Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 05:05 PM JST

PDB ID	:	26IO / pdb_000026io
EMDB ID	:	EMD-80683
Title	:	Structure of recombinant RyR2 in the open state (Ca2+ dataset)
Authors	:	Otori, Y.; Takeuchi, S.; Ogawa, H.
Deposited on	:	2026-05-01
Resolution	:	2.73 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:

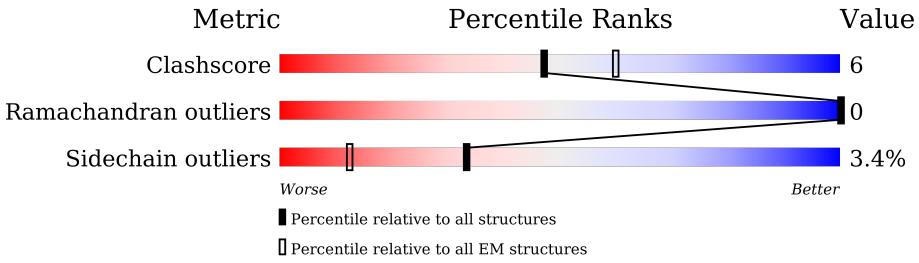
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

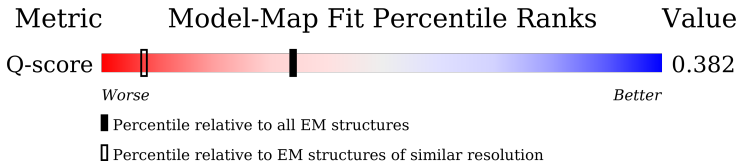
1 Overall quality at a glance

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

The reported resolution of this entry is 2.73 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.





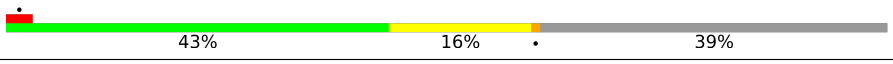
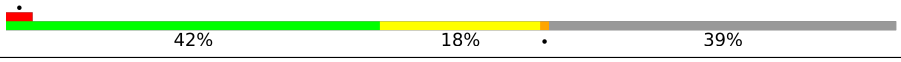
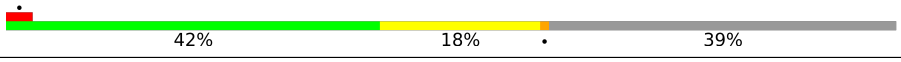
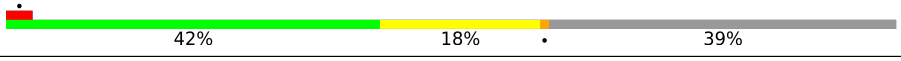
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10432 (2.23 - 3.23)

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	24% 71% 13% • 15%
1	B	4966	24% 71% 13% • 15%
1	C	4966	24% 71% 13% • 15%
1	D	4966	24% 71% 14% • 15%

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

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 275041 atoms, of which 136781 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	4217	Total	C	H	N	O	S	0	0
			67118	21505	33374	5734	6278	227		
1	B	4217	Total	C	H	N	O	S	0	0
			67119	21505	33375	5734	6278	227		
1	C	4217	Total	C	H	N	O	S	0	0
			67118	21505	33374	5734	6278	227		
1	D	4217	Total	C	H	N	O	S	0	0
			67118	21505	33374	5734	6278	227		

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

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

There are 276 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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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

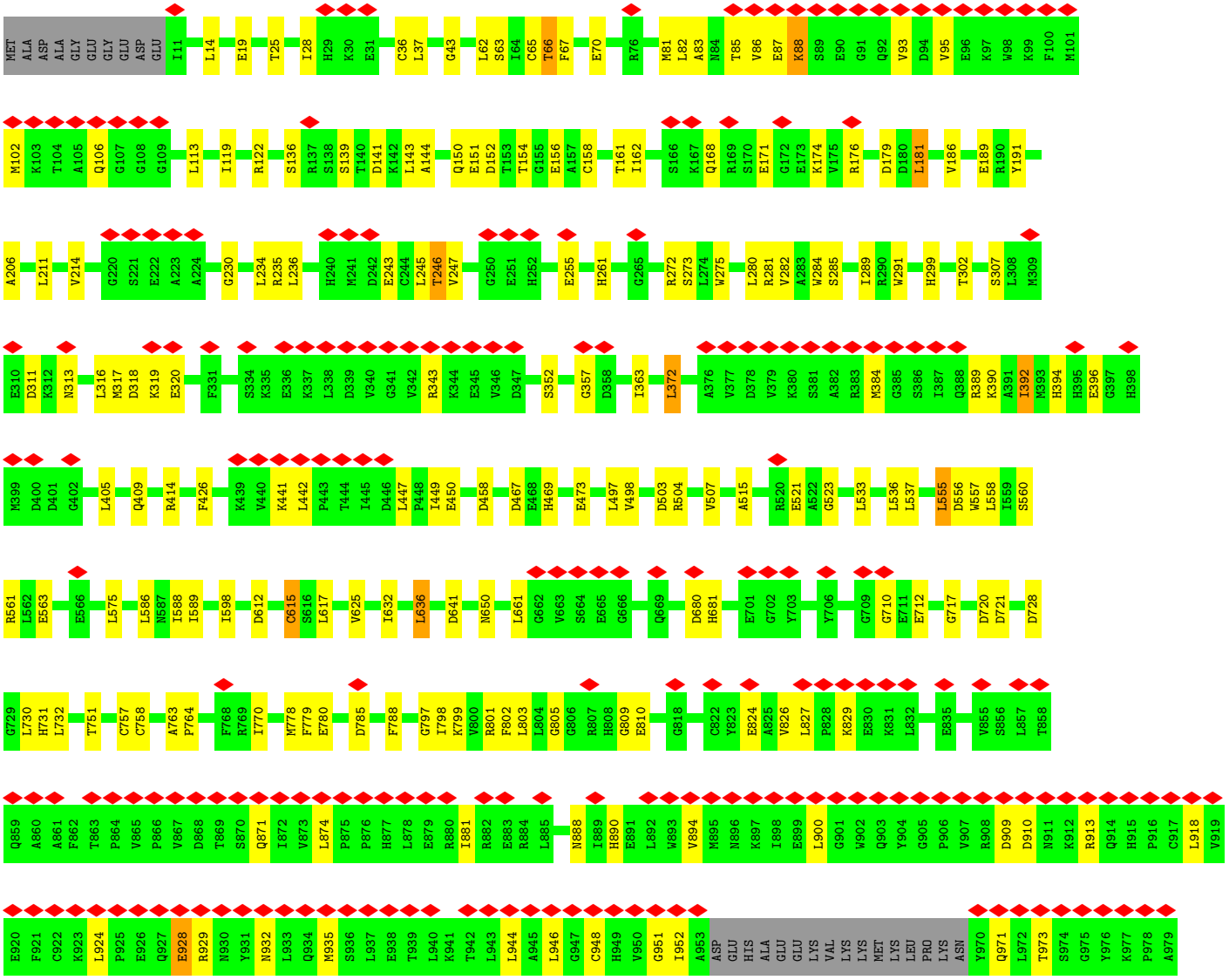
3 Residue-property plots (i)

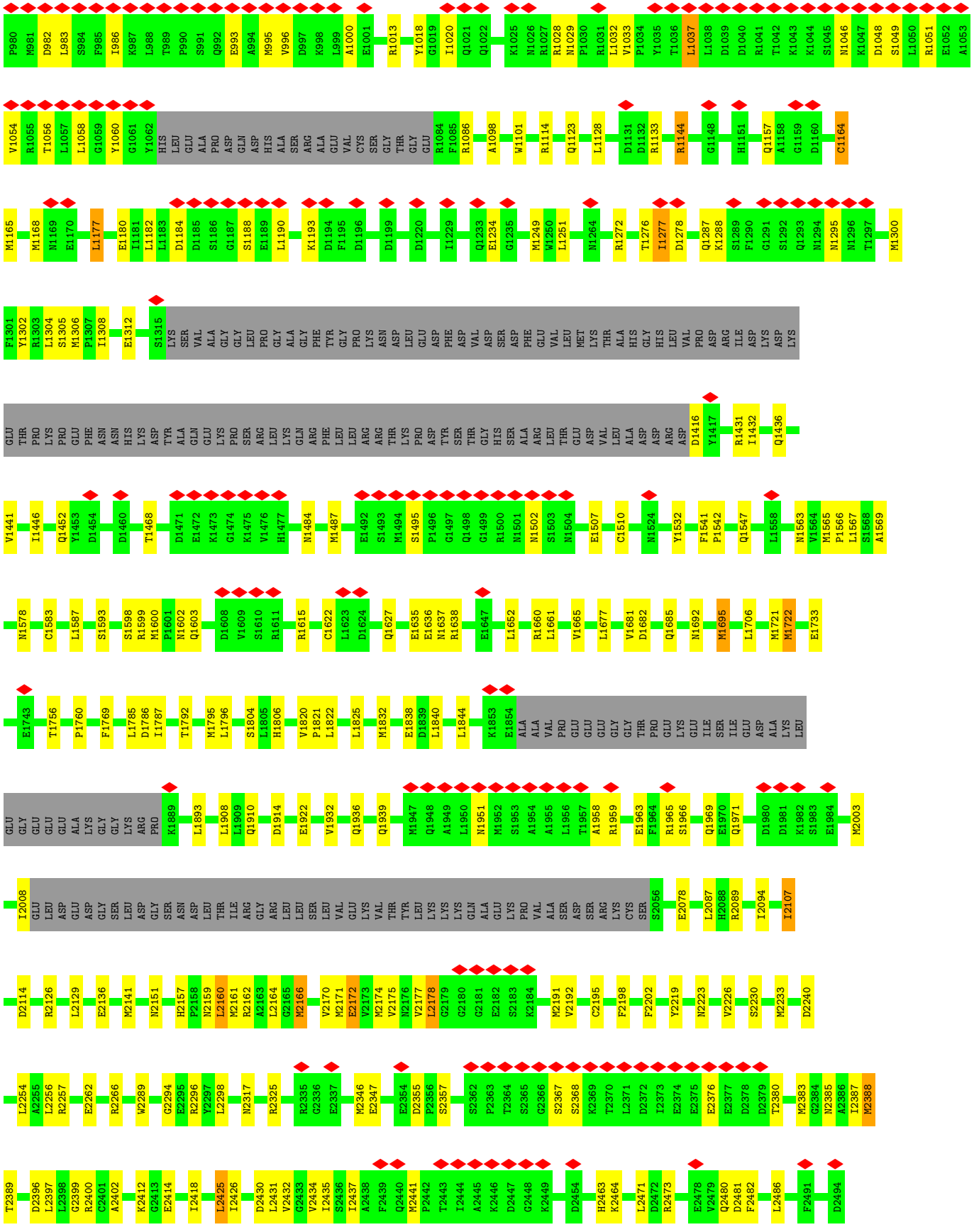
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

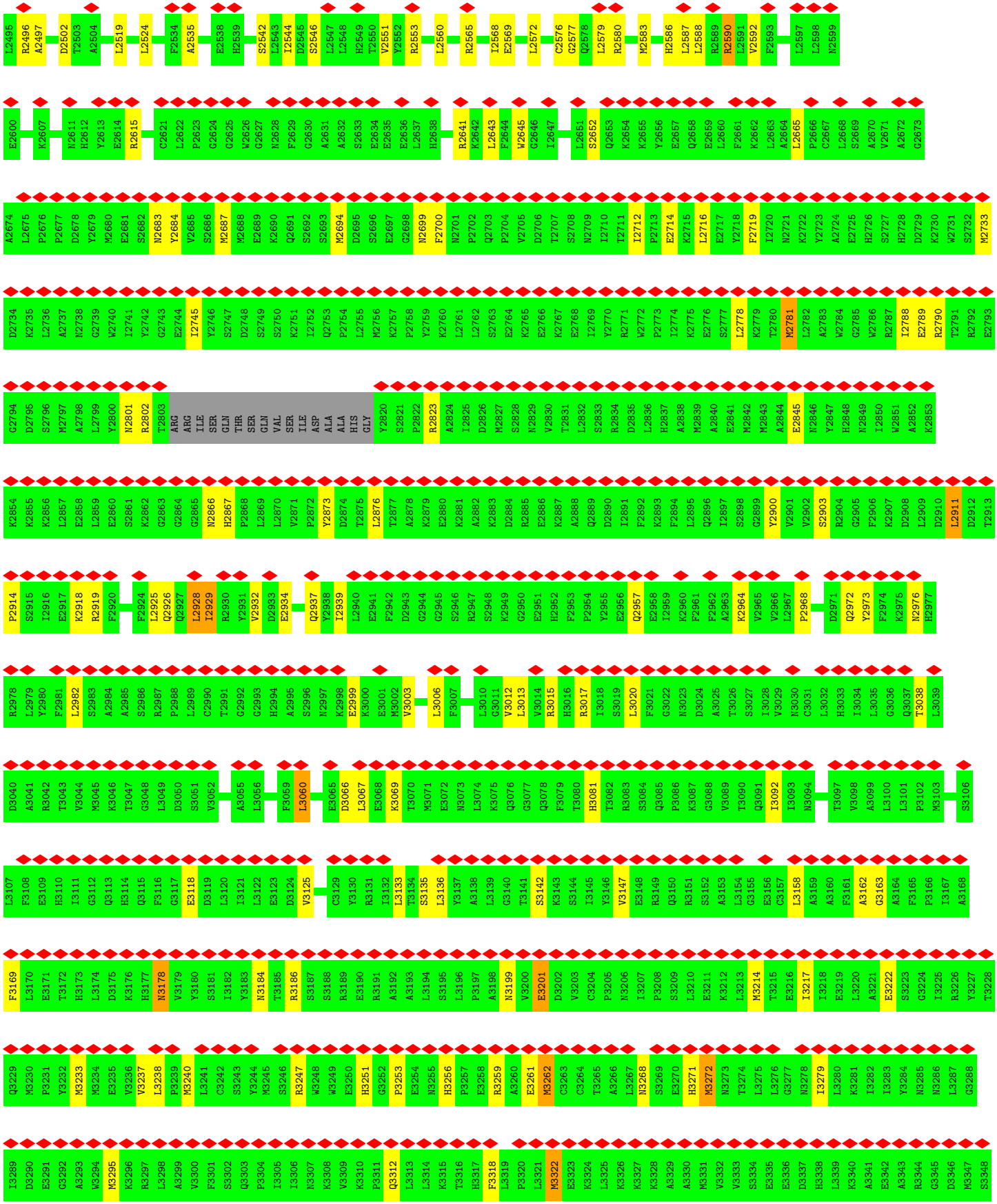
- Molecule 1: Ryanodine receptor 2

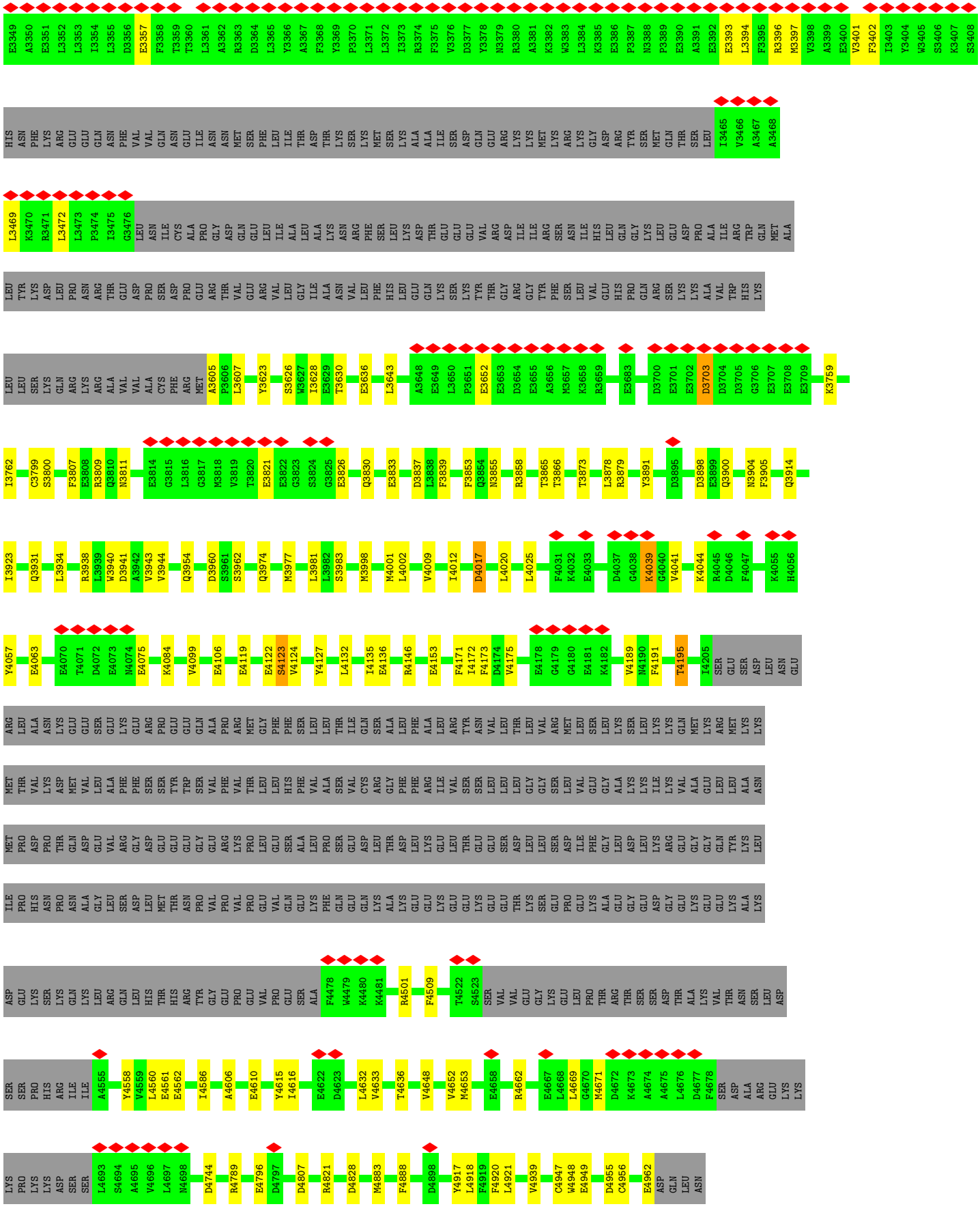
Chain A:







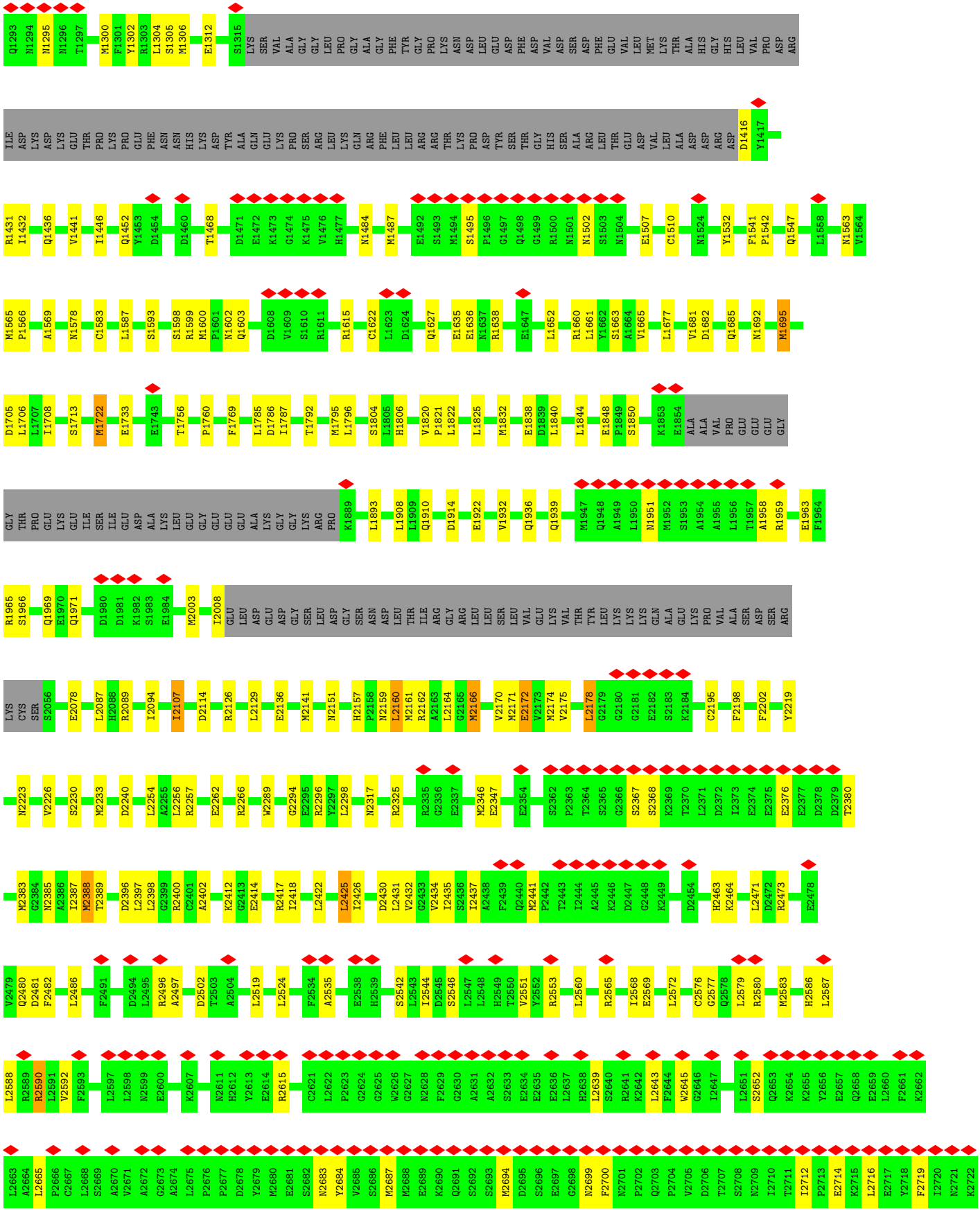

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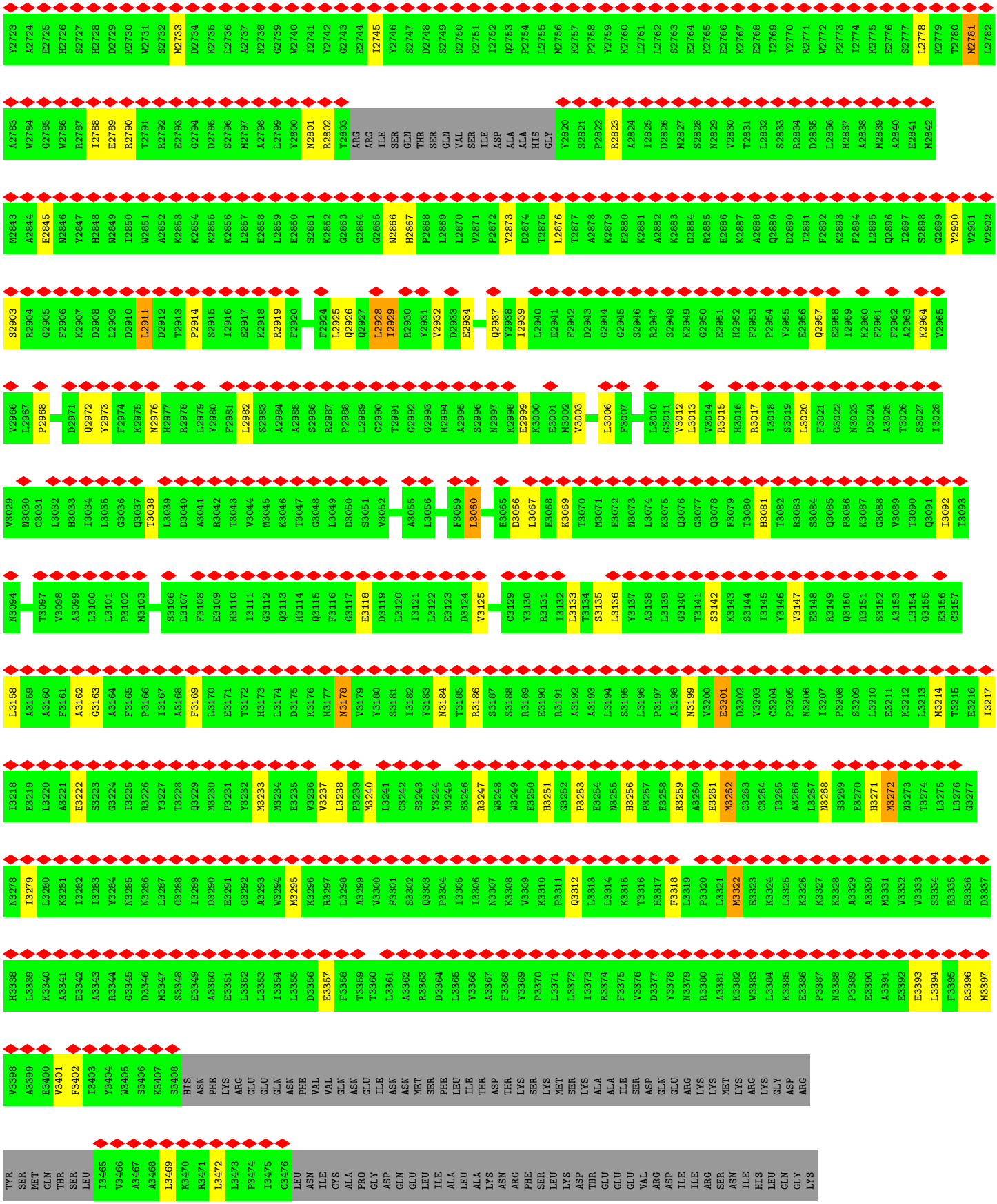


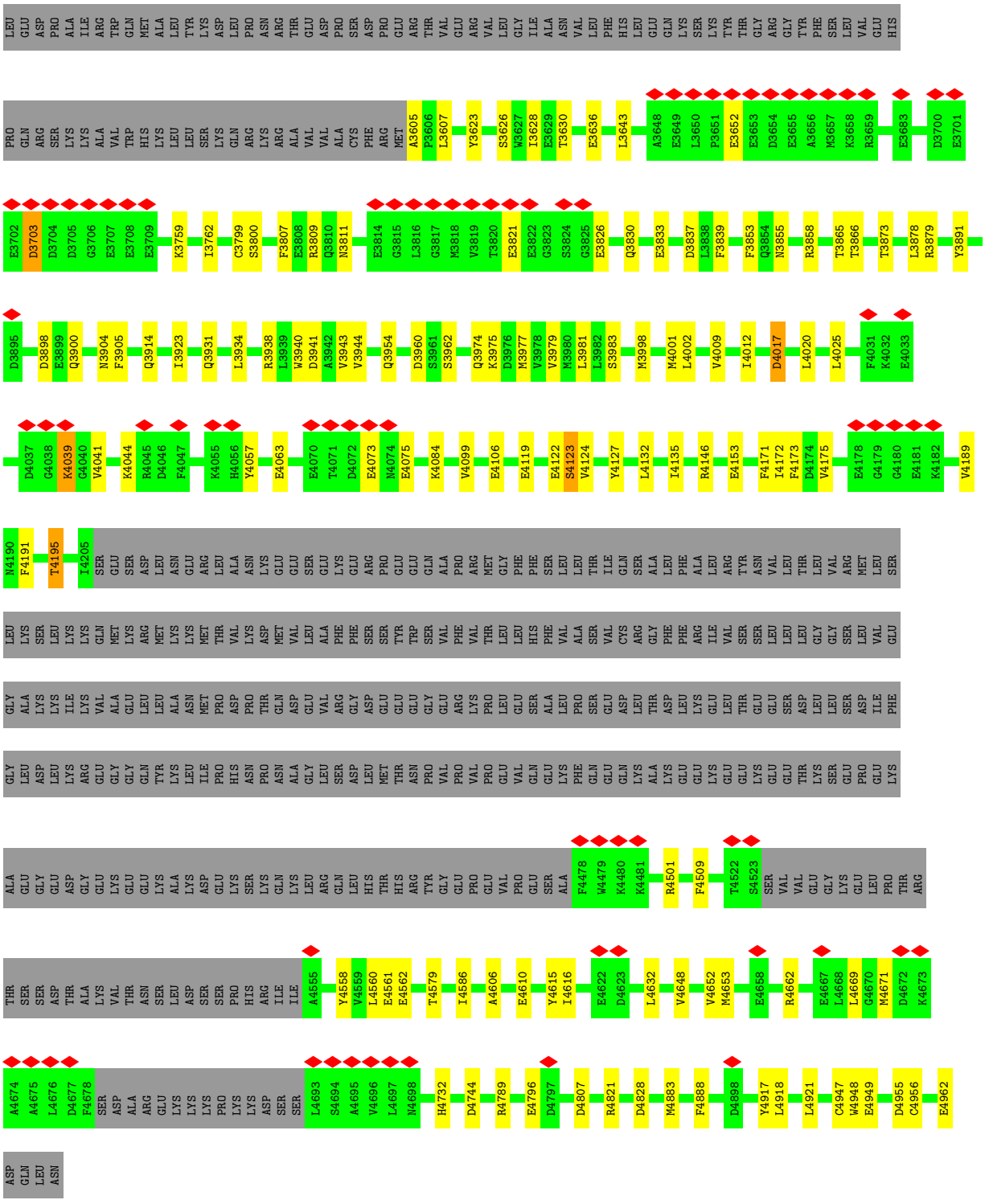
• Molecule 1: Ryanodine receptor 2

Chain B:




