Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 04:55 PM JST

PDB ID	:	26IR / pdb_000026ir
EMDB ID	:	EMD-80686
Title	:	Structure of recombinant RyR2 in complex with Ryanozole in the closed conformation (Ca2+ dataset)
Authors	:	Otori, Y.; Takeuchi, S.; Ogawa, H.
Deposited on	:	2026-05-01
Resolution	:	3.35 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:

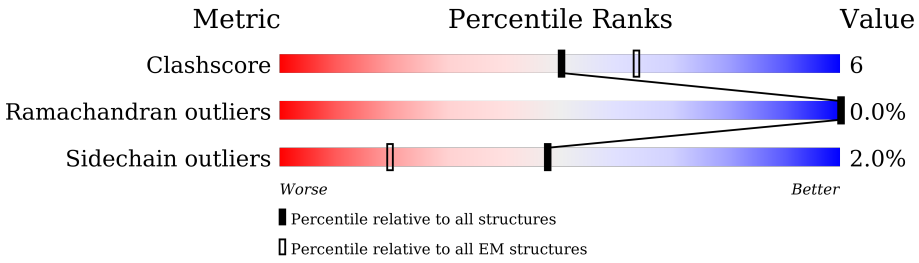
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

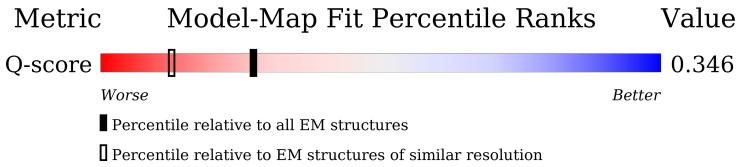
1 Overall quality at a glance

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

The reported resolution of this entry is 3.35 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.





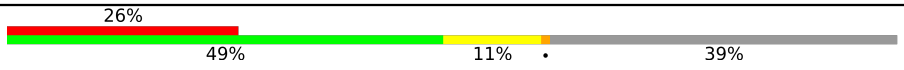
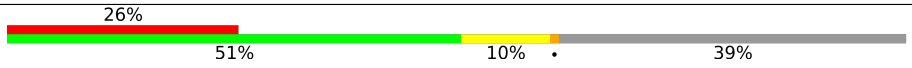
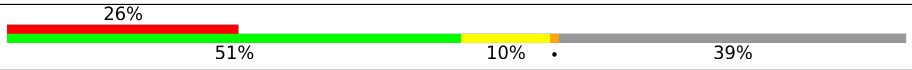
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14390 (2.85 - 3.85)

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	30% 60% 10% 30%
1	B	4966	30% 59% 11% 30%
1	C	4966	30% 60% 10% 30%
1	D	4966	30% 60% 10% 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 5 unique types of molecules in this entry. The entry contains 228528 atoms, of which 113520 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
			55452	17769	27546	4747	5200	190		
1	B	3494	Total	C	H	N	O	S	0	0
			55452	17769	27546	4747	5200	190		
1	C	3494	Total	C	H	N	O	S	0	0
			55452	17769	27546	4747	5200	190		
1	D	3494	Total	C	H	N	O	S	0	0
			55452	17769	27546	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
			1641	516	822	144	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1641	516	822	144	155	4		
2	I	107	Total	C	H	N	O	S	0	0
			1641	516	822	144	155	4		
2	J	107	Total	C	H	N	O	S	0	0
			1641	516	822	144	155	4		

There are 276 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

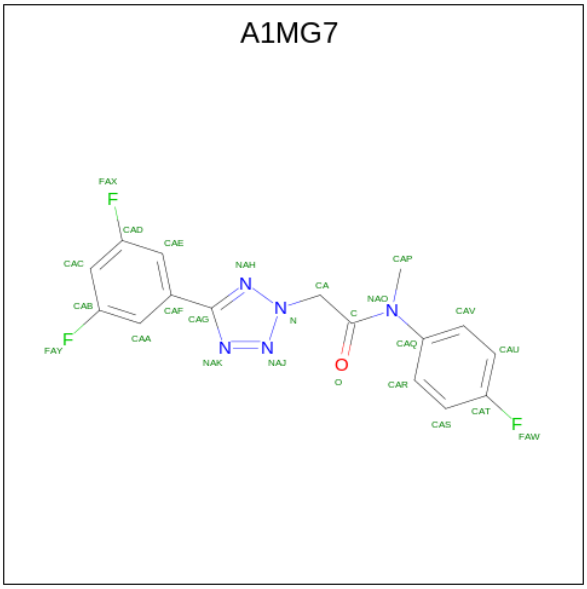
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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 CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	C	1	Total Ca 1 1	0
4	D	1	Total Ca 1 1	0

- Molecule 5 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
5	A	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
5	B	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
5	C	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
5	D	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	

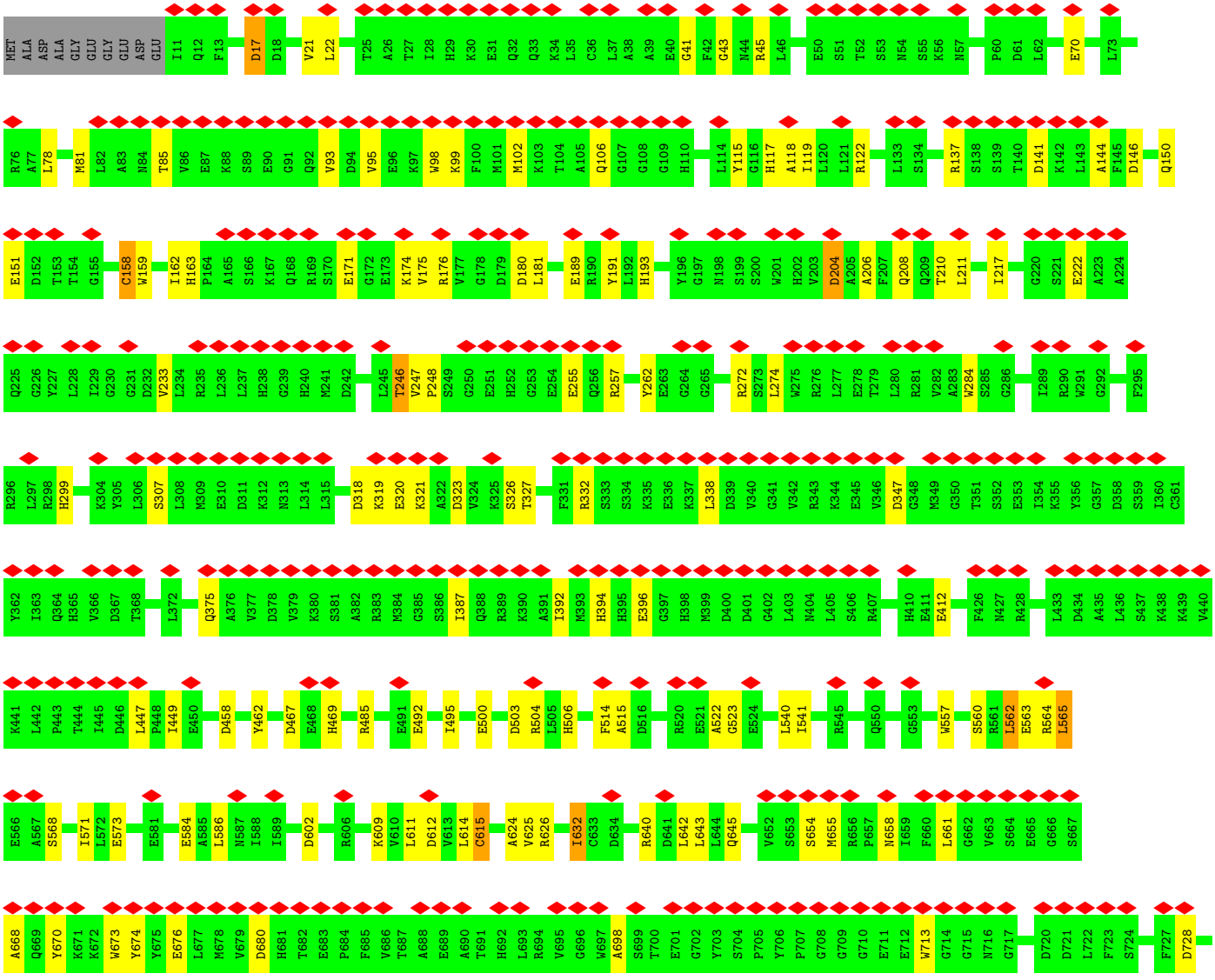
3 Residue-property plots (i)

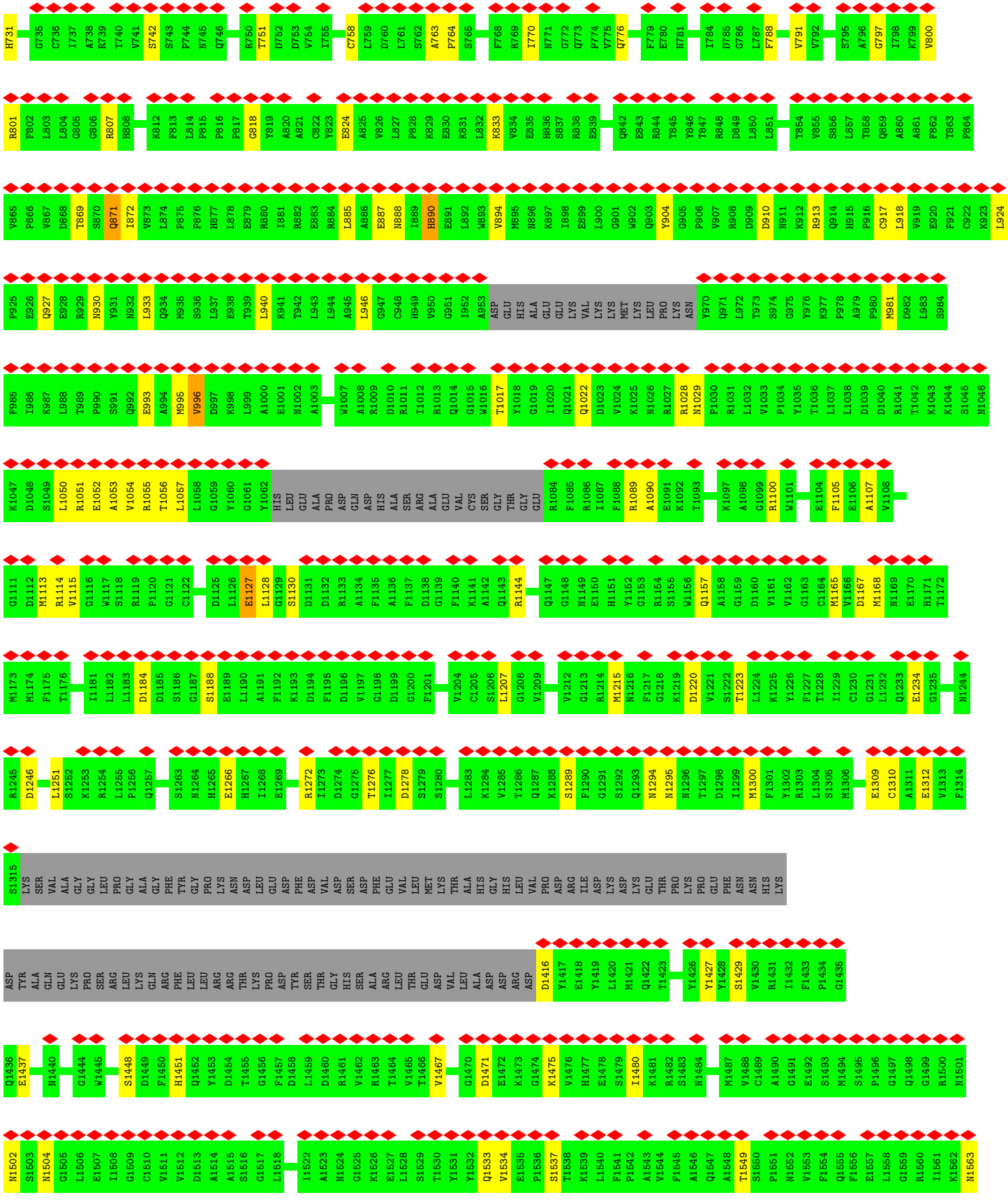
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

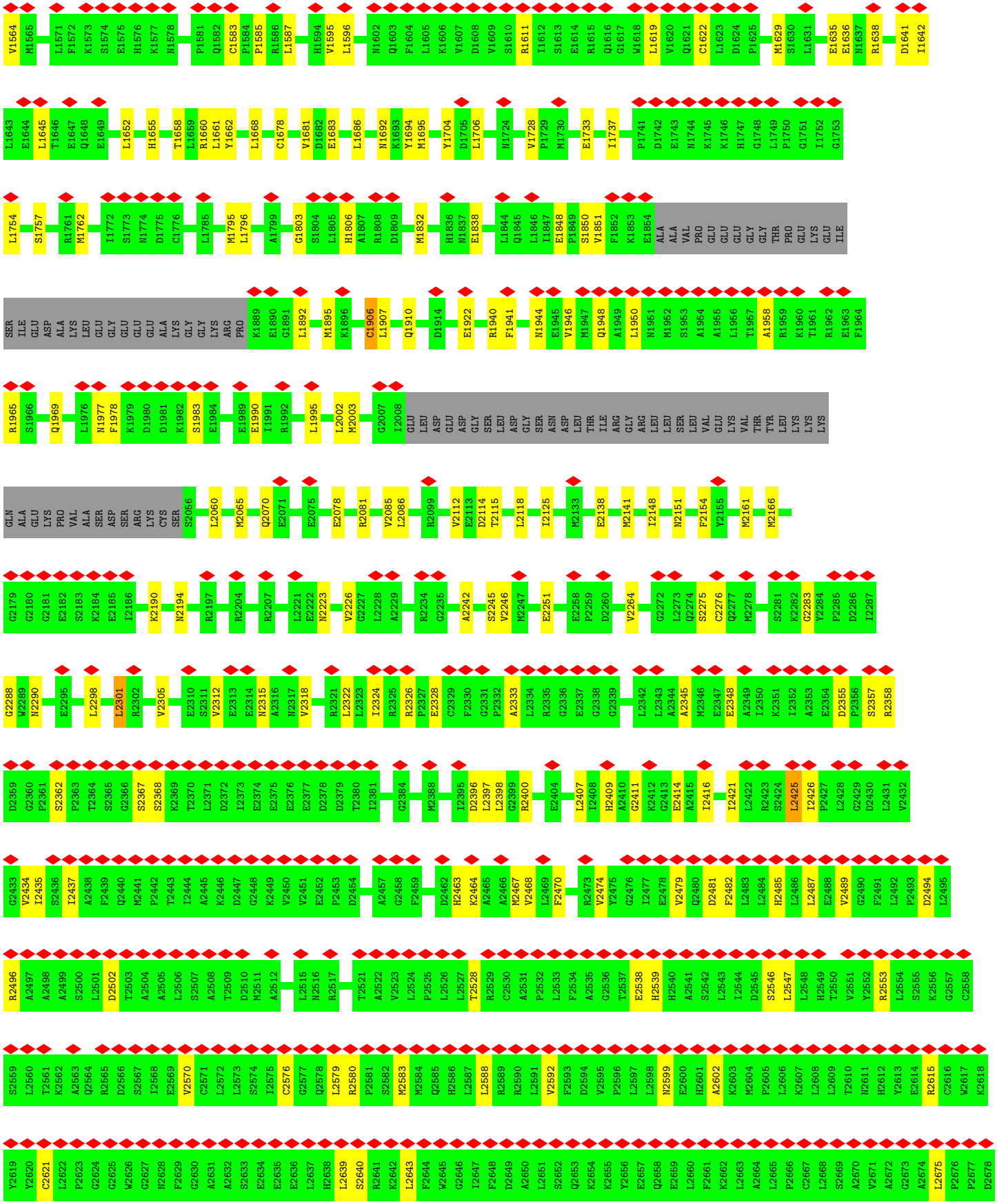
- Molecule 1: Ryanodine receptor 2

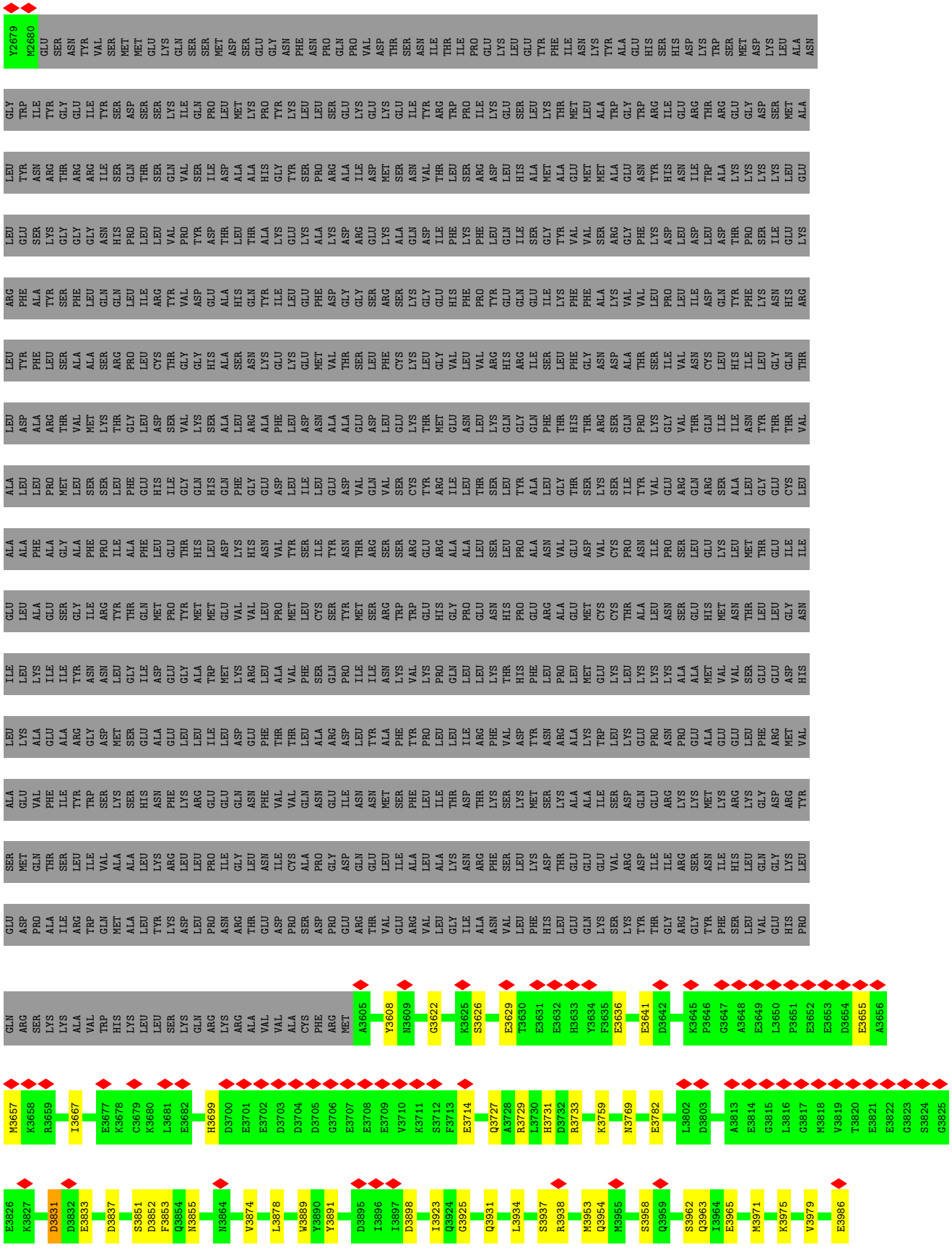
Chain A:

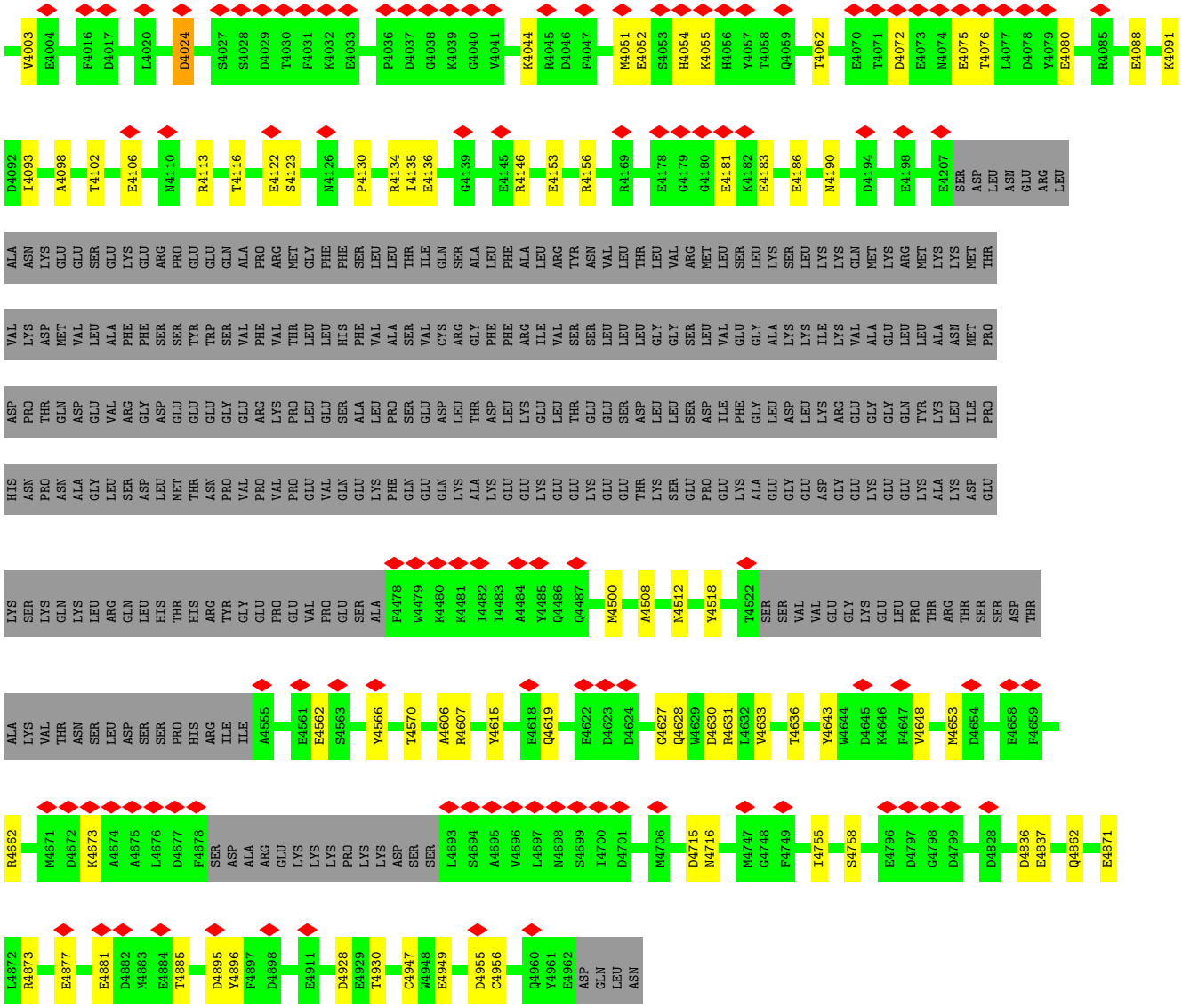





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R801 F802 L803 L804 G805 G806 R807 H808 K812 F813 L814 P815 P816 P817 G818 Y819 A820 A821 C822 Y823 E824 A825 V826 L827 P828 K829 E830 K831 L832 K833 V834 E835 H836 S837 R838 E839 Q842 E843 R844 T845 Y846 T847 R848 D849 L850 L851 T854 V855 S856 L857 T858 Q859 A860 A861 F862 T863 P864
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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 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 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 I1087 F1088 R1089 A1090 E1091 K1092 T1093 K1097 A1098 G1099 R1100 W1101 E1104 F1105 E1106 A1107 Y1108
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M1173 M1174 F1175 T1176 I1181 L1182 L1183 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1197 G1198 D1199 G1200 F1201 V1204 C1205 S1206 L1207 G1208 V1209 V1212 G1213 R1214 M1215 N1216 F1217 G1218 K1219 D1220 V1221 S1222 T1223 L1224 K1225 Y1226 F1227 T1228 I1229 C1230 G1231 L1232 Q1233 E1234 G1235 N1244
R1245 D1246 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 S1263 N1264 H1265 E1266 H1267 I1268 E1269 R1272 I1273 D1274 G1275 T1276 I1277 D1278 S1279 S1280 L1283 K1284 V1285 T1286 Q1287 K1288 S1289 F1290 G1291 S1292 Q1293 N1294 N1295 N1296 T1297 D1298 I1299 M1300 F1301 Y1302 R1303 L1304 S1305 M1306 E1309 C1310 A1311 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 Q1422 T1423 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 F1433 P1434 G1435
Q1436 E1437 N1440 G1444 W1445 S1448 D1449 F1450 H1451 Q1452 Y1453 D1454 T1455 G1456 F1457 D1458 L1459 D1460 R1461 V1462 R1463 T1464 V1465 T1466 V1467 G1470 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 I1480 K1481 R1482 S1483 N1484 M1487 V1488 C1489 A1490 G1491 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501
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V1564 M1565 L1571 F1572 K1573 S1574 E1575 H1576 K1577 N1578 P1581 Q1582 C1583 P1584 P1585 R1586 L1587 H1594 V1595 L1596 N1602 Q1603 F1604 L1605 K1606 V1607 D1608 V1609 S1610 R1611 I1612 S1613 E1614 R1615 Q1616 G1617 W1618 L1619 V1620 Q1621 C1622 L1623 D1624 P1625 M1629 S1630 L1631 E1635 E1636 N1637 R1638 D1641 I1642
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SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 E1890 G1891 L1892 M1895 K1896 C1906 L1907 Q1910 D1914 E1922 R1940 F1941 N1944 E1945 V1946 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961 R1962 E1963 F1964
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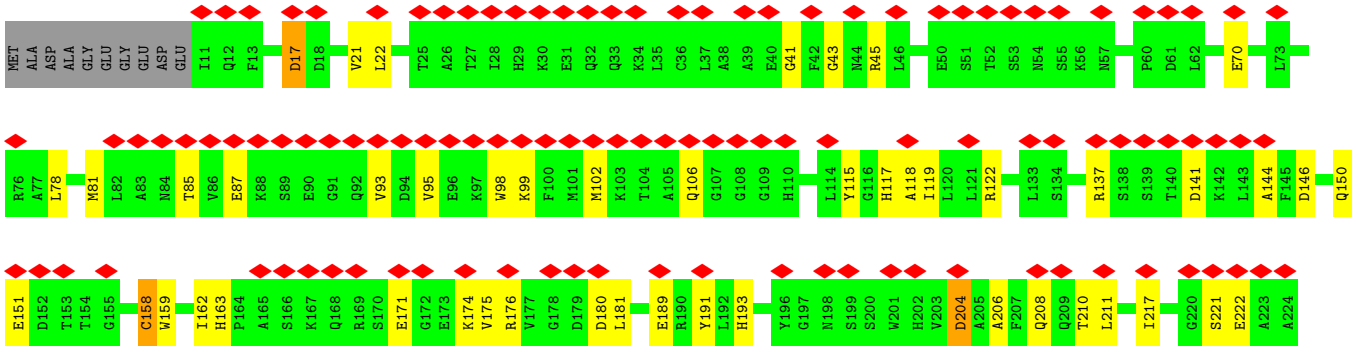

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GLY TRP ILE TYR GLY GLU ILE TYR SER ASP SER SER LYS ILE GLN PRO LEU MET LYS PRO TYR LYS LEU LEU SER GLU LYS GLU LYS GLU SER GLU LYS GLU ILE TYR ARG TRP PRO ILE LYS GLU SER LEU LYS THR MET LEU ALA TRP GLY TRP ARG ILE GLU ARG THR MET ALA
LEU TYR ASN ARG THR ARG ILE SER GLN THR SER GLN VAL SER ILE ASP 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 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 ASN ILE PHE LYS PHE LEU GLN ILE SER GLY TYR 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 GLY GLY SER GLY SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS LYS GLY GLY 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 LEU VAL ASN CYS LEU HIS ILE LEU GLY THR
LEU ASP ALA ARG THR VAL MET LYS THR GLY LEU ASP SER VAL LYS SER ALA ALA LEU ARG ALA PHE LEU ASP ASN ALA ALA GLU ASP LEU GLU LYS THR MET VAL ARG HIS THR 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 ASP VAL SER GLN LEU TYR ALA LEU LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER LEU GLU LEU PHE THR HIS SER GLN PRO VAL GLY THR SER LEU GLY GLU GLU CYS LEU
ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU HIS ILE ASN ASN VAL TYR SER ILE TYR ASN THR ARG SER SER SER ARG GLU GLU ARG GLN ASP ASN ALA ASP VAL GLN VAL SER CYS TYR ARG ILE LEU LEU THR SER LEU TYR ASP VAL CYS PRO ASN ILE PRO SER LEU GLN ARG GLU ARG ILE ARG ALA ALA LEU ASN SER LEU PRO ALA ASN VAL GLU ASP VAL CYS PRO ASN ILE SER LEU GLU ARG GLU ILE
GLU LEU 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 ASN PRO GLY VAL GLU ARG GLN ARG HIS MET VAL ASN THR LEU GLU GLU GLY
ILE LEU LYS ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LYS LEU LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS
LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU GLU ALA PHE TYR LEU LEU ILE ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL
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SER MET GLN THR SER LEU ILE VAL ALA LYS LEU ILE ASP PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU GLU GLN VAL ASP ARG ASP ILE HIS LEU GLN LEU GLY LYS VAL
GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR ASP PRO GLU ARG THR VAL GLU ARG VAL LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS TYR THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO

