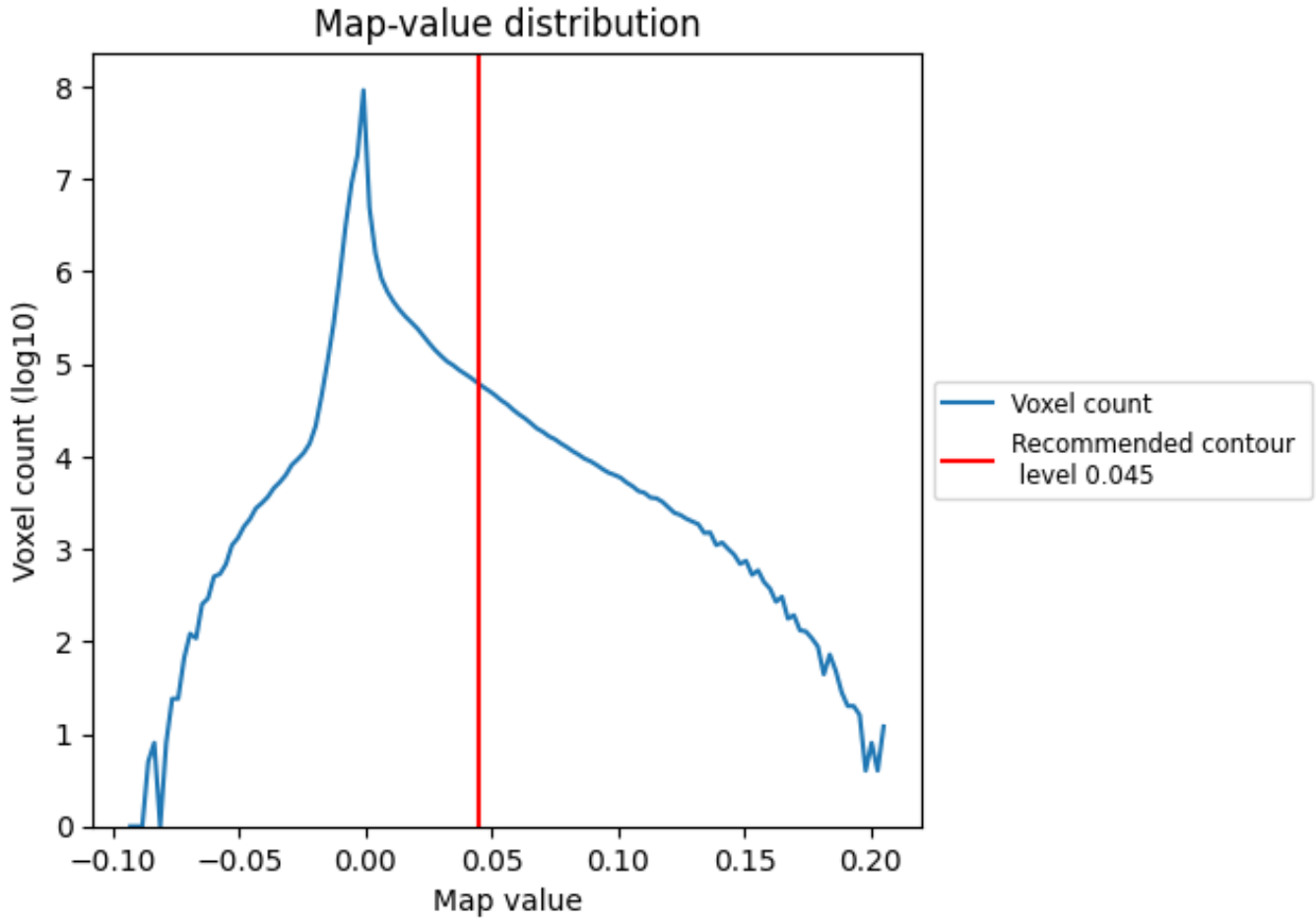
6.6 Mask visualisation (i)