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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
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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 L1893 L1908 L1909 Q1910 D1914 E1922 V1932 Q1936 Q1939 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 E1963 F1964
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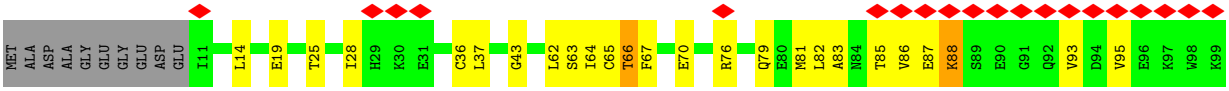

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A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 R2802 T2803 ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY Y2820 S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842
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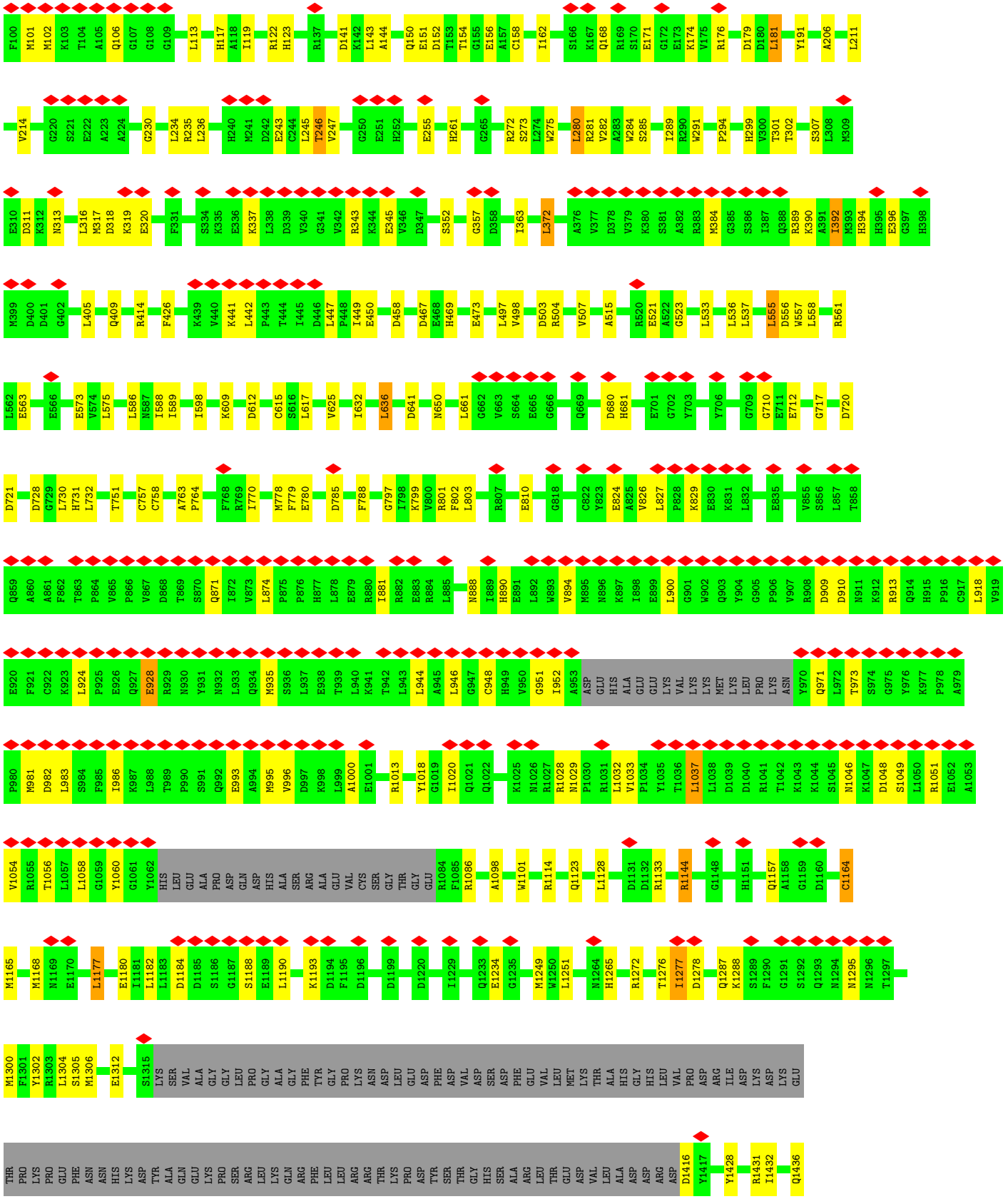


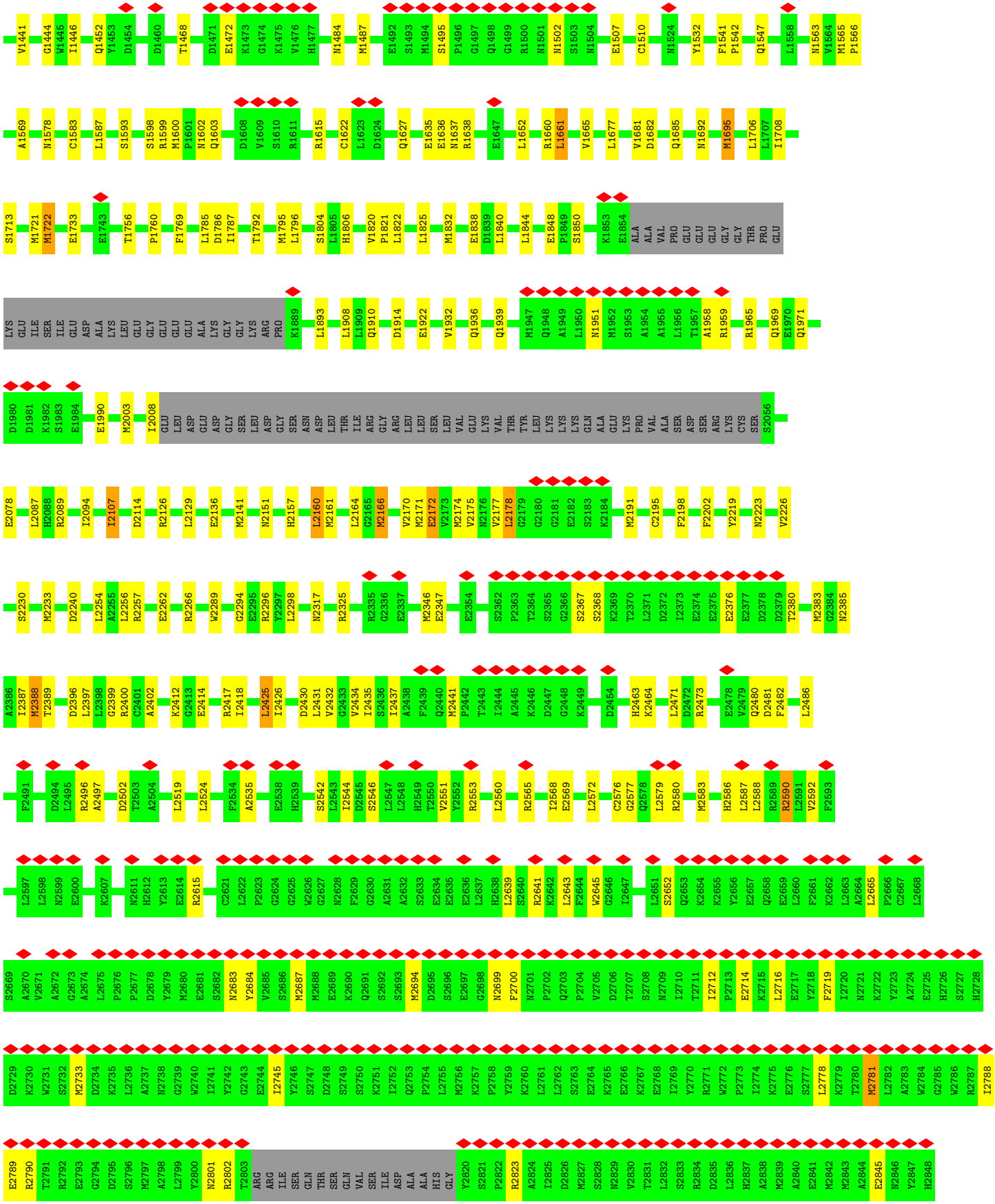
• Molecule 1: Ryanodine receptor 2

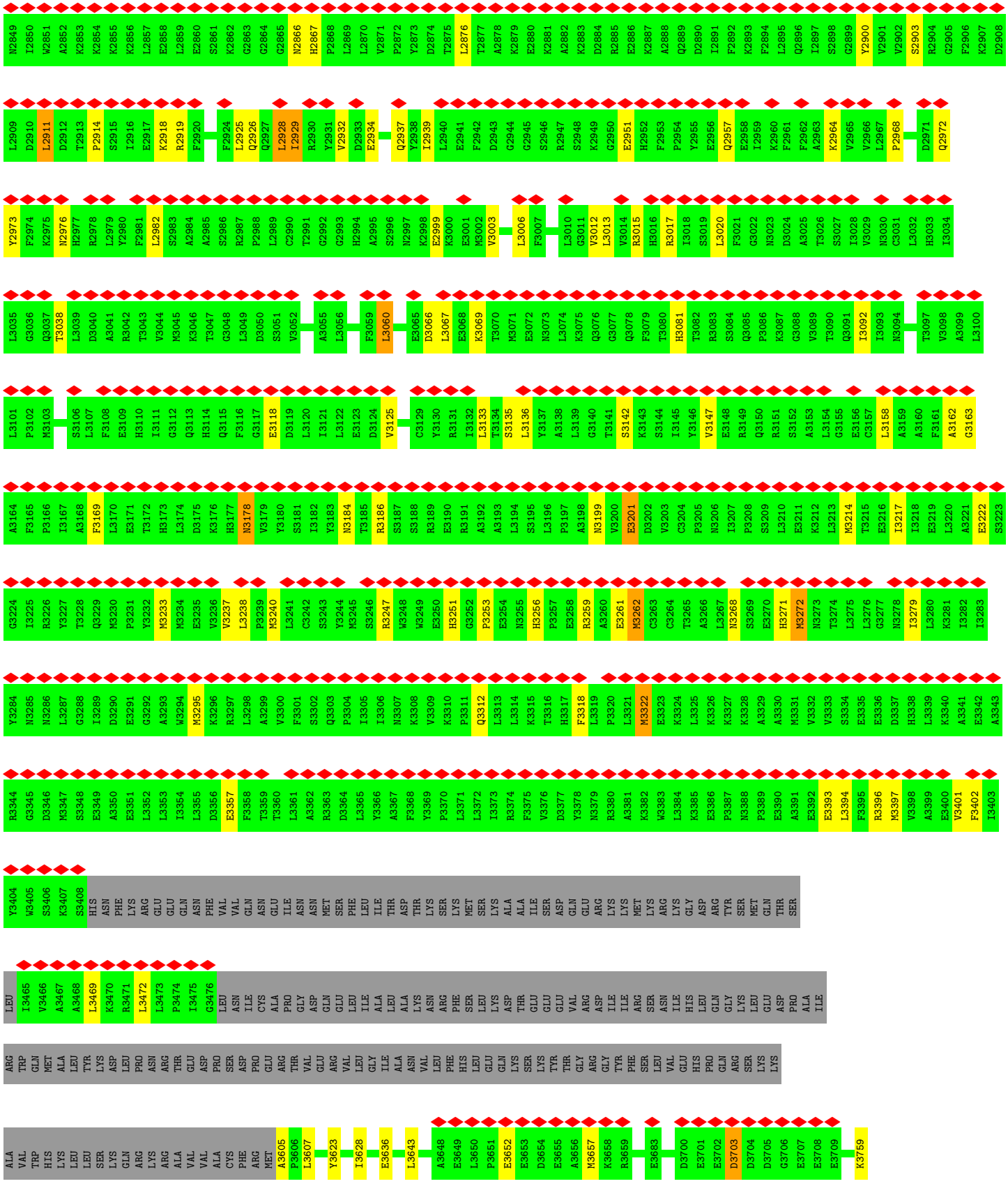
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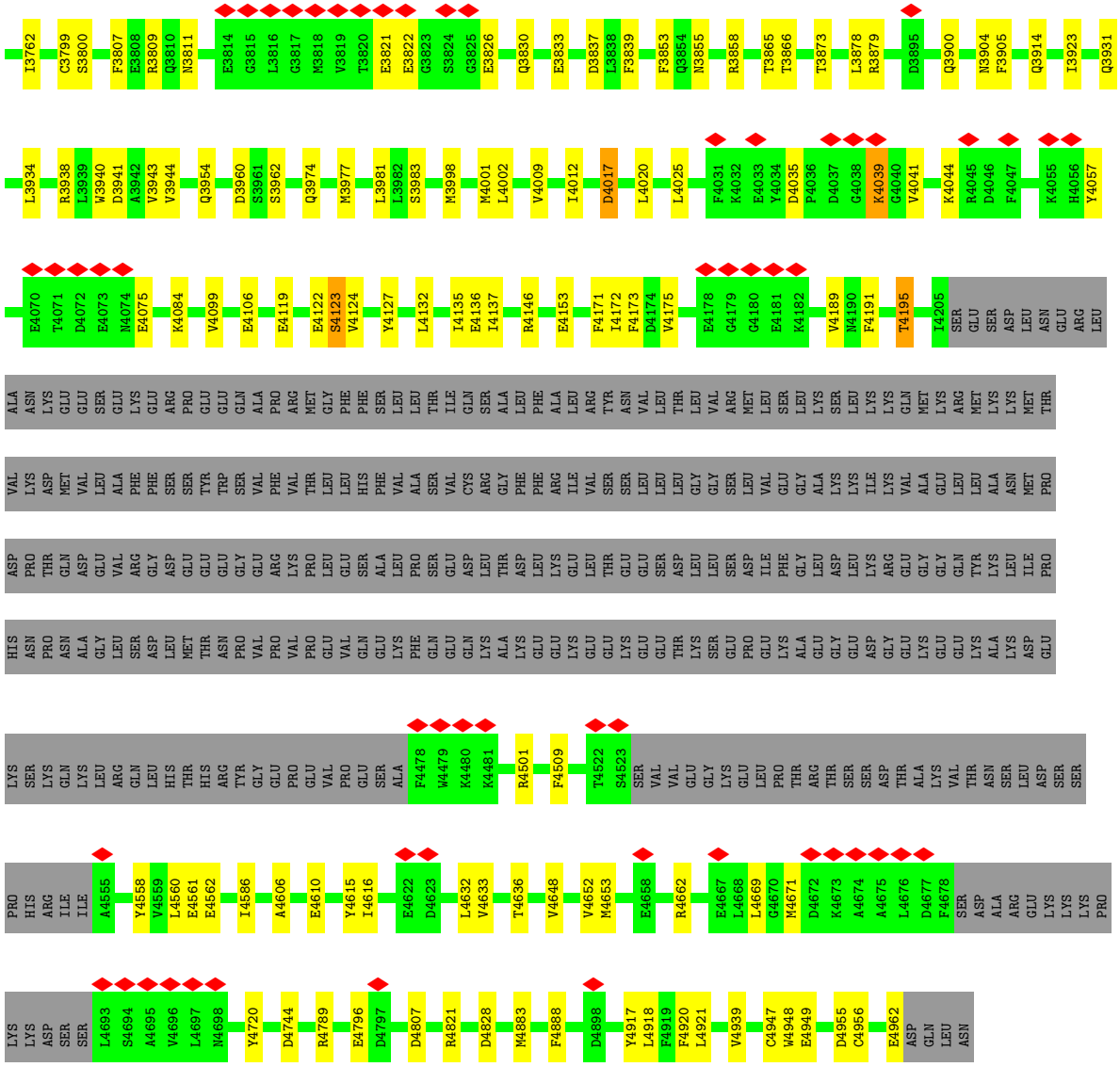





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M1300 F1301 Y1302 R1303 L1304 S1305 M1306 E1312 S1315 LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS 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 Y1428 R1431 I1432 Q1436


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LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 L1893 L1908 L1909 Q1910 D1914 E1922 V1932 Q1936 Q1939 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 R1965 Q1969 E1970 Q1971
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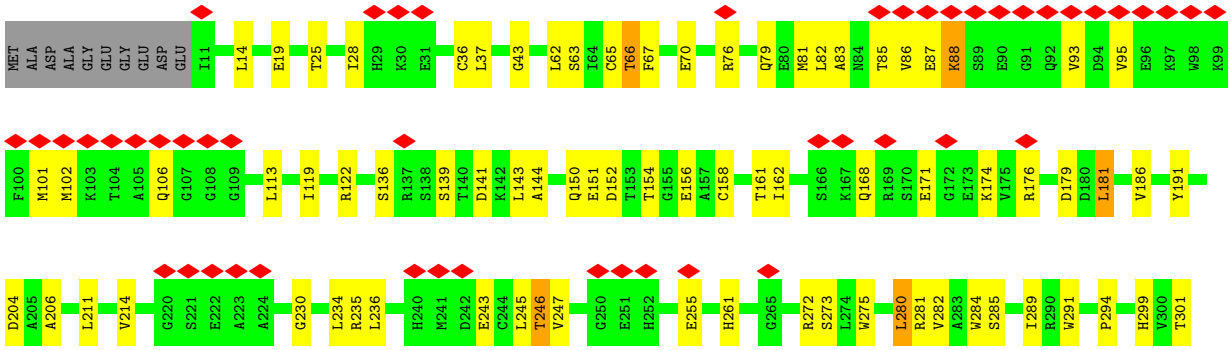

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ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP PRO SER ASP PRO GLU ARG THR VAL GLU ARG VAL LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS TYR THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS
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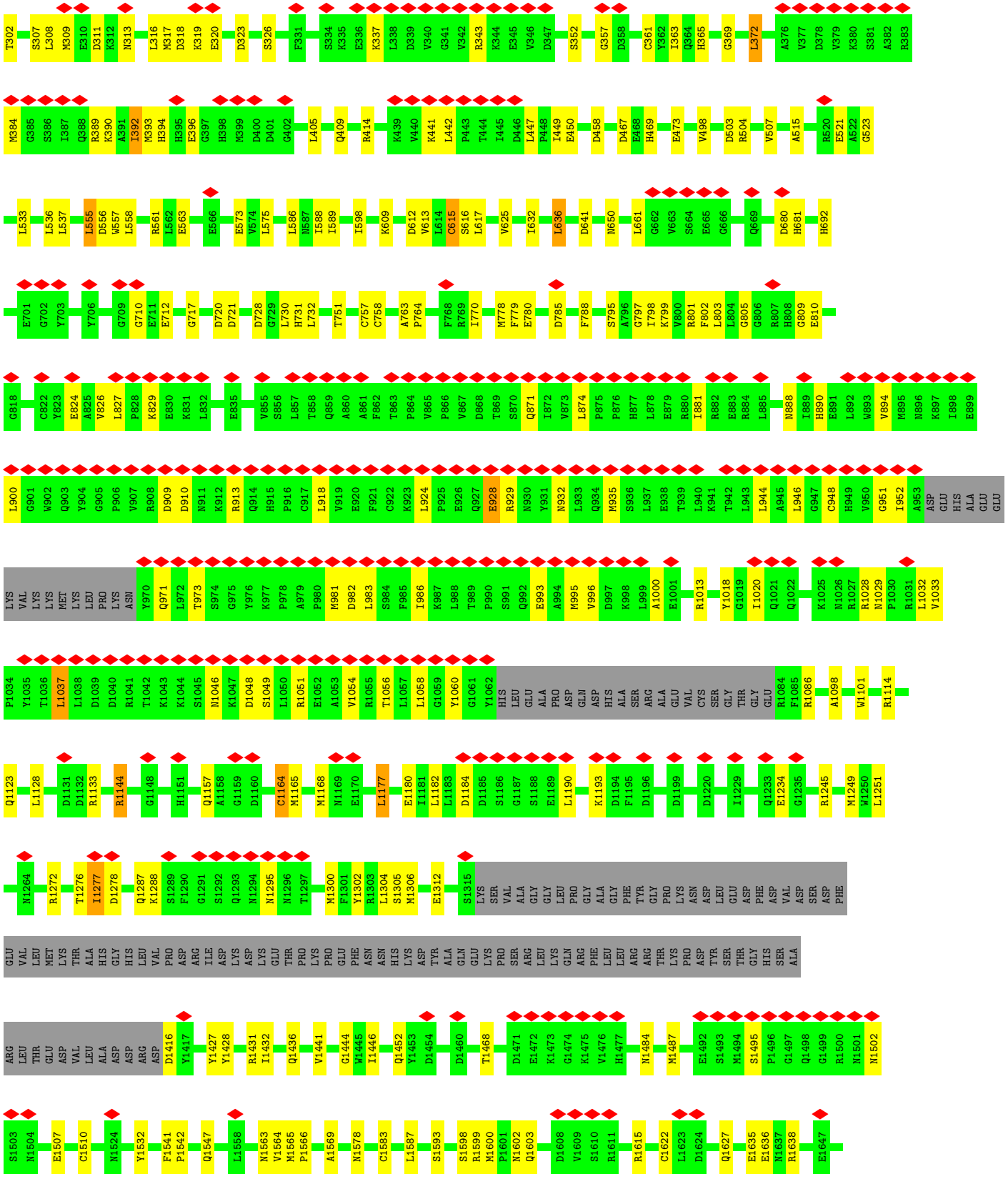


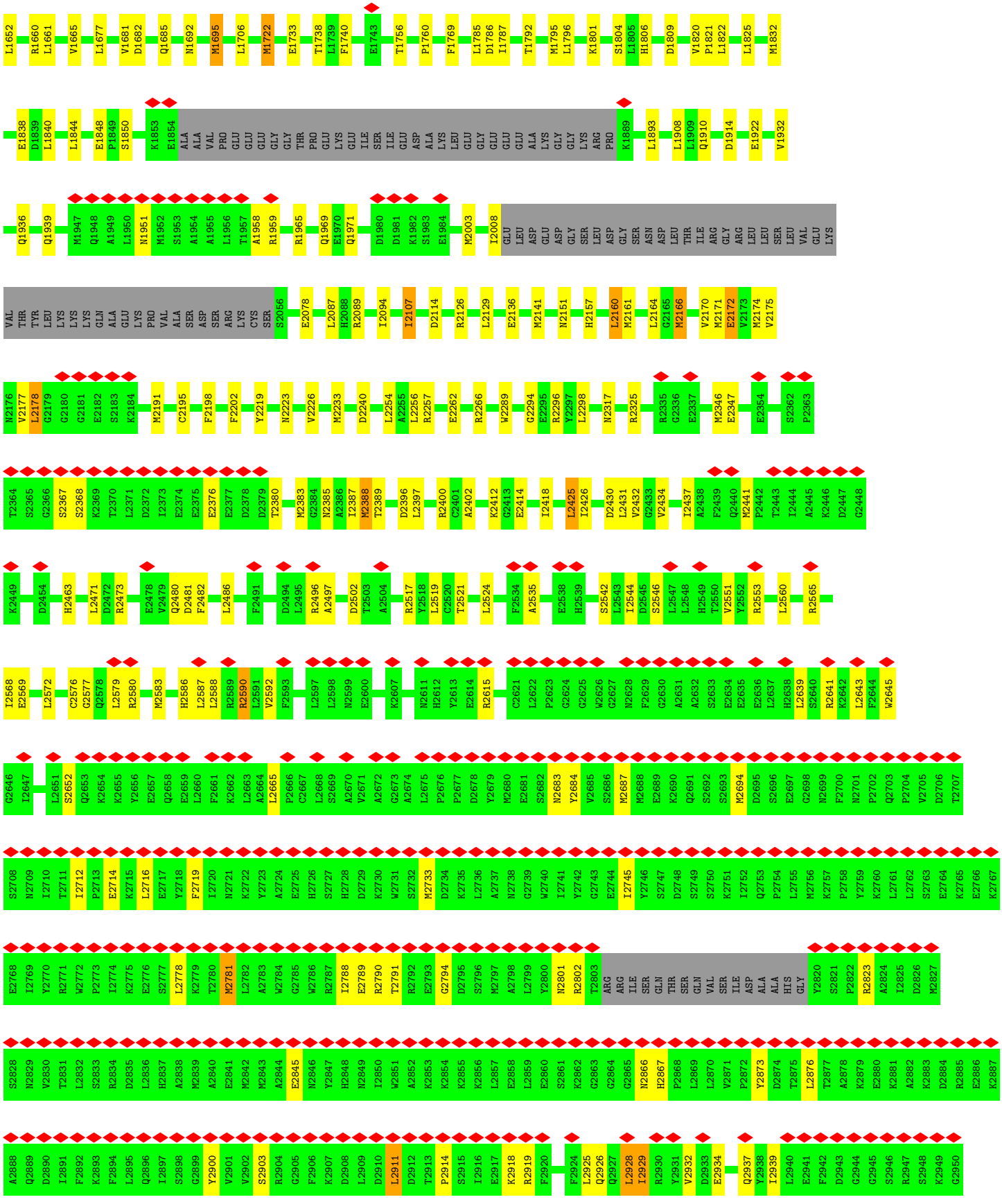
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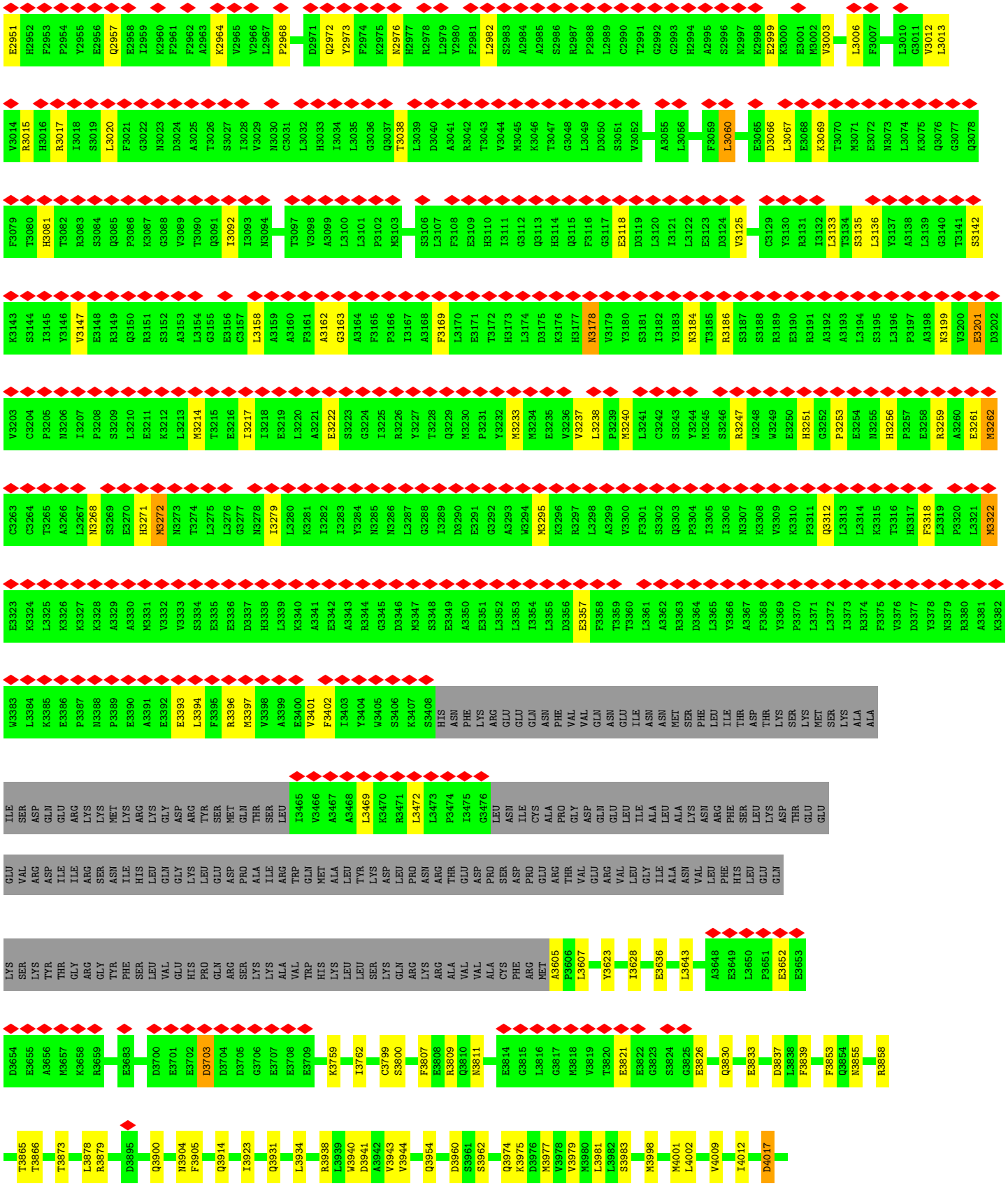
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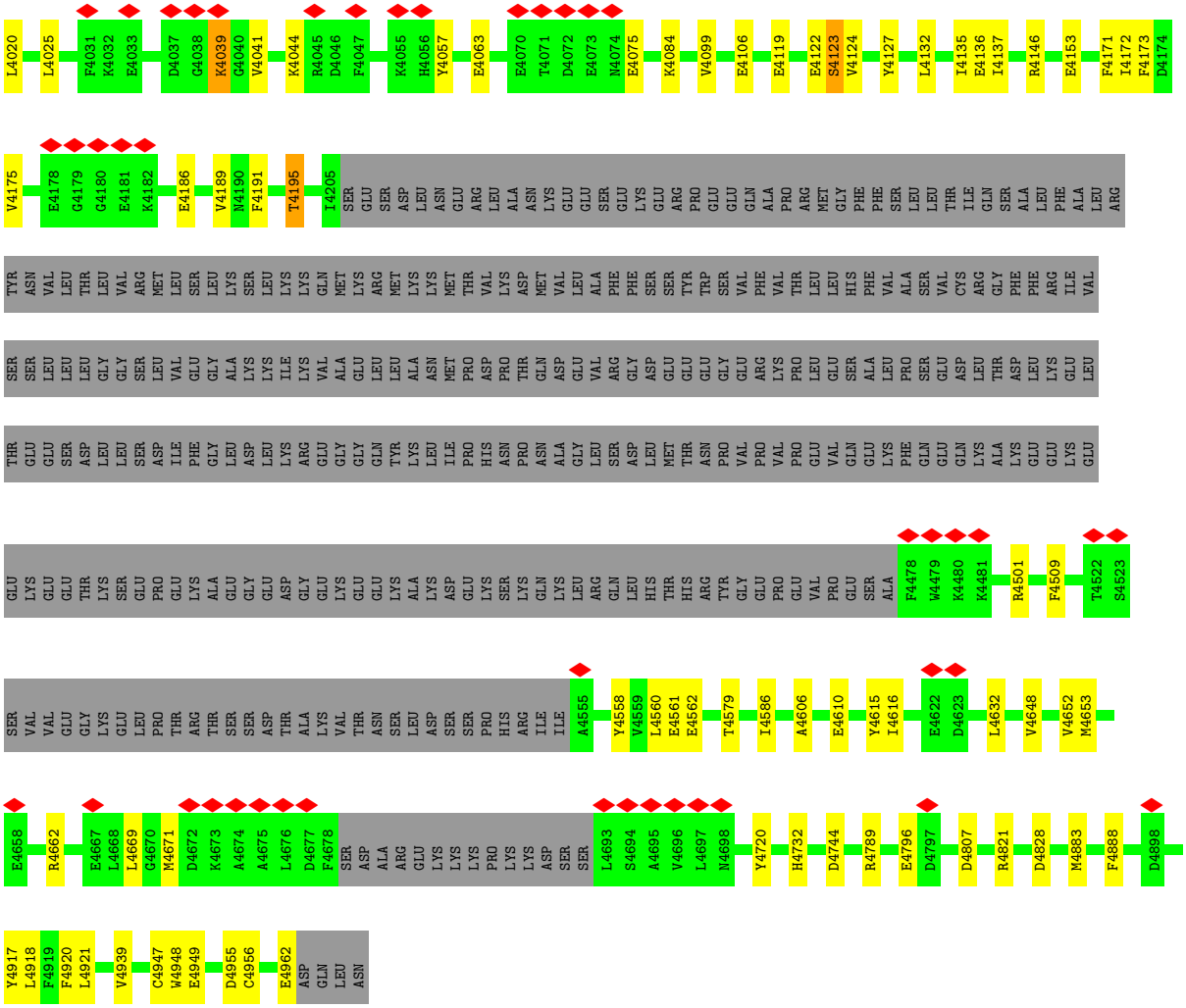