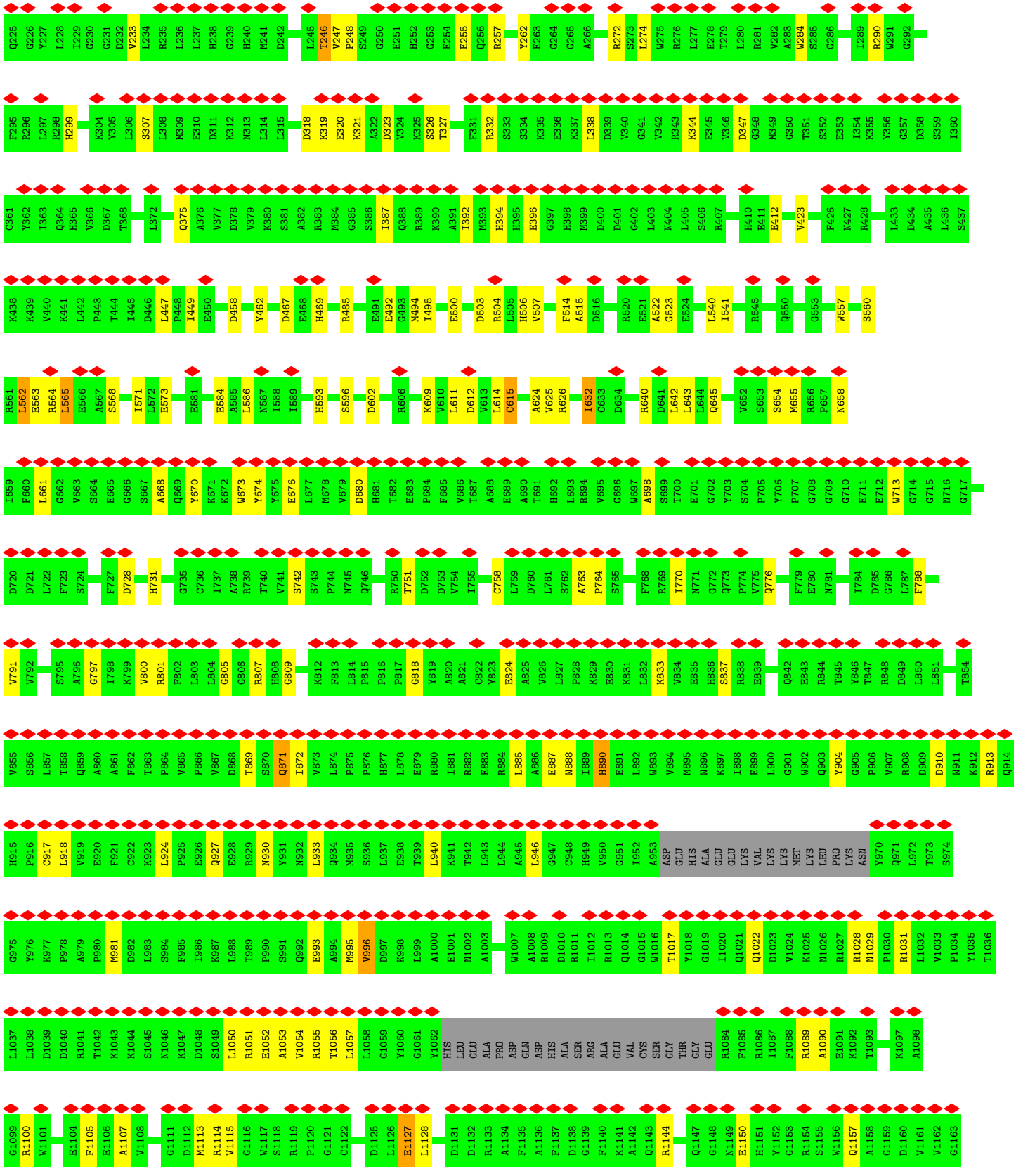


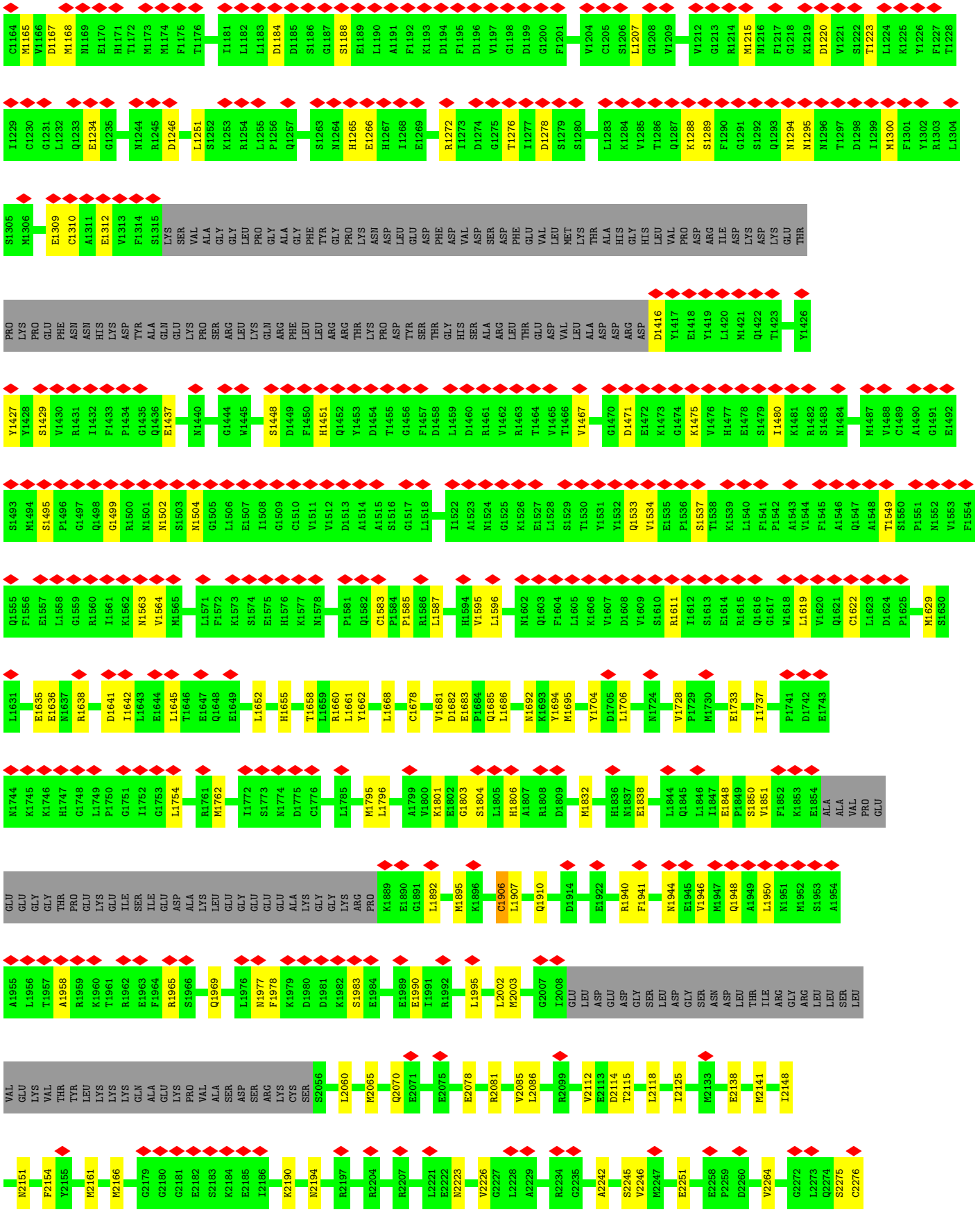
• Molecule 1: Ryanodine receptor 2

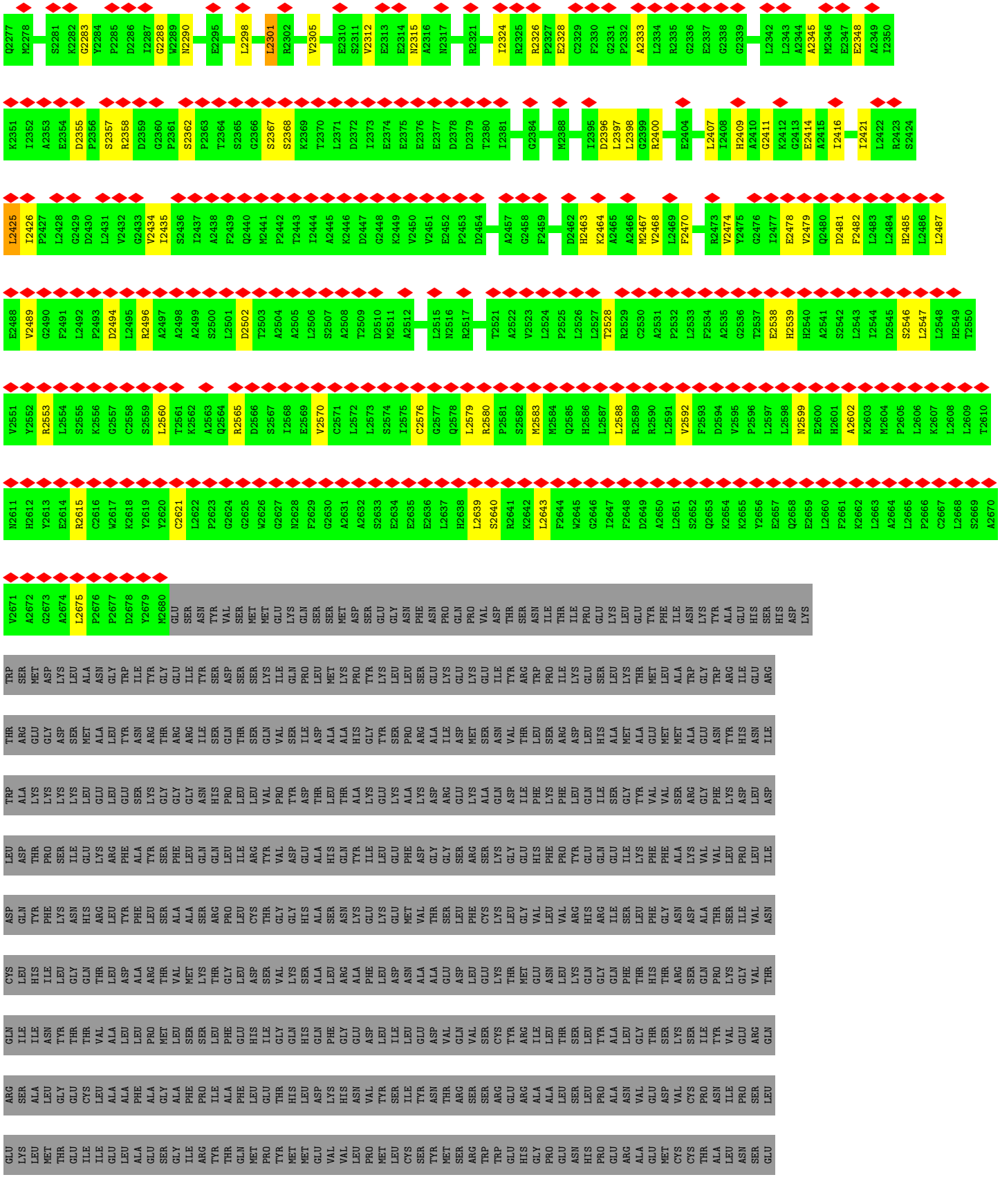
Chain B:

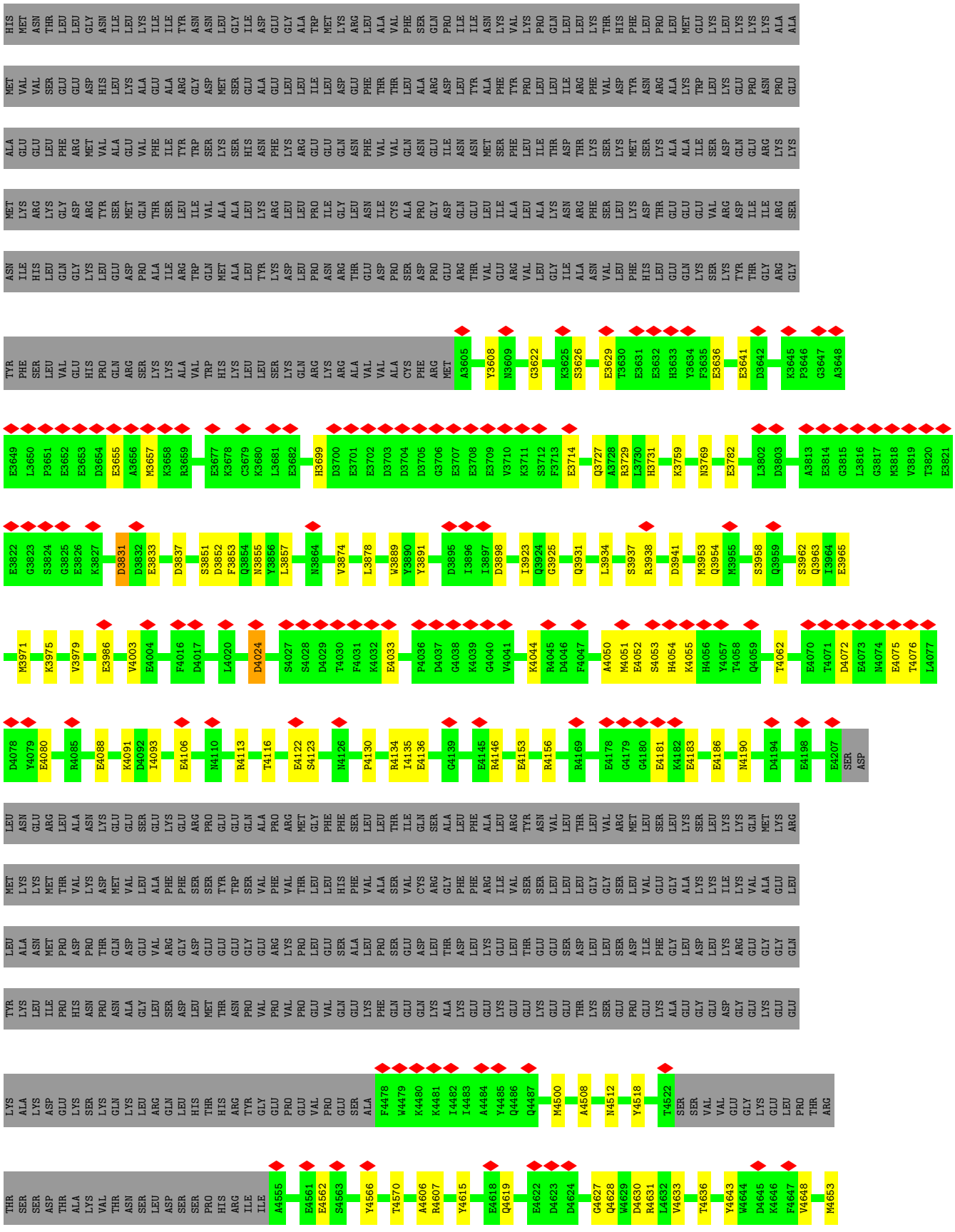


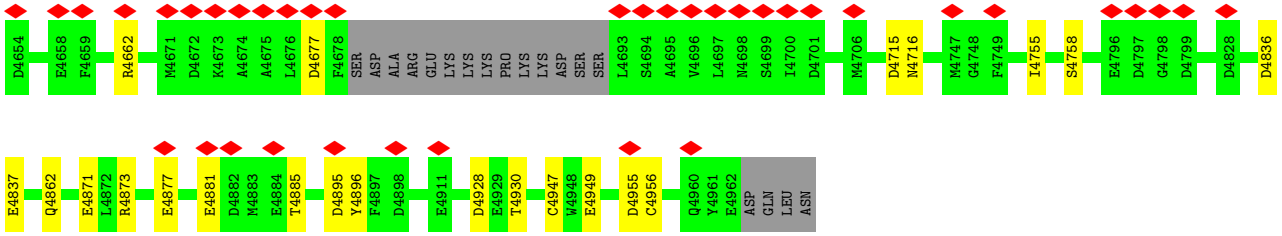



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F295 R296 L297 R298 H299 K304 Y305 L306 S307 L308 M309 E310 D311 K312 N313 L314 L315 D318 K319 E320 K321 A322 D323 V324 K325 S326 T327 F331 R332 S333 S334 K335 E336 K337 L338 D339 V340 G341 V342 R343 K344 E345 V346 D347 G348 M349 G350 T351 S352 E353 I354 K355 Y356 G357 D358 S359 I360
C361 Y362 I363 Q364 H365 V366 D367 T368 L372 Q375 A376 V377 D378 V379 K380 S381 A382 R383 M384 G385 S386 I387 Q388 R389 K390 A391 I392 M393 H394 H395 E396 G397 H398 M399 D400 D401 G402 L403 N404 L405 S406 R407 H410 E411 E412 V423 F426 N427 R428 L433 D434 A435 L436 S437
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I659 F660 L661 G662 V663 S664 E665 G666 S667 A668 Q669 Y670 K671 K672 W673 Y674 Y675 E676 L677 M678 V679 D680 H681 T682 E683 P684 F685 V686 T687 A688 E689 A690 T691 H692 L693 R694 V695 G696 W697 A698 S699 T700 E701 G702 Y703 S704 P705 Y706 P707 G708 G709 G710 E711 E712 W713 G714 G715 N716 G717
D720 D721 L722 F723 S724 F727 D728 H731 G735 C736 I737 A738 R739 T740 V741 S742 S743 P744 N745 Q746 R750 T751 D752 D753 V754 I755 C758 L759 D760 L761 S762 A763 P764 S765 F768 R769 I770 N771 G772 Q773 P774 V775 Q776 F779 E780 N781 I784 D785 G786 L787 F788
V791 V792 S796 A796 G797 I798 K799 V800 R801 P802 L803 L804 G805 G806 R807 H808 G809 K812 P813 L814 P815 P816 P817 G818 Y819 A820 A821 C822 Y823 E824 A825 V826 L827 P828 K829 E830 K831 L832 K833 V834 E835 H836 S837 R838 E839 Q842 E843 R844 T845 Y846 T847 R848 D849 L850 L851 T854
V855 S856 L857 T858 Q859 A860 A861 F862 T863 P864 V865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 R884 L885 A886 E887 N888 I889 H890 E891 L892 W893 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 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 T1017 Y1018 G1019 I1020 Q1021 Q1022 D1023 V1024 K1025 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036
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G1099 R1100 W1101 E1104 F1105 E1106 A1107 V1108 G1111 D1112 M1113 R1114 V1115 G1116 W1117 S1118 R1119 P1120 G1121 C1122 D1125 L1126 E1127 L1128 D1131 D1132 R1133 A1134 F1135 A1136 F1137 D1138 G1139 F1140 K1141 A1142 Q1143 R1144 Q1147 G1148 N1149 E1150 H1151 Y1152 G1153 R1154 S1155 W1156 Q1157 A1158 G1159 D1160 V1161 V1162 G1163




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E2488 V2489 G2490 F2491 L2492 P2493 D2494 L2495 R2496 A2497 A2498 A2499 S2500 L2501 D2502 T2503 A2504 A2505 L2506 S2507 A2508 T2509 D2510 M2511 A2512 L2515 N2516 R2517 T2521 A2522 V2523 L2524 P2525 L2526 L2527 T2528 R2529 C2530 A2531 P2532 L2533 F2534 A2535 G2536 T2537 E2538 H2539 H2540 A2541 S2542 L2543 I2544 D2545 S2546 L2547 L2548 H2549 T2550
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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 ILE TYR GLY GLU ILE TYR SER ASP SER SER LYS ILE GLN PRO LEU MET LYS PRO TYR LYS LEU GLU 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 ASP SER MET ALA LEU TYR ASN 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 SER LYS GLY 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 SER ALA 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 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 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 ALA 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 ALA ALA LEU SER LEU PRO ALA ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU
GLU LYS LEU MET THR GLU ILE ILE GLU LEU 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 GLU

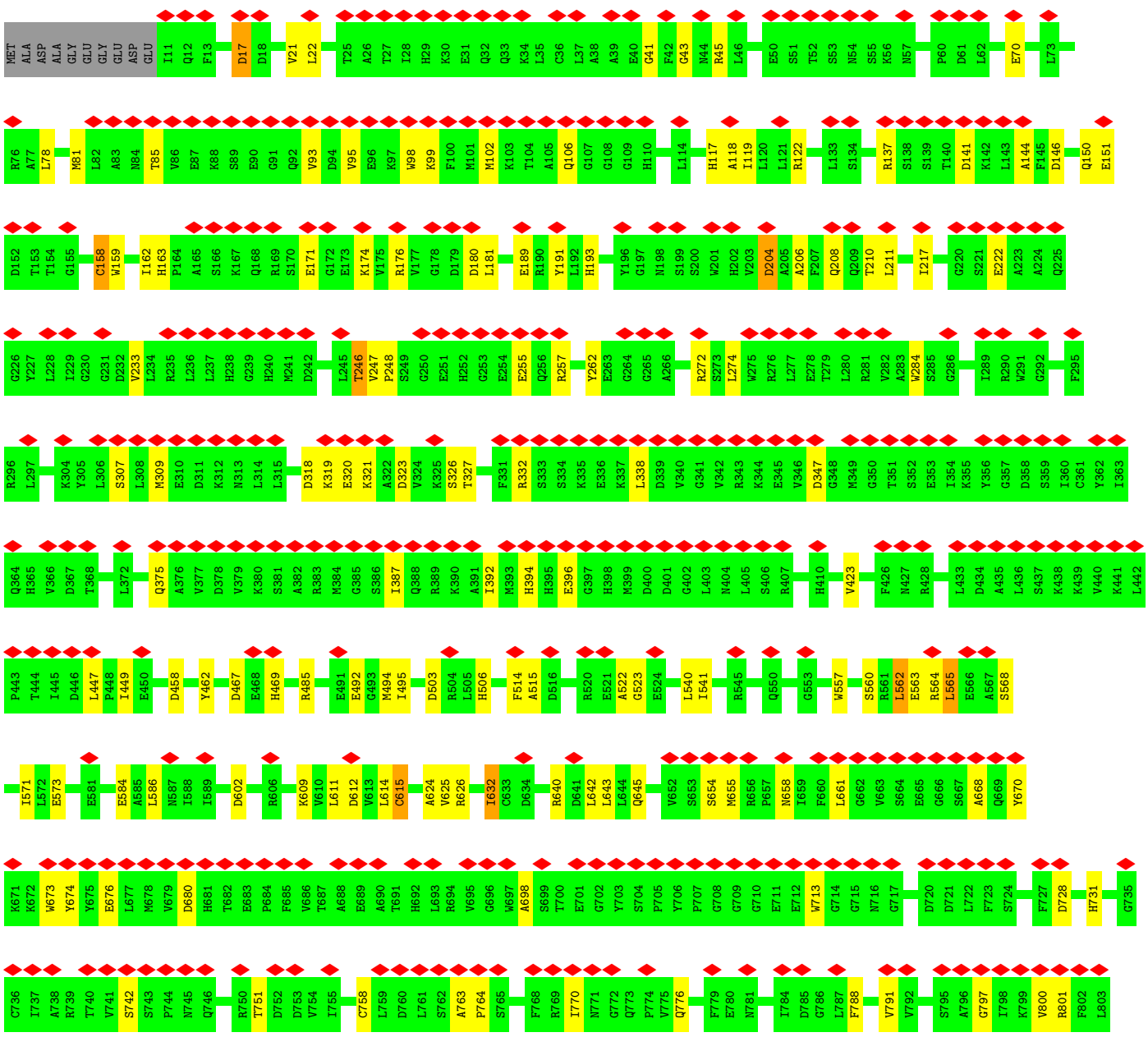

HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS LYS ALA ALA
MET VAL VAL SER GLU GLU ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE GLU ASP ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU
ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA ILE SER ASP GLN GLU LYS ARG LYS
MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU GLU ILE ARG ILE ARG ARG SER
ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP PRO GLU ARG THR VAL GLU ARG VAL LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN GLN LYS SER LYS TYR THR GLY ARG GLY
TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS LEU LEU SER LYS GLN ARG LYS ASN ALA VAL ALA CYS PHE ARG MET A3605 Y3608 M3609 G3622 K3625 S3626 E3629 T3630 E3631 E3632 H3633 Y3634 F3635 E3636 E3641 D3642 K3645 P3646 G3647 A3648
E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 E3677 K3678 C3679 K3680 L3681 E3682 H3699 D3700 E3701 E3702 D3703 D3704 D3705 G3706 E3707 E3708 E3709 V3710 K3711 S3712 F3713 E3714 Q3727 A3728 R3729 L3730 H3731 K3759 N3769 E3782 L3802 D3803 A3813 E3814 G3815 L3816 G3817 M3818 V3819 T3820 E3821
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M3971 K3975 V3979 E3986 V4003 E4004 F4016 D4017 L4020 D4024 S4027 S4028 D4029 T4030 F4031 K4032 E4033 P4036 D4037 G4038 K4039 G4040 V4041 K4044 R4045 D4046 F4047 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Y4057 T4058 Q4059 T4062 E4070 T4071 D4072 E4073 N4074 E4075 T4076 L4077
D4078 Y4079 E4080 R4085 E4088 K4091 D4092 I4093 E4106 N4110 R4113 T4116 E4122 S4123 N4126 P4130 R4134 I4135 E4136 G4139 E4145 R4146 E4153 R4156 R4169 E4178 G4179 G4180 E4181 K4182 E4183 E4186 N4190 D4194 E4198 E4207 SER ASP
LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS ARG
MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE VAL ALA SER VAL CYS ARG GLY PHE PHE ARG ILE VAL SER SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY GLY ALA ALA LYS LYS ILE LYS VAL ALA GLU GLY LEU
LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLU GLU GLY GLU ARG LYS PRO LEU GLU SER ALA LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLN
TYR LYS LEU ILE PRO HIS ASN PRO ASN GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU GLU LYS GLU GLU THR LYS SER GLU PRO GLU LYS ALA GLU GLY GLU ASP GLY GLU LYS GLU
LYS ALA LYS ASP GLU LYS LEU LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU GLN SER ALA F4478 W4479 K4480 K4481 I4482 I4483 A4484 Y4485 Q4486 Q4487 M4500 A4508 N4512 Y4518 T4522 SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG
THR SER SER ASP THR ALA LYS VAL THR ASN SER LEU ASP SER SER PRO HIS ARG ILE ILE A4555 E4561 E4562 S4563 Y4566 T4570 A4606 R4607 Y4615 E4618 Q4619 E4622 D4623 D4624 G4627 Q4628 M4629 D4630 R4631 L4632 V4633 T4636 Y4643 M4644 D4645 K4646 F4647 V4648 M4653

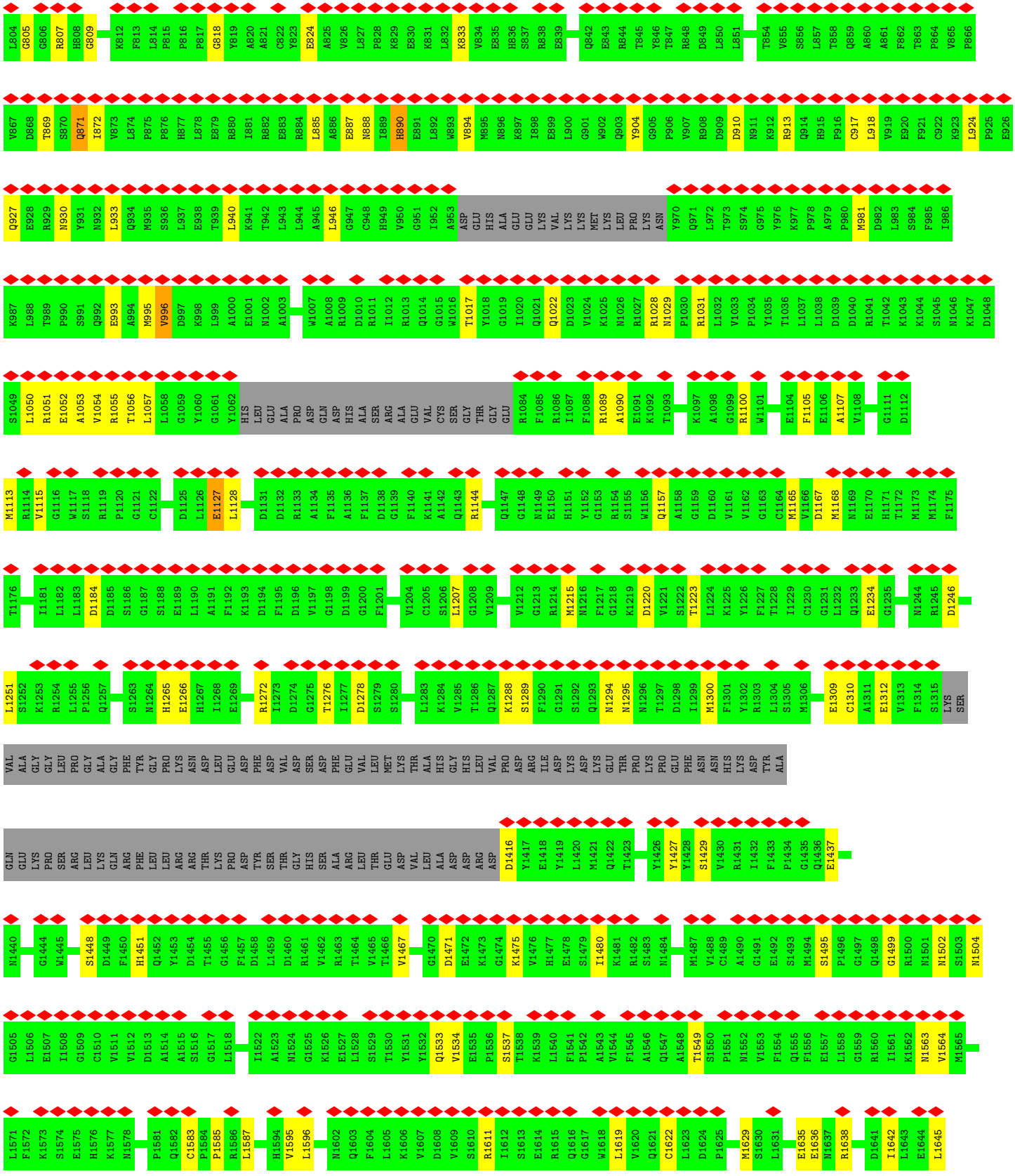


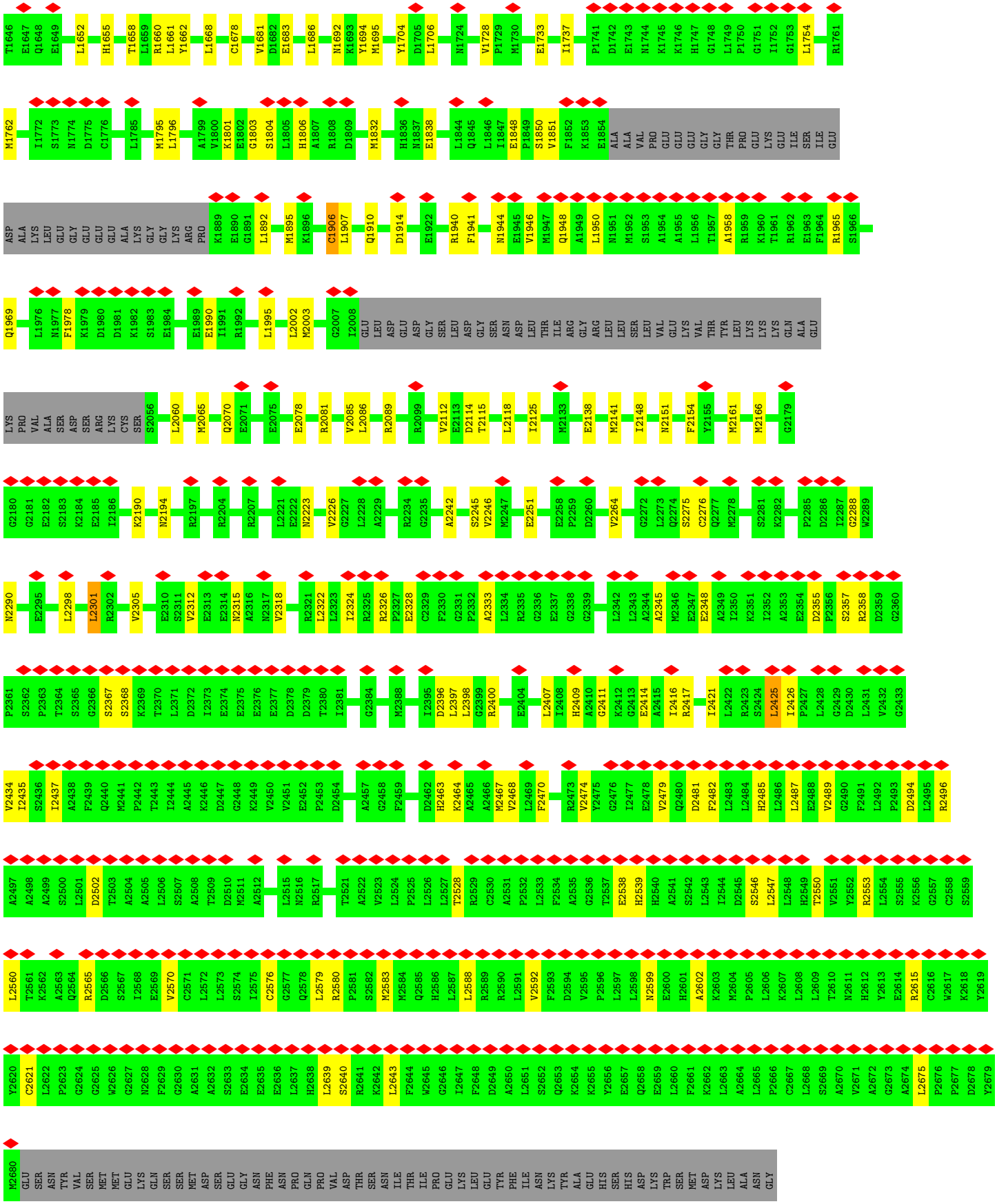
• Molecule 1: Ryanodine receptor 2

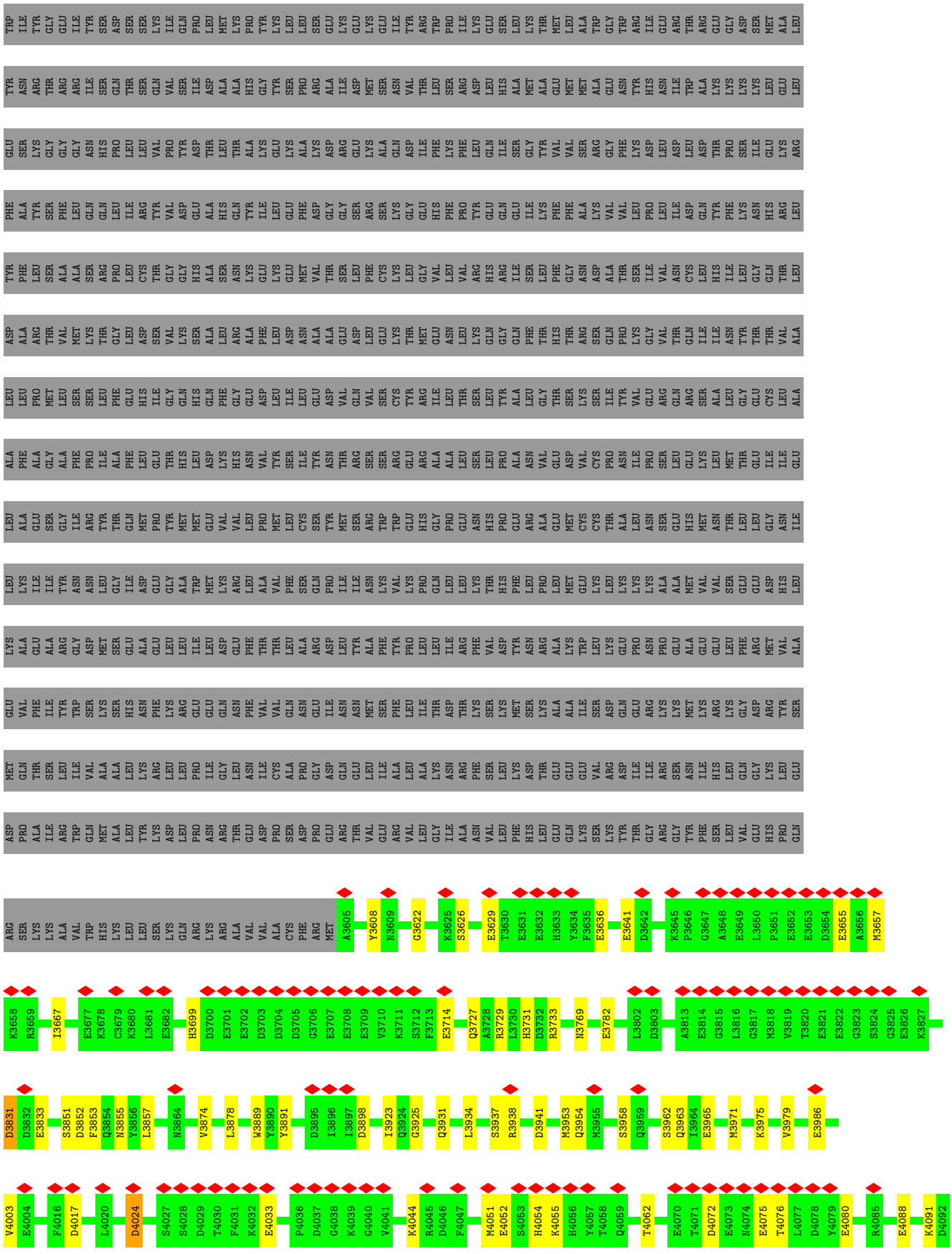
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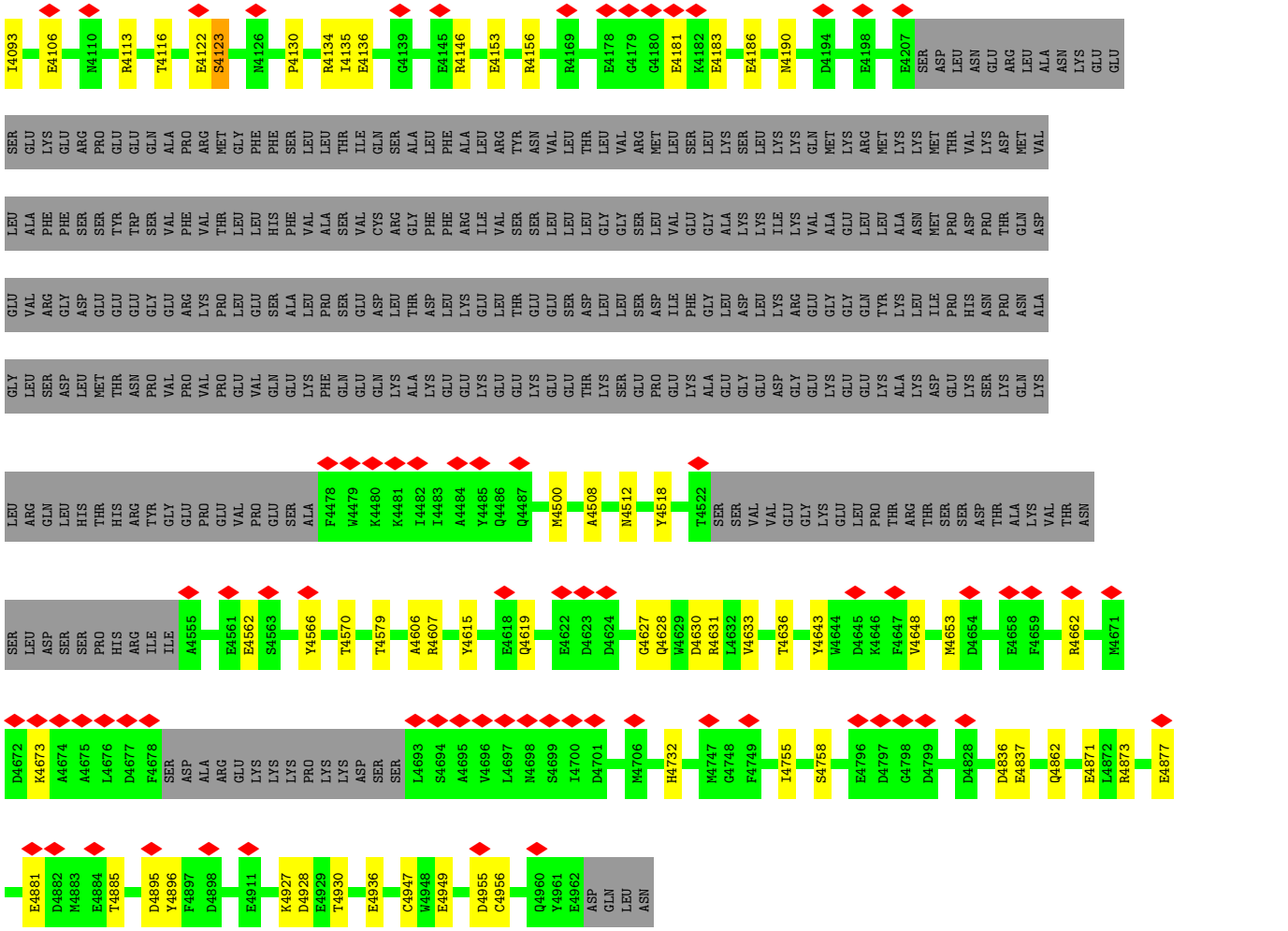