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

7 Map analysis

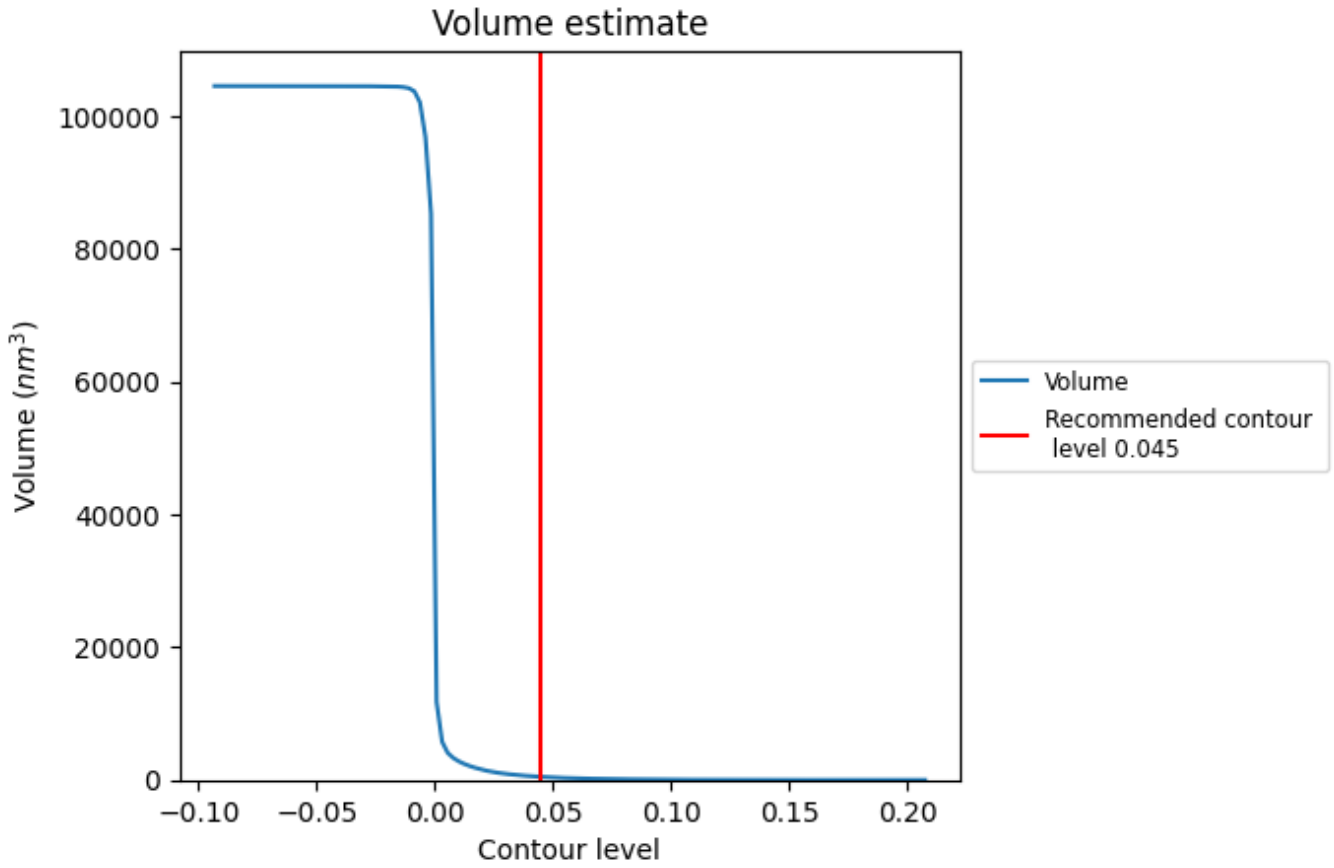
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