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LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 R1013 Y1018 G1019 I1020 Q1021 Q1022 K1025 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033
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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 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 Y1427 Y1428 R1431 I1432 Q1436 V1441 G1444 W1445 I1446 Q1452 Y1453 D1454 D1460 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 N1484 M1487 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502
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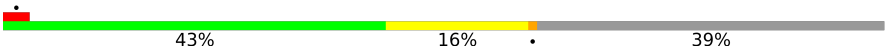

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Q1936 Q1939 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 R1965 Q1969 E1970 Q1971 D1980 D1981 K1982 S1983 E1984 M2003 I2008 GLU LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU 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 E2078 L2087 H2088 R2089 I2094 I2107 D2114 R2126 L2129 E2136 M2141 N2151 H2157 L2160 M2161 L2164 G2165 M2166 V2170 M2171 E2172 V2173 M2174 V2175
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T2364 S2365 G2366 S2367 S2368 K2369 T2370 L2371 D2372 I2373 E2374 E2375 E2376 E2377 D2378 D2379 T2380 M2383 G2384 N2385 A2386 I2387 M2388 T2389 D2396 L2397 R2400 C2401 A2402 K2412 G2413 E2414 I2418 L2425 I2426 D2430 L2431 V2432 G2433 V2434 I2437 A2438 F2439 Q2440 M2441 P2442 T2443 I2444 A2445 K2446 D2447 G2448
K2449 D2454 H2463 L2471 D2472 R2473 E2478 V2479 Q2480 D2481 F2482 L2486 F2491 D2494 L2495 R2496 A2497 D2502 T2503 A2504 R2517 Y2518 L2519 C2520 T2521 L2524 F2534 A2535 E2538 H2539 S2542 L2543 T2544 D2545 S2546 L2547 L2548 H2549 T2550 V2551 Y2552 R2553 L2560 R2565
I2568 E2569 L2572 C2576 G2577 Q2578 L2579 R2580 M2583 H2586 L2587 L2588 R2589 R2590 L2591 V2592 F2593 L2597 L2598 N2599 E2600 K2607 N2611 H2612 Y2613 E2614 R2615 C2621 L2622 P2623 G2624 G2625 W2626 G2627 N2628 F2629 G2630 A2631 A2632 S2633 E2634 E2635 E2636 L2637 H2638 L2639 S2640 R2641 K2642 L2643 F2644 W2645
G2646 I2647 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 E2681 S2682 N2683 Y2684 V2685 S2686 M2687 M2688 E2689 K2690 Q2691 S2692 S2693 M2694 D2695 S2696 E2697 G2698 N2699 F2700 N2701 P2702 Q2703 P2704 V2705 D2706 T2707
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A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 G2905 F2906 K2907 D2908 L2909 D2910 L2911 D2912 T2913 P2914 S2915 I2916 E2917 K2918 R2919 F2920 F2924 L2925 Q2926 Q2927 L2928 I2929 R2930 Y2931 V2932 D2933 E2934 Q2937 Y2938 I2939 L2940 E2941 F2942 D2943 G2944 G2945 S2946 R2947 S2948 K2949 G2950

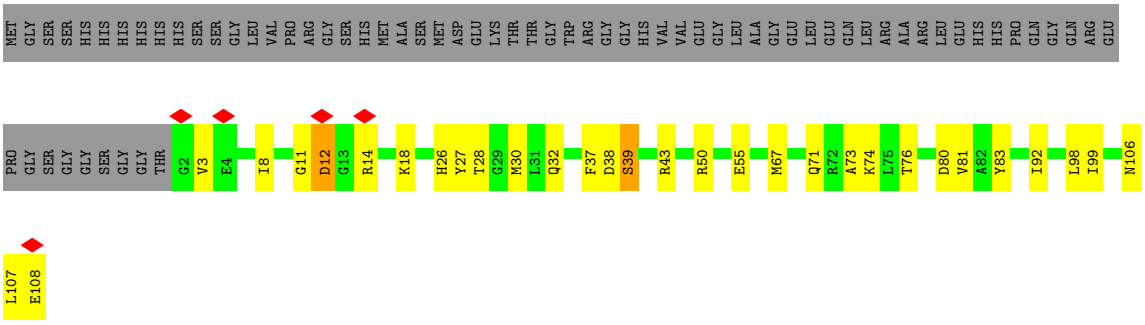

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V3014 R3015 H3016 R3017 I3018 S3019 L3020 F3021 G3022 N3023 D3024 A3025 T3026 S3027 I3028 V3029 N3030 C3031 L3032 H3033 I3034 L3035 G3036 Q3037 T3038 L3039 D3040 A3041 R3042 T3043 V3044 M3045 K3046 T3047 G3048 L3049 D3050 S3051 V3052 A3055 L3056 F3059 L3060 E3065 D3066 L3067 E3068 K3069 T3070 M3071 E3072 N3073 L3074 K3075 Q3076 G3077 Q3078
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K3143 S3144 I3145 Y3146 V3147 E3148 R3149 Q3150 R3151 S3152 A3153 L3154 G3155 E3156 C3157 L3158 A3159 A3160 F3161 A3162 G3163 A3164 F3165 P3166 I3167 A3168 F3169 L3170 E3171 T3172 H3173 L3174 D3175 K3176 H3177 N3178 V3179 Y3180 S3181 I3182 Y3183 N3184 T3185 R3186 S3187 S3188 R3189 E3190 R3191 A3192 A3193 L3194 S3195 L3196 P3197 A3198 N3199 V3200 E3201 D3202
V3203 C3204 P3205 N3206 I3207 P3208 S3209 L3210 E3211 K3212 L3213 M3214 T3215 E3216 I3217 I3218 E3219 L3220 A3221 E3222 S3223 G3224 I3225 R3226 Y3227 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 V3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 M3245 S3246 R3247 W3248 W3249 E3250 H3251 G3252 P3253 E3254 N3255 H3256 P3257 E3258 R3259 A3260 E3261 M3262
C3263 C3264 T3265 A3266 L3267 N3268 S3269 E3270 H3271 M3272 N3273 T3274 L3275 L3276 G3277 N3278 I3279 L3280 K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 A3293 W3294 M3295 K3296 R3297 L3298 A3299 V3300 F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 L3314 K3315 T3316 H3317 F3318 L3319 P3320 L3321 M3322
E3323 K3324 L3325 K3326 K3327 K3328 A3329 A3330 M3331 V3332 V3333 S3334 E3335 E3336 D3337 H3338 L3339 K3340 A3341 E3342 A3343 R3344 G3345 D3346 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357 F3358 T3359 T3360 L3361 A3362 R3363 D3364 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374 F3375 V3376 D3377 Y3378 M3379 R3380 A3381 K3382
W3383 L3384 K3385 E3386 P3387 N3388 P3389 E3390 A3391 E3392 E3393 L3394 F3395 R3396 M3397 V3398 A3399 E3400 V3401 F3402 I3403 Y3404 W3405 S3406 K3407 S3408 HIS ASN PHE LYS ARG GLU GLN GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA
ILE SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 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 ASP ILE ILE 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 SER ASP PRO GLU 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 LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET A3605 P3606 L3607 Y3623 I3628 E3636 L3643 A3648 E3649 L3650 P3651 E3652 E3653
D3654 E3655 A3656 M3657 K3658 R3659 E3683 D3700 E3701 E3702 D3703 D3704 D3705 G3706 E3707 E3708 E3709 K3759 I3762 C3799 S3800 F3807 E3808 R3809 Q3810 N3811 E3814 G3815 L3816 G3817 M3818 V3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 Q3830 E3833 D3837 L3838 F3839 F3853 Q3854 N3855 R3858
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• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

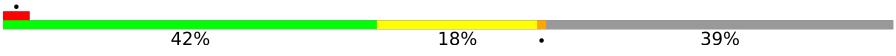
Chain G:



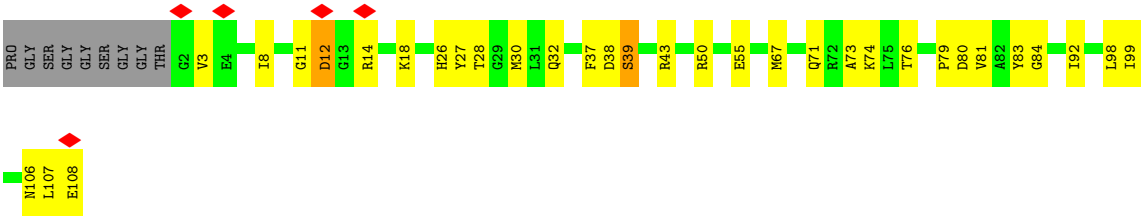


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

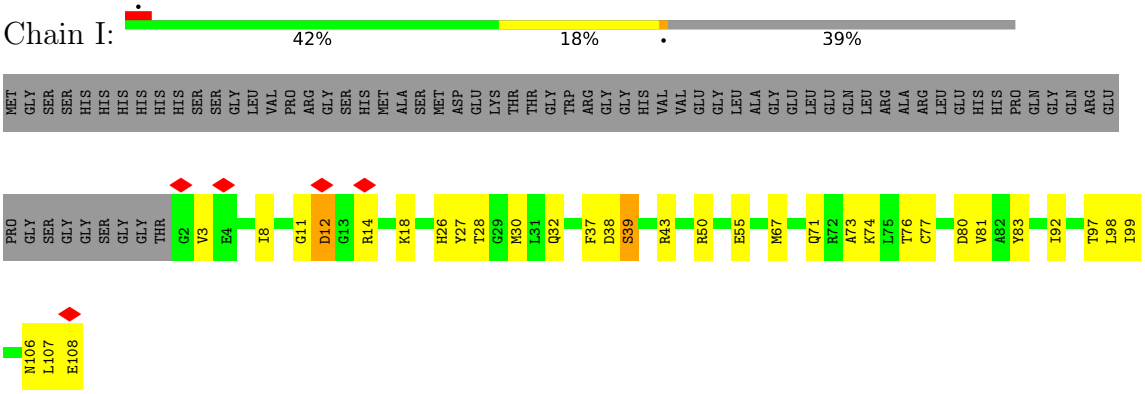
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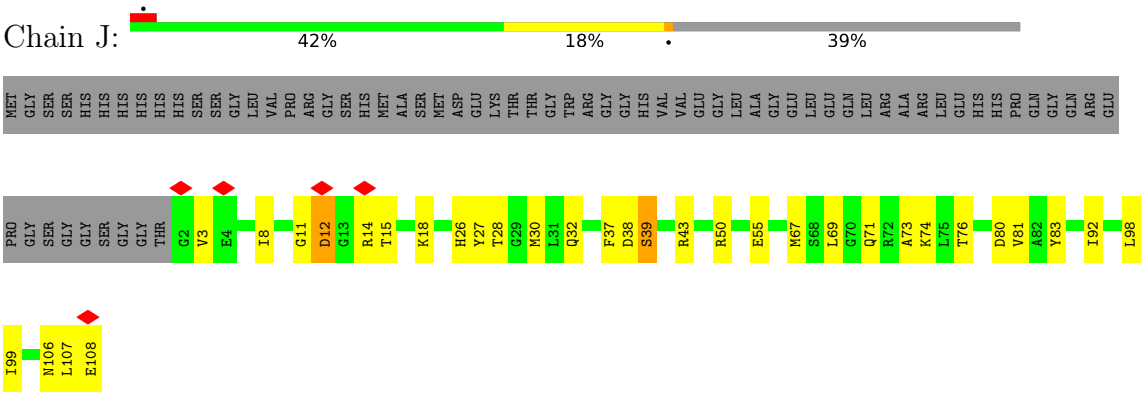