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S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 I1087 F1088 R1089 A1090 E1091 K1092 T1093 K1097 A1098 G1099 R1100 W1101 E1104 F1105 E1106 A1107 V1108 G1111 D1112
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T1176 I1181 L1182 L1183 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1197 G1198 D1199 G1200 F1201 V1204 C1205 S1206 L1207 G1208 V1209 V1212 G1213 R1214 M1215 N1216 F1217 G1218 K1219 D1220 V1221 S1222 T1223 L1224 K1225 Y1226 F1227 T1228 I1229 C1230 G1231 L1232 Q1233 E1234 G1235 N1244 R1245 D1246
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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 Q1422 T1423 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 F1433 P1434 G1435 Q1436 E1437
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T1646 E1647 Q1648 E1649 L1652 H1655 T1658 L1659 R1660 L1661 Y1662 L1668 C1678 V1681 D1682 E1683 L1686 N1692 K1693 Y1694 M1695 Y1704 D1705 L1706 N1724 V1728 P1729 M1730 E1733 I1737 P1741 D1742 E1743 N1744 K1745 K1746 H1747 G1748 L1749 P1750 G1751 I1752 G1753 L1754 R1761
M1762 I1772 S1773 N1774 D1775 C1776 L1785 M1795 L1796 A1799 V1800 K1801 E1802 G1803 S1804 L1805 H1806 A1807 R1808 D1809 M1832 H1836 N1837 E1838 L1844 Q1845 L1846 I1847 E1848 P1849 S1850 V1851 F1852 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 G1891 L1892 M1895 K1896 C1906 L1907 Q1910 D1914 E1922 R1940 F1941 N1944 E1945 V1946 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961 R1962 E1963 F1964 R1965 S1966
Q1969 L1976 N1977 F1978 K1979 D1980 D1981 K1982 S1983 E1984 E1989 E1990 I1991 R1992 L1995 L2002 M2003 G2007 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 L2060 M2065 Q2070 E2071 E2075 E2078 R2081 V2085 L2086 R2089 R2099 V2112 E2113 D2114 T2115 L2118 I2125 M2133 E2138 M2141 I2148 N2151 F2154 Y2155 M2161 M2166 G2179
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P2361 S2362 P2363 T2364 S2365 G2366 S2367 S2368 K2369 T2370 L2371 D2372 I2373 E2374 E2375 E2376 E2377 D2378 D2379 T2380 I2381 G2384 M2388 I2395 D2396 L2397 L2398 G2399 R2400 E2404 L2407 I2408 H2409 A2410 G2411 K2412 G2413 E2414 A2415 I2416 R2417 I2421 L2422 R2423 S2424 L2425 I2426 P2427 L2428 G2429 D2430 L2431 V2432 G2433
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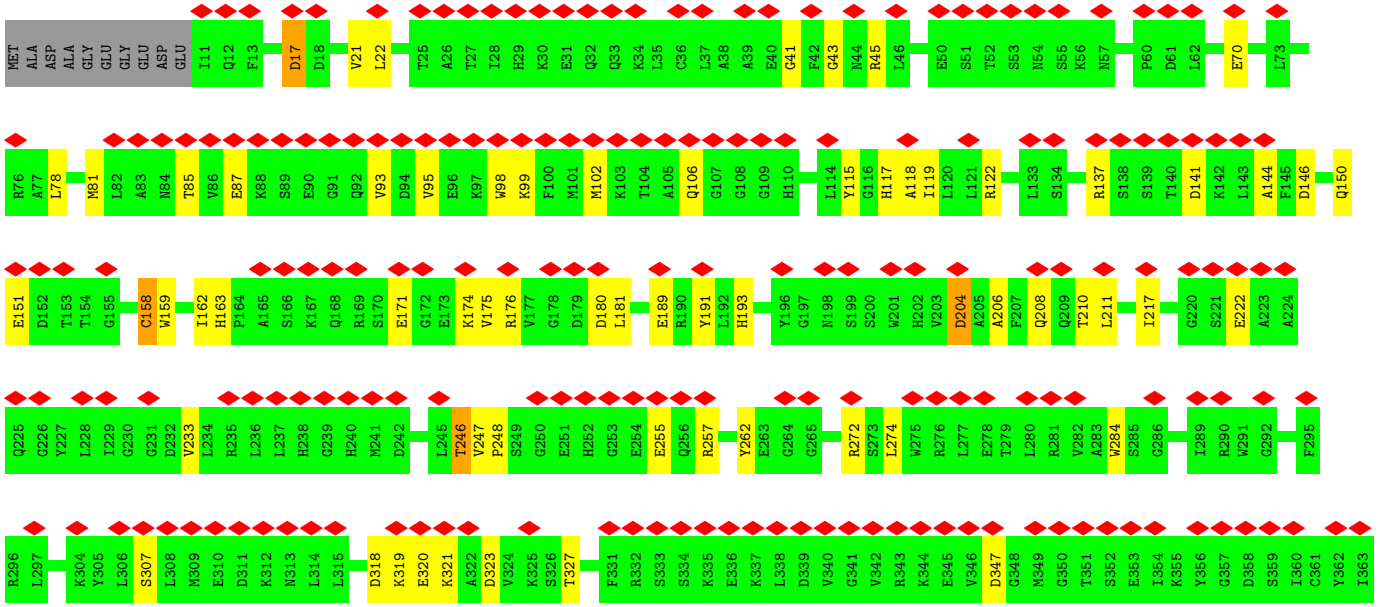

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TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY TYR SER PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG ASP ASN TYR HIS ASN ILE TRP ALA LYS LYS LYS LYS LEU GLU GLU LEU
GLU SER LYS GLY GLY GLY ASN HIS PRO LEU LEU LEU VAL PRO TYR ASP THR LEU THR ALA LYS GLU LYS ALA GLN ASP ILE PHE LYS ARG GLU ILE ASP ARG GLY PHE LYS 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 GLN ILE GLU 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 ARG HIS ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE LEU VAL ASN GLY GLN GLN THR LEU
ASP ALA ARG THR VAL MET LYS THR GLY LEU ASP GLU ALA ALA GLU LEU ARG ALA PHE LEU ASP ASN ALA LEU GLU ASP VAL GLN LYS THR MET GLU LEU VAL ARG GLN GLY GLY GLN PHE THR HIS THR ARG SER GLN PRO LYS GLY VAL THR GLN GLN ARG SER ALA LEU GLU LYS ALA LEU
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 LEU TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER LEU ILE TYR VAL GLU ARG GLN ARG SER LEU GLU LYS SER LEU LEU ALA
ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU HIS 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 LYS SER ILE TYR VAL GLU ARG GLN ARG SER LEU ILE ILE GLU
LEU 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 GLU HIS MET ASN THR LEU GLU LYS SER ILE
LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS ALA ALA MET VAL VAL SER GLU GLU GLU ASP HIS LEU
LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU ILE LEU ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS LEU PRO ALA ARG ILE GLU MET ALA GLU LEU ASN SER GLN PRO ASN PRO GLU ALA GLU ALA ALA ILE SER ASP GLN GLU ARG LEU ALA VAL GLU
GLU VAL PHE ILE SER LYS SER HIS ASN PHE LYS ARG GLU LEU LEU ILE LEU ASN GLN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA ILE SER ASP GLN GLU ARG LYS LYS MET VAL ALA PHE
MET GLN THR SER LEU ILE VAL ALA LEU LYS ARG LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU GLU GLU VAL ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU
ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP PRO GLU ARG THR VAL GLU ARG VAL LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER TYR THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN
ARG LYS LYS ALA VAL ALA CYS PHE ARG MET A3605 Y3608 N3609 G3622 K3625 S3626 E3629 T3630 E3631 E3632 H3633 Y3634 F3635 E3636 E3641 D3642 K3645 P3646 G3647 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657
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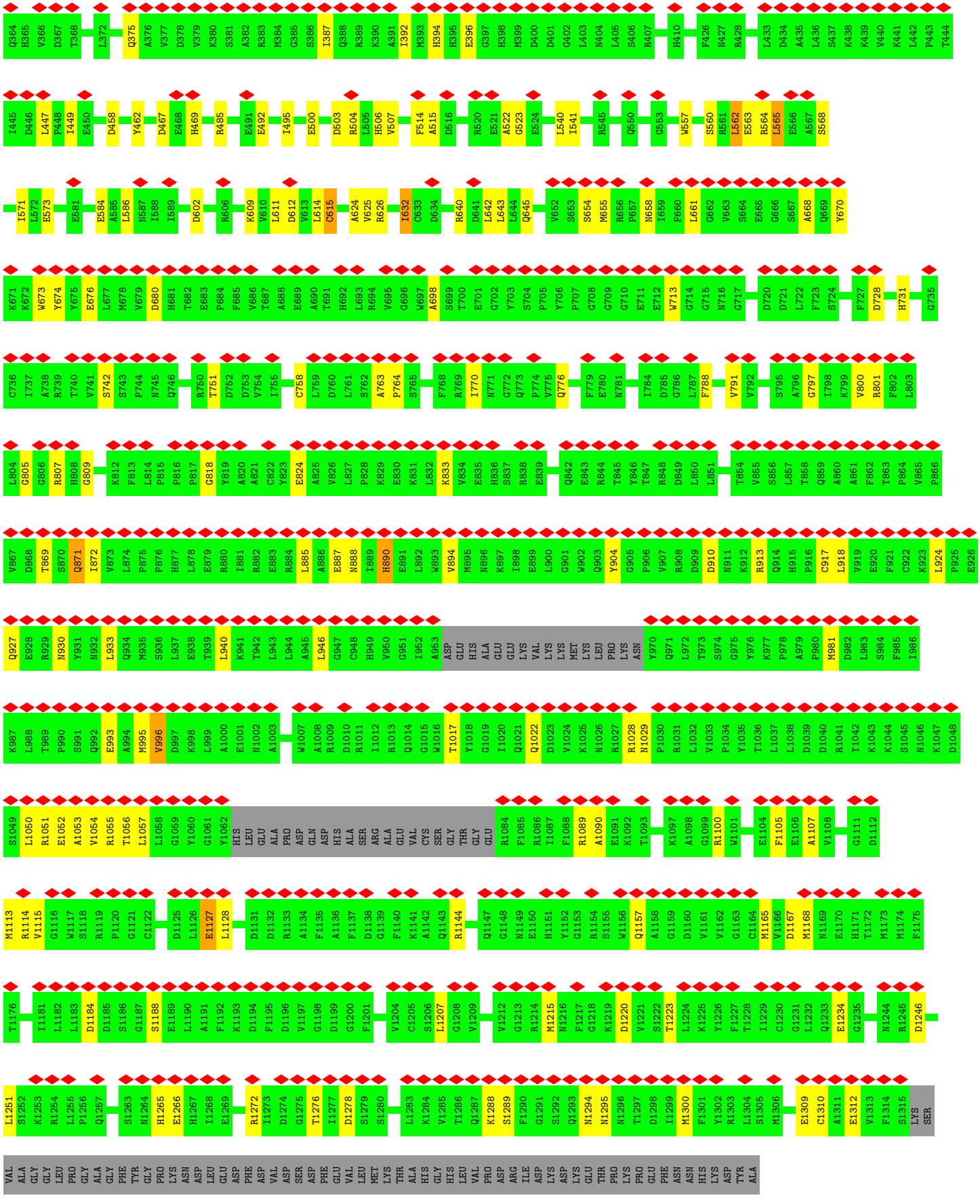


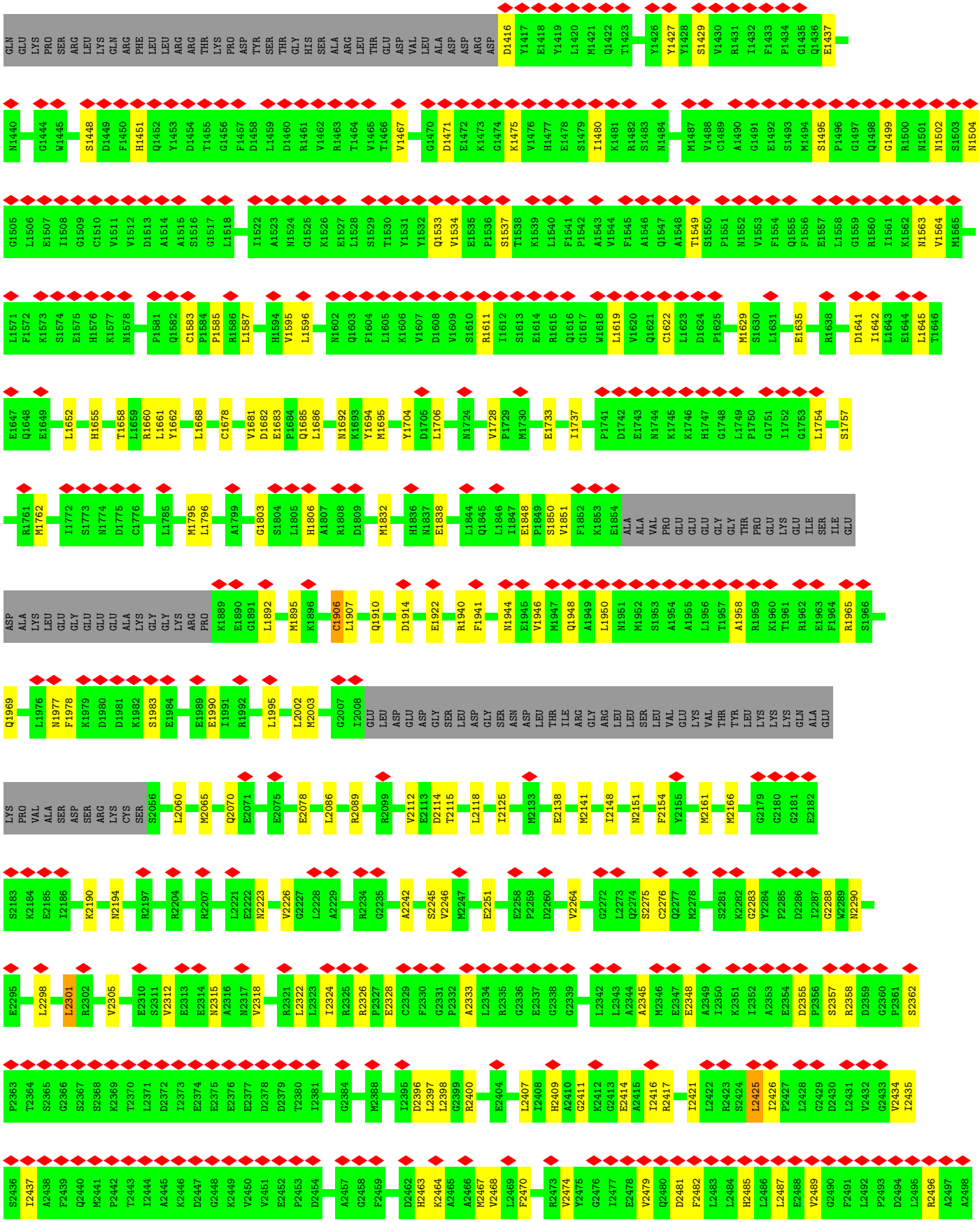
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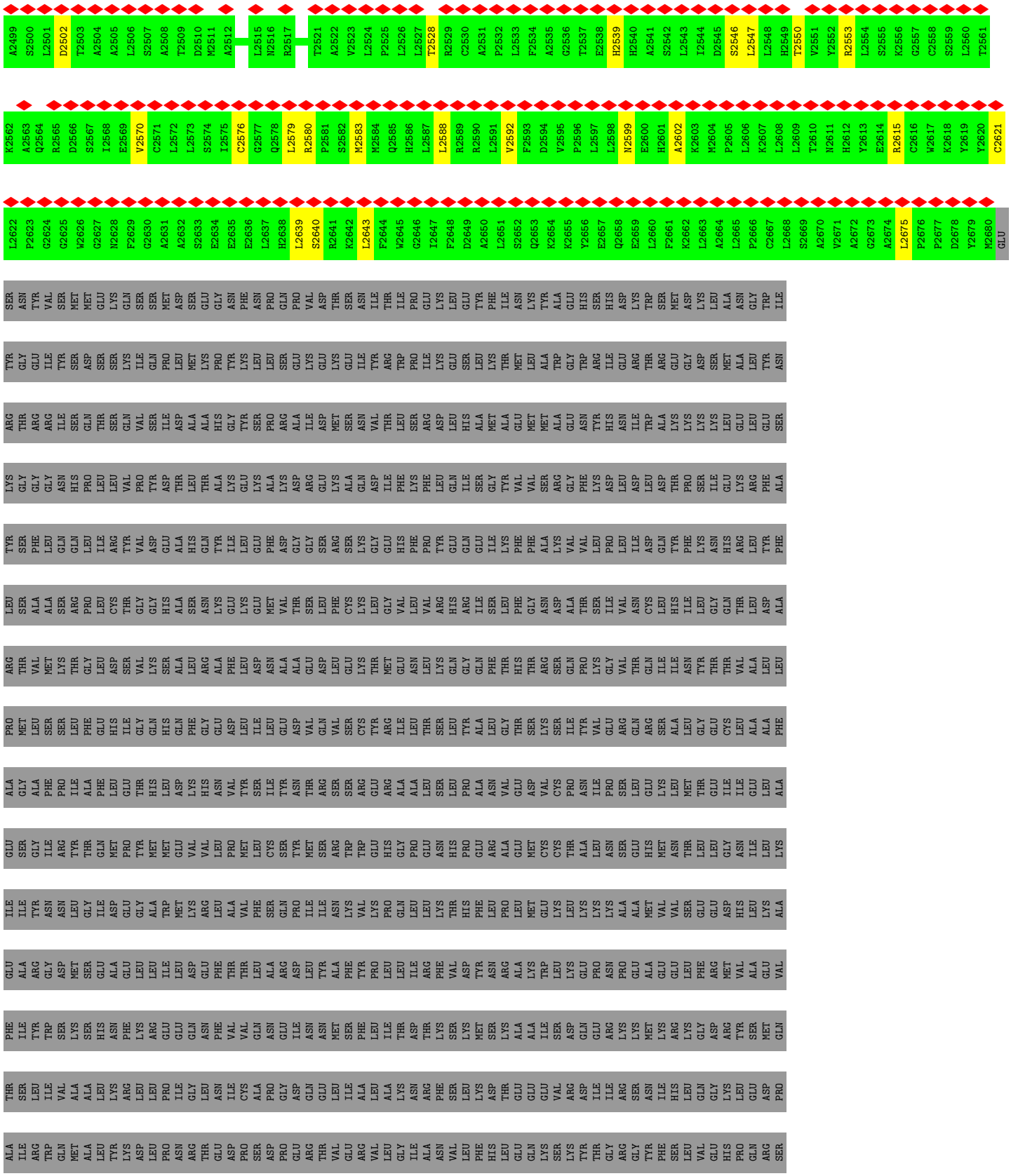
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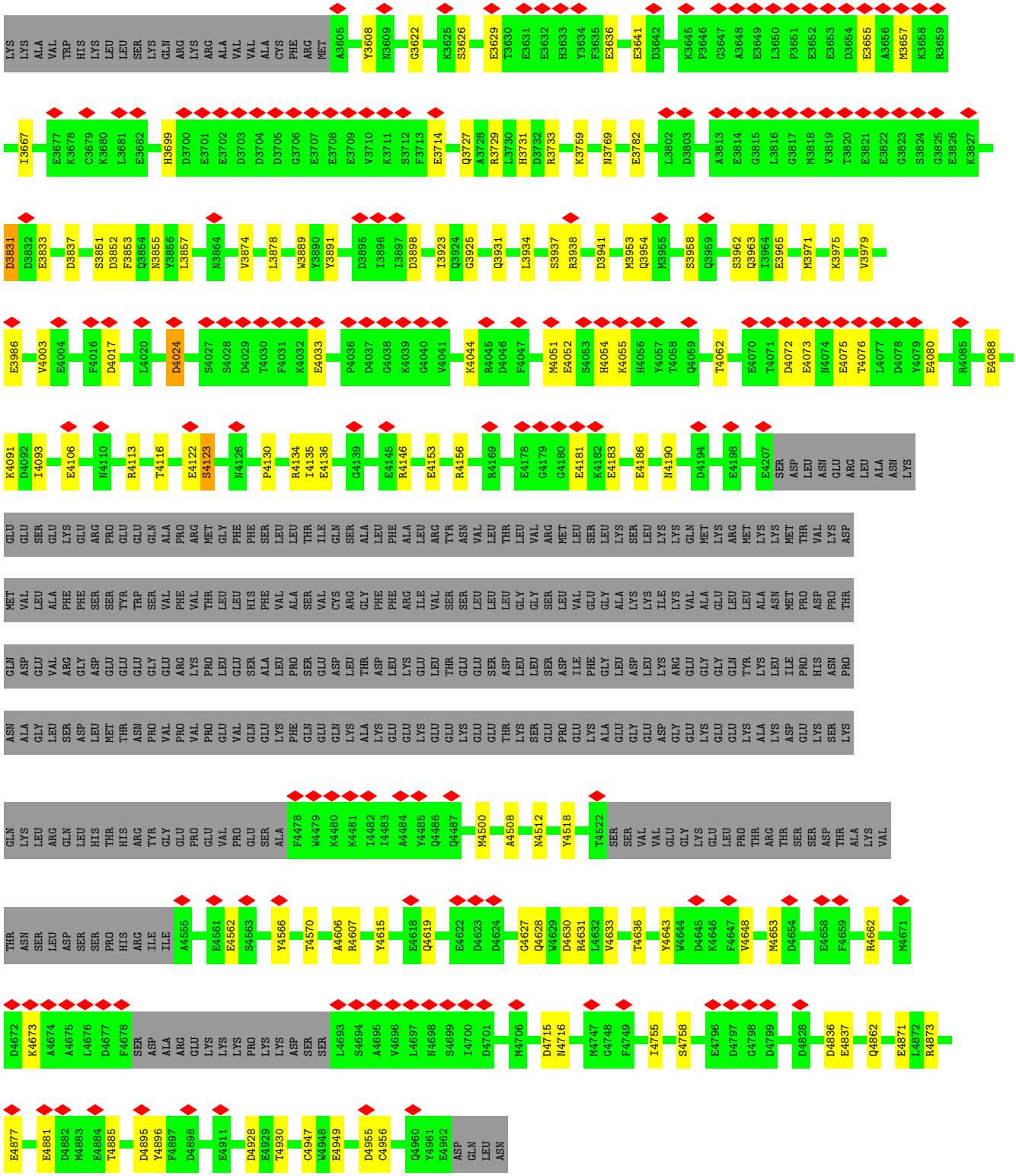





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VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA

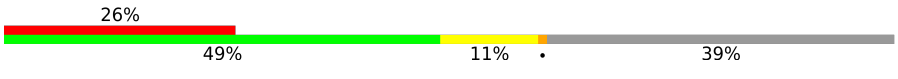

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ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 E1890 G1891 L1892 M1895 K1896 C1906 L1907 Q1910 D1914 E1922 R1940 F1941 N1944 E1945 V1946 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1969 K1960 T1961 R1962 E1963 F1964 R1965 S1966
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A2499 S2500 L2501 D2502 T2503 A2504 A2505 L2506 S2507 A2508 T2509 D2510 M2511 A2512 L2515 N2516 R2517 T2521 A2522 V2523 L2524 P2525 L2526 L2527 T2528 R2529 C2530 A2531 P2532 L2533 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 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 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 SER LYS ILE GLN PRO LEU MET LYS PRO TYR LYS LEU LEU LEU SER GLU LYS GLU LYS 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 SER GLN VAL 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 LEU 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 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 LYS GLU ASP PHE ASP GLY GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS ALA VAL VAL LEU PRO LEU ILE ASP LEU 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 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 GLN GLY GLN PHE THR HIS THR ARG SER GLN PRO LYS GLY VAL THR GLN ILE LEU ASN ASP LEU LEU 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 ALA 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 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 MET THR GLU ILE ILE GLU LEU 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 GLU HIS MET ASN THR LEU GLU GLY ASN ILE LEU LYS
ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO GLU ARG ALA GLU MET GLU LYS LEU LEU LYS LYS ALA ALA MET VAL SER GLU GLU ASP HIS LEU LEU LYS ALA
GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA MET VAL GLU GLU LEU PHE GLU ARG MET VAL ALA GLU VAL
PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN ASN PHE VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN
THR SER LEU ILE VAL ALA LEU LEU LYS ARG LEU LEU LEU PRO ILE GLY LEU ASP PRO ALA ASP GLN GLU LEU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU GLU GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN LEU GLY LYS LEU GLU ASP PRO
ALA ILE ARG TRP GLN LYS ASP LEU ARG THR VAL GLU ARG VAL LEU LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS TYR THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER

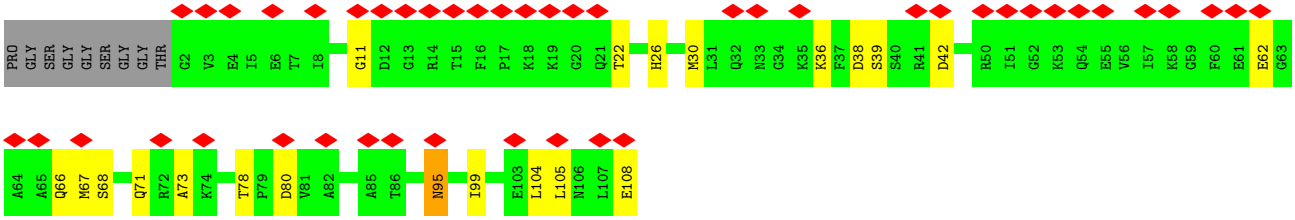


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

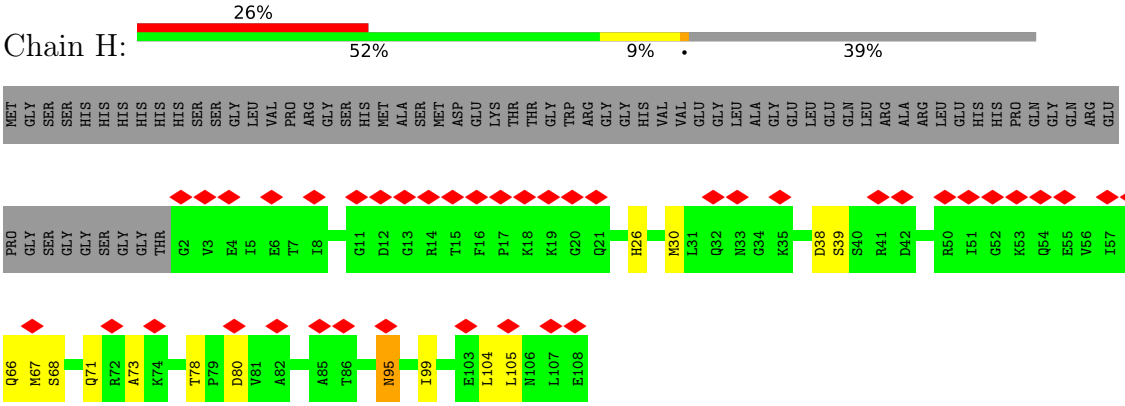
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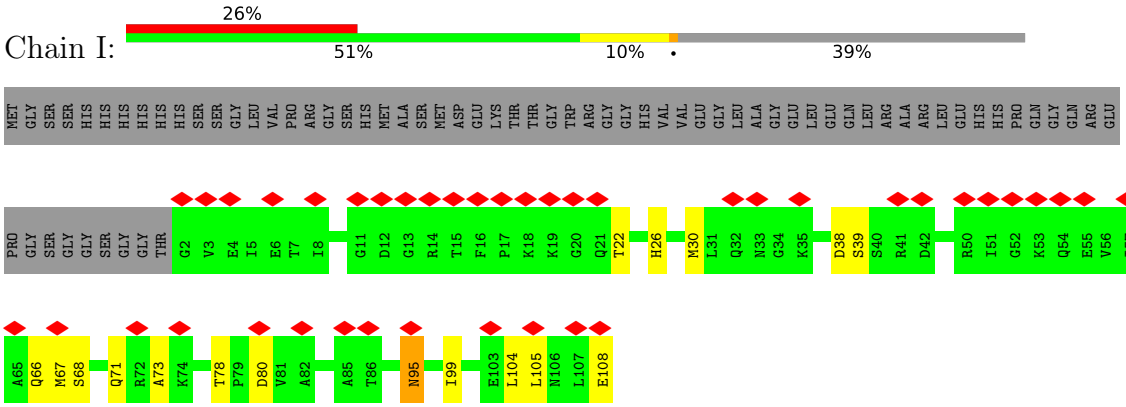