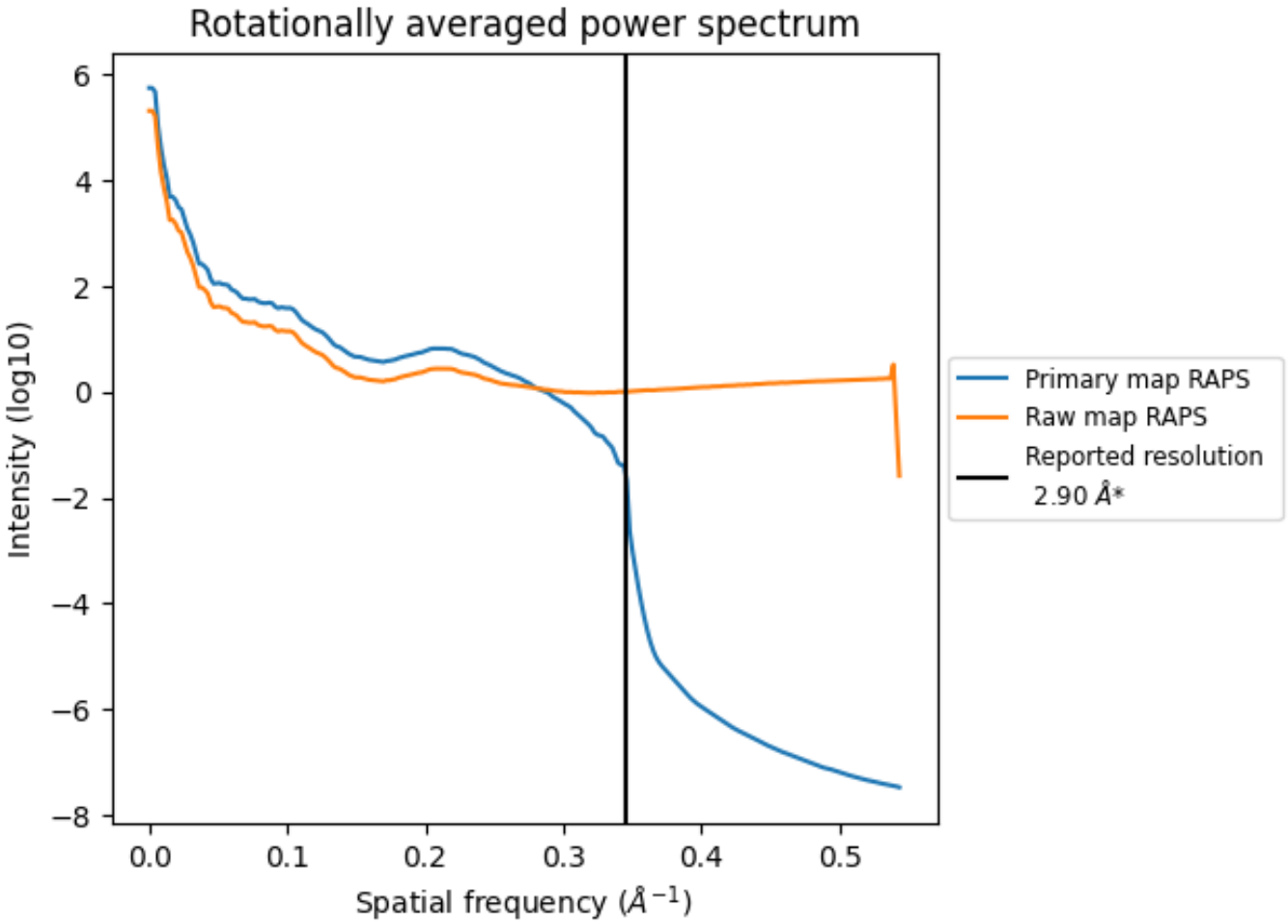
7.2 Volume estimate



The volume at the recommended contour level is 474 nm^3; this corresponds to an approximate mass of 428 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)