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	256984	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	469.504, 469.504, 469.504	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.917, 0.917, 0.917	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/34486	0.38	0/46602
1	B	0.26	0/34486	0.38	0/46602
1	C	0.26	0/34486	0.38	0/46602
1	D	0.26	0/34486	0.38	0/46602
2	G	0.23	0/835	0.42	0/1123
2	H	0.23	0/835	0.42	0/1123
2	I	0.23	0/835	0.42	0/1123
2	J	0.23	0/835	0.40	0/1123
All	All	0.26	0/141284	0.38	0/190900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33744	33374	33373	395	0
1	B	33744	33375	33373	395	0
1	C	33744	33374	33373	401	0
1	D	33744	33374	33373	404	0
2	G	819	821	821	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	819	821	821	20	0
2	I	819	821	821	21	0
2	J	819	821	821	21	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
All	All	138260	136781	136776	1651	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 (1651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1565:MET:HE2	1:B:1569:ALA:HB2	1.57	0.86
1:D:1565:MET:HE2	1:D:1569:ALA:HB2	1.57	0.86
1:B:632:ILE:HD11	1:B:1665:VAL:HG12	1.58	0.85
1:C:1565:MET:HE2	1:C:1569:ALA:HB2	1.57	0.84
1:A:1565:MET:HE2	1:A:1569:ALA:HB2	1.57	0.84
1:C:632:ILE:HD11	1:C:1665:VAL:HG12	1.58	0.83
1:A:632:ILE:HD11	1:A:1665:VAL:HG12	1.58	0.83
1:D:632:ILE:HD11	1:D:1665:VAL:HG12	1.58	0.82
1:C:615:CYS:SG	1:C:1660:ARG:NH1	2.54	0.81
1:B:612:ASP:OD1	1:B:1660:ARG:NH2	2.17	0.77
1:D:612:ASP:OD1	1:D:1660:ARG:NH2	2.17	0.77
1:A:612:ASP:OD1	1:A:1660:ARG:NH2	2.18	0.77
1:C:612:ASP:OD1	1:C:1660:ARG:NH2	2.17	0.77
1:C:3878:LEU:HD11	1:C:3938:ARG:HE	1.49	0.77
1:B:3878:LEU:HD11	1:B:3938:ARG:HE	1.49	0.76
1:A:3878:LEU:HD11	1:A:3938:ARG:HE	1.49	0.76
1:D:3878:LEU:HD11	1:D:3938:ARG:HE	1.50	0.76
1:D:3272:MET:SD	1:D:3272:MET:N	2.60	0.75
1:B:1692:ASN:ND2	1:B:1695:MET:SD	2.60	0.75
1:A:3272:MET:SD	1:A:3272:MET:N	2.60	0.74
1:C:70:GLU:OE1	1:C:122:ARG:NH1	2.21	0.74
1:C:1416:ASP:N	1:C:1563:ASN:OD1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1692:ASN:ND2	1:C:1695:MET:SD	2.60	0.74
1:D:70:GLU:OE1	1:D:122:ARG:NH1	2.20	0.74
1:B:70:GLU:OE1	1:B:122:ARG:NH1	2.20	0.74
1:B:3272:MET:SD	1:B:3272:MET:N	2.60	0.74
1:C:3272:MET:SD	1:C:3272:MET:N	2.60	0.74
1:A:1692:ASN:ND2	1:A:1695:MET:SD	2.60	0.74
1:A:70:GLU:OE1	1:A:122:ARG:NH1	2.20	0.73
1:D:1692:ASN:ND2	1:D:1695:MET:SD	2.60	0.73
1:A:1416:ASP:N	1:A:1563:ASN:OD1	2.20	0.73
1:B:1416:ASP:N	1:B:1563:ASN:OD1	2.20	0.73
1:C:4017:ASP:OD2	1:C:4123:SER:OG	2.04	0.73
1:D:1416:ASP:N	1:D:1563:ASN:OD1	2.20	0.73
1:C:4633:VAL:O	1:C:4636:THR:OG1	2.06	0.73
1:D:4017:ASP:OD2	1:D:4123:SER:OG	2.04	0.73
1:C:2542:SER:OG	1:C:2876:LEU:O	2.07	0.72
1:A:2542:SER:OG	1:A:2876:LEU:O	2.07	0.72
2:I:11:GLY:O	2:I:14:ARG:NH1	2.23	0.72
2:G:11:GLY:O	2:G:14:ARG:NH1	2.23	0.72
1:A:615:CYS:SG	1:A:1660:ARG:NH1	2.62	0.72
1:A:4017:ASP:OD2	1:A:4123:SER:OG	2.04	0.72
2:J:11:GLY:O	2:J:14:ARG:NH1	2.23	0.72
1:B:615:CYS:SG	1:B:1660:ARG:NH1	2.63	0.71
1:B:2542:SER:OG	1:B:2876:LEU:O	2.07	0.71
1:A:4633:VAL:O	1:A:4636:THR:OG1	2.06	0.71
1:D:615:CYS:SG	1:D:1660:ARG:NH1	2.63	0.71
1:D:2542:SER:OG	1:D:2876:LEU:O	2.07	0.71
1:D:281:ARG:O	1:D:285:SER:OG	2.08	0.71
1:B:4017:ASP:OD2	1:B:4123:SER:OG	2.04	0.71
2:H:11:GLY:O	2:H:14:ARG:NH1	2.23	0.71
1:A:3891:TYR:OH	1:A:3898:ASP:OD1	2.07	0.71
1:C:281:ARG:O	1:C:285:SER:OG	2.09	0.70
1:B:3938:ARG:NH1	1:B:3941:ASP:OD2	2.24	0.70
1:D:3938:ARG:NH1	1:D:3941:ASP:OD2	2.24	0.70
1:C:3938:ARG:NH1	1:C:3941:ASP:OD2	2.24	0.70
1:C:555:LEU:HD12	1:C:588:ILE:HD11	1.74	0.70
1:B:1769:PHE:O	2:H:83:TYR:OH	2.10	0.69
1:A:3938:ARG:NH1	1:A:3941:ASP:OD2	2.24	0.69
1:A:1769:PHE:O	2:G:83:TYR:OH	2.10	0.69
1:B:555:LEU:HD12	1:B:588:ILE:HD11	1.74	0.69
1:C:3233:MET:O	1:C:3237:VAL:N	2.26	0.69
1:B:2790:ARG:NH1	1:B:2900:TYR:OH	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LYS:NZ	1:C:442:LEU:O	2.26	0.69
1:B:3233:MET:O	1:B:3237:VAL:N	2.26	0.69
1:C:1769:PHE:O	2:I:83:TYR:OH	2.10	0.69
1:D:1769:PHE:O	2:J:83:TYR:OH	2.10	0.69
1:D:2385:ASN:O	1:D:2389:THR:OG1	2.06	0.69
1:B:441:LYS:NZ	1:B:442:LEU:O	2.26	0.68
1:D:4122:GLU:OE1	1:D:4122:GLU:N	2.26	0.68
1:B:4122:GLU:OE1	1:B:4122:GLU:N	2.26	0.68
1:D:555:LEU:HD12	1:D:588:ILE:HD11	1.74	0.68
1:A:555:LEU:HD12	1:A:588:ILE:HD11	1.74	0.68
1:B:2385:ASN:O	1:B:2389:THR:OG1	2.06	0.68
1:C:2790:ARG:NH1	1:C:2900:TYR:OH	2.26	0.68
1:A:3233:MET:O	1:A:3237:VAL:N	2.26	0.68
1:A:4122:GLU:N	1:A:4122:GLU:OE1	2.26	0.68
1:B:1029:ASN:OD1	1:B:1032:LEU:N	2.27	0.68
1:C:1029:ASN:OD1	1:C:1032:LEU:N	2.26	0.68
1:C:4122:GLU:N	1:C:4122:GLU:OE1	2.26	0.68
1:D:2790:ARG:NH1	1:D:2900:TYR:OH	2.26	0.68
1:B:2928:LEU:HD21	1:B:3006:LEU:HD22	1.76	0.68
1:B:3891:TYR:OH	1:B:3898:ASP:OD1	2.07	0.68
1:D:3233:MET:O	1:D:3237:VAL:N	2.26	0.68
2:J:50:ARG:N	2:J:55:GLU:OE2	2.26	0.68
1:A:2790:ARG:NH1	1:A:2900:TYR:OH	2.26	0.68
1:A:3262:MET:SD	1:A:3262:MET:N	2.67	0.68
1:A:2928:LEU:HD21	1:A:3006:LEU:HD22	1.75	0.67
1:C:3262:MET:SD	1:C:3262:MET:N	2.67	0.67
1:D:1018:TYR:O	1:D:1028:ARG:NH1	2.27	0.67
2:I:50:ARG:N	2:I:55:GLU:OE2	2.26	0.67
1:D:1029:ASN:OD1	1:D:1032:LEU:N	2.26	0.67
1:D:3262:MET:SD	1:D:3262:MET:N	2.68	0.67
1:C:2928:LEU:HD21	1:C:3006:LEU:HD22	1.75	0.67
1:D:2928:LEU:HD21	1:D:3006:LEU:HD22	1.76	0.67
1:A:441:LYS:NZ	1:A:442:LEU:O	2.27	0.67
1:D:441:LYS:NZ	1:D:442:LEU:O	2.26	0.67
1:A:281:ARG:O	1:A:285:SER:OG	2.12	0.67
1:B:2376:GLU:O	1:B:2380:THR:OG1	2.13	0.67
1:B:3262:MET:SD	1:B:3262:MET:N	2.68	0.67
1:B:3636:GLU:OE1	1:B:3636:GLU:N	2.28	0.67
1:B:1018:TYR:O	1:B:1028:ARG:NH1	2.28	0.67
1:C:2376:GLU:O	1:C:2380:THR:OG1	2.13	0.67
1:C:3636:GLU:N	1:C:3636:GLU:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3636:GLU:N	1:D:3636:GLU:OE1	2.28	0.67
2:G:50:ARG:N	2:G:55:GLU:OE2	2.27	0.67
1:A:1029:ASN:OD1	1:A:1032:LEU:N	2.27	0.67
1:C:2683:ASN:ND2	1:C:2911:LEU:O	2.28	0.67
1:A:3855:ASN:OD1	1:A:3858:ARG:NH2	2.29	0.66
1:C:2388:MET:HE1	1:C:2463:HIS:CG	2.30	0.66
1:D:4796:GLU:N	1:D:4796:GLU:OE1	2.28	0.66
1:B:1272:ARG:NH2	1:B:1583:CYS:SG	2.69	0.66
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.69	0.66
1:D:2388:MET:HE1	1:D:2463:HIS:CG	2.30	0.66
2:H:50:ARG:N	2:H:55:GLU:OE2	2.27	0.66
1:A:1018:TYR:O	1:A:1028:ARG:NH1	2.28	0.66
1:A:3636:GLU:N	1:A:3636:GLU:OE1	2.28	0.66
1:C:3855:ASN:OD1	1:C:3858:ARG:NH2	2.28	0.66
1:B:4796:GLU:OE1	1:B:4796:GLU:N	2.28	0.66
1:D:2683:ASN:ND2	1:D:2911:LEU:O	2.28	0.66
1:A:4191:PHE:O	1:A:4195:THR:OG1	2.12	0.66
1:B:2388:MET:HE1	1:B:2463:HIS:CG	2.31	0.66
1:B:3855:ASN:OD1	1:B:3858:ARG:NH2	2.29	0.66
1:D:4191:PHE:O	1:D:4195:THR:OG1	2.12	0.66
1:A:2388:MET:HE1	1:A:2463:HIS:CG	2.31	0.66
1:B:2683:ASN:ND2	1:B:2911:LEU:O	2.28	0.66
1:C:1276:THR:OG1	1:C:1278:ASP:OD1	2.11	0.66
1:C:1018:TYR:O	1:C:1028:ARG:NH1	2.28	0.66
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.68	0.66
1:A:2396:ASP:OD1	1:A:2400:ARG:NE	2.29	0.66
1:A:2683:ASN:ND2	1:A:2911:LEU:O	2.28	0.66
1:D:3855:ASN:OD1	1:D:3858:ARG:NH2	2.29	0.66
1:B:1123:GLN:OE1	1:B:1133:ARG:NH2	2.29	0.66
1:A:247:VAL:O	1:A:272:ARG:NH1	2.29	0.65
1:A:1123:GLN:OE1	1:A:1133:ARG:NH2	2.29	0.65
2:J:12:ASP:OD2	2:J:14:ARG:NH1	2.30	0.65
1:A:4796:GLU:N	1:A:4796:GLU:OE1	2.28	0.65
1:C:1123:GLN:OE1	1:C:1133:ARG:NH2	2.29	0.65
1:C:1306:MET:SD	1:C:1306:MET:N	2.70	0.65
1:C:4796:GLU:N	1:C:4796:GLU:OE1	2.28	0.65
2:H:12:ASP:OD2	2:H:14:ARG:NH1	2.30	0.65
1:A:1272:ARG:NH2	1:A:1583:CYS:SG	2.68	0.65
1:B:2396:ASP:OD1	1:B:2400:ARG:NE	2.29	0.65
1:C:247:VAL:O	1:C:272:ARG:NH1	2.29	0.65
1:D:1123:GLN:OE1	1:D:1133:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:74:LYS:NZ	2:J:76:THR:OG1	2.24	0.65
1:C:19:GLU:OE2	1:C:67:PHE:N	2.29	0.65
1:D:246:THR:OG1	1:D:247:VAL:N	2.29	0.65
1:D:247:VAL:O	1:D:272:ARG:NH1	2.29	0.65
2:J:32:GLN:N	2:J:32:GLN:OE1	2.30	0.65
1:A:19:GLU:OE2	1:A:67:PHE:N	2.30	0.65
1:B:4191:PHE:O	1:B:4195:THR:OG1	2.12	0.65
1:C:4191:PHE:O	1:C:4195:THR:OG1	2.12	0.65
1:D:1306:MET:SD	1:D:1306:MET:N	2.70	0.65
2:G:12:ASP:OD2	2:G:14:ARG:NH1	2.30	0.65
2:I:32:GLN:OE1	2:I:32:GLN:N	2.30	0.65
2:H:74:LYS:NZ	2:H:76:THR:OG1	2.24	0.65
1:A:384:MET:SD	1:A:384:MET:N	2.70	0.65
2:H:32:GLN:N	2:H:32:GLN:OE1	2.30	0.65
1:A:246:THR:OG1	1:A:247:VAL:N	2.28	0.64
1:D:25:THR:HG22	1:D:211:LEU:HD21	1.79	0.64
1:B:1306:MET:SD	1:B:1306:MET:N	2.70	0.64
1:C:299:HIS:ND1	1:C:302:THR:OG1	2.24	0.64
1:C:573:GLU:OE2	1:C:609:LYS:NZ	2.26	0.64
1:B:247:VAL:O	1:B:272:ARG:NH1	2.30	0.64
1:C:2262:GLU:OE1	1:C:2266:ARG:NH2	2.31	0.64
2:I:12:ASP:OD2	2:I:14:ARG:NH1	2.30	0.64
1:B:384:MET:N	1:B:384:MET:SD	2.70	0.64
1:B:473:GLU:N	1:B:473:GLU:OE1	2.30	0.64
1:B:4962:GLU:N	1:B:4962:GLU:OE1	2.31	0.64
1:C:25:THR:HG22	1:C:211:LEU:HD21	1.80	0.64
1:D:19:GLU:OE2	1:D:67:PHE:N	2.30	0.64
1:D:384:MET:SD	1:D:384:MET:N	2.70	0.64
2:G:32:GLN:OE1	2:G:32:GLN:N	2.30	0.64
1:A:3163:GLY:O	1:A:3247:ARG:NE	2.30	0.64
1:C:384:MET:SD	1:C:384:MET:N	2.70	0.64
1:C:473:GLU:N	1:C:473:GLU:OE1	2.30	0.64
1:D:473:GLU:N	1:D:473:GLU:OE1	2.30	0.64
1:B:2262:GLU:OE1	1:B:2266:ARG:NH2	2.31	0.64
1:C:357:GLY:N	1:C:405:LEU:O	2.31	0.64
1:C:2346:MET:HE1	1:C:2388:MET:HE3	1.80	0.64
1:C:3163:GLY:O	1:C:3247:ARG:NE	2.30	0.64
1:A:473:GLU:N	1:A:473:GLU:OE1	2.30	0.64
1:A:1306:MET:SD	1:A:1306:MET:N	2.70	0.64
1:B:357:GLY:N	1:B:405:LEU:O	2.31	0.64
1:C:4962:GLU:N	1:C:4962:GLU:OE1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2262:GLU:OE1	1:A:2266:ARG:NH2	2.31	0.64
1:B:25:THR:HG22	1:B:211:LEU:HD21	1.80	0.64
1:D:357:GLY:N	1:D:405:LEU:O	2.31	0.64
1:B:19:GLU:OE2	1:B:67:PHE:N	2.30	0.63
1:B:246:THR:OG1	1:B:247:VAL:N	2.29	0.63
1:B:3163:GLY:O	1:B:3247:ARG:NE	2.30	0.63
1:C:246:THR:OG1	1:C:247:VAL:N	2.29	0.63
1:D:2262:GLU:OE1	1:D:2266:ARG:NH2	2.31	0.63
1:D:2346:MET:HE1	1:D:2388:MET:HE3	1.80	0.63
1:A:2256:LEU:O	1:A:2257:ARG:NH1	2.32	0.63
1:A:2346:MET:HE1	1:A:2388:MET:HE3	1.80	0.63
1:B:2346:MET:HE1	1:B:2388:MET:HE3	1.80	0.63
1:C:2396:ASP:OD1	1:C:2400:ARG:NE	2.29	0.63
1:D:4962:GLU:OE1	1:D:4962:GLU:N	2.31	0.63
1:A:357:GLY:N	1:A:405:LEU:O	2.31	0.63
1:A:4962:GLU:OE1	1:A:4962:GLU:N	2.31	0.63
1:B:281:ARG:O	1:B:285:SER:OG	2.11	0.63
1:C:3268:ASN:OD1	1:C:3271:HIS:ND1	2.32	0.63
1:D:3163:GLY:O	1:D:3247:ARG:NE	2.30	0.63
1:A:25:THR:HG22	1:A:211:LEU:HD21	1.80	0.63
1:A:503:ASP:OD1	1:A:561:ARG:NH2	2.32	0.63
1:A:3393:GLU:OE1	1:A:3396:ARG:NH1	2.32	0.63
1:A:467:ASP:OD2	1:A:469:HIS:NE2	2.32	0.63
1:B:2256:LEU:O	1:B:2257:ARG:NH1	2.32	0.63
1:B:3268:ASN:OD1	1:B:3271:HIS:ND1	2.32	0.63
1:B:168:GLN:OE1	1:B:168:GLN:N	2.32	0.63
1:B:2441:MET:HE1	1:B:2497:ALA:HB1	1.81	0.63
1:C:2256:LEU:O	1:C:2257:ARG:NH1	2.32	0.63
1:B:1682:ASP:OD2	1:B:1685:GLN:NE2	2.32	0.63
1:C:467:ASP:OD2	1:C:469:HIS:NE2	2.32	0.63
1:A:1636:GLU:OE1	1:A:1638:ARG:NE	2.30	0.63
1:A:2441:MET:HE1	1:A:2497:ALA:HB1	1.81	0.63
1:D:467:ASP:OD2	1:D:469:HIS:NE2	2.32	0.63
1:A:3268:ASN:OD1	1:A:3271:HIS:ND1	2.32	0.62
1:B:3800:SER:OG	1:B:3830:GLN:O	2.17	0.62
1:A:2385:ASN:O	1:A:2389:THR:OG1	2.11	0.62
1:B:467:ASP:OD2	1:B:469:HIS:NE2	2.32	0.62
1:A:168:GLN:N	1:A:168:GLN:OE1	2.32	0.62
1:A:1682:ASP:OD2	1:A:1685:GLN:NE2	2.32	0.62
1:C:1682:ASP:OD2	1:C:1685:GLN:NE2	2.32	0.62
1:D:3268:ASN:OD1	1:D:3271:HIS:ND1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3393:GLU:OE1	1:C:3396:ARG:NH1	2.32	0.62
1:D:168:GLN:N	1:D:168:GLN:OE1	2.32	0.62
1:D:3800:SER:OG	1:D:3830:GLN:O	2.16	0.62
1:A:299:HIS:ND1	1:A:302:THR:OG1	2.23	0.62
1:C:3800:SER:OG	1:C:3830:GLN:O	2.16	0.62
1:B:3393:GLU:OE1	1:B:3396:ARG:NH1	2.32	0.62
1:A:3800:SER:OG	1:A:3830:GLN:O	2.17	0.62
1:B:151:GLU:OE1	1:B:151:GLU:N	2.32	0.62
1:C:2178:LEU:HD11	1:C:2226:VAL:HG21	1.82	0.62
1:D:2256:LEU:O	1:D:2257:ARG:NH1	2.32	0.62
1:C:168:GLN:N	1:C:168:GLN:OE1	2.32	0.62
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.72	0.62
1:C:2441:MET:HE1	1:C:2497:ALA:HB1	1.81	0.62
1:D:3393:GLU:OE1	1:D:3396:ARG:NH1	2.32	0.62
1:B:299:HIS:ND1	1:B:302:THR:OG1	2.24	0.61
1:B:503:ASP:OD1	1:B:561:ARG:NH2	2.32	0.61
1:D:2441:MET:HE1	1:D:2497:ALA:HB1	1.81	0.61
1:D:1565:MET:HE1	1:D:1578:ASN:O	2.00	0.61
1:D:2178:LEU:HD11	1:D:2226:VAL:HG21	1.82	0.61
1:C:503:ASP:OD1	1:C:561:ARG:NH2	2.32	0.61
1:C:1565:MET:HE1	1:C:1578:ASN:O	2.00	0.61
1:D:151:GLU:OE1	1:D:151:GLU:N	2.33	0.61
1:D:299:HIS:ND1	1:D:302:THR:OG1	2.24	0.61
1:A:1168:MET:SD	1:A:1168:MET:N	2.73	0.61
1:B:1168:MET:SD	1:B:1168:MET:N	2.73	0.61
1:B:1733:GLU:OE1	1:B:1733:GLU:N	2.33	0.61
1:C:2385:ASN:O	1:C:2389:THR:OG1	2.09	0.61
1:D:2396:ASP:OD1	1:D:2400:ARG:NE	2.29	0.61
1:B:1636:GLU:OE1	1:B:1638:ARG:NE	2.30	0.61
1:B:2412:LYS:NZ	1:B:2414:GLU:OE2	2.33	0.61
1:B:2178:LEU:HD11	1:B:2226:VAL:HG21	1.82	0.61
1:C:1733:GLU:N	1:C:1733:GLU:OE1	2.33	0.61
1:D:503:ASP:OD1	1:D:561:ARG:NH2	2.32	0.61
1:A:4558:TYR:OH	1:D:4789:ARG:NH1	2.33	0.61
1:B:1276:THR:OG1	1:B:1278:ASP:OD1	2.11	0.61
1:B:2502:ASP:OD2	1:B:2553:ARG:NH1	2.34	0.60
1:C:1168:MET:SD	1:C:1168:MET:N	2.73	0.60
1:C:2502:ASP:OD2	1:C:2553:ARG:NH1	2.34	0.60
1:D:641:ASP:OD1	1:D:641:ASP:N	2.34	0.60
2:G:74:LYS:NZ	2:G:76:THR:OG1	2.25	0.60
1:A:394:HIS:ND1	1:A:396:GLU:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ASP:OD1	1:A:641:ASP:N	2.34	0.60
1:A:2502:ASP:OD2	1:A:2553:ARG:NH1	2.34	0.60
1:A:151:GLU:N	1:A:151:GLU:OE1	2.34	0.60
1:A:176:ARG:N	1:A:179:ASP:OD2	2.35	0.60
1:A:1565:MET:HE1	1:A:1578:ASN:O	2.00	0.60
1:D:1682:ASP:OD2	1:D:1685:GLN:NE2	2.33	0.60
1:B:235:ARG:NE	1:B:273:SER:OG	2.32	0.60
1:C:641:ASP:OD1	1:C:641:ASP:N	2.34	0.60
1:C:1636:GLU:OE1	1:C:1638:ARG:NE	2.30	0.60
1:D:2414:GLU:OE1	1:D:2414:GLU:N	2.35	0.60
1:D:2502:ASP:OD2	1:D:2553:ARG:NH1	2.34	0.60
1:A:1733:GLU:N	1:A:1733:GLU:OE1	2.34	0.60
1:C:151:GLU:N	1:C:151:GLU:OE1	2.34	0.60
1:D:1168:MET:SD	1:D:1168:MET:N	2.73	0.60
1:D:1276:THR:OG1	1:D:1278:ASP:OD1	2.11	0.60
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.74	0.60
1:A:2114:ASP:OD1	1:A:2151:ASN:ND2	2.35	0.60
1:B:1565:MET:HE1	1:B:1578:ASN:O	2.00	0.60
1:D:176:ARG:N	1:D:179:ASP:OD2	2.35	0.60
1:D:1599:ARG:NH2	1:D:1602:ASN:OD1	2.34	0.60
1:A:1599:ARG:NH2	1:A:1602:ASN:OD1	2.34	0.60
1:A:4002:LEU:HD13	1:A:4009:VAL:HG21	1.84	0.60
1:B:394:HIS:ND1	1:B:396:GLU:O	2.34	0.60
1:B:2114:ASP:OD1	1:B:2151:ASN:ND2	2.35	0.60
1:C:2414:GLU:N	1:C:2414:GLU:OE1	2.35	0.60
1:A:2178:LEU:HD11	1:A:2226:VAL:HG21	1.82	0.60
1:C:394:HIS:ND1	1:C:396:GLU:O	2.34	0.60
1:C:2114:ASP:OD1	1:C:2151:ASN:ND2	2.35	0.60
1:A:4789:ARG:NH1	1:B:4558:TYR:OH	2.35	0.60
1:B:1599:ARG:NH2	1:B:1602:ASN:OD1	2.35	0.60
1:C:1599:ARG:NH2	1:C:1602:ASN:OD1	2.34	0.60
1:C:4002:LEU:HD13	1:C:4009:VAL:HG21	1.84	0.60
1:D:394:HIS:ND1	1:D:396:GLU:O	2.35	0.60
1:D:2233:MET:SD	1:D:2233:MET:N	2.75	0.59
1:A:409:GLN:N	1:A:409:GLN:OE1	2.35	0.59
1:B:641:ASP:N	1:B:641:ASP:OD1	2.34	0.59
1:C:4789:ARG:NH1	1:D:4558:TYR:OH	2.35	0.59
1:A:1838:GLU:N	1:A:1838:GLU:OE1	2.36	0.59
1:D:1636:GLU:OE1	1:D:1638:ARG:NE	2.30	0.59
1:A:2233:MET:SD	1:A:2233:MET:N	2.76	0.59
1:B:650:ASN:OD1	1:B:1627:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLN:N	1:B:409:GLN:OE1	2.35	0.59
1:C:1838:GLU:N	1:C:1838:GLU:OE1	2.36	0.59
1:D:4002:LEU:HD13	1:D:4009:VAL:HG21	1.84	0.59
1:A:3253:PRO:HA	1:A:3262:MET:HE1	1.85	0.59
1:B:4789:ARG:NH1	1:C:4558:TYR:OH	2.35	0.59
1:D:1733:GLU:OE1	1:D:1733:GLU:N	2.33	0.59
1:D:2114:ASP:OD1	1:D:2151:ASN:ND2	2.35	0.59
1:A:2412:LYS:NZ	1:A:2414:GLU:OE2	2.33	0.59
1:B:3253:PRO:HA	1:B:3262:MET:HE1	1.85	0.59
1:B:4002:LEU:HD13	1:B:4009:VAL:HG21	1.84	0.59
1:B:3397:MET:O	1:B:3401:VAL:HG23	2.02	0.59
1:C:3253:PRO:HA	1:C:3262:MET:HE1	1.85	0.59
1:D:409:GLN:N	1:D:409:GLN:OE1	2.35	0.59
1:D:650:ASN:OD1	1:D:1627:GLN:NE2	2.36	0.59
1:D:3253:PRO:HA	1:D:3262:MET:HE1	1.85	0.59
1:C:650:ASN:OD1	1:C:1627:GLN:NE2	2.36	0.59
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.77	0.58
1:C:2233:MET:N	1:C:2233:MET:SD	2.76	0.58
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.76	0.58
1:D:171:GLU:N	1:D:171:GLU:OE1	2.36	0.58
1:D:3397:MET:O	1:D:3401:VAL:HG23	2.03	0.58
1:A:171:GLU:OE1	1:A:171:GLU:N	2.37	0.58
1:A:650:ASN:OD1	1:A:1627:GLN:NE2	2.36	0.58
1:C:409:GLN:N	1:C:409:GLN:OE1	2.35	0.58
2:H:106:ASN:OD1	2:H:107:LEU:N	2.37	0.58
1:A:3397:MET:O	1:A:3401:VAL:HG23	2.03	0.58
1:B:3799:CYS:O	1:B:3879:ARG:NH2	2.37	0.58
1:B:2233:MET:SD	1:B:2233:MET:N	2.76	0.58
1:B:2414:GLU:N	1:B:2414:GLU:OE1	2.35	0.58
1:B:4562:GLU:N	1:B:4562:GLU:OE1	2.36	0.58
1:C:3799:CYS:O	1:C:3879:ARG:NH2	2.37	0.58
1:C:4562:GLU:N	1:C:4562:GLU:OE1	2.36	0.58
2:G:106:ASN:OD1	2:G:107:LEU:N	2.36	0.58
2:I:106:ASN:OD1	2:I:107:LEU:N	2.36	0.58
1:B:573:GLU:OE2	1:B:609:LYS:NZ	2.26	0.58
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.36	0.58
1:B:1838:GLU:OE1	1:B:1838:GLU:N	2.36	0.58
1:C:2592:VAL:HG22	1:C:2643:LEU:HB2	1.85	0.58
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.36	0.58
1:D:3799:CYS:O	1:D:3879:ARG:NH2	2.37	0.58
1:B:2592:VAL:HG22	1:B:2643:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.36	0.58
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.36	0.58
1:C:3397:MET:O	1:C:3401:VAL:HG23	2.02	0.58
1:D:102:MET:O	1:D:106:GLN:NE2	2.37	0.58
1:D:1838:GLU:OE1	1:D:1838:GLU:N	2.36	0.58
2:J:27:TYR:OH	2:J:43:ARG:NH2	2.37	0.58
2:J:106:ASN:OD1	2:J:107:LEU:N	2.36	0.58
1:B:3839:PHE:CE1	1:B:3873:THR:HG23	2.39	0.58
1:C:3839:PHE:CE1	1:C:3873:THR:HG23	2.39	0.58
1:C:102:MET:O	1:C:106:GLN:NE2	2.37	0.57
2:H:27:TYR:OH	2:H:43:ARG:NH2	2.37	0.57
1:A:102:MET:O	1:A:106:GLN:NE2	2.37	0.57
1:D:4562:GLU:OE1	1:D:4562:GLU:N	2.36	0.57
1:A:1276:THR:OG1	1:A:1278:ASP:OD1	2.11	0.57
1:B:171:GLU:N	1:B:171:GLU:OE1	2.37	0.57
1:A:235:ARG:NE	1:A:273:SER:OG	2.33	0.57
1:A:4562:GLU:OE1	1:A:4562:GLU:N	2.36	0.57
1:B:555:LEU:HD12	1:B:588:ILE:CD1	2.34	0.57
1:C:171:GLU:OE1	1:C:171:GLU:N	2.36	0.57
1:D:3839:PHE:CE1	1:D:3873:THR:HG23	2.39	0.57
2:G:27:TYR:OH	2:G:43:ARG:NH2	2.37	0.57
1:A:81:MET:HE1	1:A:102:MET:SD	2.43	0.57
1:A:555:LEU:HD12	1:A:588:ILE:CD1	2.34	0.57
1:A:2414:GLU:OE1	1:A:2414:GLU:N	2.35	0.57
1:D:1249:MET:SD	1:D:1249:MET:N	2.77	0.57
1:B:2430:ASP:O	1:B:2434:VAL:HG23	2.05	0.57
1:C:1300:MET:HE1	1:C:1302:TYR:CE1	2.40	0.57
1:B:119:ILE:HG12	1:B:162:ILE:HD11	1.87	0.57
1:C:1249:MET:SD	1:C:1249:MET:N	2.77	0.57
1:D:1300:MET:HE1	1:D:1302:TYR:CE1	2.40	0.57
1:A:2592:VAL:HG22	1:A:2643:LEU:HB2	1.85	0.57
1:C:176:ARG:N	1:C:179:ASP:OD2	2.35	0.57
1:D:1958:ALA:O	1:D:1965:ARG:NH2	2.38	0.57
1:A:318:ASP:OD1	1:A:319:LYS:N	2.38	0.57
1:A:3839:PHE:CE1	1:A:3873:THR:HG23	2.39	0.57
1:C:555:LEU:HD12	1:C:588:ILE:CD1	2.34	0.57
1:D:1603:GLN:N	1:D:1603:GLN:OE1	2.38	0.57
1:A:1603:GLN:N	1:A:1603:GLN:OE1	2.38	0.56
1:B:176:ARG:N	1:B:179:ASP:OD2	2.35	0.56
1:B:1603:GLN:OE1	1:B:1603:GLN:N	2.38	0.56
1:C:318:ASP:OD1	1:C:319:LYS:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1635:GLU:OE1	1:D:1635:GLU:N	2.38	0.56
2:I:27:TYR:OH	2:I:43:ARG:NH2	2.36	0.56
1:B:318:ASP:OD1	1:B:319:LYS:N	2.38	0.56
1:C:450:GLU:N	1:C:450:GLU:OE1	2.38	0.56
1:D:2383:MET:SD	1:D:2383:MET:N	2.78	0.56
1:A:1958:ALA:O	1:A:1965:ARG:NH2	2.38	0.56
1:A:2430:ASP:O	1:A:2434:VAL:HG23	2.05	0.56
1:A:2925:LEU:HA	1:A:2928:LEU:HD22	1.88	0.56
1:A:4153:GLU:N	1:A:4153:GLU:OE1	2.38	0.56
1:C:2383:MET:SD	1:C:2383:MET:N	2.79	0.56
1:D:996:VAL:CG2	1:D:1054:VAL:HG21	2.36	0.56
1:D:2430:ASP:O	1:D:2434:VAL:HG23	2.05	0.56
1:D:2592:VAL:HG22	1:D:2643:LEU:HB2	1.86	0.56
1:A:1300:MET:HE1	1:A:1302:TYR:CE1	2.40	0.56
1:B:1300:MET:HE1	1:B:1302:TYR:CE1	2.40	0.56
1:B:3060:LEU:HD22	1:B:3125:VAL:HG23	1.88	0.56
1:C:2430:ASP:O	1:C:2434:VAL:HG23	2.05	0.56
1:D:555:LEU:HD12	1:D:588:ILE:CD1	2.34	0.56
1:A:2939:ILE:HG21	1:A:3013:LEU:HD13	1.88	0.56
1:B:102:MET:O	1:B:106:GLN:NE2	2.37	0.56
1:C:996:VAL:CG2	1:C:1054:VAL:HG21	2.36	0.56
1:C:4153:GLU:N	1:C:4153:GLU:OE1	2.39	0.56
1:A:2383:MET:SD	1:A:2383:MET:N	2.79	0.56
1:B:2383:MET:SD	1:B:2383:MET:N	2.79	0.56
1:D:1695:MET:SD	1:D:1695:MET:N	2.79	0.56
2:J:37:PHE:CD2	2:J:92:ILE:HD11	2.41	0.56
1:B:4153:GLU:OE1	1:B:4153:GLU:N	2.39	0.56
1:C:1603:GLN:N	1:C:1603:GLN:OE1	2.38	0.56
1:D:894:VAL:HG13	1:D:918:LEU:HD13	1.87	0.56
1:D:3060:LEU:HD22	1:D:3125:VAL:HG23	1.88	0.56
1:A:894:VAL:HG13	1:A:918:LEU:HD13	1.87	0.56
1:A:3015:ARG:NH2	1:A:3066:ASP:OD1	2.39	0.56
1:A:3799:CYS:O	1:A:3879:ARG:NH2	2.37	0.56
1:B:996:VAL:CG2	1:B:1054:VAL:HG21	2.36	0.56
1:D:3981:LEU:HD22	1:D:3998:MET:SD	2.46	0.56
2:G:28:THR:HG23	2:G:39:SER:HB2	1.88	0.56
2:J:28:THR:HG23	2:J:39:SER:HB2	1.88	0.56
1:B:894:VAL:HG13	1:B:918:LEU:HD13	1.87	0.56
1:D:81:MET:HE1	1:D:102:MET:SD	2.46	0.56
1:D:318:ASP:OD1	1:D:319:LYS:N	2.38	0.56
2:G:37:PHE:CD2	2:G:92:ILE:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:MET:SD	1:A:1249:MET:N	2.77	0.56
1:B:2939:ILE:HG21	1:B:3013:LEU:HD13	1.88	0.56
1:B:3981:LEU:HD22	1:B:3998:MET:SD	2.46	0.56
1:C:1958:ALA:O	1:C:1965:ARG:NH2	2.38	0.56
1:C:3060:LEU:HD22	1:C:3125:VAL:HG23	1.88	0.56
1:D:4955:ASP:OD1	1:D:4956:CYS:N	2.39	0.56
1:A:996:VAL:CG2	1:A:1054:VAL:HG21	2.36	0.55
1:A:2376:GLU:O	1:A:2380:THR:OG1	2.23	0.55
1:B:3015:ARG:NH2	1:B:3066:ASP:OD1	2.39	0.55
1:C:2254:LEU:O	1:C:3809:ARG:NH1	2.39	0.55
1:C:2568:ILE:HD12	1:C:2569:GLU:N	2.22	0.55
1:C:2928:LEU:HD23	1:C:2929:ILE:N	2.21	0.55
1:C:3015:ARG:NH2	1:C:3066:ASP:OD1	2.39	0.55
1:D:986:ILE:HD13	1:D:1058:LEU:HB3	1.88	0.55
1:D:3015:ARG:NH2	1:D:3066:ASP:OD1	2.39	0.55
1:D:4153:GLU:N	1:D:4153:GLU:OE1	2.39	0.55
1:A:1452:GLN:OE1	1:A:1484:ASN:ND2	2.39	0.55
1:A:1487:MET:O	1:A:1532:TYR:OH	2.19	0.55
1:C:1695:MET:SD	1:C:1695:MET:N	2.79	0.55
1:C:3067:LEU:HD23	1:C:3135:SER:OG	2.06	0.55
1:D:2376:GLU:O	1:D:2380:THR:OG1	2.13	0.55
1:D:3256:HIS:HB2	1:D:3262:MET:HE3	1.88	0.55
1:D:3954:GLN:NE2	1:D:3974:GLN:OE1	2.40	0.55
2:H:28:THR:HG23	2:H:39:SER:HB2	1.88	0.55
1:A:1565:MET:HE3	1:A:1566:PRO:HG2	1.89	0.55
1:A:1695:MET:SD	1:A:1695:MET:N	2.78	0.55
1:A:2560:LEU:O	1:A:2565:ARG:NH1	2.39	0.55
1:A:2928:LEU:HD23	1:A:2929:ILE:N	2.21	0.55
1:A:3178:ASN:O	1:A:3184:ASN:ND2	2.39	0.55
1:B:1958:ALA:O	1:B:1965:ARG:NH2	2.38	0.55
1:C:3178:ASN:O	1:C:3184:ASN:ND2	2.39	0.55
1:C:3256:HIS:HB2	1:C:3262:MET:HE3	1.89	0.55
1:D:235:ARG:NE	1:D:273:SER:OG	2.38	0.55
2:I:37:PHE:CD2	2:I:92:ILE:HD11	2.41	0.55
1:A:1251:LEU:HD23	1:A:1600:MET:CE	2.37	0.55
1:B:3067:LEU:HD23	1:B:3135:SER:OG	2.06	0.55
1:C:894:VAL:HG13	1:C:918:LEU:HD13	1.87	0.55
1:C:2496:ARG:NH2	1:C:2546:SER:OG	2.39	0.55
1:C:3069:LYS:HD2	1:C:3092:ILE:HD13	1.89	0.55
1:C:4955:ASP:OD1	1:C:4956:CYS:N	2.39	0.55
1:D:2441:MET:HE1	1:D:2497:ALA:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:28:THR:HG23	2:I:39:SER:HB2	1.87	0.55
1:A:1635:GLU:N	1:A:1635:GLU:OE1	2.38	0.55
1:B:3069:LYS:HD2	1:B:3092:ILE:HD13	1.88	0.55
1:C:1565:MET:HE3	1:C:1566:PRO:HG2	1.89	0.55
1:D:2925:LEU:HA	1:D:2928:LEU:HD22	1.88	0.55
1:D:2928:LEU:HD23	1:D:2929:ILE:N	2.22	0.55
1:D:3067:LEU:HD23	1:D:3135:SER:OG	2.07	0.55
2:I:67:MET:HE1	2:I:73:ALA:HB2	1.88	0.55
1:A:2568:ILE:HD12	1:A:2569:GLU:N	2.22	0.55
1:A:3981:LEU:HD22	1:A:3998:MET:SD	2.46	0.55
1:B:81:MET:HE1	1:B:102:MET:SD	2.47	0.55
1:B:1635:GLU:N	1:B:1635:GLU:OE1	2.38	0.55
1:C:3981:LEU:HD22	1:C:3998:MET:SD	2.46	0.55
1:D:2560:LEU:O	1:D:2565:ARG:NH1	2.39	0.55
1:D:2568:ILE:HD12	1:D:2569:GLU:N	2.22	0.55
1:A:3060:LEU:HD22	1:A:3125:VAL:HG23	1.88	0.55
1:B:1565:MET:HE2	1:B:1569:ALA:CB	2.34	0.55
1:B:3178:ASN:O	1:B:3184:ASN:ND2	2.40	0.55
1:B:3222:GLU:N	1:B:3222:GLU:OE1	2.40	0.55
1:B:3626:SER:O	1:B:3630:THR:OG1	2.12	0.55
1:B:4955:ASP:OD1	1:B:4956:CYS:N	2.39	0.55
1:C:119:ILE:HG12	1:C:162:ILE:HD11	1.88	0.55
1:C:3222:GLU:N	1:C:3222:GLU:OE1	2.40	0.55
1:D:2412:LYS:NZ	1:D:2414:GLU:OE2	2.35	0.55
1:D:2665:LEU:HD11	1:D:2968:PRO:HB2	1.89	0.55
1:D:3178:ASN:OD1	1:D:3184:ASN:ND2	2.40	0.55
1:A:3222:GLU:OE1	1:A:3222:GLU:N	2.40	0.55
1:B:555:LEU:HD11	1:B:589:ILE:CD1	2.37	0.55
1:C:2441:MET:HE1	1:C:2497:ALA:CB	2.37	0.55
1:C:2925:LEU:HA	1:C:2928:LEU:HD22	1.87	0.55
1:C:3954:GLN:NE2	1:C:3974:GLN:OE1	2.40	0.55
1:C:4172:ILE:HD12	1:C:4173:PHE:N	2.22	0.55
2:I:108:GLU:OE1	2:I:108:GLU:N	2.39	0.55
1:A:555:LEU:HD11	1:A:589:ILE:CD1	2.37	0.55
1:B:1251:LEU:HD23	1:B:1600:MET:CE	2.37	0.55
1:B:2254:LEU:O	1:B:3809:ARG:NH1	2.39	0.55
1:B:3178:ASN:OD1	1:B:3184:ASN:ND2	2.40	0.55
1:C:2939:ILE:HG21	1:C:3013:LEU:HD13	1.88	0.55
1:D:1251:LEU:HD23	1:D:1600:MET:CE	2.37	0.55
2:H:67:MET:HE1	2:H:73:ALA:HB2	1.89	0.55
1:A:450:GLU:OE1	1:A:450:GLU:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:ILE:HD13	1:A:1058:LEU:HB3	1.88	0.55
1:A:2254:LEU:O	1:A:3809:ARG:NH1	2.39	0.55
1:A:3954:GLN:NE2	1:A:3974:GLN:OE1	2.40	0.55
1:B:450:GLU:OE1	1:B:450:GLU:N	2.38	0.55
1:B:2568:ILE:HD12	1:B:2569:GLU:N	2.22	0.55
1:B:2665:LEU:HD11	1:B:2968:PRO:HB2	1.89	0.55
1:C:1635:GLU:N	1:C:1635:GLU:OE1	2.38	0.55
1:D:874:LEU:HD23	1:D:944:LEU:HD11	1.89	0.55
1:D:1452:GLN:OE1	1:D:1484:ASN:ND2	2.39	0.55
1:D:1565:MET:HE3	1:D:1566:PRO:HG2	1.89	0.55
1:D:4172:ILE:HD12	1:D:4173:PHE:N	2.22	0.55
2:H:37:PHE:CD2	2:H:92:ILE:HD11	2.41	0.55
2:J:108:GLU:N	2:J:108:GLU:OE1	2.40	0.55
1:B:1452:GLN:OE1	1:B:1484:ASN:ND2	2.39	0.54
1:B:2928:LEU:HD23	1:B:2929:ILE:N	2.22	0.54
1:C:874:LEU:HD23	1:C:944:LEU:HD11	1.89	0.54
1:A:2441:MET:HE1	1:A:2497:ALA:CB	2.37	0.54
1:B:2560:LEU:O	1:B:2565:ARG:NH1	2.39	0.54
1:B:3256:HIS:HB2	1:B:3262:MET:HE3	1.89	0.54
1:C:1452:GLN:OE1	1:C:1484:ASN:ND2	2.39	0.54
1:D:313:ASN:HA	1:D:392:ILE:HG22	1.90	0.54
1:D:1565:MET:HE2	1:D:1569:ALA:CB	2.34	0.54
1:D:2254:LEU:O	1:D:3809:ARG:NH1	2.40	0.54
2:G:108:GLU:N	2:G:108:GLU:OE1	2.40	0.54
1:B:874:LEU:HD23	1:B:944:LEU:HD11	1.89	0.54
1:B:1722:MET:HE2	1:B:1760:PRO:HD3	1.89	0.54
1:B:3954:GLN:NE2	1:B:3974:GLN:OE1	2.40	0.54
1:D:2240:ASP:OD1	1:D:2296:ARG:NH2	2.40	0.54