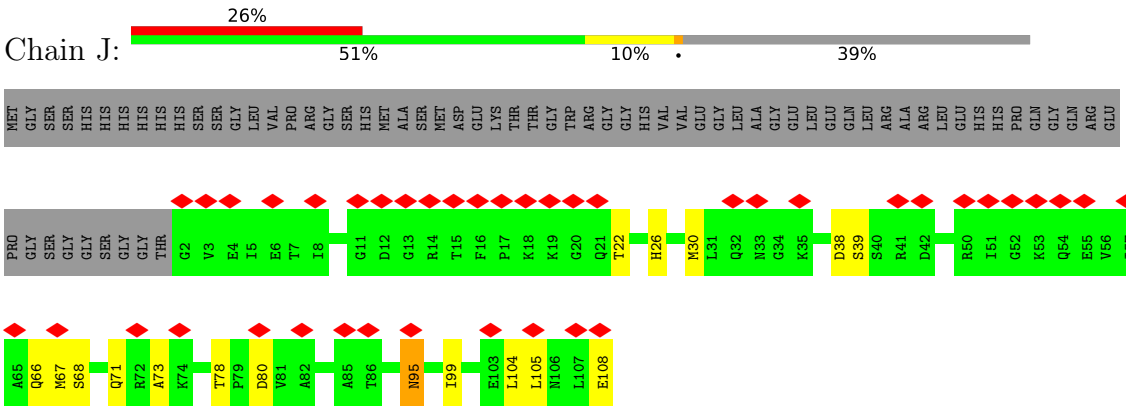
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• 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	48121	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	0.154	Depositor
Minimum map value	-0.070	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: A1MG7, ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.19	0/28516	0.34	0/38541
1	B	0.19	0/28516	0.34	0/38541
1	C	0.19	0/28516	0.34	0/38541
1	D	0.19	0/28516	0.34	0/38541
2	G	0.19	0/835	0.36	0/1123
2	H	0.19	0/835	0.36	0/1123
2	I	0.19	0/835	0.36	0/1123
2	J	0.19	0/835	0.36	0/1123
All	All	0.19	0/117404	0.34	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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) 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	B	3925	GLY	Peptide
1	C	3925	GLY	Peptide
1	D	3925	GLY	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	27546	27534	308	0
1	B	27906	27546	27534	322	0
1	C	27906	27546	27534	311	0
1	D	27906	27546	27534	313	0
2	G	819	822	821	12	0
2	H	819	822	821	9	0
2	I	819	822	821	10	0
2	J	819	822	821	10	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	25	12	0	1	0
5	B	25	12	0	1	0
5	C	25	12	0	1	0
5	D	25	12	0	1	0
All	All	115008	113520	113420	1289	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 (1289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3923:ILE:HD13	1:D:3934:LEU:HD12	1.56	0.88
1:C:3923:ILE:HD13	1:C:3934:LEU:HD12	1.56	0.87
1:A:3923:ILE:HD13	1:A:3934:LEU:HD12	1.56	0.86
1:B:3923:ILE:HD13	1:B:3934:LEU:HD12	1.57	0.86
1:C:1100:ARG:NH1	1:C:1167:ASP:OD2	2.20	0.75
1:B:1100:ARG:NH1	1:B:1167:ASP:OD2	2.20	0.75
1:D:3891:TYR:OH	1:D:3898:ASP:OD1	2.06	0.74
1:A:1100:ARG:NH1	1:A:1167:ASP:OD2	2.20	0.74
1:A:3891:TYR:OH	1:A:3898:ASP:OD1	2.05	0.73
1:B:3891:TYR:OH	1:B:3898:ASP:OD1	2.06	0.73
1:C:3891:TYR:OH	1:C:3898:ASP:OD1	2.06	0.73
1:D:1100:ARG:NH1	1:D:1167:ASP:OD2	2.20	0.73
1:D:1276:THR:OG1	1:D:1278:ASP:OD1	2.08	0.72
1:B:70:GLU:OE2	1:B:122:ARG:NH1	2.23	0.72
1:C:70:GLU:OE2	1:C:122:ARG:NH1	2.23	0.72
1:A:887:GLU:O	1:A:890:HIS:ND1	2.23	0.71
1:C:1276:THR:OG1	1:C:1278:ASP:OD1	2.08	0.71
1:A:70:GLU:OE2	1:A:122:ARG:NH1	2.23	0.71
1:D:887:GLU:O	1:D:890:HIS:ND1	2.23	0.71
1:D:4052:GLU:O	1:D:4055:LYS:NZ	2.22	0.71
1:D:70:GLU:OE2	1:D:122:ARG:NH1	2.23	0.71
1:B:1276:THR:OG1	1:B:1278:ASP:OD1	2.08	0.71
1:B:3641:GLU:OE1	1:B:3729:ARG:NH1	2.24	0.71
1:A:1276:THR:OG1	1:A:1278:ASP:OD1	2.08	0.70
1:C:3641:GLU:OE1	1:C:3729:ARG:NH1	2.24	0.70
1:D:3641:GLU:OE1	1:D:3729:ARG:NH1	2.24	0.70
1:A:670:TYR:O	1:A:673:TRP:NE1	2.24	0.70
1:A:3641:GLU:OE1	1:A:3729:ARG:NH1	2.24	0.70
1:C:670:TYR:O	1:C:673:TRP:NE1	2.24	0.70
1:D:670:TYR:O	1:D:673:TRP:NE1	2.24	0.70
1:B:4566:TYR:O	1:B:4570:THR:OG1	2.10	0.70
1:B:670:TYR:O	1:B:673:TRP:NE1	2.24	0.69
1:D:2502:ASP:OD2	1:D:2553:ARG:NH1	2.26	0.69
1:A:2580:ARG:NH1	1:A:2583:MET:SD	2.66	0.69
1:C:2580:ARG:NH1	1:C:2583:MET:SD	2.66	0.69
1:D:2580:ARG:NH1	1:D:2583:MET:SD	2.66	0.69
1:A:4052:GLU:O	1:A:4055:LYS:NZ	2.22	0.69
1:B:2502:ASP:OD2	1:B:2553:ARG:NH1	2.26	0.69
1:B:2580:ARG:NH1	1:B:2583:MET:SD	2.66	0.69
1:C:141:ASP:OD2	1:C:144:ALA:N	2.26	0.69
1:C:4928:ASP:OD1	1:C:4930:THR:OG1	2.10	0.69
1:D:1266:GLU:OE2	1:D:1294:ASN:ND2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3636:GLU:N	1:D:3636:GLU:OE1	2.26	0.69
1:B:4122:GLU:OE1	1:B:4122:GLU:N	2.26	0.69
1:C:2502:ASP:OD2	1:C:2553:ARG:NH1	2.26	0.69
1:B:323:ASP:O	1:B:327:THR:OG1	2.09	0.69
1:C:807:ARG:O	1:C:807:ARG:NH1	2.26	0.69
1:C:1266:GLU:OE2	1:C:1294:ASN:ND2	2.26	0.69
1:C:4122:GLU:N	1:C:4122:GLU:OE1	2.26	0.69
1:D:141:ASP:OD2	1:D:144:ALA:N	2.26	0.69
1:B:807:ARG:O	1:B:807:ARG:NH1	2.26	0.68
1:A:141:ASP:OD2	1:A:144:ALA:N	2.26	0.68
1:A:807:ARG:NH1	1:A:807:ARG:O	2.26	0.68
1:A:1944:ASN:O	1:A:1948:GLN:NE2	2.27	0.68
1:A:4566:TYR:O	1:A:4570:THR:OG1	2.10	0.68
1:C:887:GLU:O	1:C:890:HIS:ND1	2.23	0.68
1:D:4928:ASP:OD1	1:D:4930:THR:OG1	2.10	0.68
1:B:141:ASP:OD2	1:B:144:ALA:N	2.26	0.68
1:C:3636:GLU:N	1:C:3636:GLU:OE1	2.26	0.68
1:B:3636:GLU:OE1	1:B:3636:GLU:N	2.26	0.68
1:A:2502:ASP:OD2	1:A:2553:ARG:NH1	2.26	0.68
1:D:807:ARG:O	1:D:807:ARG:NH1	2.26	0.68
2:I:68:SER:OG	2:I:71:GLN:NE2	2.27	0.68
1:B:1266:GLU:OE2	1:B:1294:ASN:ND2	2.26	0.68
1:D:4122:GLU:OE1	1:D:4122:GLU:N	2.26	0.68
2:G:68:SER:OG	2:G:71:GLN:NE2	2.27	0.68
1:A:4122:GLU:N	1:A:4122:GLU:OE1	2.26	0.68
1:B:4052:GLU:O	1:B:4055:LYS:NZ	2.22	0.68
1:A:1266:GLU:OE2	1:A:1294:ASN:ND2	2.26	0.68
1:C:1944:ASN:O	1:C:1948:GLN:NE2	2.27	0.68
2:J:68:SER:OG	2:J:71:GLN:NE2	2.27	0.68
1:A:3636:GLU:N	1:A:3636:GLU:OE1	2.26	0.68
1:A:102:MET:O	1:A:106:GLN:NE2	2.27	0.67
1:B:887:GLU:O	1:B:890:HIS:ND1	2.23	0.67
1:C:102:MET:O	1:C:106:GLN:NE2	2.27	0.67
1:D:102:MET:O	1:D:106:GLN:NE2	2.27	0.67
2:H:68:SER:OG	2:H:71:GLN:NE2	2.27	0.67
1:A:2496:ARG:NH2	1:A:2546:SER:OG	2.28	0.67
1:A:4928:ASP:OD1	1:A:4930:THR:OG1	2.10	0.67
1:B:824:GLU:OE1	1:B:1028:ARG:NH1	2.28	0.67
1:C:824:GLU:OE1	1:C:1028:ARG:NH1	2.28	0.67
1:B:1944:ASN:O	1:B:1948:GLN:NE2	2.27	0.67
1:B:4106:GLU:OE1	1:B:4146:ARG:NE	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4566:TYR:O	1:D:4570:THR:OG1	2.10	0.67
1:D:4633:VAL:O	1:D:4636:THR:OG1	2.11	0.67
1:B:797:GLY:N	1:B:1622:CYS:O	2.28	0.67
1:B:1848:GLU:OE2	1:B:1850:SER:OG	2.12	0.67
1:B:2496:ARG:NH2	1:B:2546:SER:OG	2.28	0.67
1:C:4052:GLU:O	1:C:4055:LYS:NZ	2.22	0.67
1:D:1944:ASN:O	1:D:1948:GLN:NE2	2.27	0.67
1:A:797:GLY:N	1:A:1622:CYS:O	2.28	0.67
1:A:824:GLU:OE1	1:A:1028:ARG:NH1	2.28	0.67
1:B:102:MET:O	1:B:106:GLN:NE2	2.27	0.67
1:C:2496:ARG:NH2	1:C:2546:SER:OG	2.28	0.67
1:D:323:ASP:O	1:D:327:THR:OG1	2.09	0.67
1:D:824:GLU:OE1	1:D:1028:ARG:NH1	2.28	0.67
1:B:668:ALA:O	1:B:1017:THR:OG1	2.13	0.66
1:C:797:GLY:N	1:C:1622:CYS:O	2.28	0.66
1:D:2496:ARG:NH2	1:D:2546:SER:OG	2.28	0.66
1:A:4106:GLU:OE1	1:A:4146:ARG:NE	2.28	0.66
1:B:674:TYR:OH	1:B:676:GLU:OE2	2.11	0.66
1:C:668:ALA:O	1:C:1017:THR:OG1	2.13	0.66
1:A:1990:GLU:N	1:A:1990:GLU:OE1	2.28	0.66
1:A:668:ALA:O	1:A:1017:THR:OG1	2.13	0.66
1:B:1990:GLU:OE1	1:B:1990:GLU:N	2.28	0.66
1:C:4566:TYR:O	1:C:4570:THR:OG1	2.10	0.66
1:A:323:ASP:O	1:A:327:THR:OG1	2.09	0.66
1:A:4873:ARG:NH1	1:D:4871:GLU:OE2	2.29	0.66
1:C:1990:GLU:N	1:C:1990:GLU:OE1	2.28	0.66
1:C:2190:LYS:O	1:C:2194:ASN:ND2	2.29	0.66
1:A:807:ARG:O	1:A:1611:ARG:NH2	2.29	0.66
1:B:2190:LYS:O	1:B:2194:ASN:ND2	2.29	0.66
1:B:807:ARG:O	1:B:1611:ARG:NH2	2.30	0.65
1:B:4871:GLU:OE2	1:C:4873:ARG:NH1	2.29	0.65
1:C:4106:GLU:OE1	1:C:4146:ARG:NE	2.28	0.65
1:D:2190:LYS:O	1:D:2194:ASN:ND2	2.29	0.65
1:D:807:ARG:O	1:D:1611:ARG:NH2	2.29	0.65
1:A:2190:LYS:O	1:A:2194:ASN:ND2	2.29	0.65
1:D:4106:GLU:OE1	1:D:4146:ARG:NE	2.28	0.65
1:A:674:TYR:OH	1:A:676:GLU:OE2	2.11	0.65
1:B:189:GLU:OE1	1:B:189:GLU:N	2.30	0.65
1:C:4871:GLU:OE2	1:D:4873:ARG:NH1	2.29	0.65
1:D:797:GLY:N	1:D:1622:CYS:O	2.28	0.65
1:D:4615:TYR:OH	1:D:4627:GLY:O	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1990:GLU:N	1:D:1990:GLU:OE1	2.28	0.65
1:B:4562:GLU:N	1:B:4562:GLU:OE1	2.30	0.65
1:C:4562:GLU:N	1:C:4562:GLU:OE1	2.30	0.65
1:D:4562:GLU:OE1	1:D:4562:GLU:N	2.30	0.64
1:A:233:VAL:HG12	1:A:274:LEU:HD12	1.79	0.64
1:A:4871:GLU:OE2	1:B:4873:ARG:NH1	2.29	0.64
1:C:467:ASP:OD2	1:C:469:HIS:NE2	2.31	0.64
1:A:4562:GLU:OE1	1:A:4562:GLU:N	2.30	0.64
1:B:467:ASP:OD2	1:B:469:HIS:NE2	2.31	0.64
1:A:189:GLU:N	1:A:189:GLU:OE1	2.30	0.64
1:D:668:ALA:O	1:D:1017:THR:OG1	2.13	0.64
1:C:1220:ASP:O	1:C:1223:THR:OG1	2.15	0.64
1:D:467:ASP:OD2	1:D:469:HIS:NE2	2.31	0.64
2:I:78:THR:OG1	2:I:80:ASP:OD1	2.14	0.64
1:A:3622:GLY:O	1:A:3626:SER:OG	2.12	0.64
1:A:4615:TYR:OH	1:A:4627:GLY:O	2.12	0.64
1:C:807:ARG:O	1:C:1611:ARG:NH2	2.29	0.64
1:D:674:TYR:OH	1:D:676:GLU:OE2	2.11	0.64
1:A:573:GLU:OE1	1:A:609:LYS:NZ	2.22	0.64
1:A:1312:GLU:OE1	1:A:1537:SER:OG	2.16	0.64
1:B:233:VAL:HG12	1:B:274:LEU:HD12	1.79	0.64
1:D:2264:VAL:HG11	1:D:2301:LEU:HD13	1.80	0.63
1:D:189:GLU:N	1:D:189:GLU:OE1	2.30	0.63
1:B:222:GLU:OE1	1:B:222:GLU:N	2.31	0.63
1:D:1220:ASP:O	1:D:1223:THR:OG1	2.15	0.63
1:A:323:ASP:OD1	1:A:326:SER:OG	2.11	0.63
1:C:189:GLU:N	1:C:189:GLU:OE1	2.30	0.63
1:C:2264:VAL:HG11	1:C:2301:LEU:HD13	1.80	0.63
1:C:193:HIS:ND1	1:C:208:GLN:OE1	2.32	0.63
1:C:323:ASP:OD1	1:C:326:SER:OG	2.11	0.63
1:D:4113:ARG:O	1:D:4116:THR:OG1	2.16	0.63
1:A:222:GLU:N	1:A:222:GLU:OE1	2.31	0.63
1:A:1848:GLU:OE2	1:A:1850:SER:OG	2.12	0.63
1:B:1312:GLU:OE1	1:B:1537:SER:OG	2.16	0.63
1:B:4615:TYR:OH	1:B:4627:GLY:O	2.12	0.63
1:D:2275:SER:OG	1:D:2288:GLY:N	2.32	0.63
1:C:222:GLU:N	1:C:222:GLU:OE1	2.31	0.63
1:D:222:GLU:N	1:D:222:GLU:OE1	2.31	0.63
1:D:1848:GLU:OE2	1:D:1850:SER:OG	2.12	0.63
1:C:233:VAL:HG12	1:C:274:LEU:HD12	1.79	0.63
1:C:4113:ARG:O	1:C:4116:THR:OG1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:VAL:HG12	1:D:274:LEU:HD12	1.79	0.63
1:D:1683:GLU:OE1	1:D:1683:GLU:N	2.32	0.63
1:A:467:ASP:OD2	1:A:469:HIS:NE2	2.31	0.63
1:C:1683:GLU:N	1:C:1683:GLU:OE1	2.32	0.63
1:C:2275:SER:OG	1:C:2288:GLY:N	2.32	0.63
1:A:2275:SER:OG	1:A:2288:GLY:N	2.32	0.62
1:B:2264:VAL:HG11	1:B:2301:LEU:HD13	1.80	0.62
1:A:1220:ASP:O	1:A:1223:THR:OG1	2.15	0.62
1:C:171:GLU:OE1	1:C:171:GLU:N	2.32	0.62
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.73	0.62
1:D:4017:ASP:OD1	1:D:4123:SER:OG	2.13	0.62
1:A:4113:ARG:O	1:A:4116:THR:OG1	2.16	0.62
1:B:171:GLU:N	1:B:171:GLU:OE1	2.33	0.62
1:B:2275:SER:OG	1:B:2288:GLY:N	2.32	0.62
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.73	0.62
1:A:1683:GLU:OE1	1:A:1683:GLU:N	2.32	0.62
1:A:1234:GLU:N	1:A:1234:GLU:OE1	2.33	0.62
1:A:3923:ILE:HD11	1:A:3931:GLN:HA	1.81	0.62
1:B:193:HIS:ND1	1:B:208:GLN:OE1	2.32	0.62
1:A:564:ARG:O	1:A:568:SER:OG	2.18	0.62
1:A:2264:VAL:HG11	1:A:2301:LEU:HD13	1.80	0.62
1:D:193:HIS:ND1	1:D:208:GLN:OE1	2.32	0.62
1:D:3923:ILE:HD11	1:D:3931:GLN:HA	1.82	0.62
2:G:78:THR:OG1	2:G:80:ASP:OD1	2.14	0.62
1:B:1234:GLU:N	1:B:1234:GLU:OE1	2.33	0.62
1:B:1272:ARG:NH2	1:B:1583:CYS:SG	2.73	0.62
1:A:171:GLU:OE1	1:A:171:GLU:N	2.33	0.62
1:A:1272:ARG:NH2	1:A:1583:CYS:SG	2.73	0.62
1:B:2435:ILE:O	1:B:2464:LYS:NZ	2.25	0.62
1:C:1234:GLU:OE1	1:C:1234:GLU:N	2.33	0.62
1:C:4615:TYR:OH	1:C:4627:GLY:O	2.12	0.62
1:D:1312:GLU:OE1	1:D:1537:SER:OG	2.16	0.62
1:B:612:ASP:OD1	1:B:1660:ARG:NH2	2.33	0.61
1:B:3923:ILE:HD11	1:B:3931:GLN:HA	1.81	0.61
1:C:564:ARG:O	1:C:568:SER:OG	2.18	0.61
1:D:1234:GLU:N	1:D:1234:GLU:OE1	2.33	0.61
1:B:1246:ASP:OD1	1:B:1694:TYR:OH	2.19	0.61
1:C:674:TYR:OH	1:C:676:GLU:OE2	2.11	0.61
1:B:1662:TYR:HB2	1:B:1706:LEU:HD21	1.83	0.61
1:D:612:ASP:OD1	1:D:1660:ARG:NH2	2.33	0.61
1:C:1662:TYR:HB2	1:C:1706:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4017:ASP:OD1	1:C:4123:SER:OG	2.12	0.61
1:D:171:GLU:N	1:D:171:GLU:OE1	2.33	0.61
1:D:1662:TYR:HB2	1:D:1706:LEU:HD21	1.82	0.61
1:A:1662:TYR:HB2	1:A:1706:LEU:HD21	1.82	0.61
1:B:564:ARG:O	1:B:568:SER:OG	2.18	0.61
2:H:78:THR:OG1	2:H:80:ASP:OD1	2.14	0.61
1:D:2078:GLU:N	1:D:2078:GLU:OE1	2.34	0.61
1:A:193:HIS:ND1	1:A:208:GLN:OE1	2.32	0.61
1:A:4186:GLU:OE2	1:A:4190:ASN:ND2	2.34	0.61
1:C:612:ASP:OD1	1:C:1660:ARG:NH2	2.33	0.61
1:A:927:GLN:O	1:A:930:ASN:ND2	2.34	0.61
1:B:3851:SER:O	1:B:3855:ASN:ND2	2.34	0.61
1:B:4186:GLU:OE2	1:B:4190:ASN:ND2	2.34	0.61
1:C:3851:SER:O	1:C:3855:ASN:ND2	2.34	0.61
1:C:1848:GLU:OE2	1:C:1850:SER:OG	2.12	0.60
1:D:564:ARG:O	1:D:568:SER:OG	2.18	0.60
1:A:612:ASP:OD1	1:A:1660:ARG:NH2	2.33	0.60
1:B:1683:GLU:N	1:B:1683:GLU:OE1	2.32	0.60
1:C:1312:GLU:OE1	1:C:1537:SER:OG	2.16	0.60
1:C:3923:ILE:HD11	1:C:3931:GLN:HA	1.81	0.60
1:C:2114:ASP:OD1	1:C:2151:ASN:ND2	2.34	0.60
1:A:1127:GLU:OE1	1:A:1128:LEU:N	2.35	0.60
1:A:3851:SER:O	1:A:3855:ASN:ND2	2.34	0.60
1:B:3622:GLY:O	1:B:3626:SER:OG	2.12	0.60
1:B:1127:GLU:OE1	1:B:1128:LEU:N	2.35	0.60
1:C:927:GLN:O	1:C:930:ASN:ND2	2.34	0.60
1:C:4044:LYS:N	1:C:4075:GLU:O	2.35	0.60
1:A:2078:GLU:N	1:A:2078:GLU:OE1	2.34	0.60
1:B:1220:ASP:O	1:B:1223:THR:OG1	2.15	0.60
1:C:2078:GLU:N	1:C:2078:GLU:OE1	2.34	0.60
1:D:1127:GLU:OE1	1:D:1128:LEU:N	2.35	0.60
1:D:3851:SER:O	1:D:3855:ASN:ND2	2.34	0.60
1:A:2114:ASP:OD1	1:A:2151:ASN:ND2	2.34	0.60
1:C:323:ASP:O	1:C:327:THR:OG1	2.09	0.60
1:C:4186:GLU:OE2	1:C:4190:ASN:ND2	2.34	0.60
1:B:2078:GLU:N	1:B:2078:GLU:OE1	2.34	0.60
1:A:204:ASP:OD1	1:A:204:ASP:N	2.35	0.60
1:D:927:GLN:O	1:D:930:ASN:ND2	2.34	0.59
1:D:2114:ASP:OD1	1:D:2151:ASN:ND2	2.34	0.59
1:D:4186:GLU:OE2	1:D:4190:ASN:ND2	2.34	0.59
1:B:2114:ASP:OD1	1:B:2151:ASN:ND2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2298:LEU:HD13	1:B:2397:LEU:HD22	1.84	0.59
1:C:2298:LEU:HD13	1:C:2397:LEU:HD22	1.84	0.59
1:A:661:LEU:O	1:A:788:PHE:N	2.36	0.59
1:B:927:GLN:O	1:B:930:ASN:ND2	2.34	0.59
1:D:728:ASP:OD1	1:D:731:HIS:N	2.35	0.59
1:A:4044:LYS:N	1:A:4075:GLU:O	2.35	0.59
1:B:2242:ALA:O	1:B:2245:SER:OG	2.16	0.59
1:C:1127:GLU:OE1	1:C:1128:LEU:N	2.35	0.59
1:D:661:LEU:O	1:D:788:PHE:N	2.36	0.59
1:D:1246:ASP:OD1	1:D:1694:TYR:OH	2.19	0.59
1:D:2242:ALA:O	1:D:2245:SER:OG	2.16	0.59
1:B:394:HIS:ND1	1:B:396:GLU:O	2.36	0.59
1:B:4044:LYS:N	1:B:4075:GLU:O	2.35	0.59
1:D:946:LEU:HD12	1:D:995:MET:HE1	1.85	0.59
1:B:204:ASP:N	1:B:204:ASP:OD1	2.35	0.59
1:D:1892:LEU:HD12	1:D:1895:MET:HE1	1.85	0.59
1:C:2487:LEU:HD21	1:C:2547:LEU:HD22	1.85	0.59
1:A:728:ASP:OD1	1:A:731:HIS:N	2.35	0.59
1:C:394:HIS:ND1	1:C:396:GLU:O	2.36	0.59
1:C:946:LEU:HD12	1:C:995:MET:HE1	1.85	0.59
1:C:1246:ASP:OD1	1:C:1694:TYR:OH	2.19	0.59
1:C:1892:LEU:HD12	1:C:1895:MET:HE1	1.85	0.59
1:D:4044:LYS:N	1:D:4075:GLU:O	2.35	0.58
1:A:1892:LEU:HD12	1:A:1895:MET:HE1	1.85	0.58
1:B:4633:VAL:O	1:B:4636:THR:OG1	2.11	0.58
1:A:4633:VAL:O	1:A:4636:THR:OG1	2.11	0.58
1:B:2487:LEU:HD21	1:B:2547:LEU:HD22	1.85	0.58
1:C:3954:GLN:O	1:C:3958:SER:OG	2.16	0.58
1:D:2298:LEU:HD13	1:D:2397:LEU:HD22	1.84	0.58
1:B:713:TRP:HH2	1:B:1251:LEU:HD21	1.68	0.58
1:B:4113:ARG:O	1:B:4116:THR:OG1	2.16	0.58
1:B:4136:GLU:OE2	1:B:4146:ARG:NH1	2.36	0.58
1:C:4003:VAL:HG21	1:C:4113:ARG:HD2	1.85	0.58
1:A:2487:LEU:HD21	1:A:2547:LEU:HD22	1.85	0.58
1:D:2487:LEU:HD21	1:D:2547:LEU:HD22	1.85	0.58
1:A:4136:GLU:OE2	1:A:4146:ARG:NH1	2.36	0.58
1:D:3622:GLY:O	1:D:3626:SER:OG	2.12	0.58
1:A:394:HIS:ND1	1:A:396:GLU:O	2.36	0.58
1:A:800:VAL:O	1:A:1619:LEU:HD12	2.03	0.58
1:A:1246:ASP:OD1	1:A:1694:TYR:OH	2.19	0.58
1:B:661:LEU:O	1:B:788:PHE:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4928:ASP:OD1	1:B:4930:THR:OG1	2.10	0.58
1:C:661:LEU:O	1:C:788:PHE:N	2.36	0.58
1:D:394:HIS:ND1	1:D:396:GLU:O	2.36	0.58
1:A:2298:LEU:HD13	1:A:2397:LEU:HD22	1.84	0.58
1:C:4136:GLU:OE2	1:C:4146:ARG:NH1	2.36	0.58
1:A:3727:GLN:O	1:A:3731:HIS:ND1	2.37	0.58
1:A:4003:VAL:HG21	1:A:4113:ARG:HD2	1.85	0.58
1:B:1892:LEU:HD12	1:B:1895:MET:HE1	1.85	0.58
1:B:2588:LEU:O	1:B:2592:VAL:HG23	2.04	0.58
1:D:713:TRP:HH2	1:D:1251:LEU:HD21	1.69	0.58
1:B:800:VAL:O	1:B:1619:LEU:HD12	2.03	0.58
1:B:1692:ASN:OD1	1:B:1695:MET:N	2.37	0.58
1:C:728:ASP:OD1	1:C:731:HIS:N	2.35	0.58
1:C:800:VAL:O	1:C:1619:LEU:HD12	2.03	0.58
1:C:1692:ASN:OD1	1:C:1695:MET:N	2.37	0.58
1:D:4136:GLU:OE2	1:D:4146:ARG:NH1	2.36	0.58
1:C:2348:GLU:OE2	1:C:2358:ARG:NH2	2.37	0.57
1:A:2435:ILE:O	1:A:2464:LYS:NZ	2.25	0.57
1:A:2588:LEU:O	1:A:2592:VAL:HG23	2.04	0.57
1:C:713:TRP:HH2	1:C:1251:LEU:HD21	1.69	0.57
1:D:800:VAL:O	1:D:1619:LEU:HD12	2.03	0.57
1:D:3954:GLN:O	1:D:3958:SER:OG	2.16	0.57
1:D:4080:GLU:OE1	1:D:4080:GLU:N	2.38	0.57
1:A:713:TRP:HH2	1:A:1251:LEU:HD21	1.69	0.57
1:A:946:LEU:HD12	1:A:995:MET:HE1	1.85	0.57
1:B:4607:ARG:NH2	1:B:4643:TYR:OH	2.38	0.57
1:D:1692:ASN:OD1	1:D:1695:MET:N	2.37	0.57
1:A:910:ASP:OD1	1:A:913:ARG:NE	2.38	0.57
1:A:1692:ASN:OD1	1:A:1695:MET:N	2.37	0.57
1:B:946:LEU:HD12	1:B:995:MET:HE1	1.85	0.57
1:B:4003:VAL:HG21	1:B:4113:ARG:HD2	1.85	0.57
1:D:2414:GLU:OE1	1:D:2414:GLU:N	2.38	0.57
1:C:3727:GLN:O	1:C:3731:HIS:ND1	2.37	0.57
1:D:204:ASP:N	1:D:204:ASP:OD1	2.35	0.57
2:I:30:MET:N	2:I:99:ILE:O	2.38	0.57
1:A:2348:GLU:OE2	1:A:2358:ARG:NH2	2.37	0.57
1:B:728:ASP:OD1	1:B:731:HIS:N	2.35	0.57
1:D:4003:VAL:HG21	1:D:4113:ARG:HD2	1.85	0.57
1:B:910:ASP:OD1	1:B:913:ARG:NE	2.38	0.57
1:B:4080:GLU:OE1	1:B:4080:GLU:N	2.38	0.57
1:C:4080:GLU:N	1:C:4080:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2348:GLU:OE2	1:B:2358:ARG:NH2	2.37	0.57
1:B:3727:GLN:O	1:B:3731:HIS:ND1	2.37	0.57
1:D:2348:GLU:OE2	1:D:2358:ARG:NH2	2.37	0.57
1:D:3727:GLN:O	1:D:3731:HIS:ND1	2.37	0.57
2:J:30:MET:N	2:J:99:ILE:O	2.38	0.57
1:C:204:ASP:OD1	1:C:204:ASP:N	2.35	0.57
1:C:584:GLU:N	1:C:584:GLU:OE1	2.38	0.57
1:C:910:ASP:OD1	1:C:913:ARG:NE	2.38	0.57
1:C:2588:LEU:O	1:C:2592:VAL:HG23	2.04	0.57
1:A:3971:MET:HE3	1:A:4093:ILE:CD1	2.35	0.56
1:B:180:ASP:HB3	1:B:211:LEU:HD11	1.87	0.56
1:D:1940:ARG:NH2	1:D:3608:TYR:O	2.38	0.56
1:D:3971:MET:HE3	1:D:4093:ILE:CD1	2.35	0.56
1:D:4607:ARG:NH2	1:D:4643:TYR:OH	2.38	0.56
1:D:2588:LEU:O	1:D:2592:VAL:HG23	2.04	0.56
1:D:4153:GLU:N	1:D:4153:GLU:OE1	2.38	0.56
1:A:643:LEU:O	1:A:645:GLN:NE2	2.39	0.56
1:B:573:GLU:OE1	1:B:609:LYS:NZ	2.22	0.56
1:B:1662:TYR:CB	1:B:1706:LEU:HD21	2.36	0.56
1:B:2414:GLU:N	1:B:2414:GLU:OE1	2.38	0.56
1:B:4153:GLU:OE1	1:B:4153:GLU:N	2.38	0.56
1:C:1662:TYR:CB	1:C:1706:LEU:HD21	2.36	0.56
1:A:2414:GLU:OE1	1:A:2414:GLU:N	2.38	0.56
1:A:3629:GLU:OE1	1:A:3629:GLU:N	2.38	0.56
1:A:1940:ARG:NH2	1:A:3608:TYR:O	2.38	0.56
1:A:1958:ALA:O	1:A:1965:ARG:NH2	2.39	0.56
1:B:643:LEU:O	1:B:645:GLN:NE2	2.39	0.56
1:B:1958:ALA:O	1:B:1965:ARG:NH2	2.39	0.56
1:B:3629:GLU:N	1:B:3629:GLU:OE1	2.38	0.56
1:C:2435:ILE:O	1:C:2464:LYS:NZ	2.25	0.56
1:B:21:VAL:HG13	1:B:217:ILE:HG13	1.88	0.56
1:C:4153:GLU:N	1:C:4153:GLU:OE1	2.38	0.56
1:C:4607:ARG:NH2	1:C:4643:TYR:OH	2.38	0.56
1:D:1662:TYR:CB	1:D:1706:LEU:HD21	2.36	0.56
1:A:180:ASP:HB3	1:A:211:LEU:HD11	1.87	0.56
1:C:21:VAL:HG13	1:C:217:ILE:HG13	1.88	0.56
1:C:180:ASP:HB3	1:C:211:LEU:HD11	1.87	0.56
1:C:2414:GLU:N	1:C:2414:GLU:OE1	2.38	0.56
1:B:1940:ARG:NH2	1:B:3608:TYR:O	2.38	0.56
1:B:3971:MET:HE3	1:B:4093:ILE:CD1	2.35	0.56
1:C:2470:PHE:CE1	1:C:2474:VAL:HG21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:643:LEU:O	1:D:645:GLN:NE2	2.39	0.56
1:C:1940:ARG:NH2	1:C:3608:TYR:O	2.38	0.56
1:A:21:VAL:HG13	1:A:217:ILE:HG13	1.88	0.56
1:B:2251:GLU:N	1:B:2251:GLU:OE1	2.39	0.56
1:C:3629:GLU:OE1	1:C:3629:GLU:N	2.39	0.56
1:D:2251:GLU:N	1:D:2251:GLU:OE1	2.39	0.56
1:B:2470:PHE:CE1	1:B:2474:VAL:HG21	2.41	0.55
1:C:3971:MET:HE3	1:C:4093:ILE:CD1	2.35	0.55
1:A:2470:PHE:CE1	1:A:2474:VAL:HG21	2.41	0.55
1:B:563:GLU:N	1:B:563:GLU:OE1	2.40	0.55
1:B:1642:ILE:HD12	1:B:1695:MET:SD	2.47	0.55
1:B:1969:GLN:N	1:B:1969:GLN:OE1	2.39	0.55
1:C:1642:ILE:HD12	1:C:1695:MET:SD	2.47	0.55
1:C:1969:GLN:OE1	1:C:1969:GLN:N	2.39	0.55
1:C:2251:GLU:OE1	1:C:2251:GLU:N	2.39	0.55
1:A:557:TRP:O	1:A:560:SER:OG	2.20	0.55
1:A:1662:TYR:CB	1:A:1706:LEU:HD21	2.36	0.55
1:D:21:VAL:HG13	1:D:217:ILE:HG13	1.88	0.55
1:D:2470:PHE:CE1	1:D:2474:VAL:HG21	2.41	0.55
1:B:584:GLU:N	1:B:584:GLU:OE1	2.38	0.55
1:C:255:GLU:OE1	1:C:255:GLU:N	2.39	0.55
1:D:1958:ALA:O	1:D:1965:ARG:NH2	2.39	0.55
1:D:3629:GLU:N	1:D:3629:GLU:OE1	2.38	0.55
1:A:602:ASP:HA	1:A:642:LEU:HD21	1.88	0.55
1:A:1642:ILE:HD12	1:A:1695:MET:SD	2.47	0.55
1:C:1958:ALA:O	1:C:1965:ARG:NH2	2.39	0.55
1:C:643:LEU:O	1:C:645:GLN:NE2	2.39	0.55
1:D:233:VAL:CG1	1:D:274:LEU:HD12	2.37	0.55
1:A:3954:GLN:O	1:A:3958:SER:OG	2.16	0.55
1:A:4080:GLU:N	1:A:4080:GLU:OE1	2.38	0.55
1:A:4607:ARG:NH2	1:A:4643:TYR:OH	2.38	0.55
1:B:2125:ILE:HG23	1:B:2141:MET:HE1	1.89	0.55
1:C:503:ASP:OD1	1:C:557:TRP:NE1	2.40	0.55
1:C:1803:GLY:O	1:C:1806:HIS:ND1	2.40	0.55
1:C:2125:ILE:HG23	1:C:2141:MET:HE1	1.89	0.55
1:A:233:VAL:CG1	1:A:274:LEU:HD12	2.37	0.55
1:A:563:GLU:N	1:A:563:GLU:OE1	2.39	0.55
1:B:602:ASP:HA	1:B:642:LEU:HD21	1.88	0.55
1:B:3833:GLU:OE1	1:B:3833:GLU:N	2.39	0.55
1:D:1642:ILE:HD12	1:D:1695:MET:SD	2.47	0.55
2:H:30:MET:N	2:H:99:ILE:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1762:MET:SD	1:C:1762:MET:N	2.80	0.55
2:G:67:MET:HE1	2:G:73:ALA:CB	2.37	0.55
2:J:67:MET:HE1	2:J:73:ALA:CB	2.37	0.55