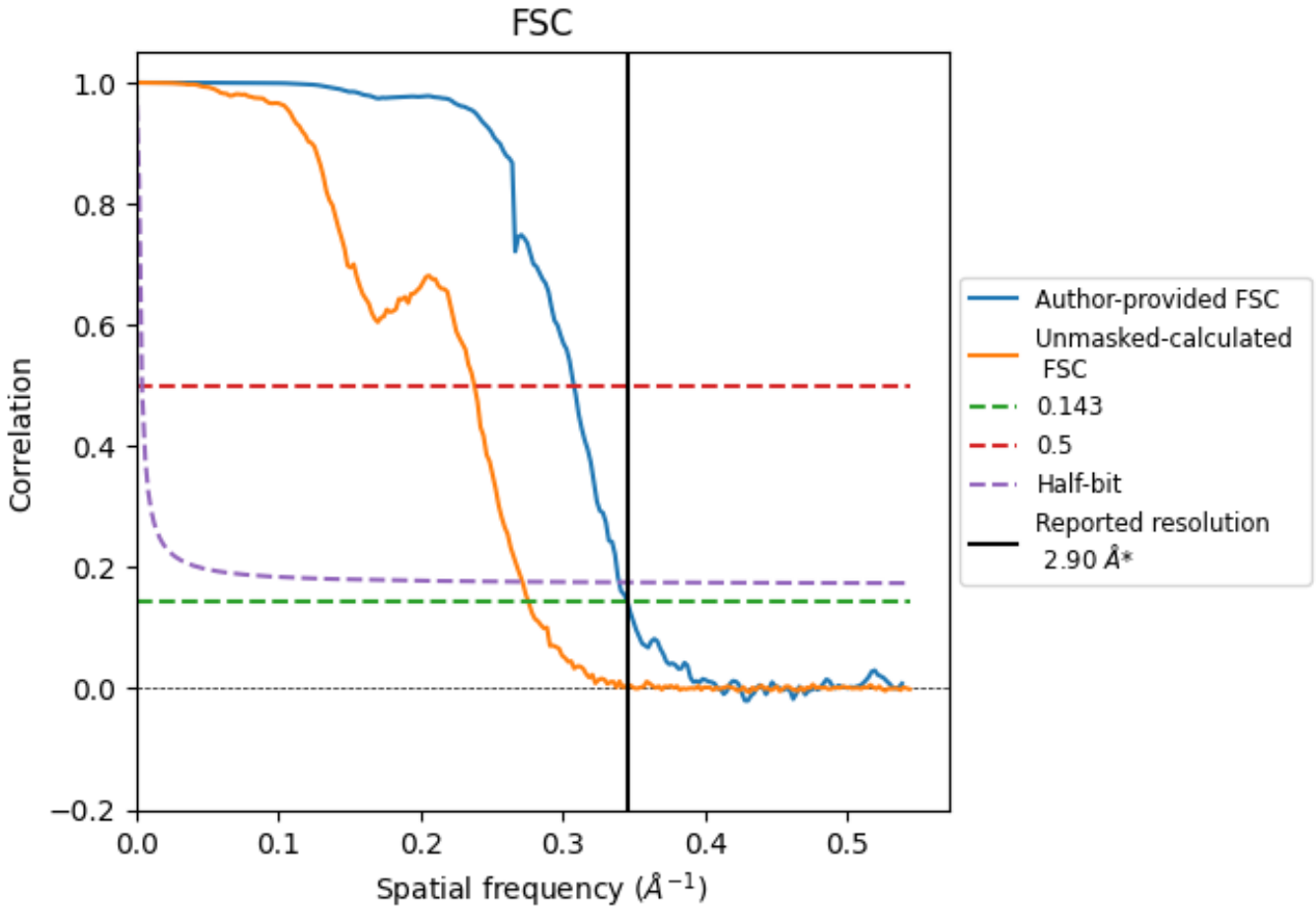


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

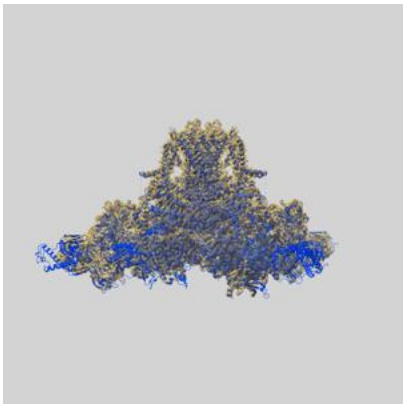
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.25	2.95
Unmasked-calculated*	3.63	4.21	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.9 by more than 10 %

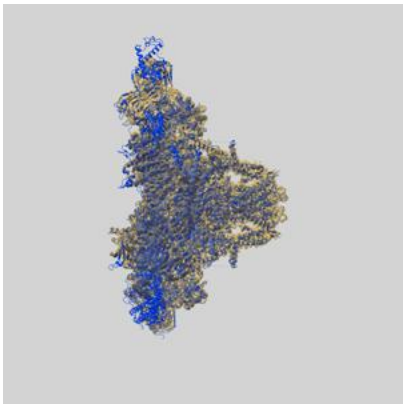
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-80687 and PDB model 26IS. Per-residue inclusion information can be found in section 3 on page 13.