1:D:3222:GLU:OE1	1:D:3222:GLU:N	2.40	0.54
1:A:81:MET:HE3	1:A:81:MET:O	2.08	0.54
1:A:3256:HIS:HB2	1:A:3262:MET:HE3	1.89	0.54
1:B:255:GLU:N	1:B:255:GLU:OE1	2.41	0.54
1:B:1565:MET:HE3	1:B:1566:PRO:HG2	1.89	0.54
1:C:2175:VAL:HG12	1:C:2219:TYR:CZ	2.42	0.54
1:C:2560:LEU:O	1:C:2565:ARG:NH1	2.39	0.54
1:D:1487:MET:O	1:D:1532:TYR:OH	2.19	0.54
1:D:2939:ILE:HG21	1:D:3013:LEU:HD13	1.88	0.54
1:A:255:GLU:N	1:A:255:GLU:OE1	2.41	0.54
1:A:2240:ASP:OD1	1:A:2296:ARG:NH2	2.40	0.54
1:B:2240:ASP:OD1	1:B:2296:ARG:NH2	2.40	0.54
1:B:2925:LEU:HA	1:B:2928:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:MET:HE1	1:C:102:MET:SD	2.47	0.54
1:C:986:ILE:HD13	1:C:1058:LEU:HB3	1.88	0.54
1:C:2240:ASP:OD1	1:C:2296:ARG:NH2	2.40	0.54
1:A:521:GLU:OE1	1:A:521:GLU:N	2.40	0.54
1:A:3067:LEU:HD23	1:A:3135:SER:OG	2.06	0.54
1:B:2441:MET:HE1	1:B:2497:ALA:CB	2.37	0.54
1:B:2588:LEU:O	1:B:2592:VAL:HG23	2.08	0.54
2:H:108:GLU:N	2:H:108:GLU:OE1	2.40	0.54
1:A:3069:LYS:HD2	1:A:3092:ILE:HD13	1.89	0.54
1:A:3136:LEU:CB	1:A:3158:LEU:HD13	2.38	0.54
1:B:810:GLU:O	1:B:1615:ARG:NH2	2.40	0.54
1:B:986:ILE:HD13	1:B:1058:LEU:HB3	1.88	0.54
1:C:36:CYS:SG	1:C:37:LEU:N	2.80	0.54
1:C:555:LEU:HD11	1:C:589:ILE:CD1	2.37	0.54
1:C:810:GLU:O	1:C:1615:ARG:NH2	2.41	0.54
1:D:555:LEU:HD11	1:D:589:ILE:CD1	2.37	0.54
1:D:1792:THR:HG21	1:D:1825:LEU:HD12	1.90	0.54
1:A:874:LEU:HD23	1:A:944:LEU:HD11	1.89	0.54
1:A:2347:GLU:OE2	1:A:2437:ILE:HD11	2.08	0.54
1:A:4955:ASP:OD1	1:A:4956:CYS:N	2.39	0.54
1:B:4172:ILE:HD12	1:B:4173:PHE:N	2.22	0.54
1:C:87:GLU:OE2	1:C:88:LYS:NZ	2.41	0.54
1:C:281:ARG:NH1	1:C:284:TRP:O	2.41	0.54
1:C:1251:LEU:HD23	1:C:1600:MET:CE	2.37	0.54
1:D:3178:ASN:O	1:D:3184:ASN:ND2	2.40	0.54
1:A:320:GLU:N	1:A:320:GLU:OE1	2.41	0.54
1:A:4172:ILE:HD12	1:A:4173:PHE:N	2.22	0.54
1:C:1792:THR:HG21	1:C:1825:LEU:HD12	1.90	0.54
1:D:3069:LYS:HD2	1:D:3092:ILE:HD13	1.89	0.54
1:B:1249:MET:SD	1:B:1249:MET:N	2.78	0.54
1:A:313:ASN:HA	1:A:392:ILE:HG22	1.90	0.53
1:A:810:GLU:O	1:A:1615:ARG:NH2	2.41	0.53
1:A:3821:GLU:OE1	1:A:3821:GLU:N	2.41	0.53
1:A:1936:GLN:NE2	1:A:3607:LEU:O	2.41	0.53
1:B:313:ASN:HA	1:B:392:ILE:HG22	1.90	0.53
1:B:1487:MET:O	1:B:1532:TYR:OH	2.19	0.53
1:B:1936:GLN:NE2	1:B:3607:LEU:O	2.41	0.53
1:B:3251:HIS:O	1:B:3262:MET:HE2	2.08	0.53
1:B:3821:GLU:N	1:B:3821:GLU:OE1	2.42	0.53
1:C:4653:MET:SD	1:C:4662:ARG:NH1	2.81	0.53
1:D:255:GLU:N	1:D:255:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2588:LEU:O	1:A:2592:VAL:HG23	2.08	0.53
1:B:320:GLU:N	1:B:320:GLU:OE1	2.41	0.53
1:B:2175:VAL:HG12	1:B:2219:TYR:CZ	2.42	0.53
1:B:3703:ASP:OD1	1:B:3703:ASP:N	2.42	0.53
1:C:1936:GLN:NE2	1:C:3607:LEU:O	2.41	0.53
1:C:2347:GLU:OE2	1:C:2437:ILE:HD11	2.08	0.53
1:C:3136:LEU:CB	1:C:3158:LEU:HD13	2.38	0.53
1:D:2175:VAL:HG12	1:D:2219:TYR:CZ	2.42	0.53
2:G:67:MET:HE1	2:G:73:ALA:HB2	1.90	0.53
2:J:67:MET:HE1	2:J:73:ALA:HB2	1.89	0.53
1:A:1177:LEU:HD23	1:A:1182:LEU:HD11	1.91	0.53
1:D:281:ARG:NH1	1:D:284:TRP:O	2.41	0.53
1:A:2175:VAL:HG12	1:A:2219:TYR:CZ	2.43	0.53
1:A:4653:MET:SD	1:A:4662:ARG:NH1	2.82	0.53
1:B:1792:THR:HG21	1:B:1825:LEU:HD12	1.90	0.53
1:C:2126:ARG:NH2	1:C:2164:LEU:O	2.42	0.53
1:C:2588:LEU:O	1:C:2592:VAL:HG23	2.08	0.53
1:D:2078:GLU:N	1:D:2078:GLU:OE1	2.42	0.53
1:D:3923:ILE:HG21	1:D:3934:LEU:HD12	1.90	0.53
1:D:4653:MET:SD	1:D:4662:ARG:NH1	2.82	0.53
1:A:900:LEU:O	1:A:913:ARG:NH2	2.42	0.53
1:A:1792:THR:HG21	1:A:1825:LEU:HD12	1.90	0.53
1:B:4653:MET:SD	1:B:4662:ARG:NH1	2.82	0.53
1:C:1722:MET:HE2	1:C:1760:PRO:HD3	1.90	0.53
1:D:320:GLU:N	1:D:320:GLU:OE1	2.41	0.53
1:D:521:GLU:N	1:D:521:GLU:OE1	2.40	0.53
1:A:3923:ILE:HG21	1:A:3934:LEU:HD12	1.90	0.53
1:B:281:ARG:NH1	1:B:284:TRP:O	2.42	0.53
1:B:2496:ARG:NH2	1:B:2546:SER:OG	2.42	0.53
1:D:450:GLU:N	1:D:450:GLU:OE1	2.38	0.53
1:D:2347:GLU:OE2	1:D:2437:ILE:HD11	2.08	0.53
1:B:1177:LEU:HD23	1:B:1182:LEU:HD11	1.91	0.53
1:B:2347:GLU:OE2	1:B:2437:ILE:HD11	2.08	0.53
1:B:3136:LEU:CB	1:B:3158:LEU:HD13	2.38	0.53
1:C:313:ASN:HA	1:C:392:ILE:HG22	1.90	0.53
1:C:3118:GLU:OE1	1:C:3118:GLU:N	2.42	0.53
1:D:87:GLU:OE2	1:D:88:LYS:NZ	2.40	0.53
1:D:181:LEU:HD21	1:D:214:VAL:HG23	1.91	0.53
1:D:2588:LEU:O	1:D:2592:VAL:HG23	2.08	0.53
1:D:3136:LEU:CB	1:D:3158:LEU:HD13	2.38	0.53
1:C:3178:ASN:OD1	1:C:3184:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:810:GLU:O	1:D:1615:ARG:NH2	2.41	0.53
1:A:3703:ASP:OD1	1:A:3703:ASP:N	2.42	0.53
1:C:900:LEU:O	1:C:913:ARG:NH2	2.42	0.53
1:C:1312:GLU:N	1:C:1312:GLU:OE1	2.42	0.53
1:C:3703:ASP:N	1:C:3703:ASP:OD1	2.42	0.53
1:D:1177:LEU:HD23	1:D:1182:LEU:HD11	1.91	0.53
1:A:2823:ARG:NH2	1:D:1502:ASN:OD1	2.43	0.52
1:C:871:GLN:OE1	1:C:871:GLN:N	2.41	0.52
1:C:1177:LEU:HD23	1:C:1182:LEU:HD11	1.91	0.52
1:C:1840:LEU:O	1:C:1844:LEU:HD23	2.10	0.52
1:C:3251:HIS:O	1:C:3262:MET:HE2	2.09	0.52
1:D:3118:GLU:N	1:D:3118:GLU:OE1	2.42	0.52
1:D:3136:LEU:HB2	1:D:3158:LEU:HD13	1.92	0.52
1:A:2126:ARG:NH2	1:A:2164:LEU:O	2.42	0.52
1:B:680:ASP:OD1	1:B:801:ARG:NH2	2.43	0.52
1:B:1796:LEU:HD22	1:B:1822:LEU:HD21	1.91	0.52
1:B:2078:GLU:N	1:B:2078:GLU:OE1	2.42	0.52
1:B:3136:LEU:HB2	1:B:3158:LEU:HD13	1.92	0.52
1:C:320:GLU:OE1	1:C:320:GLU:N	2.41	0.52
1:C:2078:GLU:N	1:C:2078:GLU:OE1	2.42	0.52
1:D:3251:HIS:O	1:D:3262:MET:HE2	2.08	0.52
1:A:119:ILE:HG12	1:A:162:ILE:HD11	1.92	0.52
1:A:3178:ASN:OD1	1:A:3184:ASN:ND2	2.42	0.52
1:C:1300:MET:HE1	1:C:1302:TYR:CZ	2.44	0.52
1:A:1565:MET:HE2	1:A:1569:ALA:CB	2.34	0.52
1:A:2078:GLU:N	1:A:2078:GLU:OE1	2.42	0.52
1:A:3251:HIS:O	1:A:3262:MET:HE2	2.09	0.52
1:B:900:LEU:O	1:B:913:ARG:NH2	2.42	0.52
1:B:1300:MET:HE1	1:B:1302:TYR:CZ	2.44	0.52
1:B:3118:GLU:N	1:B:3118:GLU:OE1	2.42	0.52
1:C:255:GLU:OE1	1:C:255:GLU:N	2.41	0.52
1:C:521:GLU:OE1	1:C:521:GLU:N	2.40	0.52
1:D:1300:MET:HE1	1:D:1302:TYR:CZ	2.45	0.52
1:A:2496:ARG:NH2	1:A:2546:SER:OG	2.42	0.52
1:B:1234:GLU:N	1:B:1234:GLU:OE1	2.42	0.52
1:B:1695:MET:SD	1:B:1695:MET:N	2.78	0.52
1:C:243:GLU:OE2	1:C:389:ARG:NH2	2.42	0.52
1:D:352:SER:O	1:D:352:SER:OG	2.26	0.52
1:D:1722:MET:HE2	1:D:1760:PRO:HD3	1.90	0.52
2:I:74:LYS:NZ	2:I:76:THR:OG1	2.37	0.52
1:A:1300:MET:HE1	1:A:1302:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1722:MET:HE2	1:A:1760:PRO:HD3	1.90	0.52
1:A:3136:LEU:HB2	1:A:3158:LEU:HD13	1.91	0.52
1:B:3923:ILE:HG21	1:B:3934:LEU:HD12	1.90	0.52
1:C:3136:LEU:HB2	1:C:3158:LEU:HD13	1.92	0.52
1:D:680:ASP:OD1	1:D:801:ARG:NH2	2.43	0.52
1:D:871:GLN:N	1:D:871:GLN:OE1	2.41	0.52
1:D:3821:GLU:OE1	1:D:3821:GLU:N	2.42	0.52
1:A:871:GLN:N	1:A:871:GLN:OE1	2.41	0.52
1:A:3118:GLU:OE1	1:A:3118:GLU:N	2.42	0.52
1:B:1840:LEU:O	1:B:1844:LEU:HD23	2.10	0.52
1:C:3923:ILE:HG21	1:C:3934:LEU:HD12	1.90	0.52
1:D:119:ILE:HG12	1:D:162:ILE:HD11	1.91	0.52
1:D:900:LEU:O	1:D:913:ARG:NH2	2.42	0.52
1:D:2694:MET:HE2	1:D:2845:GLU:OE2	2.10	0.52
1:A:181:LEU:HD21	1:A:214:VAL:HG23	1.91	0.52
1:A:1234:GLU:N	1:A:1234:GLU:OE1	2.42	0.52
1:A:1312:GLU:N	1:A:1312:GLU:OE1	2.42	0.52
1:A:1796:LEU:HD22	1:A:1822:LEU:HD21	1.91	0.52
1:B:243:GLU:OE2	1:B:389:ARG:NH2	2.42	0.52
1:B:4669:LEU:HD12	1:B:4671:MET:HE2	1.91	0.52
1:C:3821:GLU:N	1:C:3821:GLU:OE1	2.42	0.52
1:D:1796:LEU:HD22	1:D:1822:LEU:HD21	1.91	0.52
1:D:4020:LEU:HD22	1:D:4127:TYR:CD2	2.45	0.52
1:A:680:ASP:OD1	1:A:801:ARG:NH2	2.43	0.52
1:A:2136:GLU:OE1	1:A:2136:GLU:N	2.42	0.52
1:B:4020:LEU:HD22	1:B:4127:TYR:CD2	2.45	0.52
1:C:1234:GLU:OE1	1:C:1234:GLU:N	2.42	0.52
1:D:243:GLU:OE2	1:D:389:ARG:NH2	2.42	0.52
1:D:2126:ARG:NH2	1:D:2164:LEU:O	2.42	0.52
1:D:4669:LEU:HD12	1:D:4671:MET:HE2	1.91	0.52
1:A:3626:SER:O	1:A:3630:THR:OG1	2.11	0.52
1:B:2126:ARG:NH2	1:B:2164:LEU:O	2.42	0.52
1:D:1840:LEU:O	1:D:1844:LEU:HD23	2.10	0.52
1:D:2136:GLU:OE1	1:D:2136:GLU:N	2.43	0.52
1:D:2170:VAL:HG21	1:D:2198:PHE:CE2	2.45	0.52
1:D:2496:ARG:NH2	1:D:2546:SER:OG	2.42	0.52
1:B:2694:MET:HE2	1:B:2845:GLU:OE2	2.10	0.51
1:C:181:LEU:HD21	1:C:214:VAL:HG23	1.91	0.51
1:A:243:GLU:OE2	1:A:389:ARG:NH2	2.42	0.51
1:A:281:ARG:NH1	1:A:284:TRP:O	2.43	0.51
1:A:1840:LEU:O	1:A:1844:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD21	1:B:214:VAL:HG23	1.91	0.51
1:B:824:GLU:HA	1:B:1020:ILE:HD12	1.93	0.51
1:C:2412:LYS:NZ	1:C:2414:GLU:OE2	2.31	0.51
1:B:36:CYS:SG	1:B:37:LEU:N	2.83	0.51
1:B:2136:GLU:N	1:B:2136:GLU:OE1	2.43	0.51
1:B:2170:VAL:HG21	1:B:2198:PHE:CE2	2.46	0.51
1:C:2714:GLU:OE1	1:C:2714:GLU:N	2.44	0.51
1:A:2170:VAL:HG21	1:A:2198:PHE:CE2	2.46	0.51
1:B:1502:ASN:OD1	1:C:2823:ARG:NH2	2.43	0.51
1:C:680:ASP:OD1	1:C:801:ARG:NH2	2.43	0.51
1:C:2170:VAL:HG21	1:C:2198:PHE:CE2	2.46	0.51
1:C:4020:LEU:HD22	1:C:4127:TYR:CD2	2.45	0.51
1:C:4669:LEU:HD12	1:C:4671:MET:HE2	1.92	0.51
1:A:824:GLU:HA	1:A:1020:ILE:HD12	1.93	0.51
1:A:1969:GLN:OE1	1:A:1969:GLN:N	2.42	0.51
1:A:2714:GLU:OE1	1:A:2714:GLU:N	2.44	0.51
1:A:4020:LEU:HD22	1:A:4127:TYR:CD2	2.45	0.51
1:A:4669:LEU:HD12	1:A:4671:MET:HE2	1.92	0.51
1:B:826:VAL:HB	1:B:1020:ILE:HD11	1.93	0.51
1:C:563:GLU:OE1	1:C:563:GLU:N	2.43	0.51
1:D:910:ASP:OD1	1:D:913:ARG:NE	2.44	0.51
1:A:910:ASP:OD1	1:A:913:ARG:NE	2.44	0.51
1:A:1098:ALA:O	1:A:1101:TRP:NE1	2.43	0.51
1:A:1446:ILE:O	1:A:1541:PHE:N	2.43	0.51
1:A:3318:PHE:HD1	1:A:3322:MET:HE1	1.76	0.51
1:B:2480:GLN:NE2	1:B:2535:ALA:O	2.44	0.51
1:C:143:LEU:HD21	1:D:2425:LEU:HD12	1.91	0.51
1:C:1796:LEU:HD22	1:C:1822:LEU:HD21	1.91	0.51
1:D:1312:GLU:OE1	1:D:1312:GLU:N	2.42	0.51
1:A:826:VAL:HB	1:A:1020:ILE:HD11	1.93	0.51
1:C:661:LEU:O	1:C:788:PHE:N	2.43	0.51
1:D:826:VAL:HB	1:D:1020:ILE:HD11	1.93	0.51
1:B:63:SER:O	1:B:66:THR:OG1	2.29	0.51
1:B:871:GLN:N	1:B:871:GLN:OE1	2.41	0.51
1:B:3318:PHE:HD1	1:B:3322:MET:HE1	1.76	0.51
1:C:824:GLU:HA	1:C:1020:ILE:HD12	1.93	0.51
1:C:1272:ARG:NH1	1:C:1587:LEU:O	2.44	0.51
1:D:136:SER:HG	1:D:139:SER:HG	1.58	0.51
1:A:87:GLU:OE2	1:A:88:LYS:NZ	2.43	0.51
1:A:1251:LEU:HD23	1:A:1600:MET:HE3	1.93	0.51
1:A:2402:ALA:O	1:A:2473:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2480:GLN:NE2	1:A:2535:ALA:O	2.44	0.51
1:A:282:VAL:O	1:A:285:SER:OG	2.29	0.50
1:B:87:GLU:OE2	1:B:88:LYS:NZ	2.41	0.50
1:C:352:SER:O	1:C:352:SER:OG	2.26	0.50
1:D:3703:ASP:OD1	1:D:3703:ASP:N	2.42	0.50
1:A:191:TYR:N	1:A:206:ALA:O	2.44	0.50
1:D:824:GLU:HA	1:D:1020:ILE:HD12	1.93	0.50
1:C:2524:LEU:CD2	1:C:2568:ILE:HG22	2.42	0.50
1:C:3914:GLN:O	1:C:3914:GLN:NE2	2.44	0.50
1:A:2665:LEU:HD11	1:A:2968:PRO:HB2	1.93	0.50
1:A:2694:MET:HE2	1:A:2845:GLU:OE2	2.10	0.50
1:A:2716:LEU:HD21	1:A:2788:ILE:HG21	1.94	0.50
1:B:152:ASP:OD2	1:B:154:THR:OG1	2.29	0.50
1:B:910:ASP:OD1	1:B:913:ARG:NE	2.44	0.50
1:C:1502:ASN:OD1	1:D:2823:ARG:NH2	2.43	0.50
1:D:1936:GLN:NE2	1:D:3607:LEU:O	2.42	0.50
1:A:62:LEU:HD12	1:A:63:SER:N	2.27	0.50
1:A:563:GLU:OE1	1:A:563:GLU:N	2.43	0.50
1:A:2425:LEU:HD12	1:D:143:LEU:HD21	1.93	0.50
1:B:521:GLU:N	1:B:521:GLU:OE1	2.40	0.50
1:B:1272:ARG:NH1	1:B:1587:LEU:O	2.44	0.50
1:C:826:VAL:HB	1:C:1020:ILE:HD11	1.93	0.50
1:D:3318:PHE:HD1	1:D:3322:MET:HE1	1.76	0.50
1:A:797:GLY:N	1:A:1622:CYS:O	2.44	0.50
1:B:81:MET:HE3	1:B:81:MET:O	2.11	0.50
1:C:910:ASP:OD1	1:C:913:ARG:NE	2.44	0.50
1:C:3878:LEU:HD11	1:C:3938:ARG:NE	2.25	0.50
1:D:1234:GLU:N	1:D:1234:GLU:OE1	2.42	0.50
1:A:3914:GLN:O	1:A:3914:GLN:NE2	2.44	0.50
1:B:62:LEU:HD12	1:B:63:SER:N	2.27	0.50
1:C:81:MET:HE3	1:C:81:MET:O	2.11	0.50
1:C:141:ASP:OD2	1:C:144:ALA:N	2.45	0.50
1:C:797:GLY:N	1:C:1622:CYS:O	2.44	0.50
1:C:3762:ILE:HD11	1:C:3837:ASP:O	2.12	0.50
1:D:141:ASP:OD2	1:D:144:ALA:N	2.44	0.50
1:D:1251:LEU:HD23	1:D:1600:MET:HE3	1.94	0.50
1:D:2480:GLN:NE2	1:D:2535:ALA:O	2.44	0.50
1:B:563:GLU:N	1:B:563:GLU:OE1	2.43	0.50
1:C:1251:LEU:HD23	1:C:1600:MET:HE3	1.93	0.50
1:C:2136:GLU:OE1	1:C:2136:GLU:N	2.43	0.50
1:C:2480:GLN:NE2	1:C:2535:ALA:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:MET:HE3	1:D:81:MET:O	2.11	0.50
1:A:1272:ARG:NH1	1:A:1587:LEU:O	2.44	0.50
1:A:2317:ASN:ND2	1:A:2418:ILE:HD13	2.27	0.50
1:B:156:GLU:OE1	1:B:156:GLU:N	2.42	0.50
1:B:352:SER:O	1:B:352:SER:OG	2.26	0.50
1:B:2716:LEU:HD21	1:B:2788:ILE:HG21	1.94	0.50
1:C:63:SER:O	1:C:66:THR:OG1	2.29	0.50
1:D:323:ASP:OD1	1:D:326:SER:OG	2.26	0.50
1:D:3652:GLU:N	1:D:3652:GLU:OE1	2.45	0.50
1:B:797:GLY:N	1:B:1622:CYS:O	2.44	0.49
1:B:2524:LEU:CD2	1:B:2568:ILE:HG22	2.42	0.49
1:B:2714:GLU:OE1	1:B:2714:GLU:N	2.44	0.49
1:B:3839:PHE:HE1	1:B:3873:THR:HG23	1.77	0.49
1:B:3914:GLN:O	1:B:3914:GLN:NE2	2.45	0.49
1:B:4171:PHE:CE1	1:B:4175:VAL:HG11	2.47	0.49
1:C:3318:PHE:HD1	1:C:3322:MET:HE1	1.76	0.49
1:D:62:LEU:HD12	1:D:63:SER:N	2.27	0.49
1:D:1756:THR:N	1:D:1922:GLU:OE2	2.45	0.49
1:D:2402:ALA:O	1:D:2473:ARG:NH2	2.44	0.49
2:H:38:ASP:OD1	2:H:39:SER:N	2.45	0.49
1:B:141:ASP:OD2	1:B:144:ALA:N	2.45	0.49
1:B:1312:GLU:OE1	1:B:1312:GLU:N	2.42	0.49
1:C:2665:LEU:HD11	1:C:2968:PRO:HB2	1.93	0.49
1:D:36:CYS:SG	1:D:37:LEU:N	2.84	0.49
1:D:291:TRP:O	1:D:343:ARG:NH1	2.45	0.49
1:A:4821:ARG:NH1	1:D:4828:ASP:OD1	2.44	0.49
1:C:1190:LEU:HD21	1:C:1193:LYS:HD3	1.94	0.49
1:C:1722:MET:HE2	1:C:1760:PRO:CD	2.42	0.49
1:D:3914:GLN:O	1:D:3914:GLN:NE2	2.44	0.49
1:D:4171:PHE:CE1	1:D:4175:VAL:HG11	2.47	0.49
2:J:38:ASP:OD1	2:J:39:SER:N	2.45	0.49
1:A:141:ASP:OD2	1:A:144:ALA:N	2.45	0.49
1:A:363:ILE:HG22	1:A:372:LEU:HD22	1.93	0.49
1:B:555:LEU:HD11	1:B:589:ILE:HD13	1.95	0.49
1:A:555:LEU:HD11	1:A:589:ILE:HD13	1.95	0.49
1:A:1722:MET:HE2	1:A:1760:PRO:CD	2.43	0.49
1:B:1251:LEU:HD23	1:B:1600:MET:HE3	1.95	0.49
1:B:3652:GLU:N	1:B:3652:GLU:OE1	2.45	0.49
1:C:291:TRP:O	1:C:343:ARG:NH1	2.45	0.49
1:C:1969:GLN:OE1	1:C:1969:GLN:N	2.42	0.49
1:C:3652:GLU:OE1	1:C:3652:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:TRP:O	1:A:343:ARG:NH1	2.45	0.49
1:A:3833:GLU:OE1	1:A:3833:GLU:N	2.43	0.49
1:B:291:TRP:O	1:B:343:ARG:NH1	2.45	0.49
1:B:2694:MET:SD	1:B:2873:TYR:N	2.85	0.49
1:C:363:ILE:HG22	1:C:372:LEU:HD22	1.93	0.49
1:A:661:LEU:O	1:A:788:PHE:N	2.43	0.49
1:A:1190:LEU:HD21	1:A:1193:LYS:HD3	1.94	0.49
1:A:1756:THR:N	1:A:1922:GLU:OE2	2.45	0.49
1:B:363:ILE:HG22	1:B:372:LEU:HD22	1.93	0.49
1:D:363:ILE:HG22	1:D:372:LEU:HD22	1.94	0.49
1:D:2714:GLU:OE1	1:D:2714:GLU:N	2.44	0.49
2:G:38:ASP:OD1	2:G:39:SER:N	2.45	0.49
1:A:36:CYS:SG	1:A:37:LEU:N	2.84	0.49
1:A:3652:GLU:N	1:A:3652:GLU:OE1	2.45	0.49
1:B:2317:ASN:ND2	1:B:2418:ILE:HD13	2.27	0.49
1:C:1487:MET:O	1:C:1532:TYR:OH	2.19	0.49
1:C:2694:MET:HE2	1:C:2845:GLU:OE2	2.11	0.49
1:C:2716:LEU:HD21	1:C:2788:ILE:HG21	1.94	0.49
1:C:3807:PHE:O	1:C:3811:ASN:ND2	2.45	0.49
1:C:4171:PHE:CE1	1:C:4175:VAL:HG11	2.47	0.49
1:D:2317:ASN:ND2	1:D:2418:ILE:HD13	2.27	0.49
1:D:2524:LEU:CD2	1:D:2568:ILE:HG22	2.43	0.49
1:A:1502:ASN:OD1	1:B:2823:ARG:NH2	2.43	0.49
1:C:156:GLU:OE1	1:C:156:GLU:N	2.43	0.49
1:D:1969:GLN:OE1	1:D:1969:GLN:N	2.42	0.49
1:D:3762:ILE:HD11	1:D:3837:ASP:O	2.12	0.49
1:A:143:LEU:HD21	1:B:2425:LEU:HD12	1.94	0.49
1:A:2524:LEU:CD2	1:A:2568:ILE:HG22	2.42	0.49
1:A:4828:ASP:OD1	1:B:4821:ARG:NH1	2.44	0.49
1:B:282:VAL:O	1:B:285:SER:OG	2.30	0.49
1:B:3762:ILE:HD11	1:B:3837:ASP:O	2.12	0.49
1:C:2219:TYR:O	1:C:2223:ASN:ND2	2.46	0.49
1:C:2317:ASN:ND2	1:C:2418:ILE:HD13	2.27	0.49
1:A:3839:PHE:HE1	1:A:3873:THR:HG23	1.78	0.48
1:C:4610:GLU:HA	1:C:4652:VAL:HG12	1.95	0.48
1:D:993:GLU:OE2	1:D:1051:ARG:NH2	2.45	0.48
1:D:4653:MET:HB2	1:D:4671:MET:HE1	1.95	0.48
1:B:1190:LEU:HD21	1:B:1193:LYS:HD3	1.94	0.48
1:C:2402:ALA:O	1:C:2473:ARG:NH2	2.44	0.48
1:D:282:VAL:O	1:D:285:SER:OG	2.31	0.48
1:D:1722:MET:HE2	1:D:1760:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4610:GLU:HA	1:D:4652:VAL:HG12	1.96	0.48
1:A:4171:PHE:CE1	1:A:4175:VAL:HG11	2.47	0.48
1:B:4044:LYS:N	1:B:4075:GLU:O	2.45	0.48
1:C:191:TYR:N	1:C:206:ALA:O	2.46	0.48
1:C:2003:MET:SD	1:C:2003:MET:N	2.87	0.48
1:D:4039:LYS:HG2	1:D:4041:VAL:HG12	1.96	0.48
1:A:3762:ILE:HD11	1:A:3837:ASP:O	2.12	0.48
1:C:62:LEU:HD12	1:C:63:SER:N	2.27	0.48
1:C:282:VAL:O	1:C:285:SER:OG	2.31	0.48
1:C:4828:ASP:OD1	1:D:4821:ARG:NH1	2.44	0.48
1:D:1190:LEU:HD21	1:D:1193:LYS:HD3	1.94	0.48
1:B:1785:LEU:HD12	1:B:1786:ASP:N	2.29	0.48
1:B:3012:VAL:O	1:B:3017:ARG:NH2	2.46	0.48
1:C:1565:MET:HE2	1:C:1569:ALA:CB	2.34	0.48
1:D:1785:LEU:HD12	1:D:1786:ASP:N	2.29	0.48
1:A:152:ASP:OD2	1:A:154:THR:OG1	2.31	0.48
1:A:504:ARG:O	1:A:507:VAL:HG22	2.14	0.48
1:A:2003:MET:SD	1:A:2003:MET:N	2.87	0.48
1:A:4610:GLU:HA	1:A:4652:VAL:HG12	1.95	0.48
1:B:2157:HIS:O	1:B:2160:LEU:N	2.47	0.48
1:B:4610:GLU:HA	1:B:4652:VAL:HG12	1.95	0.48
1:C:235:ARG:NE	1:C:273:SER:OG	2.38	0.48
1:C:888:ASN:CG	1:C:1056:THR:HG21	2.39	0.48
1:C:1785:LEU:HD12	1:C:1786:ASP:N	2.29	0.48
1:A:1785:LEU:HD12	1:A:1786:ASP:N	2.29	0.48
1:B:888:ASN:CG	1:B:1056:THR:HG21	2.39	0.48
1:D:337:LYS:NZ	1:D:396:GLU:OE1	2.43	0.48
1:A:307:SER:CB	1:A:317:MET:HE3	2.44	0.48
1:B:2934:GLU:OE1	1:B:2937:GLN:NE2	2.46	0.48
1:B:4017:ASP:OD1	1:B:4124:VAL:HG23	2.14	0.48
1:C:2665:LEU:HD22	1:C:2964:LYS:O	2.14	0.48
1:D:4017:ASP:OD1	1:D:4124:VAL:HG23	2.14	0.48
1:D:4044:LYS:N	1:D:4075:GLU:O	2.45	0.48
1:A:2652:SER:O	1:A:2957:GLN:NE2	2.46	0.48
1:B:143:LEU:HD21	1:C:2425:LEU:HD12	1.94	0.48
1:B:3623:TYR:CE2	1:B:3628:ILE:HD11	2.49	0.48
1:C:712:GLU:OE2	1:C:1086:ARG:NH2	2.46	0.48
1:C:918:LEU:HD12	1:C:973:THR:HG23	1.96	0.48
1:C:993:GLU:OE2	1:C:1051:ARG:NH2	2.45	0.48
1:C:3012:VAL:O	1:C:3017:ARG:NH2	2.47	0.48
1:D:780:GLU:OE2	1:D:1468:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2219:TYR:O	1:D:2223:ASN:ND2	2.46	0.48
1:B:1756:THR:N	1:B:1922:GLU:OE2	2.45	0.48
1:B:2402:ALA:O	1:B:2473:ARG:NH2	2.44	0.48
1:B:2778:LEU:HD23	1:B:2781:MET:HE3	1.95	0.48
1:D:504:ARG:O	1:D:507:VAL:HG22	2.14	0.48
1:D:563:GLU:OE1	1:D:563:GLU:N	2.43	0.48
2:J:98:LEU:C	2:J:99:ILE:HD12	2.39	0.48
1:A:498:VAL:HG23	1:A:533:LEU:HD22	1.96	0.47
1:A:728:ASP:OD1	1:A:731:HIS:N	2.45	0.47
1:B:503:ASP:O	1:B:507:VAL:HG13	2.14	0.47
1:B:504:ARG:O	1:B:507:VAL:HG22	2.14	0.47
1:B:918:LEU:HD12	1:B:973:THR:HG23	1.96	0.47
1:B:4579:THR:OG1	1:B:4732:HIS:NE2	2.44	0.47
1:C:555:LEU:HD11	1:C:589:ILE:HD13	1.95	0.47
1:C:1756:THR:N	1:C:1922:GLU:OE2	2.45	0.47
1:C:2157:HIS:O	1:C:2160:LEU:N	2.47	0.47
1:C:4720:TYR:OH	1:C:4744:ASP:OD1	2.26	0.47
1:D:307:SER:CB	1:D:317:MET:HE3	2.44	0.47
1:D:447:LEU:O	1:D:449:ILE:N	2.47	0.47
1:D:797:GLY:N	1:D:1622:CYS:O	2.44	0.47
1:D:1272:ARG:NH1	1:D:1587:LEU:O	2.44	0.47
1:A:4039:LYS:HG2	1:A:4041:VAL:HG12	1.96	0.47
1:B:307:SER:CB	1:B:317:MET:HE3	2.44	0.47
1:B:4653:MET:HB2	1:B:4671:MET:HE1	1.95	0.47
1:B:4828:ASP:OD1	1:C:4821:ARG:NH1	2.44	0.47
1:C:515:ALA:HB2	1:C:523:GLY:HA3	1.96	0.47
1:C:1446:ILE:O	1:C:1541:PHE:N	2.43	0.47
1:D:498:VAL:HG23	1:D:533:LEU:HD22	1.96	0.47
1:D:918:LEU:HD12	1:D:973:THR:HG23	1.96	0.47
2:I:80:ASP:OD1	2:I:81:VAL:N	2.48	0.47
1:A:2694:MET:SD	1:A:2873:TYR:N	2.85	0.47
1:A:4653:MET:HB2	1:A:4671:MET:HE1	1.95	0.47
1:B:946:LEU:HD12	1:B:995:MET:HE1	1.97	0.47
1:C:1144:ARG:NH1	1:C:1184:ASP:OD1	2.47	0.47
1:C:2577:GLY:O	1:C:2615:ARG:NH1	2.47	0.47
1:C:4653:MET:HB2	1:C:4671:MET:HE1	1.96	0.47
1:D:2157:HIS:O	1:D:2160:LEU:N	2.46	0.47
1:D:2716:LEU:HD21	1:D:2788:ILE:HG21	1.94	0.47
1:A:712:GLU:OE2	1:A:1086:ARG:NH2	2.46	0.47
1:A:888:ASN:CG	1:A:1056:THR:HG21	2.39	0.47
1:C:504:ARG:O	1:C:507:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:ASP:O	1:D:507:VAL:HG13	2.14	0.47
1:D:2003:MET:SD	1:D:2003:MET:N	2.87	0.47
1:D:4020:LEU:HD12	1:D:4124:VAL:HG22	1.96	0.47
1:A:2577:GLY:O	1:A:2615:ARG:NH1	2.47	0.47
1:A:2665:LEU:HD22	1:A:2964:LYS:O	2.14	0.47
1:A:2778:LEU:HD23	1:A:2781:MET:HE3	1.95	0.47
1:B:447:LEU:O	1:B:449:ILE:N	2.47	0.47
1:B:498:VAL:HG23	1:B:533:LEU:HD22	1.96	0.47
1:C:4039:LYS:HG2	1:C:4041:VAL:HG12	1.96	0.47
1:D:573:GLU:OE2	1:D:609:LYS:NZ	2.35	0.47
1:D:2577:GLY:O	1:D:2615:ARG:NH1	2.47	0.47
1:A:557:TRP:O	1:A:560:SER:OG	2.27	0.47
1:A:2008:ILE:HD13	1:A:2094:ILE:HD11	1.96	0.47
1:A:2157:HIS:O	1:A:2160:LEU:N	2.47	0.47
1:A:2219:TYR:O	1:A:2223:ASN:ND2	2.46	0.47
1:A:3900:GLN:O	1:A:3904:ASN:ND2	2.45	0.47
1:B:1722:MET:HE2	1:B:1760:PRO:CD	2.44	0.47
1:C:447:LEU:O	1:C:449:ILE:N	2.47	0.47
1:C:503:ASP:O	1:C:507:VAL:HG13	2.14	0.47
1:C:3839:PHE:HE1	1:C:3873:THR:HG23	1.78	0.47
1:C:4017:ASP:OD1	1:C:4124:VAL:HG23	2.14	0.47
1:D:152:ASP:OD2	1:D:154:THR:OG1	2.32	0.47
1:D:555:LEU:HD11	1:D:589:ILE:HD13	1.95	0.47
1:D:2934:GLU:OE1	1:D:2937:GLN:NE2	2.46	0.47
2:I:38:ASP:OD1	2:I:39:SER:N	2.48	0.47
1:A:352:SER:O	1:A:352:SER:OG	2.26	0.47
1:A:447:LEU:O	1:A:449:ILE:N	2.47	0.47
1:A:4017:ASP:OD1	1:A:4124:VAL:HG23	2.14	0.47
1:B:136:SER:HG	1:B:139:SER:HG	1.61	0.47
1:B:661:LEU:O	1:B:788:PHE:N	2.43	0.47
1:B:780:GLU:OE2	1:B:1468:THR:OG1	2.31	0.47
1:B:1969:GLN:OE1	1:B:1969:GLN:N	2.42	0.47
1:B:2579:LEU:O	1:B:2615:ARG:NH1	2.45	0.47
1:B:3759:LYS:NZ	1:B:3837:ASP:OD2	2.47	0.47
1:B:3960:ASP:OD1	1:B:3962:SER:N	2.44	0.47
1:B:4020:LEU:HD12	1:B:4124:VAL:HG22	1.96	0.47
1:C:498:VAL:HG23	1:C:533:LEU:HD22	1.96	0.47
1:C:780:GLU:OE2	1:C:1468:THR:OG1	2.31	0.47
1:C:3960:ASP:OD1	1:C:3962:SER:N	2.44	0.47
1:C:4020:LEU:HD12	1:C:4124:VAL:HG22	1.96	0.47
1:D:888:ASN:CG	1:D:1056:THR:HG21	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1144:ARG:NH1	1:D:1184:ASP:OD1	2.47	0.47
2:G:80:ASP:OD1	2:G:81:VAL:N	2.48	0.47
2:H:67:MET:HE1	2:H:73:ALA:CB	2.45	0.47
2:H:80:ASP:OD1	2:H:81:VAL:N	2.47	0.47
1:A:918:LEU:HD12	1:A:973:THR:HG23	1.96	0.47
1:A:1144:ARG:NH1	1:A:1184:ASP:OD1	2.47	0.47
1:A:2972:GLN:NE2	1:A:2976:ASN:OD1	2.48	0.47
1:B:191:TYR:N	1:B:206:ALA:O	2.47	0.47
1:B:2577:GLY:O	1:B:2615:ARG:NH1	2.47	0.47
1:C:307:SER:CB	1:C:317:MET:HE3	2.44	0.47
1:C:1098:ALA:O	1:C:1101:TRP:NE1	2.43	0.47
1:D:2294:GLY:O	1:D:2298:LEU:HD23	2.15	0.47
1:D:3233:MET:SD	1:D:3233:MET:N	2.84	0.47
1:A:4020:LEU:HD12	1:A:4124:VAL:HG22	1.96	0.47
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.46	0.47
1:C:2008:ILE:HD13	1:C:2094:ILE:HD11	1.96	0.47
1:D:515:ALA:HB2	1:D:523:GLY:HA3	1.96	0.47
1:D:1446:ILE:O	1:D:1541:PHE:N	2.43	0.47
1:D:2778:LEU:HD23	1:D:2781:MET:HE3	1.95	0.47
1:B:515:ALA:HB2	1:B:523:GLY:HA3	1.97	0.47
1:B:3069:LYS:CD	1:B:3092:ILE:HD13	2.45	0.47
1:C:152:ASP:OD2	1:C:154:THR:OG1	2.32	0.47
1:C:3069:LYS:CD	1:C:3092:ILE:HD13	2.45	0.47
1:C:4606:ALA:HB1	1:C:4648:VAL:HG21	1.97	0.47
1:D:2665:LEU:HD22	1:D:2964:LYS:O	2.15	0.47
1:A:4135:ILE:HD11	1:A:4917:TYR:HA	1.97	0.46
1:B:728:ASP:OD1	1:B:731:HIS:N	2.45	0.46
1:B:2003:MET:SD	1:B:2003:MET:N	2.87	0.46
1:B:2294:GLY:O	1:B:2298:LEU:HD23	2.15	0.46
1:C:946:LEU:HD12	1:C:995:MET:HE1	1.97	0.46
1:C:2934:GLU:OE1	1:C:2937:GLN:NE2	2.46	0.46
1:C:3623:TYR:CE2	1:C:3628:ILE:HD11	2.50	0.46
1:D:661:LEU:O	1:D:788:PHE:N	2.43	0.46
1:D:2652:SER:O	1:D:2957:GLN:NE2	2.46	0.46
1:B:2911:LEU:HD23	1:B:2914:PRO:HG2	1.97	0.46
1:B:4039:LYS:HG2	1:B:4041:VAL:HG12	1.96	0.46
1:C:3940:TRP:O	1:C:3944:VAL:HG23	2.16	0.46
1:D:2801:ASN:OD1	1:D:2802:ARG:N	2.48	0.46
1:D:3839:PHE:HE1	1:D:3873:THR:HG23	1.78	0.46
2:J:67:MET:HE1	2:J:73:ALA:CB	2.45	0.46
1:A:993:GLU:OE2	1:A:1051:ARG:NH2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3012:VAL:O	1:A:3017:ARG:NH2	2.47	0.46
1:A:3623:TYR:CE2	1:A:3628:ILE:HD11	2.50	0.46
1:B:1144:ARG:NH1	1:B:1184:ASP:OD1	2.47	0.46
1:B:2972:GLN:NE2	1:B:2976:ASN:OD1	2.49	0.46
1:B:3833:GLU:OE1	1:B:3833:GLU:N	2.43	0.46
1:B:3943:VAL:HG23	1:B:3977:MET:SD	2.55	0.46
1:C:2294:GLY:O	1:C:2298:LEU:HD23	2.15	0.46
1:C:2388:MET:HE1	1:C:2463:HIS:HB3	1.98	0.46
1:C:2911:LEU:HD23	1:C:2914:PRO:HG2	1.97	0.46
1:D:156:GLU:OE1	1:D:156:GLU:N	2.43	0.46
1:D:2911:LEU:O	1:D:2911:LEU:HD22	2.15	0.46
1:D:4025:LEU:HD22	1:D:4057:TYR:CE2	2.51	0.46
2:I:67:MET:HE1	2:I:73:ALA:CB	2.44	0.46
2:J:80:ASP:OD1	2:J:81:VAL:N	2.49	0.46
1:A:946:LEU:HD12	1:A:995:MET:HE1	1.97	0.46
1:A:2911:LEU:O	1:A:2911:LEU:HD22	2.15	0.46
1:B:235:ARG:NE	1:B:273:SER:HG	2.12	0.46
1:C:1914:ASP:OD1	1:C:2089:ARG:NH1	2.47	0.46
1:C:2801:ASN:OD1	1:C:2802:ARG:N	2.49	0.46
1:D:2008:ILE:HD13	1:D:2094:ILE:HD11	1.96	0.46
1:D:2694:MET:SD	1:D:2873:TYR:N	2.85	0.46
1:D:2866:ASN:OD1	1:D:2867:HIS:N	2.48	0.46
1:D:2972:GLN:NE2	1:D:2976:ASN:OD1	2.49	0.46
2:G:67:MET:HE1	2:G:73:ALA:CB	2.45	0.46
1:B:2219:TYR:O	1:B:2223:ASN:ND2	2.46	0.46
1:B:2388:MET:HE1	1:B:2463:HIS:HB3	1.98	0.46
1:B:2665:LEU:HD22	1:B:2964:LYS:O	2.15	0.46
1:C:4025:LEU:HD22	1:C:4057:TYR:CE2	2.51	0.46
1:C:4135:ILE:HD11	1:C:4917:TYR:HA	1.97	0.46
1:D:4579:THR:OG1	1:D:4732:HIS:NE2	2.46	0.46
1:A:503:ASP:O	1:A:507:VAL:HG13	2.14	0.46
1:A:515:ALA:HB2	1:A:523:GLY:HA3	1.97	0.46
1:A:780:GLU:OE2	1:A:1468:THR:OG1	2.31	0.46
1:A:948:CYS:SG	1:A:995:MET:HE2	2.55	0.46
1:A:1304:LEU:HD12	1:A:1542:PRO:HG2	1.98	0.46
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.46	0.46
1:A:2801:ASN:OD1	1:A:2802:ARG:N	2.49	0.46
1:A:4606:ALA:HB1	1:A:4648:VAL:HG21	1.97	0.46
1:B:948:CYS:SG	1:B:995:MET:HE2	2.55	0.46
1:B:1304:LEU:HD12	1:B:1542:PRO:HG2	1.98	0.46
1:C:2778:LEU:HD23	1:C:2781:MET:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4501:ARG:NH2	1:C:4744:ASP:OD1	2.46	0.46
1:D:3943:VAL:HG23	1:D:3977:MET:SD	2.56	0.46
1:A:245:LEU:HD22	1:A:261:HIS:O	2.16	0.46
1:A:2388:MET:HE1	1:A:2463:HIS:HB3	1.98	0.46
1:A:4025:LEU:HD22	1:A:4057:TYR:CE2	2.51	0.46
1:B:2801:ASN:OD1	1:B:2802:ARG:N	2.49	0.46
1:B:2866:ASN:OD1	1:B:2867:HIS:N	2.48	0.46
1:B:2911:LEU:O	1:B:2911:LEU:HD22	2.15	0.46
1:D:3960:ASP:OD1	1:D:3962:SER:N	2.44	0.46
1:A:161:THR:HG23	1:A:186:VAL:HG12	1.97	0.46
1:A:2294:GLY:O	1:A:2298:LEU:HD23	2.15	0.46
1:A:3238:LEU:HD12	1:A:3279:ILE:HD11	1.98	0.46
1:A:3759:LYS:NZ	1:A:3837:ASP:OD2	2.48	0.46
1:B:3900:GLN:O	1:B:3904:ASN:ND2	2.45	0.46
1:B:4025:LEU:HD22	1:B:4057:TYR:CE2	2.51	0.46
1:C:2911:LEU:O	1:C:2911:LEU:HD22	2.15	0.46
1:D:2175:VAL:HG12	1:D:2219:TYR:CE2	2.51	0.46
1:D:4135:ILE:HD11	1:D:4917:TYR:HA	1.98	0.46