1:A:4153:GLU:N	1:A:4153:GLU:OE1	2.38	0.55
1:D:602:ASP:HA	1:D:642:LEU:HD21	1.88	0.55
1:C:602:ASP:HA	1:C:642:LEU:HD21	1.88	0.54
1:D:180:ASP:HB3	1:D:211:LEU:HD11	1.88	0.54
1:D:1803:GLY:O	1:D:1806:HIS:ND1	2.40	0.54
1:D:4051:MET:SD	1:D:4062:THR:HG23	2.47	0.54
2:H:67:MET:HE1	2:H:73:ALA:CB	2.37	0.54
1:A:565:LEU:HD11	1:A:1585:PRO:HG2	1.89	0.54
1:A:1946:VAL:HG13	1:A:1950:LEU:HD12	1.89	0.54
1:C:233:VAL:CG1	1:C:274:LEU:HD12	2.37	0.54
1:C:565:LEU:HD11	1:C:1585:PRO:HG2	1.89	0.54
1:C:3833:GLU:N	1:C:3833:GLU:OE1	2.39	0.54
1:D:557:TRP:O	1:D:560:SER:OG	2.20	0.54
1:D:910:ASP:OD1	1:D:913:ARG:NE	2.38	0.54
1:C:4024:ASP:OD1	1:C:4054:HIS:NE2	2.38	0.54
1:C:4051:MET:SD	1:C:4062:THR:HG23	2.48	0.54
1:D:1635:GLU:OE1	1:D:1635:GLU:N	2.40	0.54
1:A:584:GLU:N	1:A:584:GLU:OE1	2.38	0.54
1:B:1803:GLY:O	1:B:1806:HIS:ND1	2.40	0.54
1:C:563:GLU:N	1:C:563:GLU:OE1	2.39	0.54
1:A:1289:SER:O	1:A:1295:ASN:ND2	2.41	0.54
1:A:2125:ILE:HG23	1:A:2141:MET:HE1	1.89	0.54
1:A:3833:GLU:N	1:A:3833:GLU:OE1	2.39	0.54
1:C:2242:ALA:O	1:C:2245:SER:OG	2.16	0.54
1:D:43:GLY:N	1:D:458:ASP:OD2	2.41	0.54
1:D:2125:ILE:HG23	1:D:2141:MET:HE1	1.89	0.54
2:G:30:MET:N	2:G:99:ILE:O	2.38	0.54
1:A:246:THR:OG1	1:A:247:VAL:N	2.41	0.54
1:A:503:ASP:OD1	1:A:557:TRP:NE1	2.40	0.54
1:D:1946:VAL:HG13	1:D:1950:LEU:HD12	1.89	0.54
1:D:4051:MET:SD	1:D:4052:GLU:N	2.81	0.54
1:B:503:ASP:OD1	1:B:557:TRP:NE1	2.40	0.54
2:I:67:MET:HE1	2:I:73:ALA:CB	2.37	0.54
1:A:1635:GLU:OE1	1:A:1635:GLU:N	2.40	0.54
1:B:233:VAL:CG1	1:B:274:LEU:HD12	2.37	0.54
1:B:320:GLU:N	1:B:320:GLU:OE1	2.41	0.54
1:B:4051:MET:SD	1:B:4052:GLU:N	2.81	0.54
1:A:2251:GLU:OE1	1:A:2251:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4051:MET:SD	1:A:4062:THR:HG23	2.47	0.54
1:D:584:GLU:N	1:D:584:GLU:OE1	2.38	0.54
1:D:320:GLU:N	1:D:320:GLU:OE1	2.41	0.54
1:D:503:ASP:OD1	1:D:557:TRP:NE1	2.40	0.54
1:D:1289:SER:O	1:D:1295:ASN:ND2	2.41	0.54
1:A:1803:GLY:O	1:A:1806:HIS:ND1	2.40	0.53
1:B:565:LEU:HD11	1:B:1585:PRO:HG2	1.89	0.53
1:C:1448:SER:O	1:C:1451:HIS:NE2	2.41	0.53
1:D:563:GLU:N	1:D:563:GLU:OE1	2.39	0.53
1:A:4024:ASP:OD1	1:A:4054:HIS:NE2	2.39	0.53
1:B:1502:ASN:ND2	1:B:1504:ASN:OD1	2.42	0.53
1:B:4051:MET:SD	1:B:4062:THR:HG23	2.48	0.53
1:C:4051:MET:SD	1:C:4052:GLU:N	2.81	0.53
1:D:565:LEU:HD11	1:D:1585:PRO:HG2	1.89	0.53
1:D:1427:TYR:HB2	1:D:1564:VAL:HG11	1.91	0.53
2:J:67:MET:HE1	2:J:73:ALA:HB2	1.90	0.53
1:A:1762:MET:SD	1:A:1762:MET:N	2.80	0.53
1:A:1448:SER:O	1:A:1451:HIS:NE2	2.41	0.53
1:A:1502:ASN:ND2	1:A:1504:ASN:OD1	2.42	0.53
1:A:2242:ALA:O	1:A:2245:SER:OG	2.16	0.53
1:B:1762:MET:SD	1:B:1762:MET:N	2.80	0.53
1:B:1946:VAL:HG13	1:B:1950:LEU:HD12	1.89	0.53
1:D:1502:ASN:ND2	1:D:1504:ASN:OD1	2.42	0.53
2:H:67:MET:HE1	2:H:73:ALA:HB2	1.90	0.53
1:B:248:PRO:O	1:B:257:ARG:NE	2.35	0.53
1:C:1427:TYR:HB2	1:C:1564:VAL:HG11	1.91	0.53
1:C:1502:ASN:ND2	1:C:1504:ASN:OD1	2.41	0.53
1:C:1946:VAL:HG13	1:C:1950:LEU:HD12	1.89	0.53
1:A:4051:MET:SD	1:A:4052:GLU:N	2.81	0.53
1:B:1289:SER:O	1:B:1295:ASN:ND2	2.41	0.53
1:B:1635:GLU:OE1	1:B:1635:GLU:N	2.40	0.53
2:I:67:MET:HE1	2:I:73:ALA:HB2	1.90	0.53
1:A:3714:GLU:N	1:A:3714:GLU:OE1	2.42	0.53
1:C:162:ILE:O	1:C:163:HIS:ND1	2.41	0.53
1:D:162:ILE:O	1:D:163:HIS:ND1	2.41	0.53
1:D:2118:LEU:HD21	1:D:2161:MET:HE1	1.90	0.53
1:A:320:GLU:N	1:A:320:GLU:OE1	2.41	0.53
1:A:1969:GLN:OE1	1:A:1969:GLN:N	2.39	0.53
1:A:4628:GLN:OE1	1:A:4631:ARG:NH1	2.42	0.53
1:B:4024:ASP:OD1	1:B:4054:HIS:NE2	2.38	0.53
1:D:41:GLY:O	1:D:45:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:78:THR:OG1	2:J:80:ASP:OD1	2.14	0.53
1:A:41:GLY:O	1:A:45:ARG:NH1	2.42	0.53
1:A:2118:LEU:HD21	1:A:2161:MET:HE1	1.90	0.53
1:B:162:ILE:O	1:B:163:HIS:ND1	2.41	0.53
1:B:1144:ARG:NH1	1:B:1184:ASP:OD2	2.42	0.53
1:B:4628:GLN:OE1	1:B:4631:ARG:NH1	2.42	0.53
1:C:1309:GLU:OE1	1:C:1310:CYS:N	2.42	0.53
1:D:1969:GLN:N	1:D:1969:GLN:OE1	2.39	0.53
1:D:4628:GLN:OE1	1:D:4631:ARG:NH1	2.42	0.53
1:B:1309:GLU:OE1	1:B:1310:CYS:N	2.42	0.53
1:B:3954:GLN:O	1:B:3958:SER:OG	2.16	0.53
1:C:1289:SER:O	1:C:1295:ASN:ND2	2.41	0.53
1:D:1448:SER:O	1:D:1451:HIS:NE2	2.41	0.53
1:A:162:ILE:O	1:A:163:HIS:ND1	2.41	0.52
1:B:1427:TYR:HB2	1:B:1564:VAL:HG11	1.91	0.52
1:D:3833:GLU:OE1	1:D:3833:GLU:N	2.39	0.52
1:A:680:ASP:OD2	1:A:801:ARG:NE	2.42	0.52
1:B:871:GLN:C	1:B:872:ILE:HD12	2.34	0.52
1:A:728:ASP:OD2	1:A:731:HIS:ND1	2.42	0.52
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.42	0.52
1:A:4755:ILE:O	1:A:4758:SER:OG	2.26	0.52
1:B:680:ASP:OD2	1:B:801:ARG:NE	2.42	0.52
1:B:2118:LEU:HD21	1:B:2161:MET:HE1	1.90	0.52
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.42	0.52
1:C:41:GLY:O	1:C:45:ARG:NH1	2.42	0.52
1:C:680:ASP:OD2	1:C:801:ARG:NE	2.42	0.52
1:C:4633:VAL:O	1:C:4636:THR:OG1	2.11	0.52
1:A:1427:TYR:HB2	1:A:1564:VAL:HG11	1.91	0.52
1:B:320:GLU:OE2	1:B:321:LYS:NZ	2.43	0.52
1:B:1448:SER:O	1:B:1451:HIS:NE2	2.41	0.52
1:B:2592:VAL:HG21	1:B:2639:LEU:HG	1.92	0.52
1:C:320:GLU:OE1	1:C:320:GLU:N	2.41	0.52
1:D:4928:ASP:OD1	1:D:4930:THR:N	2.43	0.52
1:C:2579:LEU:O	1:C:2615:ARG:NH2	2.42	0.52
1:C:4928:ASP:OD1	1:C:4930:THR:N	2.43	0.52
1:D:151:GLU:OE1	1:D:151:GLU:N	2.43	0.52
1:D:1309:GLU:OE1	1:D:1310:CYS:N	2.42	0.52
2:G:67:MET:HE1	2:G:73:ALA:HB2	1.90	0.52
1:A:43:GLY:N	1:A:458:ASP:OD2	2.41	0.52
1:A:871:GLN:C	1:A:872:ILE:HD12	2.34	0.52
1:B:41:GLY:O	1:B:45:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLU:OE1	1:B:255:GLU:N	2.39	0.52
1:B:1655:HIS:O	1:B:1658:THR:OG1	2.24	0.52
1:C:871:GLN:C	1:C:872:ILE:HD12	2.34	0.52
1:C:1655:HIS:O	1:C:1658:THR:OG1	2.24	0.52
1:D:246:THR:OG1	1:D:247:VAL:N	2.41	0.52
1:D:462:TYR:O	1:D:485:ARG:NH1	2.43	0.52
1:D:680:ASP:OD2	1:D:801:ARG:NE	2.42	0.52
1:A:1144:ARG:NH1	1:A:1184:ASP:OD2	2.42	0.52
1:B:462:TYR:O	1:B:485:ARG:NH1	2.43	0.52
1:B:557:TRP:O	1:B:560:SER:OG	2.20	0.52
1:D:2579:LEU:O	1:D:2615:ARG:NH2	2.42	0.52
1:A:1309:GLU:OE1	1:A:1310:CYS:N	2.42	0.52
1:B:1533:GLN:NE2	1:B:1534:VAL:O	2.43	0.52
1:B:1978:PHE:CZ	1:B:1995:LEU:HD23	2.45	0.52
1:B:4928:ASP:OD1	1:B:4930:THR:N	2.43	0.52
1:C:462:TYR:O	1:C:485:ARG:NH1	2.43	0.52
1:C:2592:VAL:HG21	1:C:2639:LEU:HG	1.92	0.52
1:C:3714:GLU:N	1:C:3714:GLU:OE1	2.42	0.52
1:C:4628:GLN:OE1	1:C:4631:ARG:NH1	2.42	0.52
1:A:151:GLU:N	1:A:151:GLU:OE1	2.43	0.52
1:A:462:TYR:O	1:A:485:ARG:NH1	2.43	0.52
1:A:888:ASN:OD1	1:A:1056:THR:HG21	2.10	0.52
1:B:2112:VAL:O	1:B:2115:THR:OG1	2.27	0.52
1:B:2579:LEU:O	1:B:2615:ARG:NH2	2.42	0.52
1:C:1978:PHE:CZ	1:C:1995:LEU:HD23	2.45	0.52
1:D:255:GLU:N	1:D:255:GLU:OE1	2.39	0.52
1:D:742:SER:OG	1:D:776:GLN:OE1	2.22	0.52
1:D:871:GLN:C	1:D:872:ILE:HD12	2.34	0.52
1:B:191:TYR:N	1:B:206:ALA:O	2.43	0.52
1:C:320:GLU:OE2	1:C:321:LYS:NZ	2.43	0.52
1:C:1838:GLU:N	1:C:1838:GLU:OE1	2.43	0.52
1:C:2118:LEU:HD21	1:C:2161:MET:HE1	1.90	0.52
1:D:1144:ARG:NH1	1:D:1184:ASP:OD2	2.42	0.52
1:A:191:TYR:N	1:A:206:ALA:O	2.43	0.51
1:A:255:GLU:OE1	1:A:255:GLU:N	2.39	0.51
1:D:1089:ARG:NH1	1:D:1090:ALA:O	2.43	0.51
1:A:2592:VAL:HG21	1:A:2639:LEU:HG	1.92	0.51
1:B:1089:ARG:NH1	1:B:1090:ALA:O	2.43	0.51
1:B:3714:GLU:OE1	1:B:3714:GLU:N	2.42	0.51
1:C:1144:ARG:NH1	1:C:1184:ASP:OD2	2.42	0.51
1:A:1533:GLN:NE2	1:A:1534:VAL:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:LEU:O	1:D:1661:LEU:HD21	2.10	0.51
1:A:1089:ARG:NH1	1:A:1090:ALA:O	2.43	0.51
1:B:246:THR:OG1	1:B:247:VAL:N	2.41	0.51
1:B:611:LEU:O	1:B:1661:LEU:HD21	2.11	0.51
1:B:888:ASN:OD1	1:B:1056:THR:HG21	2.10	0.51
1:B:1022:GLN:OE1	1:B:1029:ASN:ND2	2.43	0.51
1:C:246:THR:OG1	1:C:247:VAL:N	2.41	0.51
1:C:2463:HIS:O	1:C:2467:MET:HE2	2.11	0.51
1:D:1851:VAL:HG11	1:D:2060:LEU:HD22	1.93	0.51
1:D:1978:PHE:CZ	1:D:1995:LEU:HD23	2.45	0.51
1:A:1978:PHE:CZ	1:A:1995:LEU:HD23	2.45	0.51
1:B:1851:VAL:HG11	1:B:2060:LEU:HD22	1.93	0.51
1:B:3962:SER:OG	1:B:3963:GLN:OE1	2.12	0.51
1:C:888:ASN:OD1	1:C:1056:THR:HG21	2.10	0.51
1:D:615:CYS:SG	1:D:1661:LEU:HD23	2.51	0.51
1:D:2576:CYS:O	1:D:2615:ARG:NH2	2.44	0.51
1:A:2463:HIS:O	1:A:2467:MET:HE2	2.11	0.51
1:D:1533:GLN:NE2	1:D:1534:VAL:O	2.43	0.51
1:D:2242:ALA:O	1:D:2246:VAL:HG22	2.11	0.51
1:A:611:LEU:O	1:A:1661:LEU:HD21	2.10	0.51
1:C:191:TYR:N	1:C:206:ALA:O	2.43	0.51
1:D:888:ASN:OD1	1:D:1056:THR:HG21	2.10	0.51
1:D:1838:GLU:OE1	1:D:1838:GLU:N	2.43	0.51
1:A:1838:GLU:N	1:A:1838:GLU:OE1	2.43	0.51
1:B:2223:ASN:O	1:B:2226:VAL:HG12	2.11	0.51
1:C:1533:GLN:NE2	1:C:1534:VAL:O	2.43	0.51
1:C:1851:VAL:HG11	1:C:2060:LEU:HD22	1.93	0.51
1:C:2112:VAL:O	1:C:2115:THR:OG1	2.27	0.51
1:A:4928:ASP:OD1	1:A:4930:THR:N	2.43	0.51
1:B:2576:CYS:O	1:B:2615:ARG:NH2	2.44	0.51
1:C:611:LEU:O	1:C:1661:LEU:HD21	2.10	0.51
1:C:1910:GLN:HB2	1:C:2086:LEU:HD21	1.93	0.51
1:D:2592:VAL:HG21	1:D:2639:LEU:HG	1.92	0.51
1:D:4606:ALA:HB1	1:D:4648:VAL:HG21	1.93	0.51
1:A:615:CYS:SG	1:A:1661:LEU:HD23	2.51	0.50
1:A:2242:ALA:O	1:A:2246:VAL:HG22	2.11	0.50
1:A:4606:ALA:HB1	1:A:4648:VAL:HG21	1.93	0.50
1:B:2463:HIS:O	1:B:2467:MET:HE2	2.11	0.50
1:C:43:GLY:N	1:C:458:ASP:OD2	2.41	0.50
1:D:1762:MET:SD	1:D:1762:MET:N	2.80	0.50
2:H:38:ASP:OD1	2:H:39:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLU:OE1	1:B:151:GLU:N	2.43	0.50
1:B:1838:GLU:OE1	1:B:1838:GLU:N	2.43	0.50
1:C:557:TRP:O	1:C:560:SER:OG	2.20	0.50
1:C:1089:ARG:NH1	1:C:1090:ALA:O	2.43	0.50
1:C:2242:ALA:O	1:C:2246:VAL:HG22	2.11	0.50
1:C:4072:ASP:OD1	1:C:4076:THR:N	2.42	0.50
1:D:191:TYR:N	1:D:206:ALA:O	2.43	0.50
1:D:1022:GLN:OE1	1:D:1029:ASN:ND2	2.43	0.50
1:D:2223:ASN:O	1:D:2226:VAL:HG12	2.11	0.50
1:A:2579:LEU:O	1:A:2615:ARG:NH2	2.42	0.50
1:B:728:ASP:OD2	1:B:731:HIS:ND1	2.42	0.50
1:B:4755:ILE:O	1:B:4758:SER:OG	2.26	0.50
1:C:615:CYS:SG	1:C:1661:LEU:HD23	2.51	0.50
2:G:38:ASP:OD1	2:G:39:SER:N	2.45	0.50
1:A:1851:VAL:HG11	1:A:2060:LEU:HD22	1.93	0.50
1:C:2576:CYS:O	1:C:2615:ARG:NH2	2.44	0.50
1:D:2112:VAL:O	1:D:2115:THR:OG1	2.27	0.50
1:D:2463:HIS:O	1:D:2467:MET:HE2	2.11	0.50
1:D:3714:GLU:OE1	1:D:3714:GLU:N	2.42	0.50
2:I:38:ASP:OD1	2:I:39:SER:N	2.45	0.50
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.42	0.50
1:D:1910:GLN:HB2	1:D:2086:LEU:HD21	1.93	0.50
2:J:38:ASP:OD1	2:J:39:SER:N	2.45	0.50
1:B:43:GLY:N	1:B:458:ASP:OD2	2.41	0.50
1:B:565:LEU:HD11	1:B:1585:PRO:CG	2.42	0.50
1:B:2242:ALA:O	1:B:2246:VAL:HG22	2.11	0.50
1:B:4072:ASP:OD1	1:B:4076:THR:N	2.42	0.50
1:C:640:ARG:O	1:C:645:GLN:NE2	2.45	0.50
1:D:2435:ILE:O	1:D:2464:LYS:NZ	2.25	0.50
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.42	0.50
1:A:4072:ASP:OD1	1:A:4076:THR:N	2.42	0.50
1:D:318:ASP:OD1	1:D:319:LYS:N	2.44	0.50
1:D:728:ASP:OD2	1:D:731:HIS:ND1	2.42	0.50
1:D:981:MET:O	1:D:1055:ARG:NH1	2.44	0.50
1:A:3971:MET:HE1	5:A:5003:A1MG7:CAV	2.42	0.50
1:B:615:CYS:SG	1:B:1661:LEU:HD23	2.51	0.50
1:B:640:ARG:O	1:B:645:GLN:NE2	2.45	0.50
1:C:614:LEU:HD21	1:C:632:ILE:HG21	1.94	0.50
1:C:2223:ASN:O	1:C:2226:VAL:HG12	2.11	0.50
1:C:4606:ALA:HB1	1:C:4648:VAL:HG21	1.93	0.50
1:D:4024:ASP:OD1	1:D:4054:HIS:NE2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1655:HIS:O	1:A:1658:THR:OG1	2.24	0.50
1:C:1053:ALA:O	1:C:1056:THR:OG1	2.27	0.50
1:A:318:ASP:OD1	1:A:319:LYS:N	2.44	0.49
1:A:2576:CYS:O	1:A:2615:ARG:NH2	2.44	0.49
1:D:3971:MET:HE1	5:D:5003:A1MG7:CAV	2.42	0.49
1:D:4836:ASP:OD1	1:D:4837:GLU:N	2.45	0.49
1:A:565:LEU:HD11	1:A:1585:PRO:CG	2.42	0.49
1:B:78:LEU:HD22	1:B:118:ALA:CB	2.42	0.49
1:B:3971:MET:HE1	5:B:5003:A1MG7:CAV	2.42	0.49
1:C:151:GLU:OE1	1:C:151:GLU:N	2.43	0.49
1:D:320:GLU:OE2	1:D:321:LYS:NZ	2.43	0.49
1:A:2223:ASN:O	1:A:2226:VAL:HG12	2.11	0.49
1:B:4606:ALA:HB1	1:B:4648:VAL:HG21	1.93	0.49
1:C:2599:ASN:OD1	1:C:2602:ALA:N	2.46	0.49
1:C:4130:PRO:O	1:C:4156:ARG:NH1	2.45	0.49
1:D:284:TRP:NE1	1:D:347:ASP:OD1	2.45	0.49
1:D:4630:ASP:O	1:D:4633:VAL:HG12	2.12	0.49
1:D:4755:ILE:O	1:D:4758:SER:OG	2.26	0.49
1:A:284:TRP:NE1	1:A:347:ASP:OD1	2.45	0.49
1:B:996:VAL:HG13	1:B:1050:LEU:HD11	1.94	0.49
1:B:1910:GLN:HB2	1:B:2086:LEU:HD21	1.93	0.49
1:C:1733:GLU:OE1	1:C:1733:GLU:N	2.44	0.49
1:D:565:LEU:HD11	1:D:1585:PRO:CG	2.42	0.49
1:D:640:ARG:O	1:D:645:GLN:NE2	2.45	0.49
1:D:4130:PRO:O	1:D:4156:ARG:NH1	2.45	0.49
1:A:78:LEU:HD22	1:A:118:ALA:CB	2.42	0.49
1:A:640:ARG:O	1:A:645:GLN:NE2	2.45	0.49
1:B:1053:ALA:O	1:B:1056:THR:OG1	2.27	0.49
1:B:4619:GLN:OE1	1:B:4631:ARG:NH2	2.46	0.49
1:C:248:PRO:O	1:C:257:ARG:NE	2.35	0.49
1:C:506:HIS:O	1:C:564:ARG:NH1	2.44	0.49
1:C:3962:SER:OG	1:C:3963:GLN:OE1	2.12	0.49
1:C:3971:MET:HE1	5:C:5003:A1MG7:CAV	2.42	0.49
1:C:4630:ASP:O	1:C:4633:VAL:HG12	2.12	0.49
1:D:248:PRO:O	1:D:257:ARG:NE	2.36	0.49
1:D:4072:ASP:OD1	1:D:4076:THR:N	2.42	0.49
1:A:1100:ARG:NH2	1:A:1234:GLU:O	2.45	0.49
1:A:1910:GLN:HB2	1:A:2086:LEU:HD21	1.93	0.49
1:B:869:THR:HA	1:B:872:ILE:HD13	1.95	0.49
1:C:78:LEU:HD22	1:C:118:ALA:CB	2.42	0.49
1:D:78:LEU:HD22	1:D:118:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:869:THR:HA	1:D:872:ILE:HD13	1.95	0.49
1:A:981:MET:O	1:A:1055:ARG:NH1	2.44	0.49
1:A:1022:GLN:OE1	1:A:1029:ASN:ND2	2.43	0.49
1:A:2154:PHE:HD1	1:A:2161:MET:HE2	1.78	0.49
1:A:3852:ASP:OD1	1:A:3853:PHE:N	2.46	0.49
1:B:284:TRP:NE1	1:B:347:ASP:OD1	2.45	0.49
1:B:4653:MET:SD	1:B:4662:ARG:NH1	2.86	0.49
1:C:1635:GLU:OE1	1:C:1635:GLU:N	2.40	0.49
1:A:2599:ASN:OD1	1:A:2602:ALA:N	2.46	0.49
1:A:4130:PRO:O	1:A:4156:ARG:NH1	2.45	0.49
1:A:4630:ASP:O	1:A:4633:VAL:HG12	2.12	0.49
1:A:4653:MET:SD	1:A:4662:ARG:NH1	2.86	0.49
1:A:4836:ASP:OD1	1:A:4837:GLU:N	2.45	0.49
1:B:3852:ASP:OD1	1:B:3853:PHE:N	2.46	0.49
1:C:1265:HIS:O	1:C:1288:LYS:NZ	2.40	0.49
1:C:3852:ASP:OD1	1:C:3853:PHE:N	2.46	0.49
1:D:614:LEU:HD21	1:D:632:ILE:HG21	1.94	0.49
1:D:2154:PHE:HD1	1:D:2161:MET:HE2	1.78	0.49
1:A:869:THR:HA	1:A:872:ILE:HD13	1.95	0.49
1:B:4130:PRO:O	1:B:4156:ARG:NH1	2.45	0.49
1:C:996:VAL:HG13	1:C:1050:LEU:HD11	1.94	0.49
1:D:2305:VAL:O	1:D:2312:VAL:HG22	2.13	0.49
1:A:658:ASN:OD1	1:A:833:LYS:N	2.45	0.48
1:A:2161:MET:HE3	1:A:2166:MET:CE	2.43	0.48
1:A:2426:ILE:HD13	1:A:2470:PHE:CZ	2.48	0.48
1:B:1272:ARG:NH1	1:B:1587:LEU:O	2.45	0.48
1:B:1704:TYR:OH	1:B:1795:MET:SD	2.71	0.48
1:B:2426:ILE:HD13	1:B:2470:PHE:CZ	2.49	0.48
1:C:869:THR:HA	1:C:872:ILE:HD13	1.95	0.48
1:C:1272:ARG:NH1	1:C:1587:LEU:O	2.45	0.48
1:C:4619:GLN:OE1	1:C:4631:ARG:NH2	2.46	0.48
1:D:3831:ASP:OD1	1:D:3831:ASP:N	2.46	0.48
1:D:3852:ASP:OD1	1:D:3853:PHE:N	2.46	0.48
1:A:4619:GLN:OE1	1:A:4631:ARG:NH2	2.46	0.48
1:B:614:LEU:HD21	1:B:632:ILE:HG21	1.94	0.48
1:B:2161:MET:HE3	1:B:2166:MET:CE	2.43	0.48
1:B:2305:VAL:O	1:B:2312:VAL:HG22	2.13	0.48
1:C:2305:VAL:O	1:C:2312:VAL:HG22	2.13	0.48
1:D:1100:ARG:NH2	1:D:1234:GLU:O	2.45	0.48
1:D:1272:ARG:NH1	1:D:1587:LEU:O	2.45	0.48
1:D:2599:ASN:OD1	1:D:2602:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2154:PHE:HD1	1:B:2161:MET:HE2	1.78	0.48
1:D:3962:SER:OG	1:D:3963:GLN:OE1	2.12	0.48
1:A:614:LEU:HD21	1:A:632:ILE:HG21	1.94	0.48
1:A:3831:ASP:OD1	1:A:3831:ASP:N	2.46	0.48
1:B:1733:GLU:OE1	1:B:1733:GLU:N	2.44	0.48
1:C:658:ASN:OD1	1:C:833:LYS:N	2.45	0.48
1:C:981:MET:O	1:C:1055:ARG:NH1	2.44	0.48
1:C:4836:ASP:OD1	1:C:4837:GLU:N	2.46	0.48
1:A:670:TYR:OH	1:A:818:GLY:O	2.32	0.48
1:B:658:ASN:OD1	1:B:833:LYS:N	2.45	0.48
1:B:670:TYR:OH	1:B:818:GLY:O	2.32	0.48
1:C:565:LEU:HD11	1:C:1585:PRO:CG	2.42	0.48
1:C:1157:GLN:OE1	1:C:1157:GLN:N	2.47	0.48
1:A:996:VAL:HG13	1:A:1050:LEU:HD11	1.94	0.48
1:B:4630:ASP:O	1:B:4633:VAL:HG12	2.12	0.48
1:C:4755:ILE:O	1:C:4758:SER:OG	2.26	0.48
1:B:323:ASP:OD1	1:B:326:SER:OG	2.11	0.48
1:B:1265:HIS:O	1:B:1288:LYS:NZ	2.40	0.48
1:C:981:MET:SD	1:C:981:MET:N	2.87	0.48
1:D:1704:TYR:OH	1:D:1795:MET:SD	2.71	0.48
1:A:1157:GLN:N	1:A:1157:GLN:OE1	2.47	0.48
1:C:1022:GLN:OE1	1:C:1029:ASN:ND2	2.43	0.48
1:C:4653:MET:SD	1:C:4662:ARG:NH1	2.86	0.48
1:D:885:LEU:HD11	1:D:1057:LEU:HD21	1.95	0.48
1:D:4619:GLN:OE1	1:D:4631:ARG:NH2	2.46	0.48
1:A:2305:VAL:O	1:A:2312:VAL:HG22	2.13	0.48
1:B:2599:ASN:OD1	1:B:2602:ALA:N	2.46	0.48
1:B:4836:ASP:OD1	1:B:4837:GLU:N	2.47	0.48
1:C:670:TYR:OH	1:C:818:GLY:O	2.32	0.48
1:C:1704:TYR:OH	1:C:1795:MET:SD	2.71	0.48
1:D:4653:MET:SD	1:D:4662:ARG:NH1	2.86	0.48
1:B:506:HIS:O	1:B:564:ARG:NH1	2.44	0.48
1:C:728:ASP:OD2	1:C:731:HIS:ND1	2.42	0.48
1:D:2426:ILE:HD13	1:D:2470:PHE:CZ	2.48	0.48
1:A:1704:TYR:OH	1:A:1795:MET:SD	2.71	0.47
1:C:284:TRP:NE1	1:C:347:ASP:OD1	2.45	0.47
1:C:885:LEU:HD11	1:C:1057:LEU:HD21	1.95	0.47
1:D:1157:GLN:N	1:D:1157:GLN:OE1	2.47	0.47
1:A:946:LEU:CD1	1:A:995:MET:HE1	2.44	0.47
1:C:2426:ILE:HD13	1:C:2470:PHE:CZ	2.48	0.47
1:D:658:ASN:OD1	1:D:833:LYS:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:981:MET:SD	1:D:981:MET:N	2.87	0.47
1:D:1051:ARG:HA	1:D:1054:VAL:HG22	1.96	0.47
1:A:742:SER:OG	1:A:776:GLN:OE1	2.22	0.47
1:B:1157:GLN:N	1:B:1157:GLN:OE1	2.47	0.47
1:C:1051:ARG:HA	1:C:1054:VAL:HG22	1.96	0.47
1:C:2154:PHE:HD1	1:C:2161:MET:HE2	1.78	0.47
1:D:996:VAL:HG13	1:D:1050:LEU:HD11	1.94	0.47
1:D:2161:MET:HE3	1:D:2166:MET:CE	2.43	0.47
1:C:2161:MET:HE3	1:C:2166:MET:CE	2.43	0.47
1:D:93:VAL:HG22	1:D:95:VAL:HG23	1.97	0.47
1:D:506:HIS:O	1:D:564:ARG:NH1	2.44	0.47
1:A:17:ASP:N	1:A:17:ASP:OD1	2.48	0.47
1:C:993:GLU:OE1	1:C:1051:ARG:NH1	2.48	0.47
1:D:586:LEU:CD2	1:D:625:VAL:HG21	2.45	0.47
1:A:320:GLU:OE2	1:A:321:LYS:NZ	2.43	0.47
1:B:946:LEU:CD1	1:B:995:MET:HE1	2.44	0.47
1:B:981:MET:O	1:B:1055:ARG:NH1	2.44	0.47
1:C:1100:ARG:NH2	1:C:1234:GLU:O	2.46	0.47
1:D:4508:ALA:O	1:D:4512:ASN:ND2	2.48	0.47
1:A:885:LEU:HD11	1:A:1057:LEU:HD21	1.95	0.47
1:B:885:LEU:HD11	1:B:1057:LEU:HD21	1.95	0.47
1:B:3965:GLU:OE1	1:B:3965:GLU:N	2.45	0.47
1:C:586:LEU:CD2	1:C:625:VAL:HG21	2.45	0.47
1:C:946:LEU:CD1	1:C:995:MET:HE1	2.44	0.47
1:C:4508:ALA:O	1:C:4512:ASN:ND2	2.48	0.47
2:J:62:GLU:OE2	2:J:66:GLN:NE2	2.48	0.47
1:A:1629:MET:HG3	1:A:1642:ILE:HD13	1.97	0.47
1:B:1051:ARG:HA	1:B:1054:VAL:HG22	1.96	0.47
1:B:3831:ASP:N	1:B:3831:ASP:OD1	2.46	0.47
1:C:318:ASP:OD1	1:C:319:LYS:N	2.44	0.47
1:D:670:TYR:OH	1:D:818:GLY:O	2.32	0.47
1:D:1655:HIS:O	1:D:1658:THR:OG1	2.24	0.47
1:A:93:VAL:HG22	1:A:95:VAL:HG23	1.97	0.47
1:B:1629:MET:HG3	1:B:1642:ILE:HD13	1.97	0.47
1:A:586:LEU:CD2	1:A:625:VAL:HG21	2.45	0.47
1:A:4895:ASP:OD1	1:A:4896:TYR:N	2.48	0.47
1:C:2276:CYS:SG	1:C:2290:ASN:ND2	2.88	0.47
1:D:1053:ALA:O	1:D:1056:THR:OG1	2.27	0.47
1:D:1629:MET:HG3	1:D:1642:ILE:HD13	1.97	0.47
2:H:62:GLU:OE2	2:H:66:GLN:NE2	2.48	0.47
1:A:1051:ARG:HA	1:A:1054:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2276:CYS:SG	1:A:2290:ASN:ND2	2.88	0.46
1:A:3965:GLU:OE1	1:A:3965:GLU:N	2.45	0.46
1:A:4508:ALA:O	1:A:4512:ASN:ND2	2.48	0.46
1:B:4895:ASP:OD1	1:B:4896:TYR:N	2.48	0.46
1:D:917:CYS:HA	1:D:924:LEU:HD22	1.97	0.46
1:D:946:LEU:CD1	1:D:995:MET:HE1	2.44	0.46
1:D:4895:ASP:OD1	1:D:4896:TYR:N	2.48	0.46
1:B:514:PHE:CE2	1:B:522:ALA:HB1	2.51	0.46
1:B:981:MET:SD	1:B:981:MET:N	2.87	0.46
1:C:17:ASP:N	1:C:17:ASP:OD1	2.47	0.46
1:C:624:ALA:CB	1:C:1668:LEU:HD12	2.46	0.46
1:C:2333:ALA:CB	1:C:2345:ALA:HB2	2.46	0.46
1:D:1733:GLU:OE1	1:D:1733:GLU:N	2.44	0.46
2:I:62:GLU:OE2	2:I:66:GLN:NE2	2.48	0.46
1:A:98:TRP:HD1	1:A:102:MET:HE2	1.80	0.46
1:B:624:ALA:CB	1:B:1668:LEU:HD12	2.46	0.46
1:B:917:CYS:HA	1:B:924:LEU:HD22	1.97	0.46
1:B:2276:CYS:SG	1:B:2290:ASN:ND2	2.88	0.46
1:D:1300:MET:SD	1:D:1300:MET:N	2.88	0.46
1:D:2333:ALA:CB	1:D:2345:ALA:HB2	2.46	0.46
1:A:514:PHE:CE2	1:A:522:ALA:HB1	2.51	0.46
1:A:993:GLU:OE1	1:A:1051:ARG:NH1	2.48	0.46
1:A:1300:MET:SD	1:A:1300:MET:N	2.88	0.46
1:A:2112:VAL:O	1:A:2115:THR:OG1	2.27	0.46
1:B:447:LEU:O	1:B:449:ILE:N	2.49	0.46
1:B:586:LEU:CD2	1:B:625:VAL:HG21	2.45	0.46
1:B:2333:ALA:CB	1:B:2345:ALA:HB2	2.46	0.46
1:C:98:TRP:HD1	1:C:102:MET:HE2	1.81	0.46
1:D:78:LEU:HD22	1:D:118:ALA:HB1	1.97	0.46
1:A:78:LEU:HD22	1:A:118:ALA:HB1	1.97	0.46
1:B:680:ASP:O	1:B:751:THR:HG23	2.16	0.46
1:B:1100:ARG:NH2	1:B:1234:GLU:O	2.46	0.46
1:B:1300:MET:SD	1:B:1300:MET:N	2.88	0.46
1:C:93:VAL:HG22	1:C:95:VAL:HG23	1.97	0.46
1:C:447:LEU:O	1:C:449:ILE:N	2.49	0.46
1:C:917:CYS:HA	1:C:924:LEU:HD22	1.97	0.46
1:C:1300:MET:SD	1:C:1300:MET:N	2.88	0.46
1:D:17:ASP:OD1	1:D:17:ASP:N	2.48	0.46