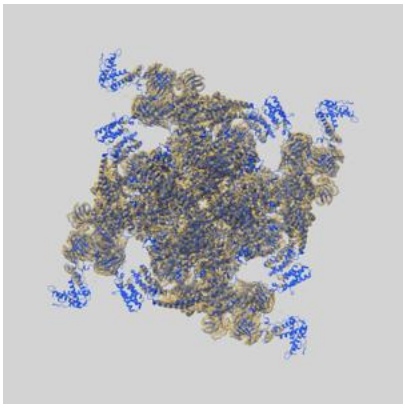
9.1 Map-model overlay



X



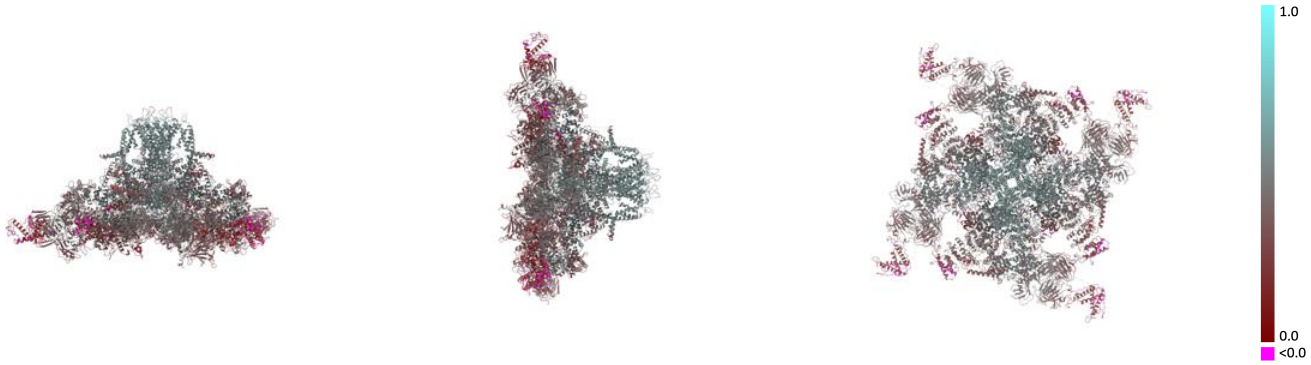
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

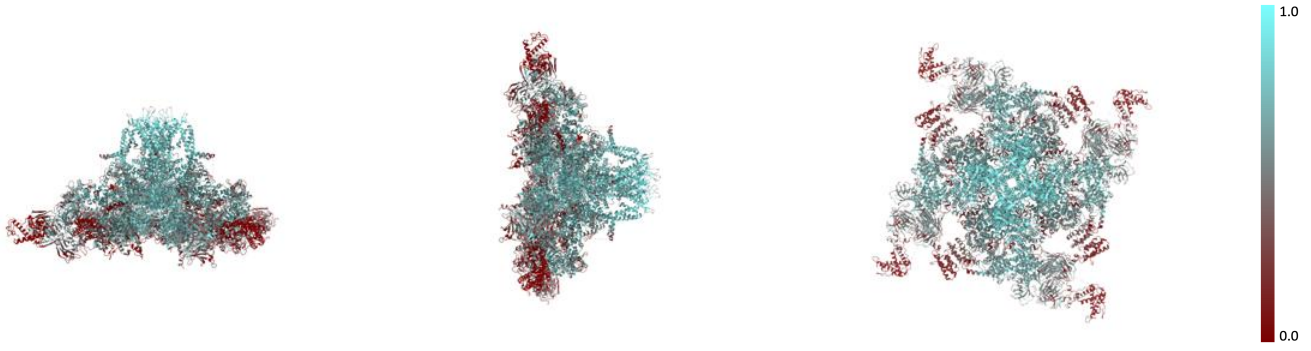
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