1:A:710:GLY:N	1:A:721:ASP:OD2	2.49	0.46
1:B:2367:SER:OG	1:B:2368:SER:N	2.49	0.46
1:B:3940:TRP:O	1:B:3944:VAL:HG23	2.16	0.46
1:A:2866:ASN:OD1	1:A:2867:HIS:N	2.48	0.46
1:A:3069:LYS:CD	1:A:3092:ILE:HD13	2.46	0.46
1:B:710:GLY:N	1:B:721:ASP:OD2	2.49	0.46
1:B:712:GLU:OE2	1:B:1086:ARG:NH2	2.46	0.46
1:C:710:GLY:N	1:C:721:ASP:OD2	2.49	0.46
1:C:3900:GLN:O	1:C:3904:ASN:ND2	2.46	0.46
1:C:3943:VAL:HG23	1:C:3977:MET:SD	2.55	0.46
1:D:191:TYR:N	1:D:206:ALA:O	2.46	0.46
1:D:946:LEU:HD12	1:D:995:MET:HE1	1.97	0.46
1:A:1056:THR:HG22	1:A:1060:TYR:CE2	2.51	0.45
1:A:2129:LEU:HD11	1:A:2172:GLU:HB3	1.98	0.45
1:A:2157:HIS:O	1:A:2161:MET:HE2	2.16	0.45
1:A:3943:VAL:HG23	1:A:3977:MET:SD	2.55	0.45
1:B:3238:LEU:HD12	1:B:3279:ILE:HD11	1.98	0.45
1:B:4135:ILE:HD11	1:B:4917:TYR:HA	1.98	0.45
1:C:948:CYS:SG	1:C:995:MET:HE2	2.55	0.45
1:C:1056:THR:HG22	1:C:1060:TYR:CE2	2.51	0.45
1:C:2586:HIS:O	1:C:2590:ARG:NH1	2.49	0.45
1:D:712:GLU:OE2	1:D:1086:ARG:NH2	2.46	0.45
1:D:1304:LEU:HD12	1:D:1542:PRO:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:MET:N	2:H:99:ILE:O	2.49	0.45
1:A:2175:VAL:HG12	1:A:2219:TYR:CE2	2.51	0.45
1:A:2432:VAL:HG22	1:A:2486:LEU:HD23	1.98	0.45
1:A:2911:LEU:HD23	1:A:2914:PRO:HG2	1.97	0.45
1:A:3940:TRP:O	1:A:3944:VAL:HG23	2.15	0.45
1:C:2432:VAL:HG22	1:C:2486:LEU:HD23	1.98	0.45
1:C:3238:LEU:HD12	1:C:3279:ILE:HD11	1.98	0.45
1:C:3833:GLU:OE1	1:C:3833:GLU:N	2.43	0.45
1:D:2157:HIS:O	1:D:2161:MET:HE2	2.16	0.45
1:A:2367:SER:OG	1:A:2368:SER:N	2.49	0.45
1:B:64:ILE:O	1:B:123:HIS:NE2	2.46	0.45
1:B:2432:VAL:HG22	1:B:2486:LEU:HD23	1.98	0.45
1:C:1304:LEU:HD12	1:C:1542:PRO:HG2	1.97	0.45
1:C:2129:LEU:HD11	1:C:2172:GLU:HB3	1.98	0.45
1:D:1786:ASP:OD1	1:D:1787:ILE:N	2.49	0.45
1:D:2388:MET:HE1	1:D:2463:HIS:HB3	1.98	0.45
1:D:2432:VAL:HG22	1:D:2486:LEU:HD23	1.99	0.45
1:D:3238:LEU:HD12	1:D:3279:ILE:HD11	1.98	0.45
1:D:3940:TRP:O	1:D:3944:VAL:HG23	2.15	0.45
1:D:4606:ALA:HB1	1:D:4648:VAL:HG21	1.97	0.45
1:A:63:SER:O	1:A:66:THR:OG1	2.35	0.45
1:C:2157:HIS:O	1:C:2161:MET:HE2	2.16	0.45
1:D:1164:CYS:C	1:D:1165:MET:HE2	2.42	0.45
1:D:2911:LEU:HD23	1:D:2914:PRO:HG2	1.97	0.45
1:D:3878:LEU:HD11	1:D:3938:ARG:NE	2.25	0.45
1:A:14:LEU:C	1:A:113:LEU:HD23	2.42	0.45
1:A:1804:SER:O	1:A:1806:HIS:ND1	2.49	0.45
1:A:2171:MET:O	1:A:2175:VAL:HG13	2.17	0.45
1:B:82:LEU:HA	1:B:85:THR:HG22	1.99	0.45
1:B:2171:MET:O	1:B:2175:VAL:HG13	2.17	0.45
1:D:710:GLY:N	1:D:721:ASP:OD2	2.50	0.45
2:G:30:MET:N	2:G:99:ILE:O	2.49	0.45
2:J:30:MET:N	2:J:99:ILE:O	2.50	0.45
1:B:3233:MET:SD	1:B:3233:MET:N	2.84	0.45
1:B:4606:ALA:HB1	1:B:4648:VAL:HG21	1.97	0.45
1:C:2972:GLN:NE2	1:C:2976:ASN:OD1	2.48	0.45
1:D:717:GLY:N	1:D:720:ASP:OD2	2.45	0.45
1:D:3900:GLN:O	1:D:3904:ASN:ND2	2.46	0.45
2:I:30:MET:N	2:I:99:ILE:O	2.49	0.45
1:A:43:GLY:N	1:A:458:ASP:OD2	2.50	0.45
1:A:2579:LEU:O	1:A:2615:ARG:NH1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:HD22	1:B:261:HIS:O	2.17	0.45
1:B:1056:THR:HG22	1:B:1060:TYR:CE2	2.51	0.45
1:B:1164:CYS:C	1:B:1165:MET:HE2	2.42	0.45
1:B:2129:LEU:HD11	1:B:2172:GLU:HB3	1.98	0.45
1:B:2157:HIS:O	1:B:2161:MET:HE2	2.16	0.45
1:B:2932:VAL:HG21	1:B:3006:LEU:HD11	1.99	0.45
1:D:728:ASP:OD1	1:D:731:HIS:N	2.44	0.45
1:D:829:LYS:NZ	1:D:1037:LEU:O	2.47	0.45
1:D:948:CYS:SG	1:D:995:MET:HE2	2.56	0.45
1:D:1056:THR:HG22	1:D:1060:TYR:CE2	2.51	0.45
1:D:1287:GLN:OE1	1:D:1288:LYS:N	2.50	0.45
1:A:4615:TYR:C	1:A:4616:ILE:HD12	2.42	0.45
1:B:2175:VAL:HG12	1:B:2219:TYR:CE2	2.51	0.45
1:C:2866:ASN:OD1	1:C:2867:HIS:N	2.48	0.45
1:D:2579:LEU:O	1:D:2615:ARG:NH1	2.45	0.45
1:D:3069:LYS:CD	1:D:3092:ILE:HD13	2.46	0.45
1:D:3623:TYR:CE2	1:D:3628:ILE:HD11	2.50	0.45
1:D:3759:LYS:NZ	1:D:3837:ASP:OD2	2.48	0.45
1:A:83:ALA:HA	1:A:86:VAL:HG23	1.99	0.45
1:A:1164:CYS:C	1:A:1165:MET:HE2	2.42	0.45
1:A:1951:ASN:OD1	1:A:1951:ASN:N	2.50	0.45
1:B:83:ALA:HA	1:B:86:VAL:HG23	1.99	0.45
1:B:929:ARG:NH2	1:B:932:ASN:OD1	2.47	0.45
1:B:1287:GLN:OE1	1:B:1288:LYS:N	2.50	0.45
1:B:1446:ILE:O	1:B:1541:PHE:N	2.43	0.45
1:B:3807:PHE:O	1:B:3811:ASN:ND2	2.44	0.45
1:B:4106:GLU:OE1	1:B:4146:ARG:NH1	2.50	0.45
1:C:82:LEU:HA	1:C:85:THR:HG22	1.99	0.45
1:D:2129:LEU:HD11	1:D:2172:GLU:HB3	1.98	0.45
1:B:2652:SER:O	1:B:2957:GLN:NE2	2.46	0.45
1:C:1971:GLN:NE2	1:C:3605:ALA:O	2.45	0.45
1:C:2367:SER:OG	1:C:2368:SER:N	2.49	0.45
1:C:2579:LEU:O	1:C:2615:ARG:NH1	2.45	0.45
1:C:3759:LYS:NZ	1:C:3837:ASP:OD2	2.48	0.45
1:D:2171:MET:O	1:D:2175:VAL:HG13	2.17	0.45
1:D:4501:ARG:NH2	1:D:4744:ASP:OD1	2.47	0.45
1:A:829:LYS:NZ	1:A:1037:LEU:O	2.47	0.44
1:A:1432:ILE:HG12	1:A:1441:VAL:HG11	1.99	0.44
1:A:2388:MET:HE2	1:A:2388:MET:O	2.18	0.44
1:B:982:ASP:OD1	1:B:983:LEU:N	2.50	0.44
1:C:14:LEU:C	1:C:113:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ALA:HA	1:C:86:VAL:HG23	1.99	0.44
1:C:1287:GLN:OE1	1:C:1288:LYS:N	2.50	0.44
1:D:1432:ILE:HG12	1:D:1441:VAL:HG11	1.99	0.44
1:A:156:GLU:OE1	1:A:156:GLU:N	2.44	0.44
1:A:982:ASP:OD1	1:A:983:LEU:N	2.50	0.44
1:A:2426:ILE:HD11	1:A:2431:LEU:HD11	2.00	0.44
1:A:2982:LEU:HB2	1:A:3038:THR:HG23	1.99	0.44
1:B:993:GLU:OE2	1:B:1051:ARG:NH2	2.45	0.44
1:C:1277:ILE:HD12	1:C:1278:ASP:N	2.32	0.44
1:C:2175:VAL:HG12	1:C:2219:TYR:CE2	2.51	0.44
1:C:2982:LEU:HB2	1:C:3038:THR:HG23	1.98	0.44
1:D:2932:VAL:HG21	1:D:3006:LEU:HD11	1.99	0.44
1:D:4615:TYR:C	1:D:4616:ILE:HD12	2.42	0.44
2:H:98:LEU:C	2:H:99:ILE:HD12	2.42	0.44
1:A:2932:VAL:HG21	1:A:3006:LEU:HD11	1.99	0.44
1:A:4106:GLU:OE1	1:A:4146:ARG:NH1	2.50	0.44
1:B:2719:PHE:CE2	1:B:2778:LEU:HD21	2.53	0.44
1:B:3878:LEU:HD11	1:B:3938:ARG:NE	2.25	0.44
1:C:1708:ILE:O	1:C:1713:SER:N	2.49	0.44
1:C:2652:SER:O	1:C:2957:GLN:NE2	2.46	0.44
1:C:4615:TYR:C	1:C:4616:ILE:HD12	2.42	0.44
1:D:3012:VAL:O	1:D:3017:ARG:NH2	2.46	0.44
1:A:2719:PHE:CE2	1:A:2778:LEU:HD21	2.53	0.44
1:B:2008:ILE:HD13	1:B:2094:ILE:HD11	1.98	0.44
1:B:2388:MET:HE2	1:B:2388:MET:O	2.18	0.44
1:C:1164:CYS:C	1:C:1165:MET:HE2	2.42	0.44
1:C:2171:MET:O	1:C:2175:VAL:HG13	2.17	0.44
1:C:2230:SER:OG	1:C:2233:MET:SD	2.74	0.44
1:C:2932:VAL:HG21	1:C:3006:LEU:HD11	1.99	0.44
1:D:63:SER:O	1:D:66:THR:OG1	2.34	0.44
1:D:982:ASP:OD1	1:D:983:LEU:N	2.50	0.44
1:A:1820:VAL:HG12	1:A:1821:PRO:HD3	2.00	0.44
1:A:2087:LEU:HD21	1:A:3643:LEU:HD21	2.00	0.44
1:A:2919:ARG:NE	1:A:2999:GLU:OE2	2.51	0.44
1:B:14:LEU:C	1:B:113:LEU:HD23	2.42	0.44
1:B:1432:ILE:HG12	1:B:1441:VAL:HG11	1.99	0.44
1:B:1804:SER:O	1:B:1806:HIS:ND1	2.49	0.44
1:C:245:LEU:HD22	1:C:261:HIS:O	2.17	0.44
1:C:1432:ILE:HG12	1:C:1441:VAL:HG11	1.99	0.44
1:C:1951:ASN:OD1	1:C:1951:ASN:N	2.51	0.44
1:C:1959:ARG:O	1:C:1959:ARG:NE	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2435:ILE:O	1:C:2464:LYS:NZ	2.42	0.44
1:D:1277:ILE:HD12	1:D:1278:ASP:N	2.33	0.44
1:D:1436:GLN:NE2	1:D:1547:GLN:O	2.50	0.44
2:I:98:LEU:C	2:I:99:ILE:HD12	2.42	0.44
1:A:1287:GLN:OE1	1:A:1288:LYS:N	2.50	0.44
1:A:2934:GLU:OE1	1:A:2937:GLN:NE2	2.46	0.44
1:B:1848:GLU:OE2	1:B:1850:SER:OG	2.35	0.44
1:B:2087:LEU:HD21	1:B:3643:LEU:HD21	2.00	0.44
1:D:14:LEU:C	1:D:113:LEU:HD23	2.42	0.44
1:D:82:LEU:HA	1:D:85:THR:HG22	1.99	0.44
1:D:1098:ALA:O	1:D:1101:TRP:NE1	2.43	0.44
1:D:2166:MET:O	1:D:2170:VAL:HG23	2.18	0.44
1:D:2388:MET:O	1:D:2388:MET:HE2	2.18	0.44
2:G:98:LEU:C	2:G:99:ILE:HD12	2.42	0.44
1:A:4044:LYS:N	1:A:4075:GLU:O	2.45	0.44
1:B:1959:ARG:O	1:B:1959:ARG:NE	2.51	0.44
1:C:64:ILE:O	1:C:123:HIS:NE2	2.47	0.44
1:C:337:LYS:NZ	1:C:396:GLU:OE1	2.45	0.44
1:C:982:ASP:OD1	1:C:983:LEU:N	2.50	0.44
1:C:1804:SER:O	1:C:1806:HIS:ND1	2.49	0.44
1:C:2388:MET:HE2	1:C:2388:MET:O	2.18	0.44
1:C:2641:ARG:NH1	1:C:2918:LYS:O	2.50	0.44
1:D:83:ALA:HA	1:D:86:VAL:HG23	1.99	0.44
1:D:2426:ILE:HD11	1:D:2431:LEU:HD11	2.00	0.44
1:A:82:LEU:HA	1:A:85:THR:HG22	2.00	0.44
1:A:2174:MET:HE1	1:A:2178:LEU:HD13	2.00	0.44
1:A:2289:TRP:CZ2	1:A:2387:ILE:HG23	2.53	0.44
1:A:2586:HIS:O	1:A:2590:ARG:NH1	2.50	0.44
1:B:1820:VAL:HG12	1:B:1821:PRO:HD3	2.00	0.44
1:C:2087:LEU:HD21	1:C:3643:LEU:HD21	2.00	0.44
1:C:2426:ILE:HD11	1:C:2431:LEU:HD11	2.00	0.44
1:C:2719:PHE:CE2	1:C:2778:LEU:HD21	2.53	0.44
1:C:4106:GLU:OE1	1:C:4146:ARG:NH1	2.51	0.44
1:D:245:LEU:HD22	1:D:261:HIS:O	2.17	0.44
1:D:721:ASP:OD1	1:D:721:ASP:N	2.50	0.44
1:D:1951:ASN:OD1	1:D:1951:ASN:N	2.50	0.44
1:D:4720:TYR:OH	1:D:4744:ASP:OD1	2.26	0.44
1:A:1959:ARG:NE	1:A:1959:ARG:O	2.51	0.44
1:A:2435:ILE:O	1:A:2464:LYS:NZ	2.41	0.44
1:B:1951:ASN:N	1:B:1951:ASN:OD1	2.51	0.44
1:B:3142:SER:HB3	1:B:3147:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:ASP:OD1	1:C:721:ASP:N	2.51	0.44
1:C:728:ASP:OD1	1:C:731:HIS:N	2.45	0.44
1:D:3833:GLU:OE1	1:D:3833:GLU:N	2.43	0.44
1:A:136:SER:HG	1:A:139:SER:HG	1.65	0.43
1:B:557:TRP:O	1:B:560:SER:OG	2.27	0.43
1:B:2166:MET:O	1:B:2170:VAL:HG23	2.18	0.43
1:B:3931:GLN:NE2	1:B:3983:SER:O	2.51	0.43
1:B:4615:TYR:C	1:B:4616:ILE:HD12	2.42	0.43
1:D:1427:TYR:HB2	1:D:1564:VAL:HG11	2.00	0.43
1:D:1959:ARG:NE	1:D:1959:ARG:O	2.51	0.43
1:D:2586:HIS:O	1:D:2590:ARG:NH1	2.50	0.43
2:H:79:PRO:O	2:H:84:GLY:N	2.46	0.43
1:A:3402:PHE:CG	1:A:3469:LEU:HD22	2.54	0.43
1:B:1786:ASP:OD1	1:B:1787:ILE:N	2.49	0.43
1:B:2586:HIS:O	1:B:2590:ARG:NH1	2.50	0.43
1:C:1820:VAL:HG12	1:C:1821:PRO:HD3	2.00	0.43
1:C:3142:SER:HB3	1:C:3147:VAL:HG21	2.00	0.43
1:D:1820:VAL:HG12	1:D:1821:PRO:HD3	2.00	0.43
1:D:3402:PHE:CG	1:D:3469:LEU:HD22	2.54	0.43
1:B:829:LYS:NZ	1:B:1037:LEU:O	2.47	0.43
1:B:1157:GLN:N	1:B:1157:GLN:OE1	2.52	0.43
1:B:2166:MET:HE1	1:B:2202:PHE:CD1	2.53	0.43
1:B:2426:ILE:HD11	1:B:2431:LEU:HD11	2.00	0.43
1:C:43:GLY:N	1:C:458:ASP:OD2	2.50	0.43
1:D:1157:GLN:N	1:D:1157:GLN:OE1	2.51	0.43
1:D:2719:PHE:CE2	1:D:2778:LEU:HD21	2.53	0.43
1:A:1277:ILE:HD12	1:A:1278:ASP:N	2.33	0.43
1:C:4136:GLU:O	1:C:4917:TYR:OH	2.33	0.43
1:D:43:GLY:N	1:D:458:ASP:OD2	2.50	0.43
1:D:909:ASP:OD1	1:D:910:ASP:N	2.52	0.43
2:I:77:CYS:O	2:I:97:THR:OG1	2.27	0.43
1:A:1157:GLN:N	1:A:1157:GLN:OE1	2.51	0.43
1:A:2166:MET:HE1	1:A:2202:PHE:CD1	2.53	0.43
1:B:1277:ILE:HD12	1:B:1278:ASP:N	2.33	0.43
1:B:1914:ASP:OD1	1:B:2089:ARG:NH1	2.47	0.43
1:B:2289:TRP:CZ2	1:B:2387:ILE:HG23	2.53	0.43
1:B:2919:ARG:NE	1:B:2999:GLU:OE2	2.51	0.43
1:B:2982:LEU:HB2	1:B:3038:THR:HG23	1.99	0.43
1:C:615:CYS:SG	1:C:1661:LEU:HD22	2.57	0.43
1:C:1436:GLN:NE2	1:C:1547:GLN:O	2.50	0.43
1:C:3133:LEU:HD21	1:C:3169:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3402:PHE:CG	1:C:3469:LEU:HD22	2.53	0.43
1:D:805:GLY:N	1:D:809:GLY:O	2.47	0.43
1:D:929:ARG:NH2	1:D:932:ASN:OD1	2.47	0.43
1:D:1738:THR:OG1	1:D:1740:PHE:O	2.33	0.43
1:D:2289:TRP:CZ2	1:D:2387:ILE:HG23	2.53	0.43
1:A:2230:SER:OG	1:A:2233:MET:SD	2.74	0.43
1:B:275:TRP:CH2	1:B:316:LEU:HD21	2.54	0.43
1:B:3133:LEU:HD21	1:B:3169:PHE:CD1	2.53	0.43
1:C:2166:MET:O	1:C:2170:VAL:HG23	2.18	0.43
1:C:2174:MET:HE1	1:C:2178:LEU:HD13	2.00	0.43
1:C:4044:LYS:N	1:C:4075:GLU:O	2.45	0.43
1:D:1804:SER:O	1:D:1806:HIS:ND1	2.49	0.43
1:D:1914:ASP:OD1	1:D:2089:ARG:NH1	2.47	0.43
1:D:3931:GLN:NE2	1:D:3983:SER:O	2.51	0.43
1:A:3142:SER:HB3	1:A:3147:VAL:HG21	2.00	0.43
1:A:3931:GLN:NE2	1:A:3983:SER:O	2.52	0.43
1:B:1971:GLN:NE2	1:B:3605:ALA:O	2.45	0.43
1:B:2435:ILE:O	1:B:2464:LYS:NZ	2.41	0.43
1:D:4106:GLU:OE1	1:D:4146:ARG:NH1	2.51	0.43
1:A:275:TRP:CH2	1:A:316:LEU:HD21	2.53	0.43
1:A:3807:PHE:O	1:A:3811:ASN:ND2	2.44	0.43
1:A:4099:VAL:HG22	1:A:4132:LEU:HD23	2.01	0.43
1:B:3402:PHE:CG	1:B:3469:LEU:HD22	2.54	0.43
1:C:275:TRP:CH2	1:C:316:LEU:HD21	2.54	0.43
1:C:1848:GLU:OE2	1:C:1850:SER:OG	2.35	0.43
1:D:2087:LEU:HD21	1:D:3643:LEU:HD21	2.00	0.43
1:D:2641:ARG:NH1	1:D:2918:LYS:O	2.50	0.43
1:A:3133:LEU:HD21	1:A:3169:PHE:CD1	2.53	0.43
1:B:43:GLY:N	1:B:458:ASP:OD2	2.50	0.43
1:B:924:LEU:HD22	1:B:928:GLU:OE2	2.19	0.43
1:B:4883:MET:HE1	1:B:4888:PHE:HD1	1.83	0.43
1:C:2166:MET:HE1	1:C:2202:PHE:CD1	2.53	0.43
1:C:2289:TRP:CZ2	1:C:2387:ILE:HG23	2.53	0.43
1:C:3931:GLN:NE2	1:C:3983:SER:O	2.51	0.43
1:D:3394:LEU:HG	1:D:3472:LEU:HD11	2.01	0.43
1:A:717:GLY:N	1:A:720:ASP:OD2	2.45	0.43
1:A:805:GLY:N	1:A:809:GLY:O	2.47	0.43
1:B:1436:GLN:NE2	1:B:1547:GLN:O	2.50	0.43
1:B:2174:MET:HE1	1:B:2178:LEU:HD13	2.00	0.43
1:C:2919:ARG:NE	1:C:2999:GLU:OE2	2.51	0.43
1:D:2919:ARG:NE	1:D:2999:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3142:SER:HB3	1:D:3147:VAL:HG21	2.00	0.43
1:D:4136:GLU:O	1:D:4917:TYR:OH	2.34	0.43
2:G:67:MET:HE2	2:G:71:GLN:O	2.19	0.43
1:A:3878:LEU:HD11	1:A:3938:ARG:NE	2.25	0.42
1:B:3162:ALA:HB2	1:B:3240:MET:HE1	2.01	0.42
1:C:681:HIS:O	1:C:799:LYS:N	2.52	0.42
1:C:3394:LEU:HG	1:C:3472:LEU:HD11	2.01	0.42
1:D:802:PHE:O	1:D:803:LEU:HD23	2.20	0.42
1:D:2166:MET:HE1	1:D:2202:PHE:CD1	2.53	0.42
1:D:2982:LEU:HB2	1:D:3038:THR:HG23	1.99	0.42
1:D:3133:LEU:HD21	1:D:3169:PHE:CD1	2.53	0.42
1:D:4099:VAL:HG22	1:D:4132:LEU:HD23	2.01	0.42
1:A:721:ASP:OD1	1:A:721:ASP:N	2.51	0.42
1:A:2641:ARG:NH1	1:A:2918:LYS:O	2.50	0.42
1:A:4001:MET:SD	1:A:4002:LEU:HD22	2.60	0.42
1:B:556:ASP:OD1	1:B:557:TRP:N	2.52	0.42
1:B:4099:VAL:HG22	1:B:4132:LEU:HD23	2.01	0.42
1:C:1721:MET:SD	1:C:2126:ARG:NH1	2.90	0.42
1:C:1939:GLN:NE2	1:C:1971:GLN:OE1	2.52	0.42
1:C:4001:MET:SD	1:C:4002:LEU:HD22	2.59	0.42
1:C:4883:MET:HE1	1:C:4888:PHE:HD1	1.84	0.42
1:D:1801:LYS:O	1:D:1804:SER:OG	2.32	0.42
1:D:1939:GLN:NE2	1:D:1971:GLN:OE1	2.52	0.42
1:A:1033:VAL:HG21	1:A:1037:LEU:HD12	2.02	0.42
1:A:2107:ILE:HD12	1:A:2107:ILE:O	2.20	0.42
1:A:2166:MET:O	1:A:2170:VAL:HG23	2.18	0.42
1:A:2355:ASP:CG	1:A:2357:SER:HG	2.28	0.42
1:A:3162:ALA:HB2	1:A:3240:MET:HE1	2.01	0.42
1:B:2107:ILE:O	1:B:2107:ILE:HD12	2.19	0.42
1:B:4001:MET:SD	1:B:4002:LEU:HD22	2.60	0.42
1:C:730:LEU:CD1	2:I:8:ILE:HG23	2.50	0.42
1:C:802:PHE:O	1:C:803:LEU:HD23	2.20	0.42
1:C:1000:ALA:HB1	1:C:1046:ASN:ND2	2.34	0.42
1:D:275:TRP:CH2	1:D:316:LEU:HD21	2.54	0.42
1:D:2551:VAL:CG1	1:D:2572:LEU:HD13	2.50	0.42
1:D:3162:ALA:HB2	1:D:3240:MET:HE1	2.01	0.42
1:D:4001:MET:SD	1:D:4002:LEU:HD22	2.60	0.42
2:I:8:ILE:HD11	2:I:74:LYS:HB2	1.99	0.42
1:A:2551:VAL:CG1	1:A:2572:LEU:HD13	2.50	0.42
1:A:4883:MET:HE1	1:A:4888:PHE:HD1	1.83	0.42
1:C:4035:ASP:OD1	1:C:4039:LYS:NZ	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:ASP:OD1	1:D:557:TRP:N	2.52	0.42
1:D:785:ASP:OD1	1:D:785:ASP:N	2.53	0.42
1:D:4883:MET:HE1	1:D:4888:PHE:HD1	1.84	0.42
1:A:189:GLU:OE1	1:B:2417:ARG:NH2	2.52	0.42
1:A:909:ASP:OD1	1:A:910:ASP:N	2.52	0.42
1:A:929:ARG:NH2	1:A:932:ASN:OD1	2.47	0.42
1:B:365:HIS:O	1:B:369:GLY:N	2.46	0.42
1:C:1157:GLN:OE1	1:C:1157:GLN:N	2.52	0.42
1:D:1848:GLU:OE2	1:D:1850:SER:OG	2.35	0.42
1:A:3960:ASP:OD1	1:A:3962:SER:N	2.44	0.42
1:B:721:ASP:N	1:B:721:ASP:OD1	2.51	0.42
1:B:805:GLY:N	1:B:809:GLY:O	2.47	0.42
1:B:951:GLY:C	1:B:952:ILE:HD12	2.45	0.42
1:B:1098:ALA:O	1:B:1101:TRP:NE1	2.43	0.42
1:B:1708:ILE:O	1:B:1713:SER:N	2.47	0.42
1:B:3259:ARG:O	1:B:3261:GLU:N	2.53	0.42
1:C:785:ASP:OD1	1:C:785:ASP:N	2.53	0.42
1:C:1428:TYR:OH	1:C:1444:GLY:O	2.36	0.42
1:D:230:GLY:CA	1:D:289:ILE:HD11	2.50	0.42
1:A:924:LEU:HD22	1:A:928:GLU:OE2	2.19	0.42
1:A:3214:MET:HA	1:A:3217:ILE:HG22	2.02	0.42
1:B:2481:ASP:OD1	1:B:2482:PHE:N	2.52	0.42
1:C:230:GLY:CA	1:C:289:ILE:HD11	2.50	0.42
1:C:3214:MET:HA	1:C:3217:ILE:HG22	2.02	0.42
1:C:3233:MET:SD	1:C:3233:MET:N	2.84	0.42
1:D:1000:ALA:HB1	1:D:1046:ASN:ND2	2.34	0.42
1:D:4186:GLU:OE1	1:D:4948:TRP:NE1	2.51	0.42
1:A:1939:GLN:NE2	1:A:1971:GLN:OE1	2.53	0.42
1:B:586:LEU:HD21	1:B:625:VAL:HG21	2.02	0.42
1:B:2230:SER:OG	1:B:2233:MET:SD	2.74	0.42
1:B:3214:MET:HA	1:B:3217:ILE:HG22	2.02	0.42
1:C:951:GLY:C	1:C:952:ILE:HD12	2.45	0.42
1:C:1265:HIS:O	1:C:1288:LYS:NZ	2.48	0.42
1:D:2107:ILE:HD12	1:D:2107:ILE:O	2.19	0.42
1:D:2174:MET:HE1	1:D:2178:LEU:HD13	2.00	0.42
1:D:2580:ARG:NH2	1:D:2583:MET:SD	2.93	0.42
1:A:598:ILE:HG12	1:A:636:LEU:HD23	2.02	0.42
1:A:951:GLY:C	1:A:952:ILE:HD12	2.45	0.42
1:A:2481:ASP:OD1	1:A:2482:PHE:N	2.52	0.42
1:A:3394:LEU:HG	1:A:3472:LEU:HD11	2.01	0.42
1:B:117:HIS:O	1:B:162:ILE:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLY:CA	1:B:289:ILE:HD11	2.50	0.42
1:B:1000:ALA:HB1	1:B:1046:ASN:ND2	2.34	0.42
1:C:1431:ARG:NH2	1:C:1507:GLU:OE1	2.53	0.42
1:C:3162:ALA:HB2	1:C:3240:MET:HE1	2.01	0.42
1:D:732:LEU:HD22	1:D:779:PHE:CE2	2.55	0.42
1:D:1431:ARG:NH2	1:D:1507:GLU:OE1	2.53	0.42
1:D:3199:ASN:O	1:D:3201:GLU:N	2.52	0.42
1:A:1287:GLN:NE2	1:A:1295:ASN:OD1	2.53	0.42
1:B:802:PHE:O	1:B:803:LEU:HD23	2.20	0.42
1:B:2925:LEU:HD21	1:B:3003:VAL:HG22	2.02	0.42
1:C:93:VAL:HG12	1:C:95:VAL:HG23	2.02	0.42
1:C:2551:VAL:CG1	1:C:2572:LEU:HD13	2.50	0.42
1:C:3259:ARG:O	1:C:3261:GLU:N	2.53	0.42
1:A:230:GLY:CA	1:A:289:ILE:HD11	2.50	0.41
1:A:730:LEU:CD1	2:G:8:ILE:HG23	2.50	0.41
1:A:1914:ASP:OD1	1:A:2089:ARG:NH1	2.47	0.41
1:A:3259:ARG:O	1:A:3261:GLU:N	2.53	0.41
1:C:924:LEU:HD22	1:C:928:GLU:OE2	2.20	0.41
1:D:924:LEU:HD22	1:D:928:GLU:OE2	2.19	0.41
1:D:1287:GLN:NE2	1:D:1295:ASN:OD1	2.53	0.41
1:D:2481:ASP:OD1	1:D:2482:PHE:N	2.52	0.41
1:A:93:VAL:HG12	1:A:95:VAL:HG23	2.03	0.41
1:A:2580:ARG:NH2	1:A:2583:MET:SD	2.93	0.41
1:A:3199:ASN:O	1:A:3201:GLU:N	2.52	0.41
1:A:4501:ARG:NH2	1:A:4744:ASP:OD1	2.50	0.41
1:B:1033:VAL:HG21	1:B:1037:LEU:HD12	2.02	0.41
1:B:2789:GLU:N	1:B:2789:GLU:OE1	2.53	0.41
1:C:281:ARG:NH2	1:C:345:GLU:OE1	2.52	0.41
1:C:598:ILE:HG12	1:C:636:LEU:HD23	2.02	0.41
1:C:909:ASP:OD1	1:C:910:ASP:N	2.52	0.41
1:C:1287:GLN:NE2	1:C:1295:ASN:OD1	2.53	0.41
1:C:1792:THR:HG21	1:C:1825:LEU:CD1	2.50	0.41
1:C:2107:ILE:HD12	1:C:2107:ILE:O	2.19	0.41
1:C:4099:VAL:HG22	1:C:4132:LEU:HD23	2.02	0.41
1:D:730:LEU:CD1	2:J:8:ILE:HG23	2.50	0.41
1:D:2716:LEU:HD13	1:D:2778:LEU:HD22	2.02	0.41
1:D:2925:LEU:HD21	1:D:3003:VAL:HG22	2.02	0.41
1:D:3807:PHE:O	1:D:3811:ASN:ND2	2.45	0.41
1:A:681:HIS:O	1:A:799:LYS:N	2.52	0.41
1:A:1786:ASP:OD1	1:A:1787:ILE:N	2.49	0.41
1:A:1792:THR:HG21	1:A:1825:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LEU:CD1	2:H:8:ILE:HG23	2.50	0.41
1:B:3394:LEU:HG	1:B:3472:LEU:HD11	2.01	0.41
1:C:586:LEU:HD21	1:C:625:VAL:HG21	2.02	0.41
1:C:1786:ASP:OD1	1:C:1787:ILE:N	2.49	0.41
1:D:3214:MET:HA	1:D:3217:ILE:HG22	2.02	0.41
2:H:67:MET:HE2	2:H:71:GLN:O	2.21	0.41
1:A:732:LEU:HD22	1:A:779:PHE:CE2	2.55	0.41
1:A:785:ASP:OD1	1:A:785:ASP:N	2.53	0.41
1:A:1431:ARG:NH2	1:A:1507:GLU:OE1	2.53	0.41
1:A:4020:LEU:HD22	1:A:4127:TYR:CE2	2.56	0.41
1:B:426:PHE:HB2	1:B:497:LEU:HD21	2.03	0.41
1:B:2398:LEU:HB3	1:B:2422:LEU:HD22	2.03	0.41
1:B:4189:VAL:HG11	1:B:4948:TRP:CH2	2.55	0.41
1:B:4949:GLU:OE1	1:B:4949:GLU:N	2.53	0.41
1:C:117:HIS:O	1:C:162:ILE:HD12	2.20	0.41
1:C:426:PHE:HB2	1:C:497:LEU:HD21	2.02	0.41
1:C:2789:GLU:N	1:C:2789:GLU:OE1	2.53	0.41
1:D:951:GLY:C	1:D:952:ILE:HD12	2.45	0.41
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.85	0.41
1:A:586:LEU:HD21	1:A:625:VAL:HG21	2.02	0.41
1:A:1436:GLN:NE2	1:A:1547:GLN:O	2.50	0.41
1:A:2789:GLU:OE1	1:A:2789:GLU:N	2.53	0.41
1:B:1939:GLN:NE2	1:B:1971:GLN:OE1	2.52	0.41
1:B:2580:ARG:NH2	1:B:2583:MET:SD	2.93	0.41
1:C:2481:ASP:OD1	1:C:2482:PHE:N	2.52	0.41
1:C:2925:LEU:HD21	1:C:3003:VAL:HG22	2.02	0.41
1:C:4189:VAL:HG11	1:C:4948:TRP:CH2	2.55	0.41
1:D:4020:LEU:HD22	1:D:4127:TYR:CE2	2.56	0.41
1:A:1000:ALA:HB1	1:A:1046:ASN:ND2	2.34	0.41
1:B:1431:ARG:NH2	1:B:1507:GLU:OE1	2.53	0.41
1:B:1663:SER:OG	1:B:1705:ASP:OD2	2.28	0.41
1:C:732:LEU:HD22	1:C:779:PHE:CE2	2.55	0.41
1:C:1048:ASP:OD1	1:C:1049:SER:N	2.54	0.41
1:C:4020:LEU:HD22	1:C:4127:TYR:CE2	2.56	0.41
1:D:93:VAL:HG12	1:D:95:VAL:HG23	2.02	0.41
1:D:2367:SER:OG	1:D:2368:SER:N	2.49	0.41
1:D:3975:LYS:O	1:D:3979:VAL:HG23	2.21	0.41
2:I:67:MET:HE2	2:I:71:GLN:O	2.20	0.41
1:A:802:PHE:O	1:A:803:LEU:HD23	2.20	0.41
1:A:1048:ASP:OD1	1:A:1049:SER:N	2.54	0.41
1:A:2399:GLY:O	1:A:2473:ARG:NE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4949:GLU:OE1	1:A:4949:GLU:N	2.53	0.41
1:B:93:VAL:HG12	1:B:95:VAL:HG23	2.02	0.41
1:C:2399:GLY:O	1:C:2473:ARG:NE	2.50	0.41
1:C:2716:LEU:HD13	1:C:2778:LEU:HD22	2.02	0.41
1:C:2951:GLU:OE1	1:C:2951:GLU:N	2.54	0.41
1:D:3259:ARG:O	1:D:3261:GLU:N	2.53	0.41
1:D:4949:GLU:OE1	1:D:4949:GLU:N	2.53	0.41
1:A:1184:ASP:N	1:A:1188:SER:O	2.51	0.41
1:A:4189:VAL:HG11	1:A:4948:TRP:CH2	2.56	0.41
1:B:785:ASP:OD1	1:B:785:ASP:N	2.52	0.41
1:B:1792:THR:HG21	1:B:1825:LEU:CD1	2.50	0.41
1:C:763:ALA:HB3	1:C:764:PRO:C	2.46	0.41
1:C:1033:VAL:HG21	1:C:1037:LEU:HD12	2.02	0.41
1:C:2580:ARG:NH2	1:C:2583:MET:SD	2.93	0.41
1:D:680:ASP:O	1:D:751:THR:HG23	2.20	0.41
1:A:798:ILE:O	1:A:798:ILE:HD12	2.21	0.41
1:A:1721:MET:SD	1:A:2126:ARG:NH1	2.91	0.41
1:A:1963:GLU:O	1:A:1966:SER:OG	2.39	0.41
1:A:2716:LEU:HD13	1:A:2778:LEU:HD22	2.03	0.41
1:A:4136:GLU:O	1:A:4917:TYR:OH	2.34	0.41
1:B:299:HIS:O	1:B:303:GLY:N	2.47	0.41
1:B:598:ILE:HG12	1:B:636:LEU:HD23	2.02	0.41
1:B:2551:VAL:CG1	1:B:2572:LEU:HD13	2.50	0.41
1:B:2699:ASN:OD1	1:B:2700:PHE:N	2.54	0.41
1:B:4020:LEU:HD22	1:B:4127:TYR:CE2	2.56	0.41
1:B:4073:GLU:OE1	1:B:4073:GLU:N	2.50	0.41
1:C:556:ASP:OD1	1:C:557:TRP:N	2.52	0.41
1:C:1184:ASP:N	1:C:1188:SER:O	2.50	0.41
1:C:1472:GLU:OE1	1:C:1472:GLU:N	2.51	0.41
1:C:1990:GLU:OE1	1:C:1990:GLU:N	2.47	0.41
1:C:2177:VAL:HG21	1:C:2191:MET:CG	2.51	0.41
1:C:4949:GLU:N	1:C:4949:GLU:OE1	2.53	0.41
1:D:681:HIS:O	1:D:799:LYS:N	2.52	0.41
1:D:763:ALA:HB3	1:D:764:PRO:C	2.46	0.41
1:D:1792:THR:HG21	1:D:1825:LEU:CD1	2.50	0.41
1:D:1971:GLN:NE2	1:D:3605:ALA:O	2.46	0.41
1:A:680:ASP:O	1:A:751:THR:HG23	2.21	0.41
1:A:1971:GLN:NE2	1:A:3605:ALA:O	2.46	0.41
1:B:763:ALA:HB3	1:B:764:PRO:C	2.46	0.41
1:B:909:ASP:OD1	1:B:910:ASP:N	2.52	0.41
1:B:1265:HIS:O	1:B:1288:LYS:NZ	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:GLN:NE2	1:B:1295:ASN:OD1	2.53	0.41
1:B:4501:ARG:NH2	1:B:4744:ASP:OD1	2.50	0.41
1:C:981:MET:SD	1:C:1056:THR:HG23	2.61	0.41
1:C:3822:GLU:N	1:C:3822:GLU:OE1	2.54	0.41
1:D:798:ILE:O	1:D:798:ILE:HD12	2.21	0.41
1:D:1428:TYR:OH	1:D:1444:GLY:O	2.37	0.41
1:D:2791:THR:HG23	1:D:2794:GLY:H	1.86	0.41
1:A:763:ALA:HB3	1:A:764:PRO:C	2.46	0.40
1:A:1637:ASN:OD1	1:A:1637:ASN:N	2.54	0.40
1:A:2925:LEU:HD21	1:A:3003:VAL:HG22	2.02	0.40
1:B:1048:ASP:OD1	1:B:1049:SER:N	2.54	0.40
1:B:3199:ASN:O	1:B:3201:GLU:N	2.52	0.40
1:C:280:LEU:HD21	1:C:294:PRO:HG2	2.03	0.40
1:C:2161:MET:HE2	1:C:2161:MET:H	1.86	0.40
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.85	0.40
1:D:101:MET:SD	1:D:102:MET:N	2.95	0.40
1:D:204:ASP:N	1:D:204:ASP:OD1	2.53	0.40
1:D:280:LEU:HD21	1:D:294:PRO:HG2	2.03	0.40
1:D:308:LEU:HD22	1:D:393:MET:HG2	2.03	0.40
1:D:1432:ILE:HD12	1:D:1432:ILE:H	1.86	0.40
1:D:2517:ARG:O	1:D:2521:THR:OG1	2.21	0.40
1:D:2789:GLU:OE1	1:D:2789:GLU:N	2.54	0.40
1:D:4189:VAL:HG11	1:D:4948:TRP:CH2	2.55	0.40
1:A:1432:ILE:HD12	1:A:1432:ILE:H	1.86	0.40
1:A:2177:VAL:HG21	1:A:2191:MET:CG	2.52	0.40
1:B:308:LEU:HD22	1:B:393:MET:HG2	2.03	0.40
1:B:717:GLY:N	1:B:720:ASP:OD2	2.44	0.40
1:C:680:ASP:O	1:C:751:THR:HG23	2.20	0.40
1:C:717:GLY:N	1:C:720:ASP:OD2	2.45	0.40
1:C:2592:VAL:HG21	1:C:2639:LEU:HG	2.03	0.40
1:D:598:ILE:HG12	1:D:636:LEU:HD23	2.02	0.40
1:D:692:HIS:N	1:D:795:SER:OG	2.53	0.40
1:D:2388:MET:HE2	1:D:2388:MET:C	2.47	0.40
1:D:2951:GLU:OE1	1:D:2951:GLU:N	2.54	0.40
2:J:8:ILE:HD11	2:J:74:LYS:HB2	2.03	0.40
2:J:15:THR:HB	2:J:69:LEU:HD23	2.03	0.40
1:A:556:ASP:OD1	1:A:557:TRP:N	2.52	0.40
1:A:2699:ASN:OD1	1:A:2700:PHE:N	2.54	0.40
1:B:732:LEU:HD22	1:B:779:PHE:CE2	2.55	0.40
1:B:3975:LYS:O	1:B:3979:VAL:HG23	2.21	0.40
1:C:3199:ASN:O	1:C:3201:GLU:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:MET:SD	1:D:309:MET:N	2.84	0.40
1:D:613:VAL:O	1:D:616:SER:OG	2.27	0.40
1:D:1033:VAL:HG21	1:D:1037:LEU:HD12	2.02	0.40
1:D:1048:ASP:OD1	1:D:1049:SER:N	2.54	0.40
1:D:2161:MET:HE2	1:D:2161:MET:H	1.86	0.40
1:D:2592:VAL:HG21	1:D:2639:LEU:HG	2.03	0.40
1:A:426:PHE:HB2	1:A:497:LEU:HD21	2.03	0.40
1:A:2388:MET:HE2	1:A:2388:MET:C	2.47	0.40
1:A:3038:THR:O	1:A:3038:THR:HG22	2.22	0.40
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.85	0.40
1:B:280:LEU:HD21	1:B:294:PRO:HG2	2.04	0.40
1:C:829:LYS:NZ	1:C:1037:LEU:O	2.48	0.40
1:C:2699:ASN:OD1	1:C:2700:PHE:N	2.54	0.40
1:C:3038:THR:O	1:C:3038:THR:HG22	2.21	0.40
1:D:365:HIS:O	1:D:369:GLY:N	2.46	0.40
1:D:981:MET:SD	1:D:1056:THR:HG23	2.61	0.40
1:D:1245:ARG:NH1	1:D:1809:ASP:O	2.55	0.40
1:D:2177:VAL:HG21	1:D:2191:MET:CG	2.52	0.40
2:J:67:MET:HE2	2:J:71:GLN:O	2.21	0.40
1:A:1308:ILE:HD11	1:A:1567:LEU:CD1	2.52	0.40
1:A:2174:MET:HE1	1:A:2192:VAL:HG13	2.03	0.40
1:B:101:MET:SD	1:B:102:MET:N	2.95	0.40
1:B:1963:GLU:O	1:B:1966:SER:OG	2.40	0.40
1:B:2161:MET:HE2	1:B:2161:MET:H	1.87	0.40
1:B:2592:VAL:HG21	1:B:2639:LEU:HG	2.03	0.40
1:C:101:MET:SD	1:C:102:MET:N	2.95	0.40
1:C:1637:ASN:OD1	1:C:1637:ASN:N	2.55	0.40
1:C:3657:MET:HA	1:C:3657:MET:HE3	2.04	0.40
1:D:161:THR:HG23	1:D:186:VAL:HG12	2.04	0.40
1:D:586:LEU:HD21	1:D:625:VAL:HG21	2.02	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	4193/4966 (84%)	4044 (96%)	149 (4%)	0	100	100
1	B	4193/4966 (84%)	4044 (96%)	149 (4%)	0	100	100
1	C	4193/4966 (84%)	4044 (96%)	149 (4%)	0	100	100
1	D	4193/4966 (84%)	4044 (96%)	149 (4%)	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
2	J	105/176 (60%)	99 (94%)	6 (6%)	0	100	100
All	All	17192/20568 (84%)	16572 (96%)	620 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3695/4355 (85%)	3572 (97%)	123 (3%)	33	55
1	B	3695/4355 (85%)	3570 (97%)	125 (3%)	32	55
1	C	3695/4355 (85%)	3569 (97%)	126 (3%)	32	55
1	D	3695/4355 (85%)	3567 (96%)	128 (4%)	32	54
2	G	88/140 (63%)	83 (94%)	5 (6%)	18	34
2	H	88/140 (63%)	83 (94%)	5 (6%)	18	34
2	I	88/140 (63%)	83 (94%)	5 (6%)	18	34
2	J	88/140 (63%)	83 (94%)	5 (6%)	18	34
All	All	15132/17980 (84%)	14610 (97%)	522 (3%)	33	55