1:D:98:TRP:HD1	1:D:102:MET:HE2	1.81	0.46
1:D:626:ARG:NH2	1:D:1668:LEU:O	2.48	0.46
1:D:993:GLU:OE1	1:D:1051:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:SER:OG	1:B:776:GLN:OE1	2.22	0.46
1:B:993:GLU:OE1	1:B:1051:ARG:NH1	2.48	0.46
1:C:2425:LEU:HB3	1:C:2426:ILE:HD12	1.98	0.46
1:A:2333:ALA:CB	1:A:2345:ALA:HB2	2.46	0.46
1:B:93:VAL:HG22	1:B:95:VAL:HG23	1.97	0.46
1:C:78:LEU:HD22	1:C:118:ALA:HB1	1.97	0.46
1:C:680:ASP:O	1:C:751:THR:HG23	2.16	0.46
1:D:2276:CYS:SG	1:D:2290:ASN:ND2	2.88	0.46
1:D:2312:VAL:HG23	1:D:2315:ASN:HB2	1.98	0.46
2:G:62:GLU:OE2	2:G:66:GLN:NE2	2.48	0.46
1:A:506:HIS:O	1:A:564:ARG:NH1	2.44	0.46
1:A:1906:CYS:SG	1:A:1907:LEU:N	2.89	0.46
1:A:2070:GLN:HA	1:A:3657:MET:HE3	1.98	0.46
1:A:3878:LEU:HD21	1:A:3938:ARG:HH21	1.81	0.46
1:D:2425:LEU:HB3	1:D:2426:ILE:HD12	1.98	0.46
1:A:447:LEU:O	1:A:449:ILE:N	2.49	0.46
1:B:17:ASP:OD1	1:B:17:ASP:N	2.47	0.46
1:B:2425:LEU:HB3	1:B:2426:ILE:HD12	1.98	0.46
1:C:1629:MET:HG3	1:C:1642:ILE:HD13	1.97	0.46
1:C:2312:VAL:HG23	1:C:2315:ASN:HB2	1.98	0.46
1:A:981:MET:SD	1:A:981:MET:N	2.87	0.46
1:A:1733:GLU:OE1	1:A:1733:GLU:N	2.44	0.46
1:B:2434:VAL:HG11	1:B:2467:MET:HE3	1.98	0.46
1:B:3655:GLU:OE1	1:B:3655:GLU:N	2.49	0.46
1:C:2355:ASP:CG	1:C:2357:SER:HG	2.24	0.46
1:C:4895:ASP:OD1	1:C:4896:TYR:N	2.48	0.46
1:D:624:ALA:CB	1:D:1668:LEU:HD12	2.46	0.46
1:B:1906:CYS:SG	1:B:1907:LEU:N	2.89	0.45
1:B:3937:SER:OG	1:B:3938:ARG:N	2.49	0.45
1:C:1636:GLU:OE1	1:C:1638:ARG:NE	2.40	0.45
1:A:624:ALA:CB	1:A:1668:LEU:HD12	2.46	0.45
1:B:1636:GLU:OE1	1:B:1638:ARG:NE	2.40	0.45
1:B:2070:GLN:HA	1:B:3657:MET:HE3	1.98	0.45
1:C:514:PHE:CE2	1:C:522:ALA:HB1	2.50	0.45
1:D:119:ILE:HD13	1:D:162:ILE:HD11	1.99	0.45
1:D:247:VAL:O	1:D:272:ARG:NH1	2.47	0.45
1:D:514:PHE:CE2	1:D:522:ALA:HB1	2.51	0.45
1:D:2434:VAL:HG11	1:D:2467:MET:HE3	1.98	0.45
1:A:917:CYS:HA	1:A:924:LEU:HD22	1.97	0.45
1:A:1272:ARG:NH1	1:A:1587:LEU:O	2.45	0.45
1:B:119:ILE:HD13	1:B:162:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2312:VAL:HG23	1:B:2315:ASN:HB2	1.98	0.45
1:B:4508:ALA:O	1:B:4512:ASN:ND2	2.48	0.45
1:C:1906:CYS:SG	1:C:1907:LEU:N	2.89	0.45
1:C:2434:VAL:HG11	1:C:2467:MET:HE3	1.98	0.45
1:A:2312:VAL:HG23	1:A:2315:ASN:HB2	1.98	0.45
1:B:78:LEU:HD22	1:B:118:ALA:HB1	1.97	0.45
1:C:3878:LEU:HD21	1:C:3938:ARG:HH21	1.81	0.45
1:D:2640:SER:HB3	1:D:2675:LEU:HD21	1.98	0.45
1:D:3878:LEU:HD21	1:D:3938:ARG:HH21	1.81	0.45
1:D:3965:GLU:OE1	1:D:3965:GLU:N	2.45	0.45
2:I:95:ASN:OD1	2:I:95:ASN:N	2.50	0.45
1:A:1437:GLU:N	1:A:1549:THR:OG1	2.49	0.45
1:A:2425:LEU:HB3	1:A:2426:ILE:HD12	1.98	0.45
1:B:98:TRP:HD1	1:B:102:MET:HE2	1.80	0.45
1:D:680:ASP:O	1:D:751:THR:HG23	2.16	0.45
1:A:680:ASP:O	1:A:751:THR:HG23	2.16	0.45
1:C:119:ILE:HD13	1:C:162:ILE:HD11	1.99	0.45
1:D:208:GLN:OE1	1:D:210:THR:OG1	2.31	0.45
1:D:447:LEU:O	1:D:449:ILE:N	2.49	0.45
2:H:95:ASN:N	2:H:95:ASN:OD1	2.50	0.45
1:A:1636:GLU:OE1	1:A:1638:ARG:NE	2.40	0.45
1:B:247:VAL:O	1:B:272:ARG:NH1	2.47	0.45
1:B:3878:LEU:HD21	1:B:3938:ARG:HH21	1.81	0.45
1:C:3831:ASP:OD1	1:C:3831:ASP:N	2.46	0.45
2:J:95:ASN:N	2:J:95:ASN:OD1	2.50	0.45
1:A:3975:LYS:O	1:A:3979:VAL:HG23	2.17	0.45
1:B:4088:GLU:OE1	1:B:4091:LYS:NZ	2.50	0.45
1:A:119:ILE:HD13	1:A:162:ILE:HD11	1.99	0.45
1:B:1437:GLU:N	1:B:1549:THR:OG1	2.49	0.45
1:B:2640:SER:HB3	1:B:2675:LEU:HD21	1.98	0.45
1:C:309:MET:SD	1:C:309:MET:N	2.85	0.45
1:C:2367:SER:OG	1:C:2368:SER:N	2.49	0.45
1:D:3975:LYS:O	1:D:3979:VAL:HG23	2.17	0.45
1:A:248:PRO:O	1:A:257:ARG:NE	2.36	0.45
1:B:87:GLU:OE1	1:B:87:GLU:N	2.48	0.45
1:C:2070:GLN:HA	1:C:3657:MET:HE3	1.98	0.45
1:D:1471:ASP:OD1	1:D:1475:LYS:N	2.49	0.45
1:A:272:ARG:O	1:A:299:HIS:NE2	2.39	0.44
1:A:1681:VAL:HG11	1:A:1686:LEU:HD21	2.00	0.44
1:A:2640:SER:HB3	1:A:2675:LEU:HD21	1.98	0.44
1:A:3937:SER:OG	1:A:3938:ARG:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1906:CYS:SG	1:D:1907:LEU:N	2.89	0.44
1:D:2283:GLY:O	1:D:2362:SER:N	2.48	0.44
1:B:21:VAL:HG22	1:B:217:ILE:HD11	1.99	0.44
1:B:208:GLN:OE1	1:B:210:THR:OG1	2.31	0.44
1:B:3975:LYS:O	1:B:3979:VAL:HG23	2.17	0.44
1:C:99:LYS:HA	1:C:102:MET:HE3	1.99	0.44
1:D:99:LYS:HA	1:D:102:MET:HE3	1.99	0.44
1:D:2070:GLN:HA	1:D:3657:MET:HE3	1.98	0.44
1:D:4088:GLU:OE1	1:D:4091:LYS:NZ	2.50	0.44
1:A:21:VAL:HG22	1:A:217:ILE:HD11	1.99	0.44
1:B:2355:ASP:CG	1:B:2357:SER:HG	2.24	0.44
1:C:85:THR:HB	1:C:102:MET:HE1	1.99	0.44
1:C:2640:SER:HB3	1:C:2675:LEU:HD21	1.98	0.44
1:C:3975:LYS:O	1:C:3979:VAL:HG23	2.17	0.44
1:D:3937:SER:OG	1:D:3938:ARG:N	2.49	0.44
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.91	0.44
1:A:626:ARG:NH2	1:A:1668:LEU:O	2.48	0.44
1:A:1105:PHE:CB	1:A:1115:VAL:HG21	2.47	0.44
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.50	0.44
1:A:1595:VAL:HG13	1:A:1595:VAL:O	2.18	0.44
1:A:2396:ASP:OD1	1:A:2400:ARG:NE	2.51	0.44
1:B:1471:ASP:OD1	1:B:1475:LYS:N	2.49	0.44
1:B:1681:VAL:HG11	1:B:1686:LEU:HD21	2.00	0.44
1:C:1681:VAL:HG11	1:C:1686:LEU:HD21	1.99	0.44
1:D:1105:PHE:CB	1:D:1115:VAL:HG21	2.47	0.44
1:D:1437:GLU:N	1:D:1549:THR:OG1	2.49	0.44
2:G:95:ASN:OD1	2:G:95:ASN:N	2.50	0.44
1:A:2434:VAL:HG11	1:A:2467:MET:HE3	1.98	0.44
1:C:3937:SER:OG	1:C:3938:ARG:N	2.50	0.44
1:A:1053:ALA:O	1:A:1056:THR:OG1	2.27	0.44
1:B:78:LEU:HD21	1:B:159:TRP:CG	2.53	0.44
1:C:1105:PHE:CB	1:C:1115:VAL:HG21	2.47	0.44
1:C:1595:VAL:HG13	1:C:1595:VAL:O	2.18	0.44
1:C:4033:GLU:OE1	1:C:4033:GLU:N	2.49	0.44
1:D:78:LEU:HD21	1:D:159:TRP:CG	2.53	0.44
1:D:1681:VAL:HG11	1:D:1686:LEU:HD21	2.00	0.44
1:A:99:LYS:HA	1:A:102:MET:HE3	1.99	0.44
1:A:2485:HIS:O	1:A:2489:VAL:HG22	2.18	0.44
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.50	0.44
1:B:2367:SER:OG	1:B:2368:SER:N	2.49	0.44
1:B:2538:GLU:OE1	1:B:2538:GLU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.91	0.44
1:C:247:VAL:O	1:C:272:ARG:NH1	2.47	0.44
1:C:1437:GLU:N	1:C:1549:THR:OG1	2.49	0.44
1:C:4927:LYS:NZ	1:C:4936:GLU:OE1	2.45	0.44
1:D:85:THR:HB	1:D:102:MET:HE1	1.99	0.44
1:D:2324:ILE:HD13	1:D:2421:ILE:HG21	2.00	0.44
1:D:2485:HIS:O	1:D:2489:VAL:HG22	2.18	0.44
2:J:22:THR:N	2:J:108:GLU:OXT	2.48	0.44
1:A:3962:SER:OG	1:A:3963:GLN:OE1	2.12	0.44
1:A:4955:ASP:OD1	1:A:4956:CYS:N	2.50	0.44
1:B:654:SER:O	1:B:837:SER:OG	2.25	0.44
1:B:1105:PHE:CB	1:B:1115:VAL:HG21	2.47	0.44
1:C:742:SER:OG	1:C:776:GLN:OE1	2.22	0.44
1:C:4955:ASP:OD1	1:C:4956:CYS:N	2.50	0.44
1:D:1595:VAL:O	1:D:1595:VAL:HG13	2.18	0.44
1:D:2396:ASP:OD1	1:D:2400:ARG:NE	2.51	0.44
1:A:4181:GLU:OE1	1:A:4181:GLU:N	2.50	0.44
1:B:85:THR:HB	1:B:102:MET:HE1	1.99	0.44
1:C:21:VAL:HG22	1:C:217:ILE:HD11	1.99	0.44
1:D:573:GLU:OE1	1:D:609:LYS:NZ	2.22	0.44
1:D:3655:GLU:OE1	1:D:3655:GLU:N	2.49	0.44
1:A:2283:GLY:O	1:A:2362:SER:N	2.48	0.43
1:B:318:ASP:OD1	1:B:319:LYS:N	2.44	0.43
1:B:1595:VAL:HG13	1:B:1595:VAL:O	2.18	0.43
1:B:4955:ASP:OD1	1:B:4956:CYS:N	2.50	0.43
1:A:85:THR:HB	1:A:102:MET:HE1	1.99	0.43
1:B:2396:ASP:OD1	1:B:2400:ARG:NE	2.51	0.43
1:A:78:LEU:HD21	1:A:159:TRP:CG	2.53	0.43
1:A:654:SER:C	1:A:655:MET:HE2	2.43	0.43
1:C:332:ARG:NH2	1:C:338:LEU:O	2.48	0.43
1:C:2528:THR:HG21	1:C:2570:VAL:HG12	2.00	0.43
1:C:2538:GLU:OE1	1:C:2538:GLU:N	2.48	0.43
1:D:763:ALA:HB3	1:D:764:PRO:C	2.43	0.43
1:A:763:ALA:HB3	1:A:764:PRO:C	2.43	0.43
1:A:4088:GLU:OE1	1:A:4091:LYS:NZ	2.50	0.43
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.91	0.43
1:B:332:ARG:NH2	1:B:338:LEU:O	2.48	0.43
1:B:626:ARG:NH2	1:B:1668:LEU:O	2.48	0.43
1:C:78:LEU:HD21	1:C:159:TRP:CG	2.53	0.43
1:C:2324:ILE:HD13	1:C:2421:ILE:HG21	2.00	0.43
1:A:2528:THR:HG21	1:A:2570:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2538:GLU:OE1	1:A:2538:GLU:N	2.47	0.43
1:A:3655:GLU:OE1	1:A:3655:GLU:N	2.49	0.43
1:B:137:ARG:N	1:B:146:ASP:OD2	2.51	0.43
1:B:2528:THR:HG21	1:B:2570:VAL:HG12	2.01	0.43
1:C:904:TYR:HB2	1:C:918:LEU:HD22	2.00	0.43
1:C:1029:ASN:OD1	1:C:1031:ARG:N	2.48	0.43
1:C:2396:ASP:OD1	1:C:2400:ARG:NE	2.51	0.43
1:C:2485:HIS:O	1:C:2489:VAL:HG22	2.18	0.43
1:A:904:TYR:HB2	1:A:918:LEU:HD22	2.00	0.43
1:B:2324:ILE:HD13	1:B:2421:ILE:HG21	2.00	0.43
1:C:1914:ASP:OD1	1:C:2089:ARG:NH1	2.48	0.43
1:C:3622:GLY:O	1:C:3626:SER:OG	2.13	0.43
1:C:3655:GLU:OE1	1:C:3655:GLU:N	2.49	0.43
1:D:21:VAL:HG22	1:D:217:ILE:HD11	1.99	0.43
1:D:1757:SER:N	1:D:1922:GLU:OE2	2.49	0.43
1:D:2528:THR:HG21	1:D:2570:VAL:HG12	2.01	0.43
1:B:272:ARG:O	1:B:299:HIS:NE2	2.40	0.43
1:B:1801:LYS:O	1:B:1804:SER:OG	2.36	0.43
1:B:2485:HIS:O	1:B:2489:VAL:HG22	2.18	0.43
1:C:2560:LEU:O	1:C:2565:ARG:NH1	2.51	0.43
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.91	0.43
1:C:763:ALA:HB3	1:C:764:PRO:C	2.43	0.43
1:A:500:GLU:OE1	1:A:504:ARG:NH1	2.50	0.43
1:A:2355:ASP:CG	1:A:2357:SER:HG	2.25	0.43
1:B:99:LYS:HA	1:B:102:MET:HE3	1.99	0.43
1:B:763:ALA:HB3	1:B:764:PRO:C	2.43	0.43
1:B:2283:GLY:O	1:B:2362:SER:N	2.48	0.43
1:C:495:ILE:HD13	1:C:540:LEU:HD23	2.01	0.43
1:C:654:SER:C	1:C:655:MET:HE2	2.43	0.43
1:A:698:ALA:HB2	1:A:791:VAL:HG11	2.01	0.43
1:D:495:ILE:HD13	1:D:540:LEU:HD23	2.01	0.43
1:D:654:SER:C	1:D:655:MET:HE2	2.43	0.43
1:D:904:TYR:HB2	1:D:918:LEU:HD22	2.00	0.43
1:A:611:LEU:HD22	1:A:1661:LEU:HD11	2.01	0.42
1:B:221:SER:OG	1:B:222:GLU:OE1	2.33	0.42
1:B:1107:ALA:HB1	1:B:1113:MET:CE	2.49	0.42
1:B:1184:ASP:N	1:B:1188:SER:O	2.49	0.42
1:B:2464:LYS:O	1:B:2468:VAL:HG23	2.19	0.42
1:B:4134:ARG:C	1:B:4135:ILE:HD13	2.44	0.42
1:B:4949:GLU:OE1	1:B:4949:GLU:N	2.52	0.42
1:C:611:LEU:HD22	1:C:1661:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:LEU:HD22	1:C:1661:LEU:HD22	2.01	0.42
1:D:3923:ILE:HD13	1:D:3934:LEU:CD1	2.40	0.42
1:D:4181:GLU:OE1	1:D:4181:GLU:N	2.50	0.42
1:A:1416:ASP:N	1:A:1563:ASN:OD1	2.52	0.42
1:A:2324:ILE:HD13	1:A:2421:ILE:HG21	2.00	0.42
1:B:611:LEU:HD22	1:B:1661:LEU:HD11	2.01	0.42
1:C:174:LYS:O	1:C:176:ARG:NE	2.53	0.42
1:C:573:GLU:OE1	1:C:609:LYS:NZ	2.22	0.42
1:C:2437:ILE:O	1:C:2464:LYS:NZ	2.42	0.42
2:G:22:THR:N	2:G:108:GLU:OXT	2.48	0.42
1:A:174:LYS:O	1:A:176:ARG:NE	2.53	0.42
1:A:562:LEU:HA	1:A:571:ILE:HD13	2.01	0.42
1:A:4134:ARG:C	1:A:4135:ILE:HD13	2.44	0.42
1:B:1416:ASP:N	1:B:1563:ASN:OD1	2.52	0.42
1:C:626:ARG:NH2	1:C:1668:LEU:O	2.48	0.42
1:C:1801:LYS:O	1:C:1804:SER:OG	2.36	0.42
1:C:2464:LYS:O	1:C:2468:VAL:HG23	2.19	0.42
1:C:4134:ARG:C	1:C:4135:ILE:HD13	2.44	0.42
1:D:1416:ASP:N	1:D:1563:ASN:OD1	2.52	0.42
1:D:1495:SER:O	1:D:1499:GLY:N	2.51	0.42
1:A:624:ALA:HB2	1:A:1668:LEU:HD12	2.02	0.42
1:B:654:SER:C	1:B:655:MET:HE2	2.43	0.42
1:B:1107:ALA:HB1	1:B:1113:MET:HE3	2.01	0.42
1:C:3941:ASP:N	1:C:3941:ASP:OD1	2.52	0.42
1:C:4181:GLU:OE1	1:C:4181:GLU:N	2.50	0.42
1:D:4955:ASP:OD1	1:D:4956:CYS:N	2.50	0.42
2:H:104:LEU:HD23	2:H:105:LEU:N	2.35	0.42
1:A:2464:LYS:O	1:A:2468:VAL:HG23	2.19	0.42
1:A:4881:GLU:O	1:A:4885:THR:HG22	2.20	0.42
1:B:495:ILE:HD13	1:B:540:LEU:HD23	2.01	0.42
1:B:624:ALA:HB2	1:B:1668:LEU:HD12	2.02	0.42
1:B:2560:LEU:O	1:B:2565:ARG:NH1	2.51	0.42
1:C:1107:ALA:HB1	1:C:1113:MET:CE	2.50	0.42
1:D:614:LEU:HD22	1:D:1661:LEU:HD22	2.01	0.42
1:D:1107:ALA:HB1	1:D:1113:MET:CE	2.49	0.42
1:D:3874:VAL:HG11	1:D:3937:SER:OG	2.20	0.42
1:A:2494:ASP:OD1	1:A:2494:ASP:N	2.53	0.42
1:C:137:ARG:N	1:C:146:ASP:OD2	2.51	0.42
1:C:698:ALA:HB2	1:C:791:VAL:HG11	2.01	0.42
1:D:805:GLY:N	1:D:809:GLY:O	2.51	0.42
1:D:3941:ASP:OD1	1:D:3941:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:ALA:HB2	1:B:791:VAL:HG11	2.01	0.42
1:B:3941:ASP:OD1	1:B:3941:ASP:N	2.52	0.42
1:B:4033:GLU:OE1	1:B:4033:GLU:N	2.49	0.42
1:C:4881:GLU:O	1:C:4885:THR:HG22	2.20	0.42
1:D:611:LEU:HD22	1:D:1661:LEU:HD11	2.01	0.42
1:D:1107:ALA:HB1	1:D:1113:MET:HE3	2.01	0.42
1:D:1645:LEU:O	1:D:1652:LEU:HD22	2.20	0.42
1:D:2326:ARG:NH1	1:D:2328:GLU:OE2	2.53	0.42
1:D:4033:GLU:OE1	1:D:4033:GLU:N	2.49	0.42
1:A:332:ARG:NH2	1:A:338:LEU:O	2.48	0.42
1:A:495:ILE:HD13	1:A:540:LEU:HD23	2.01	0.42
1:A:1645:LEU:O	1:A:1652:LEU:HD22	2.20	0.42
1:B:2002:LEU:HD12	1:B:2003:MET:N	2.35	0.42
1:C:805:GLY:N	1:C:809:GLY:O	2.51	0.42
1:C:1416:ASP:N	1:C:1563:ASN:OD1	2.52	0.42
1:C:2411:GLY:HA2	1:C:2416:ILE:HD11	2.02	0.42
1:C:3874:VAL:HG11	1:C:3937:SER:OG	2.20	0.42
1:D:4134:ARG:C	1:D:4135:ILE:HD13	2.44	0.42
2:G:104:LEU:HD23	2:G:105:LEU:N	2.35	0.42
1:A:1052:GLU:O	1:A:1056:THR:HG23	2.20	0.42
1:A:4949:GLU:N	1:A:4949:GLU:OE1	2.53	0.42
1:B:4881:GLU:O	1:B:4885:THR:HG22	2.20	0.42
1:D:515:ALA:HB2	1:D:523:GLY:HA3	2.02	0.42
1:D:562:LEU:HA	1:D:571:ILE:HD13	2.01	0.42
1:D:2355:ASP:CG	1:D:2357:SER:HG	2.28	0.42
1:D:4881:GLU:O	1:D:4885:THR:HG22	2.20	0.42
1:A:515:ALA:HB2	1:A:523:GLY:HA3	2.02	0.42
1:A:1107:ALA:HB1	1:A:1113:MET:CE	2.50	0.42
1:B:562:LEU:HA	1:B:571:ILE:HD13	2.01	0.42
1:B:1645:LEU:O	1:B:1652:LEU:HD22	2.20	0.42
1:B:2592:VAL:HG22	1:B:2643:LEU:HB2	2.02	0.42
1:B:3874:VAL:HG11	1:B:3937:SER:OG	2.20	0.42
1:C:208:GLN:OE1	1:C:210:THR:OG1	2.31	0.42
1:C:1052:GLU:O	1:C:1056:THR:HG23	2.20	0.42
1:D:137:ARG:N	1:D:146:ASP:OD2	2.52	0.42
1:D:2002:LEU:HD12	1:D:2003:MET:N	2.35	0.42
1:D:2437:ILE:O	1:D:2464:LYS:NZ	2.42	0.42
1:D:3759:LYS:NZ	1:D:3837:ASP:OD2	2.49	0.42
2:I:104:LEU:HD23	2:I:105:LEU:N	2.34	0.42
1:A:4098:ALA:O	1:A:4102:THR:OG1	2.31	0.41
1:B:904:TYR:HB2	1:B:918:LEU:HD22	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:LEU:HA	1:C:571:ILE:HD13	2.01	0.41
1:C:1645:LEU:O	1:C:1652:LEU:HD22	2.20	0.41
1:C:2494:ASP:OD1	1:C:2494:ASP:N	2.53	0.41
1:D:87:GLU:OE1	1:D:87:GLU:N	2.48	0.41
1:D:698:ALA:HB2	1:D:791:VAL:HG11	2.01	0.41
1:D:1052:GLU:O	1:D:1056:THR:HG23	2.20	0.41
1:A:247:VAL:O	1:A:272:ARG:NH1	2.47	0.41
1:A:1107:ALA:HB1	1:A:1113:MET:HE3	2.01	0.41
1:A:1737:ILE:HG13	1:A:1754:LEU:HD23	2.02	0.41
1:A:2326:ARG:NH1	1:A:2328:GLU:OE2	2.53	0.41
1:B:1467:VAL:O	1:B:1480:ILE:HD12	2.21	0.41
1:B:1977:ASN:O	1:B:1983:SER:OG	2.35	0.41
1:C:4088:GLU:OE1	1:C:4091:LYS:NZ	2.50	0.41
1:D:81:MET:O	1:D:85:THR:HG22	2.20	0.41
1:D:2464:LYS:O	1:D:2468:VAL:HG23	2.19	0.41
1:B:115:TYR:CZ	1:B:175:VAL:HG12	2.56	0.41
1:B:614:LEU:HD22	1:B:1661:LEU:HD22	2.01	0.41
1:B:1029:ASN:OD1	1:B:1031:ARG:N	2.48	0.41
1:B:2411:GLY:HA2	1:B:2416:ILE:HD11	2.02	0.41
1:C:4579:THR:OG1	1:C:4732:HIS:NE2	2.46	0.41
1:D:1737:ILE:HG13	1:D:1754:LEU:HD23	2.02	0.41
1:D:4949:GLU:N	1:D:4949:GLU:OE1	2.53	0.41
1:A:81:MET:O	1:A:85:THR:HG22	2.20	0.41
1:A:208:GLN:OE1	1:A:210:THR:OG1	2.31	0.41
1:A:375:GLN:OE1	1:A:392:ILE:HD13	2.21	0.41
1:A:2411:GLY:HA2	1:A:2416:ILE:HD11	2.02	0.41
1:B:307:SER:HB3	1:B:327:THR:HG22	2.03	0.41
1:B:4181:GLU:OE1	1:B:4181:GLU:N	2.50	0.41
1:C:2592:VAL:HG22	1:C:2643:LEU:HB2	2.02	0.41
1:C:4949:GLU:N	1:C:4949:GLU:OE1	2.53	0.41
1:D:1977:ASN:O	1:D:1983:SER:OG	2.35	0.41
1:A:412:GLU:OE1	1:A:412:GLU:N	2.47	0.41
1:A:1184:ASP:N	1:A:1188:SER:O	2.49	0.41
1:A:1977:ASN:O	1:A:1983:SER:OG	2.35	0.41
1:A:3874:VAL:HG11	1:A:3937:SER:OG	2.20	0.41
1:C:375:GLN:OE1	1:C:392:ILE:HD13	2.21	0.41
1:C:624:ALA:HB2	1:C:1668:LEU:HD12	2.01	0.41
1:D:307:SER:HB3	1:D:327:THR:HG22	2.02	0.41
1:D:2592:VAL:HG22	1:D:2643:LEU:HB2	2.02	0.41
2:J:104:LEU:HD23	2:J:105:LEU:N	2.35	0.41
1:A:614:LEU:HD22	1:A:1661:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:O	1:B:176:ARG:NE	2.53	0.41
1:B:375:GLN:OE1	1:B:392:ILE:HD13	2.21	0.41
1:B:3971:MET:HE3	1:B:4093:ILE:HD12	2.03	0.41
1:C:2002:LEU:HD12	1:C:2003:MET:N	2.35	0.41
1:D:115:TYR:CZ	1:D:175:VAL:HG12	2.56	0.41
1:D:375:GLN:OE1	1:D:392:ILE:HD13	2.21	0.41
1:D:1641:ASP:OD1	1:D:1642:ILE:N	2.54	0.41
1:A:115:TYR:CZ	1:A:175:VAL:HG12	2.56	0.41
1:A:1641:ASP:OD1	1:A:1642:ILE:N	2.54	0.41
1:A:4715:ASP:OD1	1:A:4716:ASN:N	2.54	0.41
1:B:515:ALA:HB2	1:B:523:GLY:HA3	2.02	0.41
1:B:4715:ASP:OD1	1:B:4716:ASN:N	2.54	0.41
1:C:81:MET:O	1:C:85:THR:HG22	2.20	0.41
1:C:2326:ARG:NH1	1:C:2328:GLU:OE2	2.53	0.41
1:C:2496:ARG:HG2	1:C:2550:THR:HG21	2.03	0.41
1:D:174:LYS:O	1:D:176:ARG:NE	2.53	0.41
1:D:890:HIS:O	1:D:894:VAL:HG23	2.21	0.41
1:D:1467:VAL:O	1:D:1480:ILE:HD12	2.21	0.41
1:A:1471:ASP:OD1	1:A:1475:LYS:N	2.49	0.41
1:A:2367:SER:OG	1:A:2368:SER:N	2.49	0.41
1:B:805:GLY:N	1:B:809:GLY:O	2.50	0.41
1:B:3853:PHE:HD1	1:B:3857:LEU:HD23	1.86	0.41
1:D:3667:ILE:HG21	1:D:3733:ARG:O	2.21	0.41
1:D:4715:ASP:OD1	1:D:4716:ASN:N	2.54	0.41
1:A:1467:VAL:O	1:A:1480:ILE:HD12	2.21	0.41
1:A:2002:LEU:HD12	1:A:2003:MET:N	2.35	0.41
1:A:2437:ILE:O	1:A:2464:LYS:NZ	2.42	0.41
1:A:3759:LYS:NZ	1:A:3837:ASP:OD2	2.49	0.41
1:B:81:MET:O	1:B:85:THR:HG22	2.20	0.41
1:B:412:GLU:OE1	1:B:412:GLU:N	2.47	0.41
1:B:504:ARG:O	1:B:507:VAL:HG22	2.21	0.41
1:B:1052:GLU:O	1:B:1056:THR:HG23	2.20	0.41
1:B:1495:SER:O	1:B:1499:GLY:N	2.51	0.41
1:B:1737:ILE:HG13	1:B:1754:LEU:HD23	2.02	0.41
1:B:2481:ASP:OD1	1:B:2482:PHE:N	2.54	0.41
1:B:2494:ASP:N	1:B:2494:ASP:OD1	2.53	0.41
1:B:3759:LYS:NZ	1:B:3837:ASP:OD2	2.49	0.41
1:C:423:VAL:HG22	1:C:494:MET:HE1	2.03	0.41
1:C:1107:ALA:HB1	1:C:1113:MET:HE3	2.01	0.41
1:C:1467:VAL:O	1:C:1480:ILE:HD12	2.21	0.41
1:C:1471:ASP:OD1	1:C:1475:LYS:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2318:VAL:O	1:C:2322:LEU:HD13	2.21	0.41
1:C:3667:ILE:HG21	1:C:3733:ARG:O	2.21	0.41
1:D:1265:HIS:O	1:D:1288:LYS:NZ	2.40	0.41
1:D:2481:ASP:OD1	1:D:2482:PHE:N	2.54	0.41
1:D:3971:MET:HE3	1:D:4093:ILE:HD12	2.03	0.41
1:B:1682:ASP:OD1	1:B:1685:GLN:N	2.46	0.41
1:C:515:ALA:HB2	1:C:523:GLY:HA3	2.02	0.41
1:C:3853:PHE:HD1	1:C:3857:LEU:HD23	1.86	0.41
1:C:3971:MET:HE3	1:C:4093:ILE:HD12	2.03	0.41
1:D:624:ALA:HB2	1:D:1668:LEU:HD12	2.02	0.41
1:D:1184:ASP:N	1:D:1188:SER:O	2.49	0.41
2:G:36:LYS:NZ	2:G:42:ASP:OD2	2.43	0.41
1:A:3971:MET:HE3	1:A:4093:ILE:HD12	2.03	0.40
1:B:593:HIS:O	1:B:596:SER:OG	2.30	0.40
1:B:1144:ARG:N	1:B:1150:GLU:O	2.46	0.40
1:C:307:SER:HB3	1:C:327:THR:HG22	2.02	0.40
1:D:504:ARG:O	1:D:507:VAL:HG22	2.21	0.40
1:D:2496:ARG:HG2	1:D:2550:THR:HG21	2.03	0.40
1:A:137:ARG:N	1:A:146:ASP:OD2	2.52	0.40
1:A:890:HIS:O	1:A:894:VAL:HG23	2.21	0.40
1:A:3667:ILE:HG21	1:A:3733:ARG:O	2.21	0.40
1:B:189:GLU:OE2	1:C:2417:ARG:NE	2.55	0.40
1:C:189:GLU:OE2	1:D:2417:ARG:NE	2.55	0.40
1:C:1737:ILE:HG13	1:C:1754:LEU:HD23	2.02	0.40
1:C:3965:GLU:OE1	1:C:3965:GLU:N	2.45	0.40
1:D:500:GLU:OE1	1:D:504:ARG:NH1	2.50	0.40
1:D:2324:ILE:CD1	1:D:2421:ILE:HG21	2.52	0.40
1:A:1757:SER:N	1:A:1922:GLU:OE2	2.49	0.40
1:A:2081:ARG:O	1:A:2085:VAL:HG23	2.21	0.40
1:A:2318:VAL:O	1:A:2322:LEU:HD13	2.21	0.40
1:A:2324:ILE:CD1	1:A:2421:ILE:HG21	2.52	0.40
1:A:2592:VAL:HG22	1:A:2643:LEU:HB2	2.02	0.40
1:B:290:ARG:NH1	1:B:344:LYS:O	2.51	0.40
1:B:423:VAL:HG22	1:B:494:MET:HE1	2.03	0.40
1:B:2081:ARG:O	1:B:2085:VAL:HG23	2.21	0.40
1:B:2326:ARG:NH1	1:B:2328:GLU:OE2	2.53	0.40
1:B:2478:GLU:N	1:B:2478:GLU:OE1	2.55	0.40
1:C:2481:ASP:OD1	1:C:2482:PHE:N	2.54	0.40
1:D:1682:ASP:OD1	1:D:1685:GLN:N	2.46	0.40
1:D:1914:ASP:OD1	1:D:2089:ARG:NH1	2.48	0.40
1:D:2318:VAL:O	1:D:2322:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4073:GLU:OE1	1:D:4073:GLU:N	2.47	0.40
2:G:11:GLY:O	2:G:68:SER:OG	2.29	0.40
1:A:307:SER:HB3	1:A:327:THR:HG22	2.02	0.40
1:A:1127:GLU:O	1:A:1130:SER:OG	2.33	0.40
1:A:2481:ASP:OD1	1:A:2482:PHE:N	2.54	0.40
1:B:500:GLU:OE1	1:B:504:ARG:NH1	2.50	0.40
1:B:1251:LEU:H	1:B:1251:LEU:HD23	1.87	0.40
1:C:1495:SER:O	1:C:1499:GLY:N	2.51	0.40
1:D:2411:GLY:HA2	1:D:2416:ILE:HD11	2.02	0.40
1:D:3853:PHE:HD1	1:D:3857:LEU:HD23	1.86	0.40
2:I:22:THR:N	2:I:108:GLU:OXT	2.48	0.40
1:B:1641:ASP:OD1	1:B:1642:ILE:N	2.54	0.40
1:B:4050:ALA:O	1:B:4053:SER:OG	2.36	0.40
1:C:890:HIS:O	1:C:894:VAL:HG23	2.21	0.40
1:C:2081:ARG:O	1:C:2085:VAL:HG23	2.21	0.40
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.50	0.40
1:D:1251:LEU:HD23	1:D:1251:LEU:H	1.87	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%)	3363 (97%)	111 (3%)	0	100	100
1	B	3474/4966 (70%)	3366 (97%)	107 (3%)	1 (0%)	100	100
1	C	3474/4966 (70%)	3364 (97%)	110 (3%)	0	100	100
1	D	3474/4966 (70%)	3363 (97%)	111 (3%)	0	100	100
2	G	105/176 (60%)	99 (94%)	6 (6%)	0	100	100
2	H	105/176 (60%)	99 (94%)	6 (6%)	0	100	100
2	I	105/176 (60%)	99 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	105/176 (60%)	99 (94%)	6 (6%)	0	100	100
All	All	14316/20568 (70%)	13852 (97%)	463 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4677	ASP