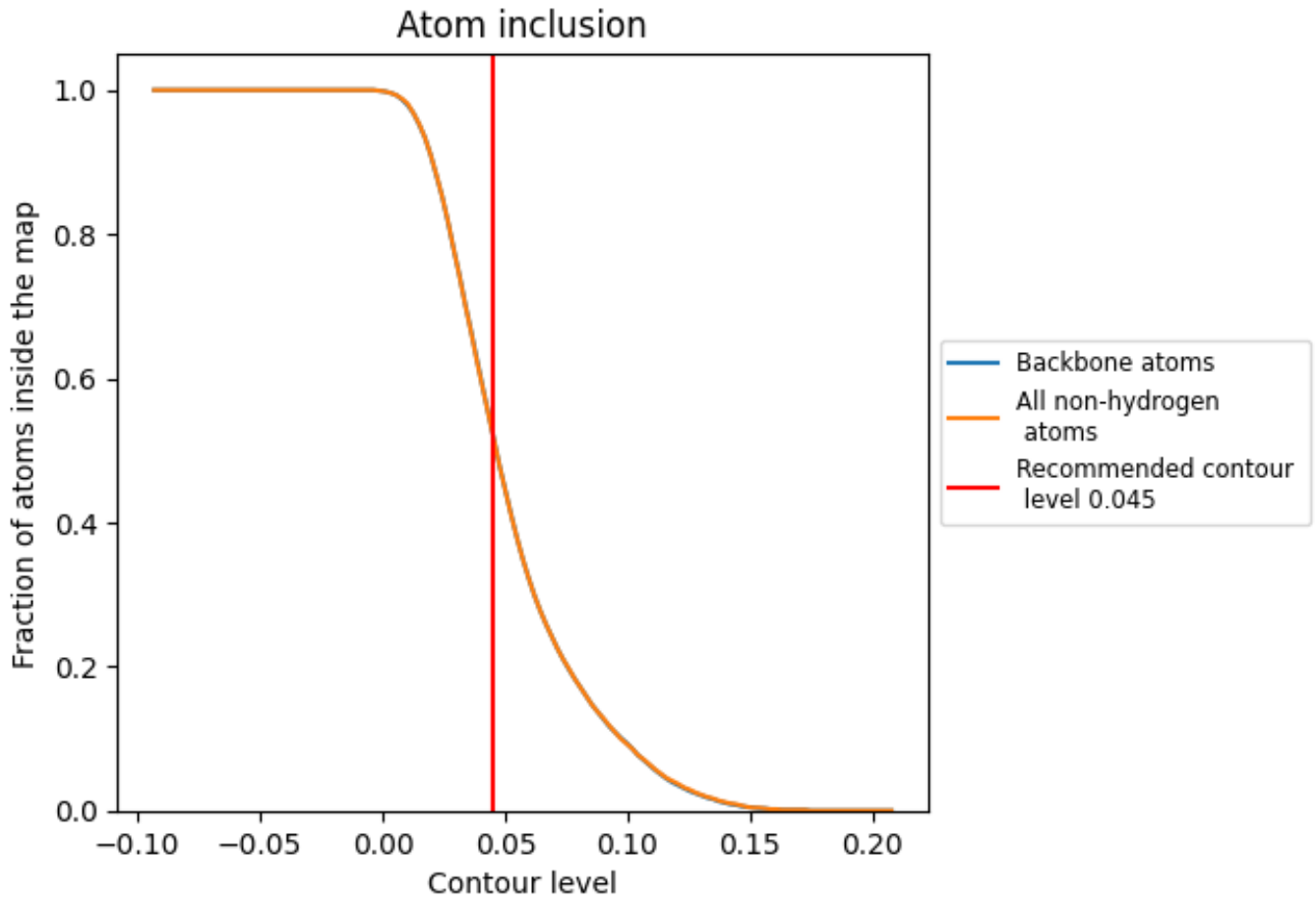
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5210	0.3970
A	0.5310	0.3960
B	0.5310	0.3970
C	0.5310	0.3960
D	0.5310	0.3960
G	0.5130	0.4030
H	0.5130	0.4080
I	0.5120	0.4050
J	0.5130	0.4030