All (522) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	65	CYS
1	A	66	THR
1	A	88	LYS
1	A	174	LYS
1	A	181	LEU
1	A	234	LEU
1	A	236	LEU
1	A	246	THR
1	A	280	LEU
1	A	311	ASP
1	A	372	LEU
1	A	390	LYS
1	A	392	ILE
1	A	414	ARG
1	A	536	LEU
1	A	537	LEU
1	A	555	LEU
1	A	558	LEU
1	A	575	LEU
1	A	615	CYS
1	A	617	LEU
1	A	636	LEU
1	A	757	CYS
1	A	758	CYS
1	A	770	ILE
1	A	778	MET
1	A	827	LEU
1	A	881	ILE
1	A	890	HIS
1	A	928	GLU
1	A	935	MET
1	A	971	GLN
1	A	1013	ARG
1	A	1037	LEU
1	A	1144	ARG
1	A	1164	CYS
1	A	1177	LEU
1	A	1180	GLU
1	A	1277	ILE
1	A	1305	SER
1	A	1495	SER
1	A	1510	CYS

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Mol	Chain	Res	Type
1	A	1593	SER
1	A	1598	SER
1	A	1652	LEU
1	A	1661	LEU
1	A	1677	LEU
1	A	1681	VAL
1	A	1695	MET
1	A	1706	LEU
1	A	1722	MET
1	A	1795	MET
1	A	1832	MET
1	A	1893	LEU
1	A	1908	LEU
1	A	1910	GLN
1	A	1932	VAL
1	A	2107	ILE
1	A	2141	MET
1	A	2160	LEU
1	A	2166	MET
1	A	2172	GLU
1	A	2178	LEU
1	A	2195	CYS
1	A	2325	ARG
1	A	2388	MET
1	A	2397	LEU
1	A	2425	LEU
1	A	2471	LEU
1	A	2519	LEU
1	A	2544	ILE
1	A	2576	CYS
1	A	2587	LEU
1	A	2590	ARG
1	A	2645	TRP
1	A	2684	TYR
1	A	2687	MET
1	A	2712	ILE
1	A	2733	MET
1	A	2745	ILE
1	A	2781	MET
1	A	2903	SER
1	A	2911	LEU
1	A	2926	GLN