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%)	2996 (98%)	61 (2%)	48	65
1	B	3057/4355 (70%)	2997 (98%)	60 (2%)	48	65
1	C	3057/4355 (70%)	2996 (98%)	61 (2%)	48	65
1	D	3057/4355 (70%)	2996 (98%)	61 (2%)	48	65
2	G	88/140 (63%)	86 (98%)	2 (2%)	44	62
2	H	88/140 (63%)	86 (98%)	2 (2%)	44	62
2	I	88/140 (63%)	86 (98%)	2 (2%)	44	62
2	J	88/140 (63%)	86 (98%)	2 (2%)	44	62
All	All	12580/17980 (70%)	12329 (98%)	251 (2%)	48	65

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

Mol	Chain	Res	Type
1	A	17	ASP
1	A	22	LEU
1	A	117	HIS
1	A	158	CYS
1	A	181	LEU
1	A	204	ASP
1	A	246	THR

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Mol	Chain	Res	Type
1	A	262	TYR
1	A	387	ILE
1	A	492	GLU
1	A	541	ILE
1	A	562	LEU
1	A	565	LEU
1	A	615	CYS
1	A	632	ILE
1	A	758	CYS
1	A	770	ILE
1	A	871	GLN
1	A	890	HIS
1	A	933	LEU
1	A	940	LEU
1	A	996	VAL
1	A	1127	GLU
1	A	1165	MET
1	A	1168	MET
1	A	1207	LEU
1	A	1215	MET
1	A	1429	SER
1	A	1596	LEU
1	A	1678	CYS
1	A	1728	VAL
1	A	1796	LEU
1	A	1832	MET
1	A	1906	CYS
1	A	1941	PHE
1	A	2065	MET
1	A	2138	GLU
1	A	2148	ILE
1	A	2301	LEU
1	A	2398	LEU
1	A	2407	LEU
1	A	2409	HIS
1	A	2425	LEU
1	A	2479	VAL
1	A	2539	HIS
1	A	2621	CYS
1	A	3699	HIS
1	A	3782	GLU
1	A	3831	ASP

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Mol	Chain	Res	Type
1	A	3889	TRP
1	A	3953	MET
1	A	3986	GLU
1	A	4024	ASP
1	A	4123	SER
1	A	4183	GLU
1	A	4500	MET
1	A	4518	TYR
1	A	4673	LYS
1	A	4862	GLN
1	A	4877	GLU
1	A	4947	CYS
1	B	17	ASP
1	B	22	LEU
1	B	117	HIS
1	B	158	CYS
1	B	181	LEU
1	B	204	ASP
1	B	246	THR
1	B	262	TYR
1	B	387	ILE
1	B	492	GLU
1	B	541	ILE
1	B	562	LEU
1	B	565	LEU
1	B	615	CYS
1	B	632	ILE
1	B	758	CYS
1	B	770	ILE
1	B	871	GLN
1	B	890	HIS
1	B	933	LEU
1	B	940	LEU
1	B	996	VAL
1	B	1127	GLU
1	B	1165	MET
1	B	1168	MET
1	B	1207	LEU
1	B	1215	MET
1	B	1429	SER
1	B	1596	LEU
1	B	1678	CYS

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Mol	Chain	Res	Type
1	B	1728	VAL
1	B	1796	LEU
1	B	1832	MET
1	B	1906	CYS
1	B	1941	PHE
1	B	2065	MET
1	B	2138	GLU
1	B	2148	ILE
1	B	2301	LEU
1	B	2398	LEU
1	B	2407	LEU
1	B	2409	HIS
1	B	2425	LEU
1	B	2479	VAL
1	B	2539	HIS
1	B	2621	CYS
1	B	3699	HIS
1	B	3782	GLU
1	B	3831	ASP
1	B	3889	TRP
1	B	3953	MET
1	B	3986	GLU
1	B	4024	ASP
1	B	4123	SER
1	B	4183	GLU
1	B	4500	MET
1	B	4518	TYR
1	B	4862	GLN
1	B	4877	GLU
1	B	4947	CYS
1	C	17	ASP
1	C	22	LEU
1	C	117	HIS
1	C	158	CYS
1	C	181	LEU
1	C	204	ASP
1	C	246	THR
1	C	262	TYR
1	C	387	ILE
1	C	492	GLU
1	C	541	ILE
1	C	562	LEU

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Mol	Chain	Res	Type
1	C	565	LEU
1	C	615	CYS
1	C	632	ILE
1	C	758	CYS
1	C	770	ILE
1	C	871	GLN
1	C	890	HIS
1	C	933	LEU
1	C	940	LEU
1	C	996	VAL
1	C	1127	GLU
1	C	1165	MET
1	C	1168	MET
1	C	1207	LEU
1	C	1215	MET
1	C	1429	SER
1	C	1596	LEU
1	C	1678	CYS
1	C	1728	VAL
1	C	1796	LEU
1	C	1832	MET
1	C	1906	CYS
1	C	1941	PHE
1	C	2065	MET
1	C	2138	GLU
1	C	2148	ILE
1	C	2301	LEU
1	C	2398	LEU
1	C	2407	LEU
1	C	2409	HIS
1	C	2425	LEU
1	C	2479	VAL
1	C	2539	HIS
1	C	2621	CYS
1	C	3699	HIS
1	C	3782	GLU
1	C	3831	ASP
1	C	3889	TRP
1	C	3953	MET
1	C	3986	GLU
1	C	4024	ASP
1	C	4123	SER

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Mol	Chain	Res	Type
1	C	4183	GLU
1	C	4500	MET
1	C	4518	TYR
1	C	4673	LYS
1	C	4862	GLN
1	C	4877	GLU
1	C	4947	CYS
1	D	17	ASP
1	D	22	LEU
1	D	117	HIS
1	D	158	CYS
1	D	181	LEU
1	D	204	ASP
1	D	246	THR
1	D	262	TYR
1	D	387	ILE
1	D	492	GLU
1	D	541	ILE
1	D	562	LEU
1	D	565	LEU
1	D	615	CYS
1	D	632	ILE
1	D	758	CYS
1	D	770	ILE
1	D	871	GLN
1	D	890	HIS
1	D	933	LEU
1	D	940	LEU
1	D	996	VAL
1	D	1127	GLU
1	D	1165	MET
1	D	1168	MET
1	D	1207	LEU
1	D	1215	MET
1	D	1429	SER
1	D	1596	LEU
1	D	1678	CYS
1	D	1728	VAL
1	D	1796	LEU
1	D	1832	MET
1	D	1906	CYS
1	D	1941	PHE

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Mol	Chain	Res	Type
1	D	2065	MET
1	D	2138	GLU
1	D	2148	ILE
1	D	2301	LEU
1	D	2398	LEU
1	D	2407	LEU
1	D	2409	HIS
1	D	2425	LEU
1	D	2479	VAL
1	D	2539	HIS
1	D	2621	CYS
1	D	3699	HIS
1	D	3782	GLU
1	D	3831	ASP
1	D	3889	TRP
1	D	3953	MET
1	D	3986	GLU
1	D	4024	ASP
1	D	4123	SER
1	D	4183	GLU
1	D	4500	MET
1	D	4518	TYR
1	D	4673	LYS
1	D	4862	GLN
1	D	4877	GLU
1	D	4947	CYS
2	G	26	HIS
2	G	95	ASN
2	H	26	HIS
2	H	95	ASN
2	I	26	HIS
2	I	95	ASN
2	J	26	HIS
2	J	95	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	313	ASN
1	A	681	HIS
1	A	1294	ASN

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Mol	Chain	Res	Type
1	A	1627	GLN
1	A	2090	GLN
1	A	2208	GLN
1	A	2485	HIS
1	A	3633	HIS
1	A	3924	GLN
1	A	4107	HIS
1	B	198	ASN
1	B	313	ASN
1	B	681	HIS
1	B	1294	ASN
1	B	2090	GLN
1	B	2208	GLN
1	B	2480	GLN
1	B	2485	HIS
1	B	3633	HIS
1	B	3924	GLN
1	B	3991	ASN
1	B	4107	HIS
1	B	4512	ASN
1	C	198	ASN
1	C	313	ASN
1	C	681	HIS
1	C	1294	ASN
1	C	1627	GLN
1	C	2090	GLN
1	C	2208	GLN
1	C	2485	HIS
1	C	3633	HIS
1	C	3924	GLN
1	C	3991	ASN
1	C	4074	ASN
1	C	4107	HIS
1	C	4512	ASN
1	D	198	ASN
1	D	313	ASN
1	D	681	HIS
1	D	1294	ASN
1	D	1627	GLN
1	D	1904	GLN
1	D	2090	GLN
1	D	2208	GLN

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Mol	Chain	Res	Type
1	D	2485	HIS
1	D	3633	HIS
1	D	3924	GLN
1	D	3991	ASN
1	D	4107	HIS
1	D	4512	ASN
2	G	71	GLN
2	H	71	GLN
2	I	71	GLN
2	J	71	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 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	$\#\|Z\|>2$
5	A1MG7	C	5003	-	27,27,27	1.60	6 (22%)	36,38,38	2.42	11 (30%)
5	A1MG7	D	5003	-	27,27,27	1.61	6 (22%)	36,38,38	2.41	10 (27%)
5	A1MG7	B	5003	-	27,27,27	1.60	6 (22%)	36,38,38	2.41	11 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	A1MG7	A	5003	-	27,27,27	1.61	6 (22%)	36,38,38	2.41	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
5	A1MG7	C	5003	-	-	0/16/16/16	0/3/3/3
5	A1MG7	D	5003	-	-	0/16/16/16	0/3/3/3
5	A1MG7	B	5003	-	-	0/16/16/16	0/3/3/3
5	A1MG7	A	5003	-	-	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)
5	A	5003	A1MG7	C-NAO	4.92	1.45	1.35
5	B	5003	A1MG7	C-NAO	4.92	1.45	1.35
5	D	5003	A1MG7	C-NAO	4.92	1.45	1.35
5	C	5003	A1MG7	C-NAO	4.88	1.45	1.35
5	A	5003	A1MG7	N-NAH	3.11	1.37	1.33
5	B	5003	A1MG7	N-NAH	3.11	1.37	1.33
5	C	5003	A1MG7	N-NAH	3.11	1.37	1.33
5	D	5003	A1MG7	N-NAH	3.11	1.37	1.33
5	A	5003	A1MG7	N-NAJ	2.82	1.36	1.32
5	C	5003	A1MG7	N-NAJ	2.82	1.36	1.32
5	D	5003	A1MG7	N-NAJ	2.82	1.36	1.32
5	B	5003	A1MG7	NAK-NAJ	2.79	1.36	1.32
5	B	5003	A1MG7	N-NAJ	2.78	1.36	1.32
5	A	5003	A1MG7	NAK-NAJ	2.77	1.36	1.32
5	D	5003	A1MG7	NAK-NAJ	2.77	1.36	1.32
5	C	5003	A1MG7	NAK-NAJ	2.75	1.36	1.32
5	B	5003	A1MG7	CAF-CAG	2.67	1.51	1.47
5	A	5003	A1MG7	CAF-CAG	2.67	1.51	1.47
5	C	5003	A1MG7	CAF-CAG	2.67	1.51	1.47
5	D	5003	A1MG7	CAF-CAG	2.67	1.51	1.47
5	A	5003	A1MG7	O-C	-2.04	1.18	1.23
5	D	5003	A1MG7	O-C	-2.04	1.18	1.23
5	C	5003	A1MG7	O-C	-2.01	1.18	1.23
5	B	5003	A1MG7	O-C	-2.00	1.18	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	5003	A1MG7	CAG-NAH-N	7.32	107.50	101.70
5	C	5003	A1MG7	CAG-NAH-N	7.32	107.50	101.70
5	D	5003	A1MG7	CAG-NAH-N	7.32	107.50	101.70
5	B	5003	A1MG7	CAG-NAH-N	7.30	107.47	101.70
5	A	5003	A1MG7	NAH-N-NAJ	-6.73	108.33	114.03
5	C	5003	A1MG7	NAH-N-NAJ	-6.73	108.33	114.03
5	D	5003	A1MG7	NAH-N-NAJ	-6.73	108.33	114.03
5	B	5003	A1MG7	NAH-N-NAJ	-6.71	108.34	114.03
5	C	5003	A1MG7	CA-N-NAJ	5.62	126.95	122.59
5	A	5003	A1MG7	CA-N-NAJ	5.57	126.92	122.59
5	D	5003	A1MG7	CA-N-NAJ	5.57	126.92	122.59
5	B	5003	A1MG7	CA-N-NAJ	5.57	126.91	122.59
5	C	5003	A1MG7	NAH-CAG-NAK	-3.39	108.83	112.00
5	A	5003	A1MG7	NAH-CAG-NAK	-3.38	108.85	112.00
5	D	5003	A1MG7	NAH-CAG-NAK	-3.38	108.85	112.00
5	B	5003	A1MG7	NAH-CAG-NAK	-3.37	108.85	112.00
5	D	5003	A1MG7	CAE-CAD-CAC	-2.83	119.95	123.52
5	B	5003	A1MG7	CAE-CAD-CAC	-2.80	119.98	123.52
5	C	5003	A1MG7	CAE-CAD-CAC	-2.79	120.00	123.52
5	A	5003	A1MG7	CAE-CAD-CAC	-2.78	120.00	123.52
5	B	5003	A1MG7	CAC-CAB-CAA	-2.75	120.04	123.52
5	C	5003	A1MG7	CAC-CAB-CAA	-2.75	120.05	123.52
5	A	5003	A1MG7	CAC-CAB-CAA	-2.73	120.07	123.52
5	D	5003	A1MG7	CAC-CAB-CAA	-2.73	120.07	123.52
5	B	5003	A1MG7	CAD-CAC-CAB	2.61	120.19	116.13
5	C	5003	A1MG7	CAD-CAC-CAB	2.58	120.14	116.13
5	D	5003	A1MG7	CAD-CAC-CAB	2.58	120.14	116.13
5	A	5003	A1MG7	CAD-CAC-CAB	2.57	120.12	116.13
5	B	5003	A1MG7	N-NAJ-NAK	2.22	107.82	105.99
5	A	5003	A1MG7	N-NAJ-NAK	2.22	107.81	105.99
5	D	5003	A1MG7	N-NAJ-NAK	2.22	107.81	105.99
5	B	5003	A1MG7	CAF-CAG-NAK	2.21	126.54	123.96
5	C	5003	A1MG7	CAF-CAG-NAK	2.18	126.51	123.96
5	C	5003	A1MG7	N-NAJ-NAK	2.18	107.78	105.99
5	A	5003	A1MG7	CAF-CAG-NAK	2.17	126.49	123.96
5	D	5003	A1MG7	CAF-CAG-NAK	2.17	126.49	123.96
5	C	5003	A1MG7	CAG-NAK-NAJ	2.08	107.57	105.91
5	A	5003	A1MG7	CAG-NAK-NAJ	2.02	107.52	105.91
5	D	5003	A1MG7	CAG-NAK-NAJ	2.02	107.52	105.91
5	B	5003	A1MG7	CAG-NAK-NAJ	2.01	107.52	105.91
5	B	5003	A1MG7	CAU-CAT-CAS	-2.01	120.15	122.83
5	C	5003	A1MG7	CAU-CAT-CAS	-2.01	120.15	122.83

There are no chirality outliers.

There are no torsion outliers.

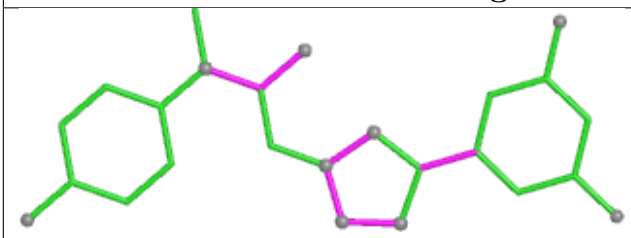
There are no ring outliers.

4 monomers are involved in 4 short contacts:

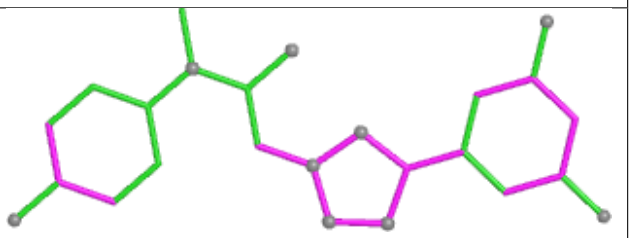
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5003	A1MG7	1	0
5	D	5003	A1MG7	1	0
5	B	5003	A1MG7	1	0
5	A	5003	A1MG7	1	0

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.

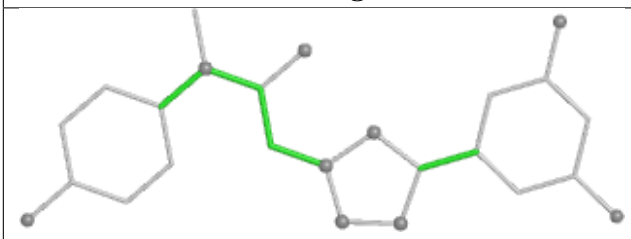
Ligand A1MG7 C 5003



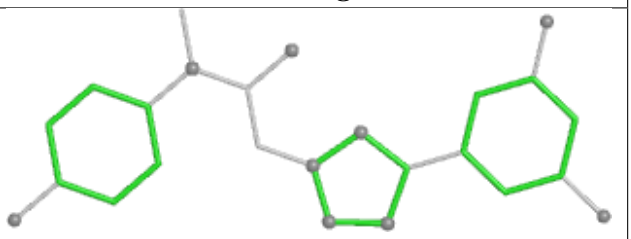
Bond lengths



Bond angles

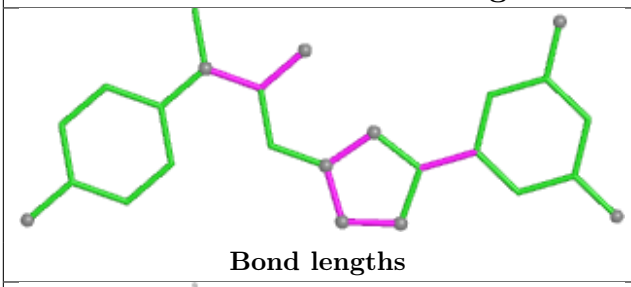


Torsions

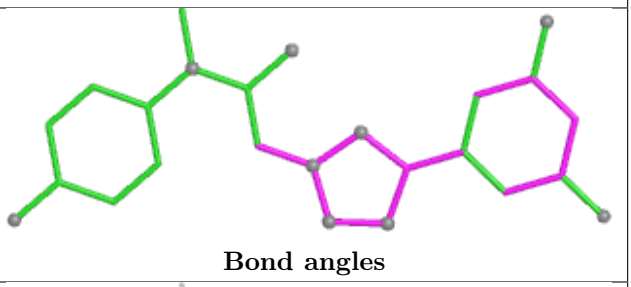


Rings

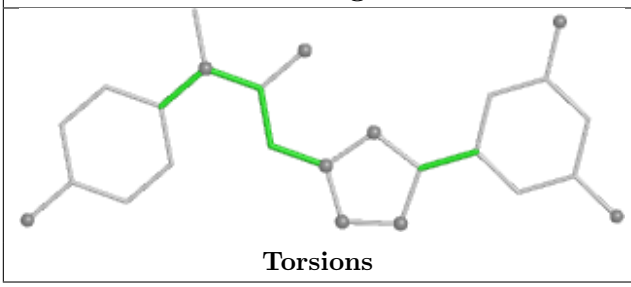
Ligand A1MG7 D 5003



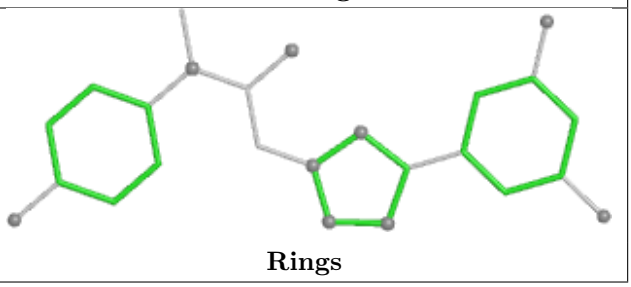
Bond lengths



Bond angles

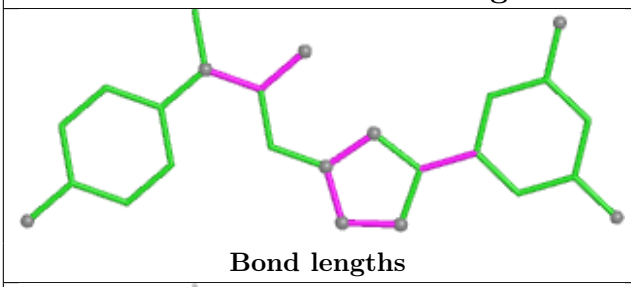


Torsions

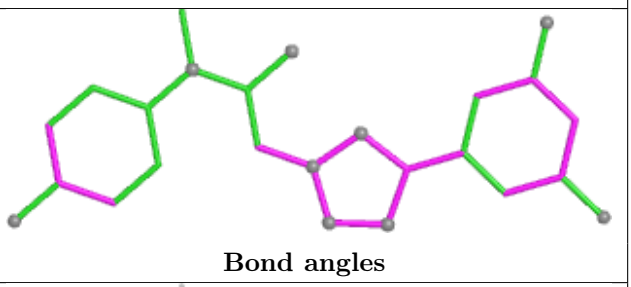


Rings

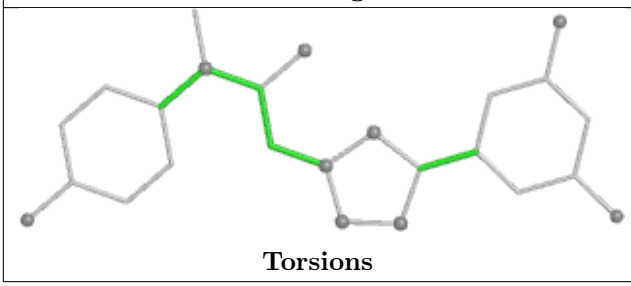
Ligand A1MG7 B 5003



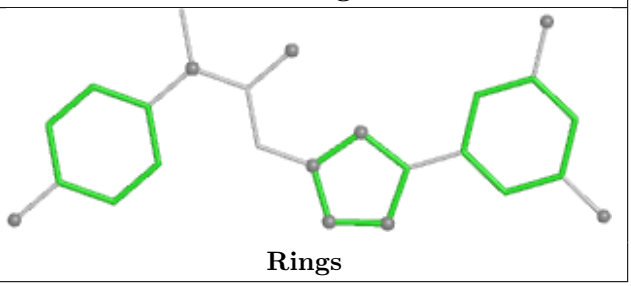
Bond lengths



Bond angles

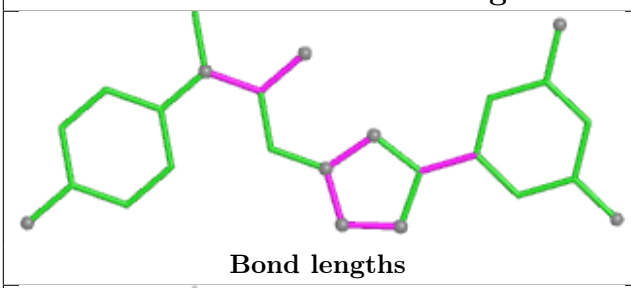


Torsions

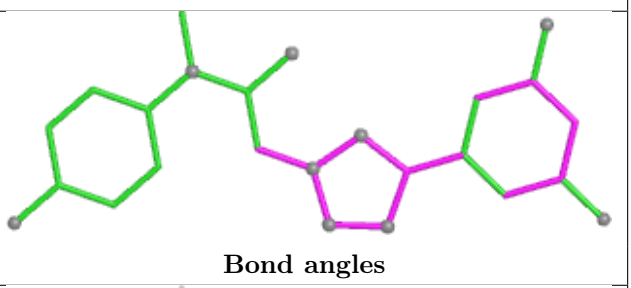


Rings

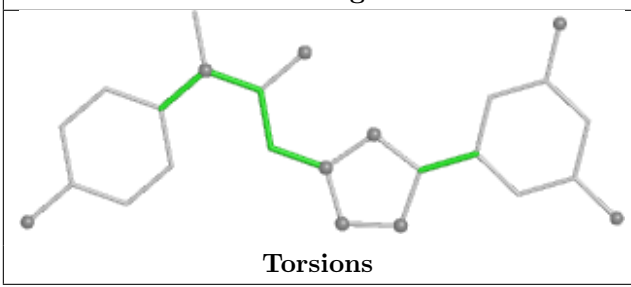
Ligand A1MG7 A 5003



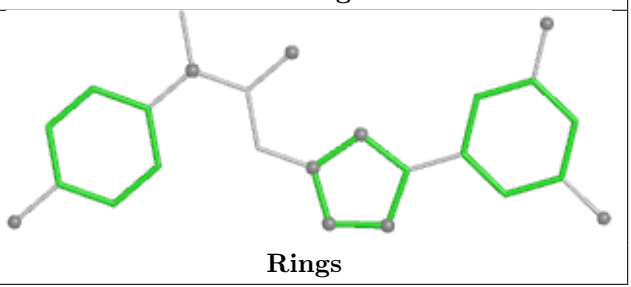
Bond lengths



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.

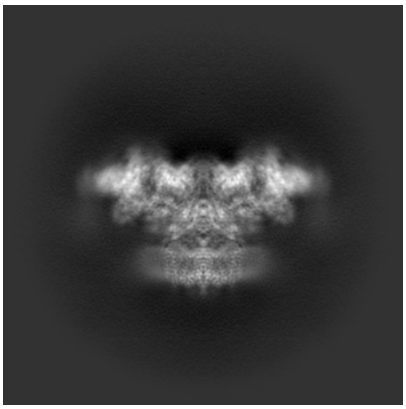
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-80686. These allow visual inspection of the internal detail of the map and identification of artifacts.

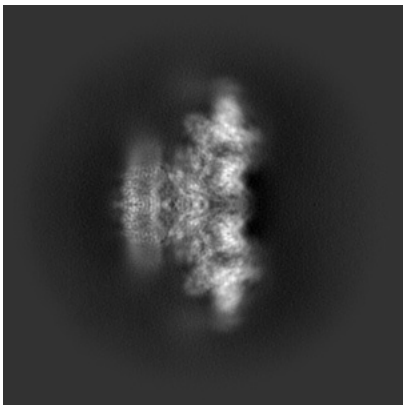
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

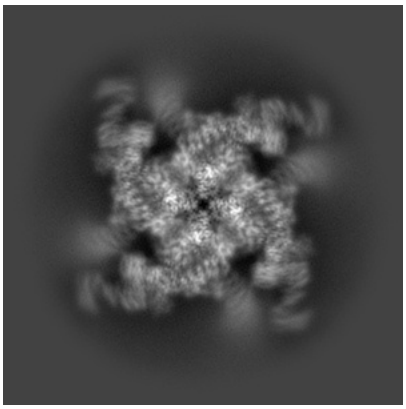
6.1.1 Primary map



X

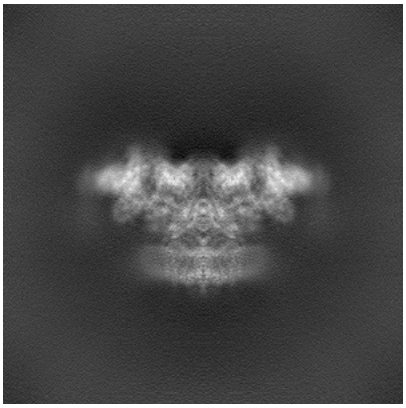


Y

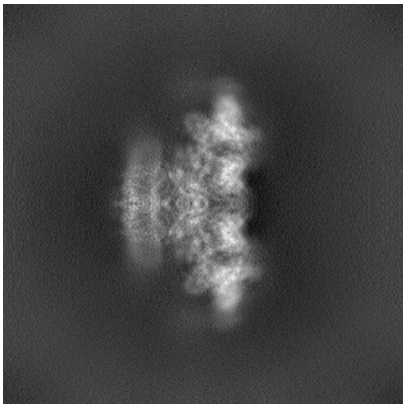


Z

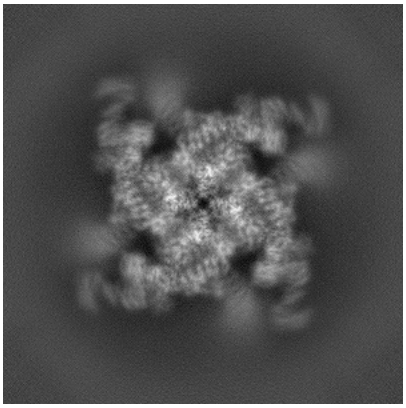
6.1.2 Raw map



X



Y

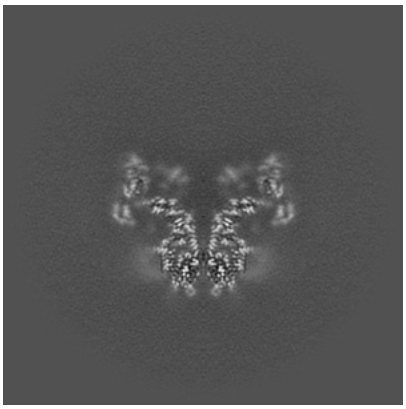


Z

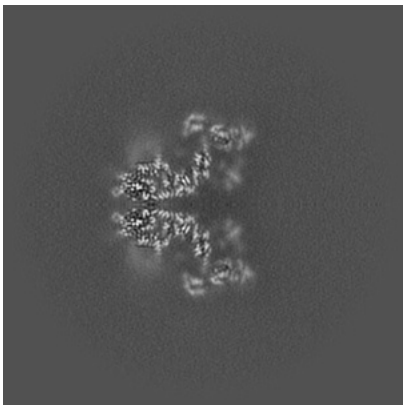
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

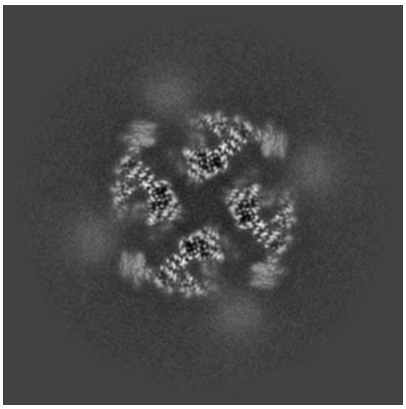
6.2.1 Primary map



X Index: 256

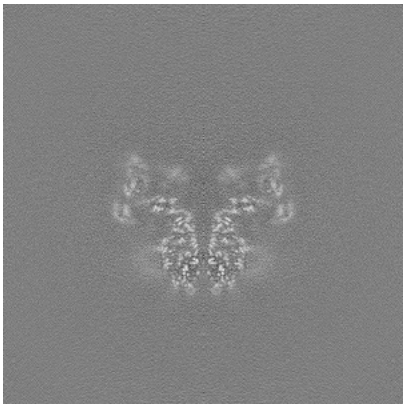


Y Index: 256

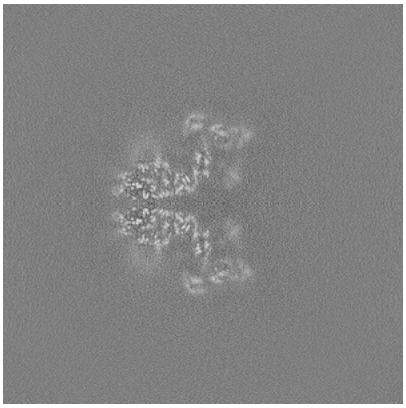


Z Index: 256

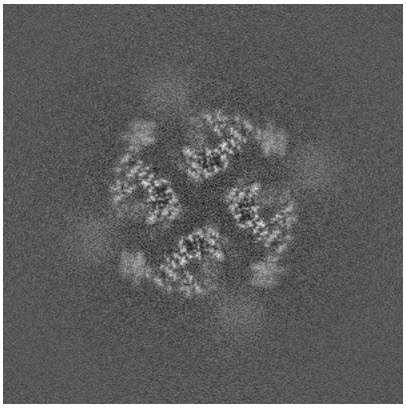
6.2.2 Raw map



X Index: 256



Y Index: 256

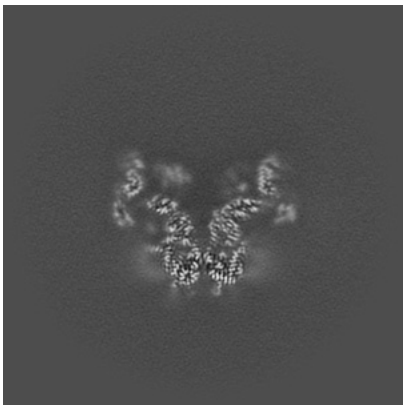


Z Index: 256

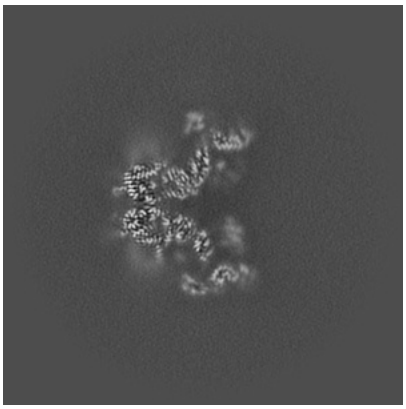
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

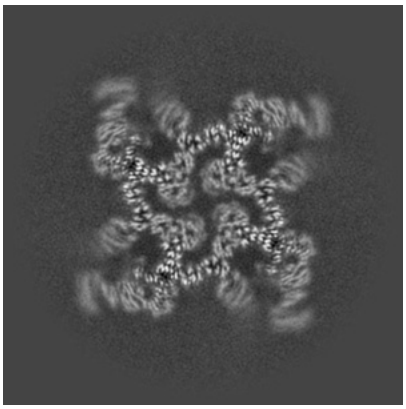
6.3.1 Primary map



X Index: 252

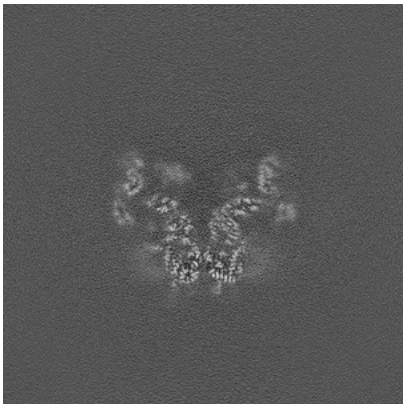


Y Index: 260

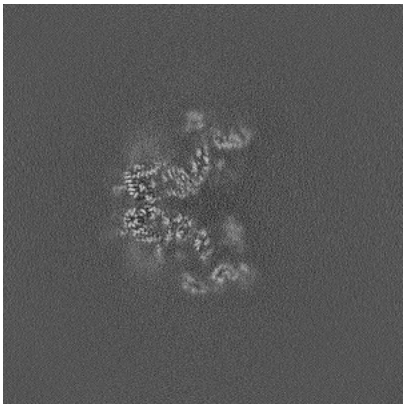


Z Index: 289

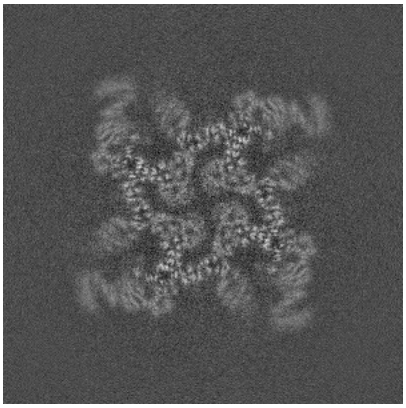
6.3.2 Raw map



X Index: 252



Y Index: 260

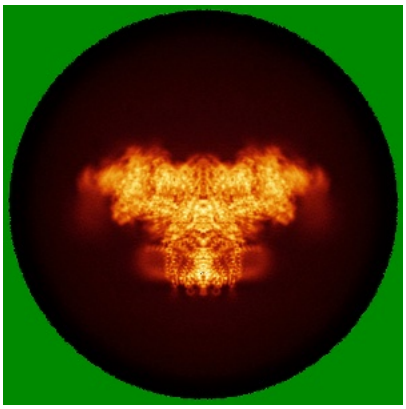


Z Index: 289

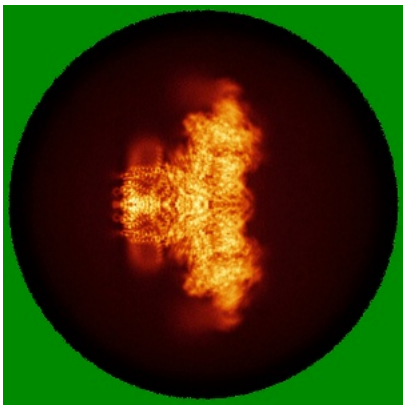
The images above show the largest variance slices of the map in three orthogonal directions.

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

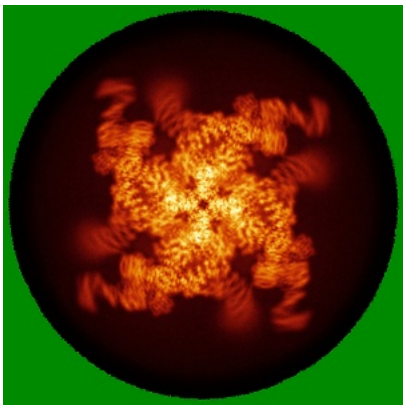
6.4.1 Primary map



X

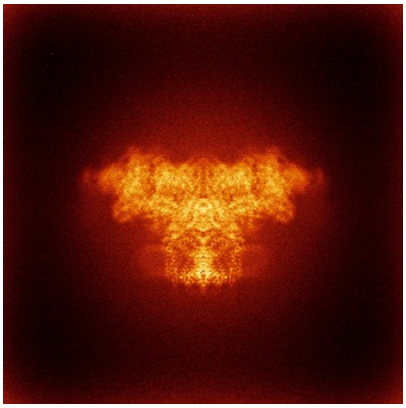


Y

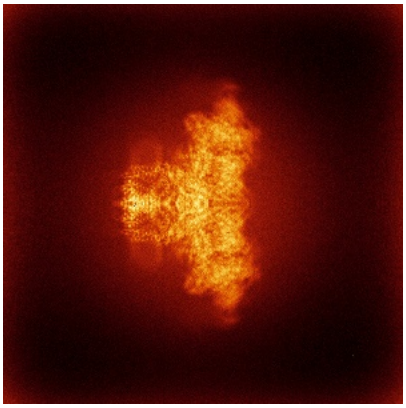


Z

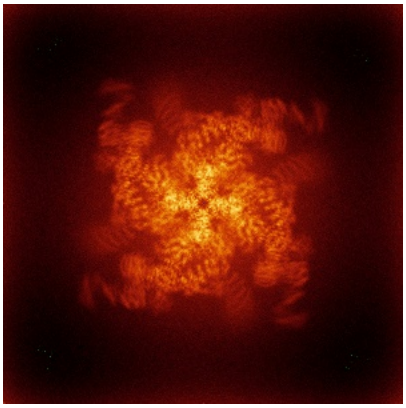
6.4.2 Raw map



X



Y

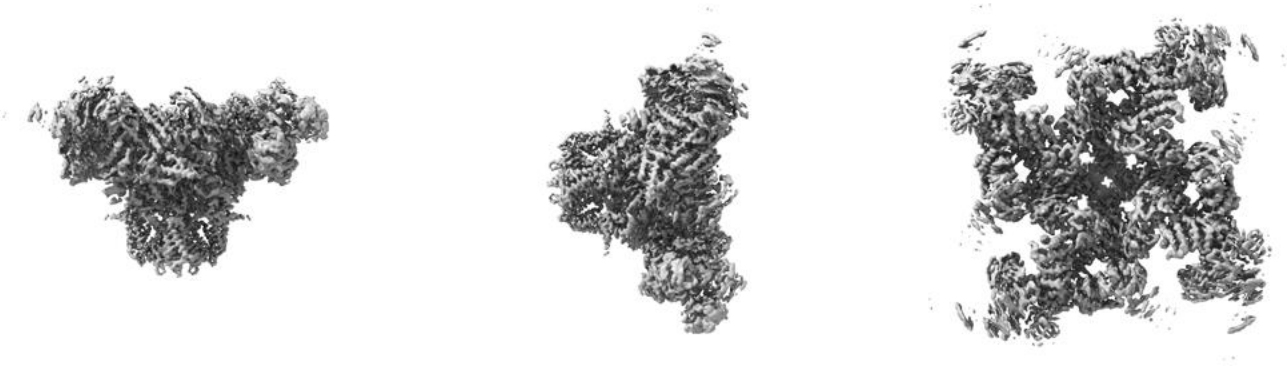


Z

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.

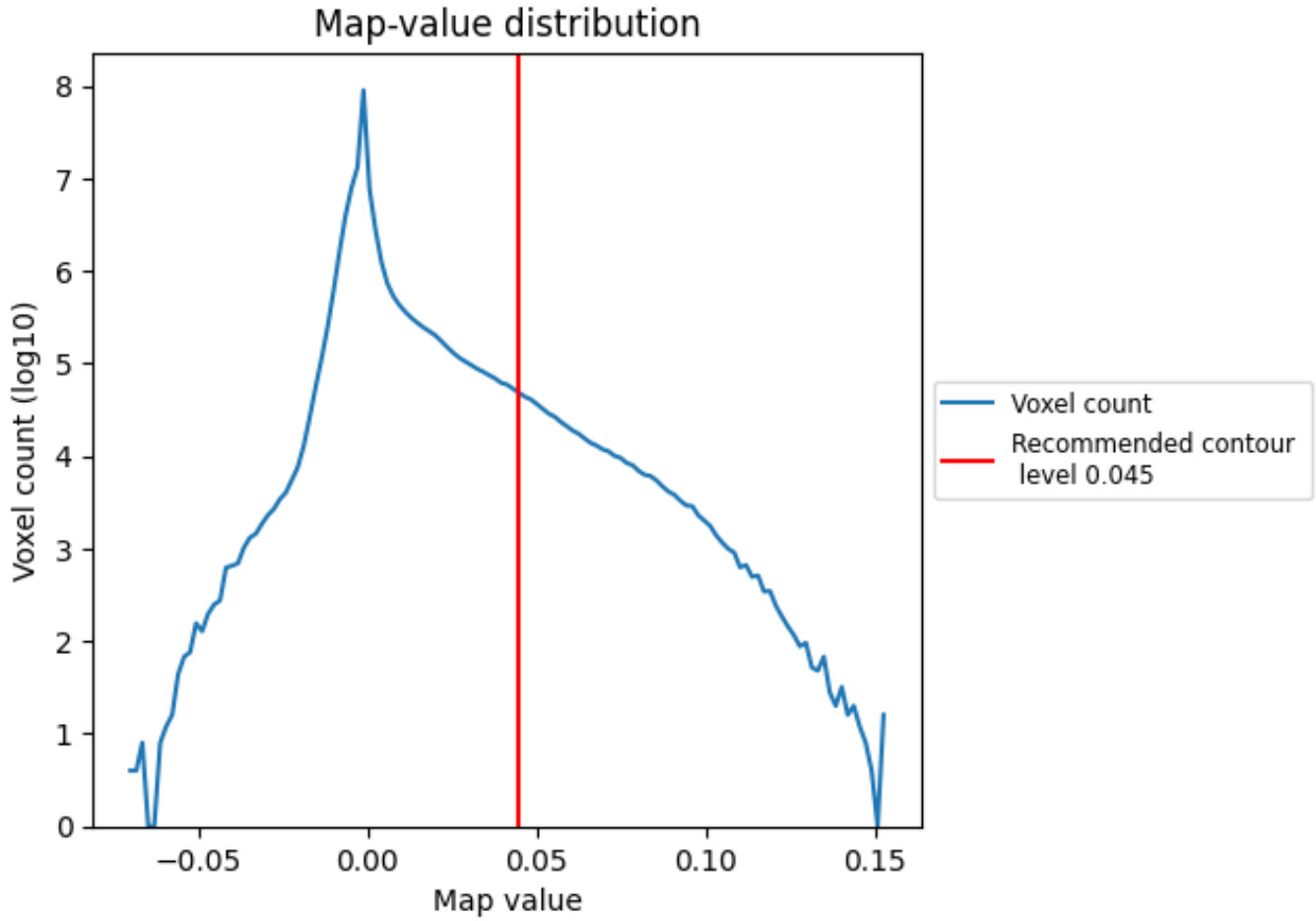
6.6 Mask visualisation (i)

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

7 Map analysis

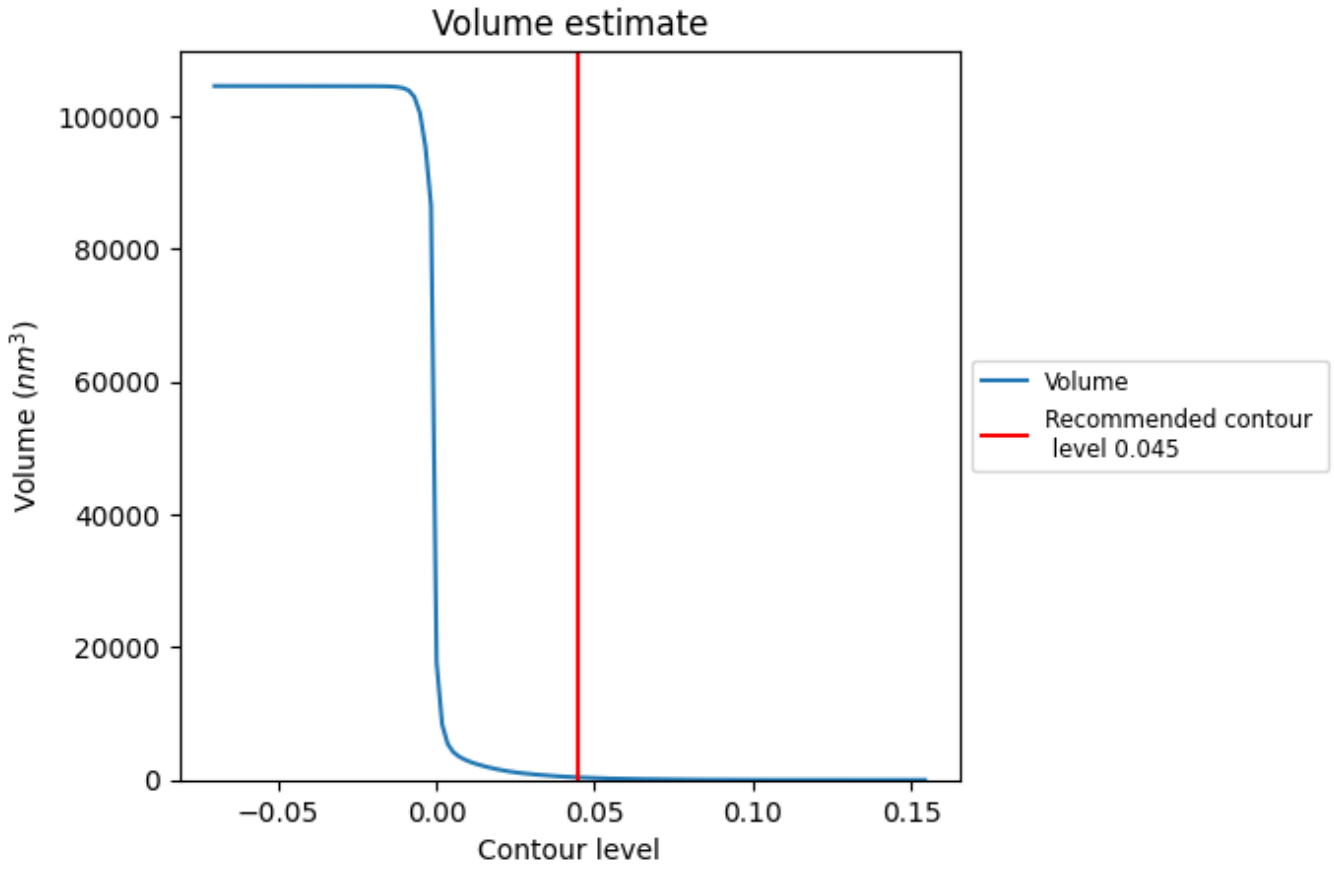
This section contains the results of statistical analysis of the map.

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.

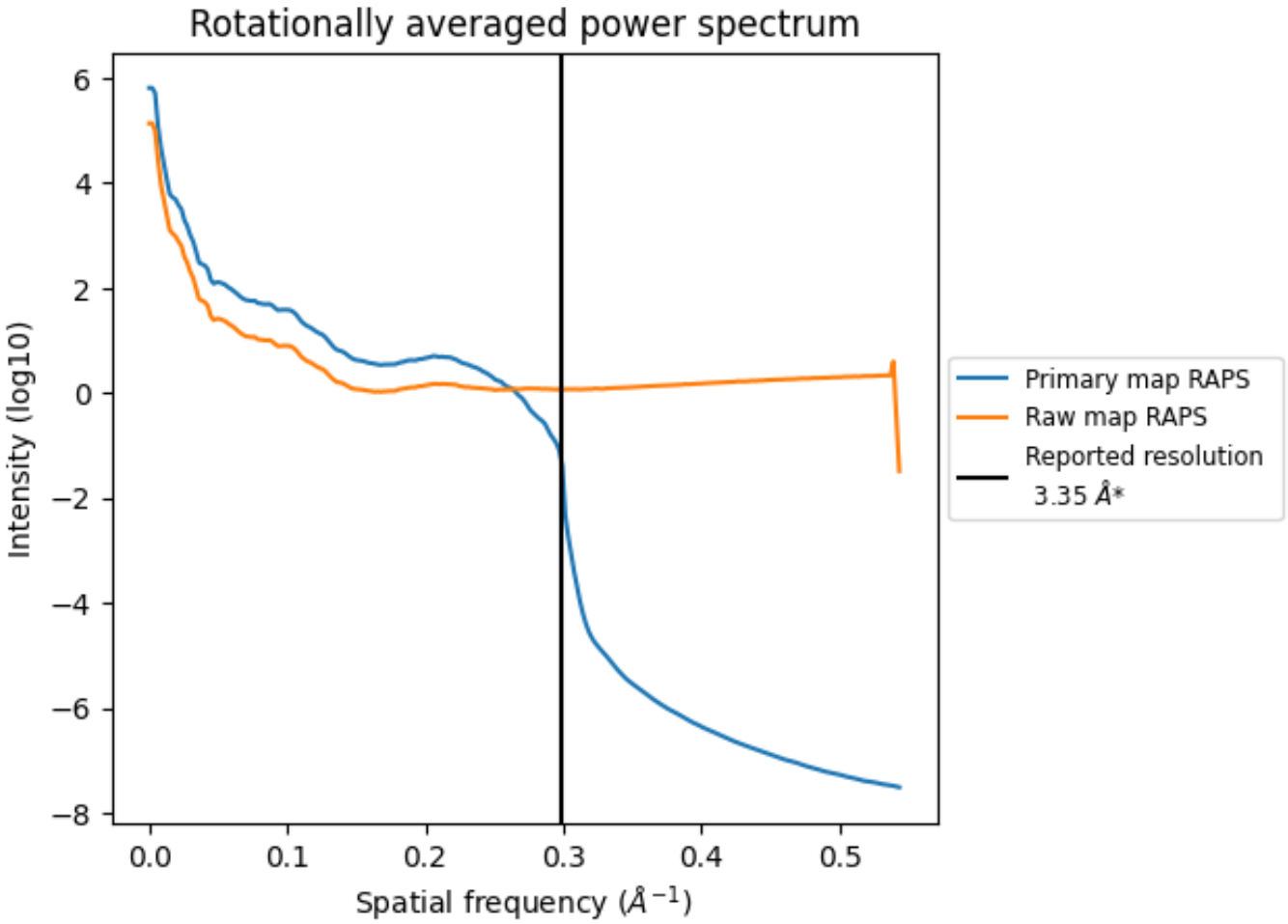
7.2 Volume estimate



The volume at the recommended contour level is 387 nm^3; this corresponds to an approximate mass of 350 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)

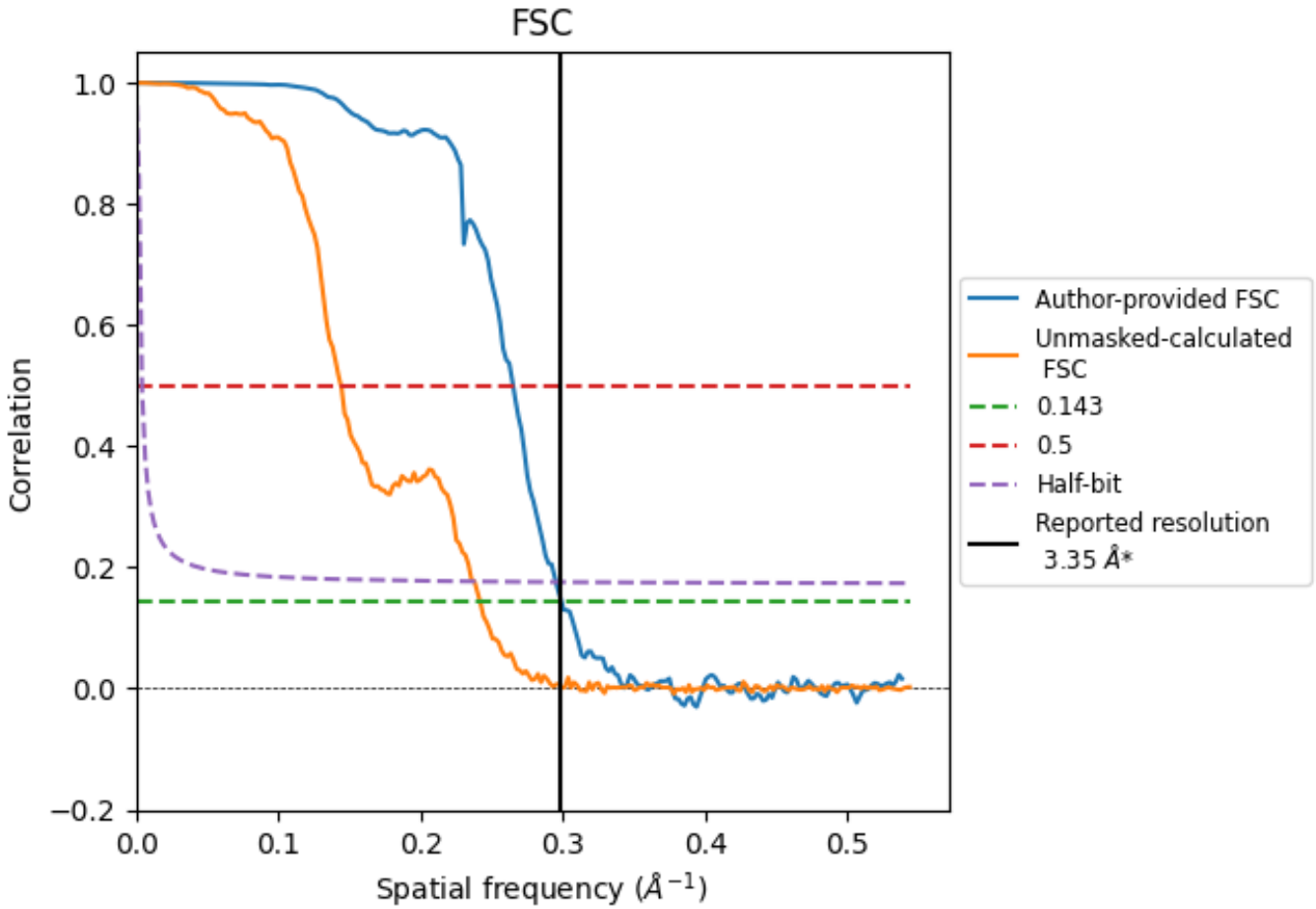


*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

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 0.299 Å^{-1}

8.2 Resolution estimates (i)

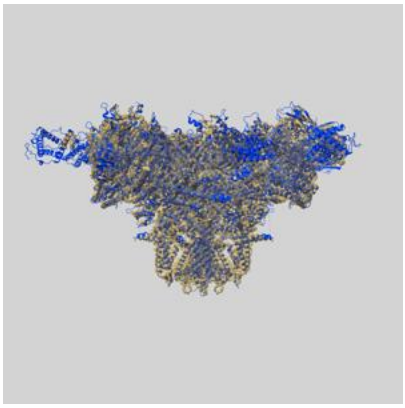
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.78	3.39
Unmasked-calculated*	4.14	6.95	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.35 by more than 10 %

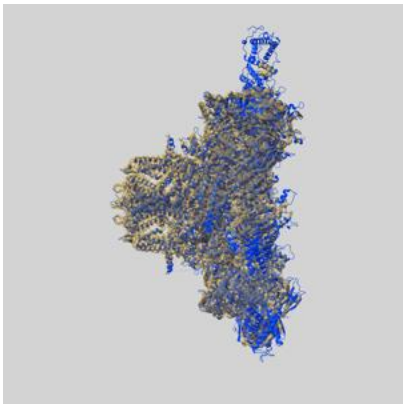
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-80686 and PDB model 26IR. Per-residue inclusion information can be found in section 3 on page 13.

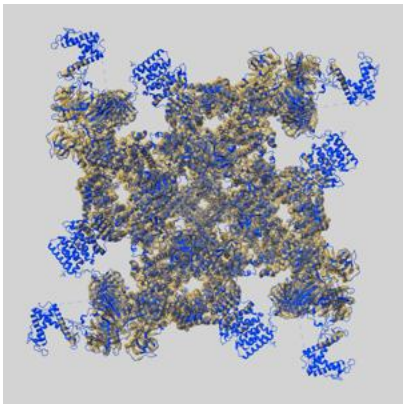
9.1 Map-model overlay



X



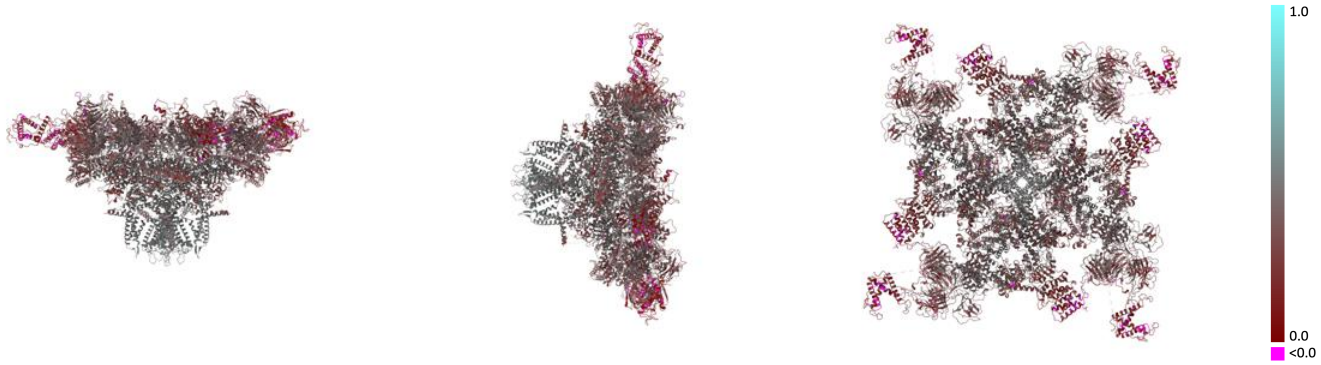
Y



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.

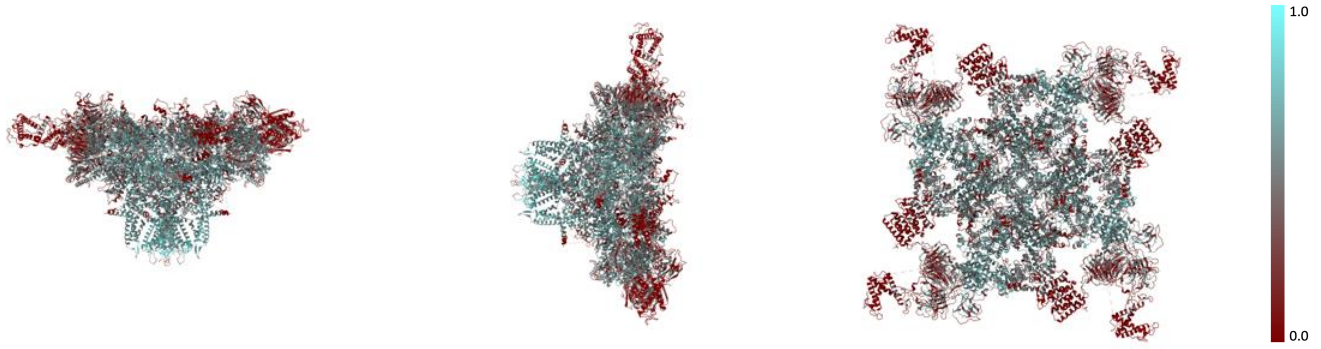
9.2 Q-score mapped to coordinate model (i)



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.

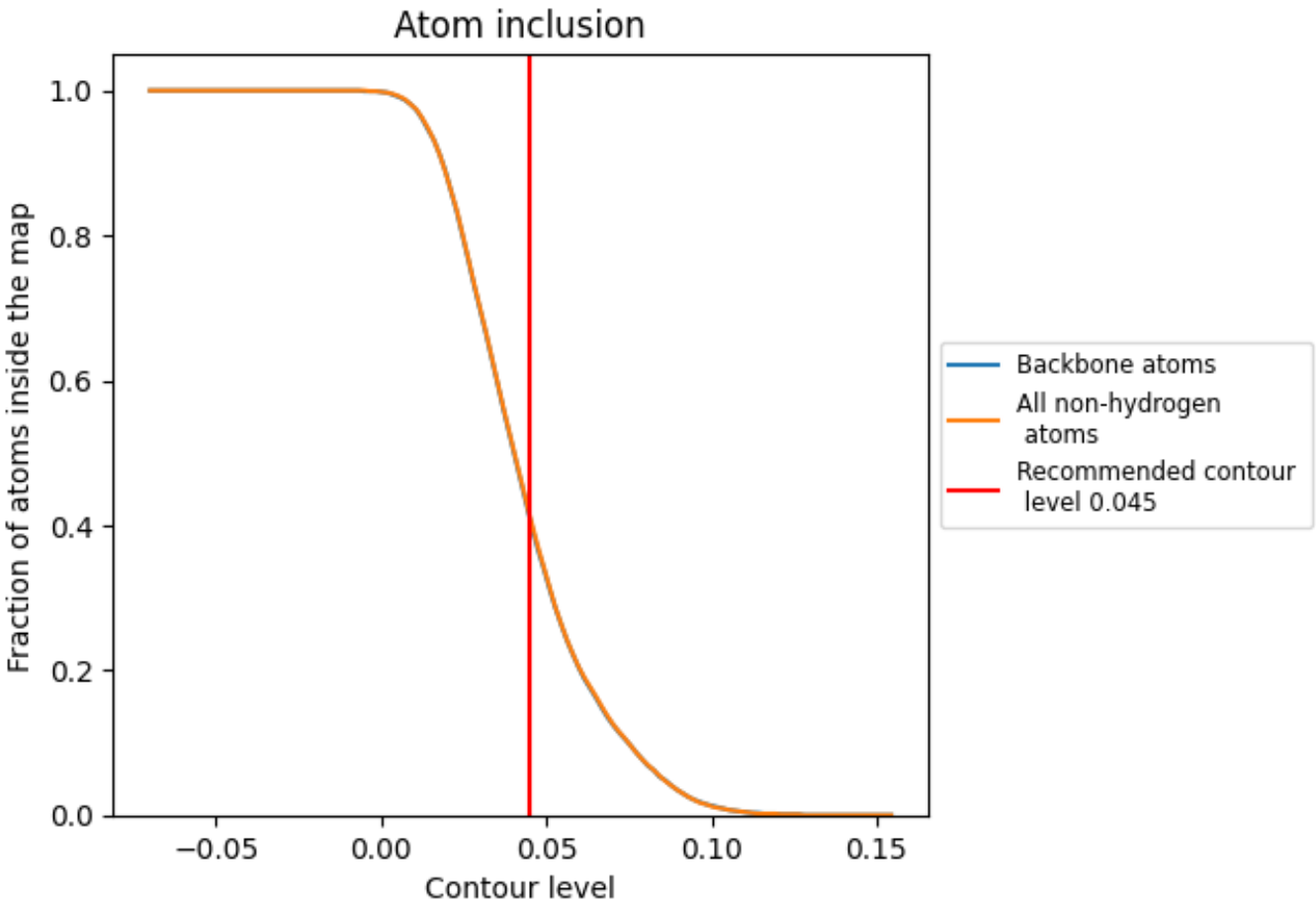
9.3 Atom inclusion mapped to coordinate model (i)



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, 41% of all backbone atoms, 41% 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	0.4130	0.3460
A	0.4200	0.3460
B	0.4200	0.3460
C	0.4200	0.3460
D	0.4200	0.3460
G	0.3980	0.3640
H	0.3980	0.3650
I	0.3980	0.3670
J	0.3980	0.3680