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Mol	Chain	Res	Type
1	A	2928	LEU
1	A	2929	ILE
1	A	2973	TYR
1	A	3020	LEU
1	A	3060	LEU
1	A	3081	HIS
1	A	3178	ASN
1	A	3186	ARG
1	A	3201	GLU
1	A	3262	MET
1	A	3272	MET
1	A	3295	MET
1	A	3312	GLN
1	A	3322	MET
1	A	3357	GLU
1	A	3703	ASP
1	A	3826	GLU
1	A	3853	PHE
1	A	3865	THR
1	A	3866	THR
1	A	3905	PHE
1	A	4012	ILE
1	A	4017	ASP
1	A	4039	LYS
1	A	4063	GLU
1	A	4084	LYS
1	A	4119	GLU
1	A	4123	SER
1	A	4195	THR
1	A	4509	PHE
1	A	4560	LEU
1	A	4561	GLU
1	A	4586	ILE
1	A	4632	LEU
1	A	4807	ASP
1	A	4918	LEU
1	A	4921	LEU
1	A	4947	CYS
1	B	28	ILE
1	B	65	CYS
1	B	66	THR
1	B	76	ARG

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Mol	Chain	Res	Type
1	B	79	GLN
1	B	88	LYS
1	B	174	LYS
1	B	181	LEU
1	B	234	LEU
1	B	236	LEU
1	B	246	THR
1	B	280	LEU
1	B	311	ASP
1	B	372	LEU
1	B	390	LYS
1	B	392	ILE
1	B	414	ARG
1	B	536	LEU
1	B	537	LEU
1	B	555	LEU
1	B	558	LEU
1	B	575	LEU
1	B	615	CYS
1	B	617	LEU
1	B	636	LEU
1	B	757	CYS
1	B	758	CYS
1	B	770	ILE
1	B	778	MET
1	B	827	LEU
1	B	881	ILE
1	B	890	HIS
1	B	928	GLU
1	B	935	MET
1	B	971	GLN
1	B	1013	ARG
1	B	1037	LEU
1	B	1144	ARG
1	B	1164	CYS
1	B	1177	LEU
1	B	1180	GLU
1	B	1277	ILE
1	B	1305	SER
1	B	1495	SER
1	B	1510	CYS
1	B	1593	SER

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Mol	Chain	Res	Type
1	B	1598	SER
1	B	1652	LEU
1	B	1661	LEU
1	B	1677	LEU
1	B	1681	VAL
1	B	1695	MET
1	B	1706	LEU
1	B	1722	MET
1	B	1795	MET
1	B	1832	MET
1	B	1893	LEU
1	B	1908	LEU
1	B	1910	GLN
1	B	1932	VAL
1	B	2107	ILE
1	B	2141	MET
1	B	2160	LEU
1	B	2166	MET
1	B	2172	GLU
1	B	2178	LEU
1	B	2195	CYS
1	B	2325	ARG
1	B	2388	MET
1	B	2397	LEU
1	B	2425	LEU
1	B	2471	LEU
1	B	2519	LEU
1	B	2544	ILE
1	B	2576	CYS
1	B	2587	LEU
1	B	2590	ARG
1	B	2645	TRP
1	B	2684	TYR
1	B	2687	MET
1	B	2712	ILE
1	B	2733	MET
1	B	2745	ILE
1	B	2781	MET
1	B	2903	SER
1	B	2911	LEU
1	B	2926	GLN
1	B	2928	LEU

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Mol	Chain	Res	Type
1	B	2929	ILE
1	B	2973	TYR
1	B	3020	LEU
1	B	3060	LEU
1	B	3081	HIS
1	B	3178	ASN
1	B	3186	ARG
1	B	3201	GLU
1	B	3262	MET
1	B	3272	MET
1	B	3295	MET
1	B	3312	GLN
1	B	3322	MET
1	B	3357	GLU
1	B	3703	ASP
1	B	3826	GLU
1	B	3853	PHE
1	B	3865	THR
1	B	3866	THR
1	B	3905	PHE
1	B	4012	ILE
1	B	4017	ASP
1	B	4039	LYS
1	B	4063	GLU
1	B	4084	LYS
1	B	4119	GLU
1	B	4123	SER
1	B	4195	THR
1	B	4509	PHE
1	B	4560	LEU
1	B	4561	GLU
1	B	4586	ILE
1	B	4632	LEU
1	B	4807	ASP
1	B	4918	LEU
1	B	4921	LEU
1	B	4947	CYS
1	C	28	ILE
1	C	65	CYS
1	C	66	THR
1	C	76	ARG
1	C	79	GLN

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Mol	Chain	Res	Type
1	C	88	LYS
1	C	174	LYS
1	C	181	LEU
1	C	234	LEU
1	C	236	LEU
1	C	246	THR
1	C	280	LEU
1	C	301	THR
1	C	311	ASP
1	C	372	LEU
1	C	390	LYS
1	C	392	ILE
1	C	414	ARG
1	C	536	LEU
1	C	537	LEU
1	C	555	LEU
1	C	558	LEU
1	C	575	LEU
1	C	617	LEU
1	C	636	LEU
1	C	757	CYS
1	C	758	CYS
1	C	770	ILE
1	C	778	MET
1	C	827	LEU
1	C	881	ILE
1	C	890	HIS
1	C	928	GLU
1	C	935	MET
1	C	971	GLN
1	C	1013	ARG
1	C	1037	LEU
1	C	1144	ARG
1	C	1164	CYS
1	C	1177	LEU
1	C	1180	GLU
1	C	1277	ILE
1	C	1305	SER
1	C	1495	SER
1	C	1510	CYS
1	C	1593	SER
1	C	1598	SER

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Mol	Chain	Res	Type
1	C	1652	LEU
1	C	1661	LEU
1	C	1677	LEU
1	C	1681	VAL
1	C	1695	MET
1	C	1706	LEU
1	C	1722	MET
1	C	1795	MET
1	C	1832	MET
1	C	1893	LEU
1	C	1908	LEU
1	C	1910	GLN
1	C	1932	VAL
1	C	2107	ILE
1	C	2141	MET
1	C	2160	LEU
1	C	2166	MET
1	C	2172	GLU
1	C	2178	LEU
1	C	2195	CYS
1	C	2325	ARG
1	C	2388	MET
1	C	2397	LEU
1	C	2417	ARG
1	C	2425	LEU
1	C	2471	LEU
1	C	2519	LEU
1	C	2544	ILE
1	C	2576	CYS
1	C	2587	LEU
1	C	2590	ARG
1	C	2645	TRP
1	C	2684	TYR
1	C	2687	MET
1	C	2712	ILE
1	C	2733	MET
1	C	2745	ILE
1	C	2781	MET
1	C	2903	SER
1	C	2911	LEU
1	C	2926	GLN
1	C	2928	LEU

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Mol	Chain	Res	Type
1	C	2929	ILE
1	C	2973	TYR
1	C	3020	LEU
1	C	3060	LEU
1	C	3081	HIS
1	C	3178	ASN
1	C	3186	ARG
1	C	3201	GLU
1	C	3262	MET
1	C	3272	MET
1	C	3295	MET
1	C	3312	GLN
1	C	3322	MET
1	C	3357	GLU
1	C	3703	ASP
1	C	3826	GLU
1	C	3853	PHE
1	C	3865	THR
1	C	3866	THR
1	C	3905	PHE
1	C	4012	ILE
1	C	4017	ASP
1	C	4039	LYS
1	C	4084	LYS
1	C	4119	GLU
1	C	4123	SER
1	C	4137	ILE
1	C	4195	THR
1	C	4509	PHE
1	C	4560	LEU
1	C	4561	GLU
1	C	4586	ILE
1	C	4632	LEU
1	C	4807	ASP
1	C	4918	LEU
1	C	4921	LEU
1	C	4947	CYS
1	D	28	ILE
1	D	65	CYS
1	D	66	THR
1	D	76	ARG
1	D	79	GLN

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Mol	Chain	Res	Type
1	D	88	LYS
1	D	174	LYS
1	D	181	LEU
1	D	234	LEU
1	D	236	LEU
1	D	246	THR
1	D	280	LEU
1	D	301	THR
1	D	311	ASP
1	D	361	CYS
1	D	372	LEU
1	D	390	LYS
1	D	392	ILE
1	D	414	ARG
1	D	536	LEU
1	D	537	LEU
1	D	555	LEU
1	D	558	LEU
1	D	575	LEU
1	D	615	CYS
1	D	617	LEU
1	D	636	LEU
1	D	757	CYS
1	D	758	CYS
1	D	770	ILE
1	D	778	MET
1	D	827	LEU
1	D	881	ILE
1	D	890	HIS
1	D	928	GLU
1	D	935	MET
1	D	971	GLN
1	D	1013	ARG
1	D	1037	LEU
1	D	1144	ARG
1	D	1164	CYS
1	D	1177	LEU
1	D	1180	GLU
1	D	1277	ILE
1	D	1305	SER
1	D	1495	SER
1	D	1510	CYS

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Mol	Chain	Res	Type
1	D	1593	SER
1	D	1598	SER
1	D	1652	LEU
1	D	1661	LEU
1	D	1677	LEU
1	D	1681	VAL
1	D	1695	MET
1	D	1706	LEU
1	D	1722	MET
1	D	1795	MET
1	D	1832	MET
1	D	1893	LEU
1	D	1908	LEU
1	D	1910	GLN
1	D	1932	VAL
1	D	2107	ILE
1	D	2141	MET
1	D	2160	LEU
1	D	2166	MET
1	D	2172	GLU
1	D	2178	LEU
1	D	2195	CYS
1	D	2325	ARG
1	D	2388	MET
1	D	2397	LEU
1	D	2425	LEU
1	D	2471	LEU
1	D	2519	LEU
1	D	2544	ILE
1	D	2576	CYS
1	D	2587	LEU
1	D	2590	ARG
1	D	2645	TRP
1	D	2684	TYR
1	D	2687	MET
1	D	2712	ILE
1	D	2733	MET
1	D	2745	ILE
1	D	2781	MET
1	D	2903	SER
1	D	2911	LEU
1	D	2926	GLN

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Mol	Chain	Res	Type
1	D	2928	LEU
1	D	2929	ILE
1	D	2973	TYR
1	D	3020	LEU
1	D	3060	LEU
1	D	3081	HIS
1	D	3178	ASN
1	D	3186	ARG
1	D	3201	GLU
1	D	3262	MET
1	D	3272	MET
1	D	3295	MET
1	D	3312	GLN
1	D	3322	MET
1	D	3357	GLU
1	D	3703	ASP
1	D	3826	GLU
1	D	3853	PHE
1	D	3865	THR
1	D	3866	THR
1	D	3905	PHE
1	D	4012	ILE
1	D	4017	ASP
1	D	4039	LYS
1	D	4063	GLU
1	D	4084	LYS
1	D	4119	GLU
1	D	4123	SER
1	D	4137	ILE
1	D	4195	THR
1	D	4509	PHE
1	D	4560	LEU
1	D	4561	GLU
1	D	4586	ILE
1	D	4632	LEU
1	D	4807	ASP
1	D	4918	LEU
1	D	4921	LEU
1	D	4947	CYS
2	G	3	VAL
2	G	12	ASP
2	G	18	LYS

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Mol	Chain	Res	Type
2	G	26	HIS
2	G	39	SER
2	H	3	VAL
2	H	12	ASP
2	H	18	LYS
2	H	26	HIS
2	H	39	SER
2	I	3	VAL
2	I	12	ASP
2	I	18	LYS
2	I	26	HIS
2	I	39	SER
2	J	3	VAL
2	J	12	ASP
2	J	18	LYS
2	J	26	HIS
2	J	39	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	208	GLN
1	A	313	ASN
1	A	457	GLN
1	A	531	ASN
1	A	651	HIS
1	A	746	GLN
1	A	1267	HIS
1	A	1723	ASN
1	A	2117	ASN
1	A	2208	GLN
1	A	2210	GLN
1	A	2703	GLN
1	A	2952	HIS
1	A	2972	GLN
1	A	2976	ASN
1	A	3317	HIS
1	A	3774	GLN
1	A	3948	HIS
1	A	4008	ASN
1	A	4190	ASN

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Mol	Chain	Res	Type
1	A	4635	ASN
1	A	4765	GLN
1	A	4960	GLN
1	B	23	GLN
1	B	208	GLN
1	B	313	ASN
1	B	531	ASN
1	B	651	HIS
1	B	1267	HIS
1	B	1723	ASN
1	B	2117	ASN
1	B	2208	GLN
1	B	2703	GLN
1	B	2753	GLN
1	B	2952	HIS
1	B	2972	GLN
1	B	3317	HIS
1	B	3917	ASN
1	B	3931	GLN
1	B	3948	HIS
1	B	4008	ASN
1	B	4190	ASN
1	B	4765	GLN
1	B	4960	GLN
1	C	23	GLN
1	C	29	HIS
1	C	457	GLN
1	C	531	ASN
1	C	651	HIS
1	C	1267	HIS
1	C	1294	ASN
1	C	1723	ASN
1	C	2117	ASN
1	C	2208	GLN
1	C	2210	GLN
1	C	2703	GLN
1	C	2952	HIS
1	C	2972	GLN
1	C	3285	ASN
1	C	3317	HIS
1	C	3931	GLN
1	C	3948	HIS

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Mol	Chain	Res	Type
1	C	4008	ASN
1	C	4190	ASN
1	C	4765	GLN
1	C	4960	GLN
1	D	23	GLN
1	D	313	ASN
1	D	531	ASN
1	D	651	HIS
1	D	971	GLN
1	D	1267	HIS
1	D	1723	ASN
1	D	2117	ASN
1	D	2208	GLN
1	D	2210	GLN
1	D	2703	GLN
1	D	2952	HIS
1	D	2972	GLN
1	D	2976	ASN
1	D	3285	ASN
1	D	3317	HIS
1	D	3931	GLN
1	D	3948	HIS
1	D	4008	ASN
1	D	4190	ASN
1	D	4765	GLN
1	D	4960	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

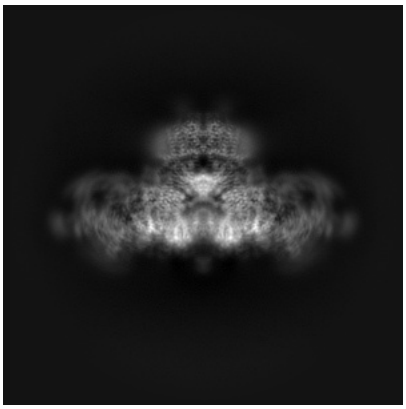
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-80683. These allow visual inspection of the internal detail of the map and identification of artifacts.

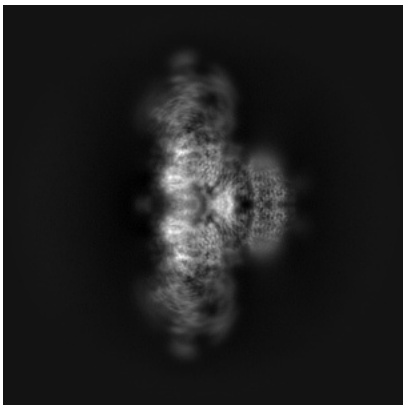
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

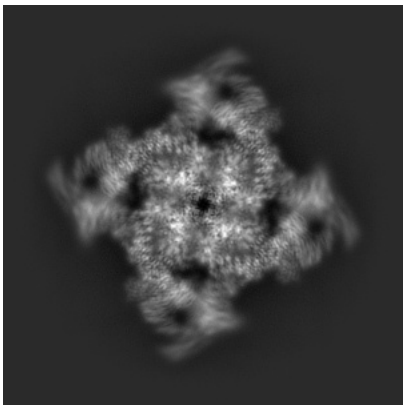
6.1.1 Primary map



X

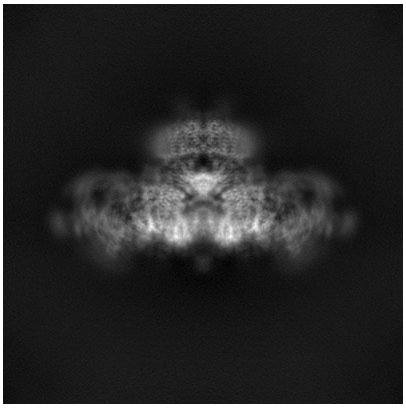


Y

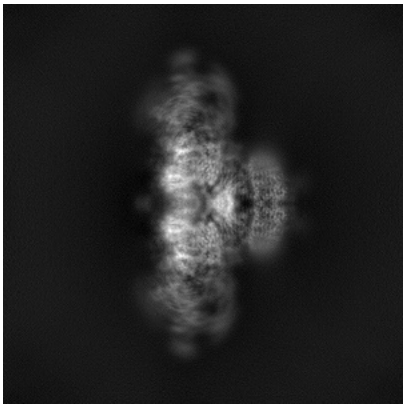


Z

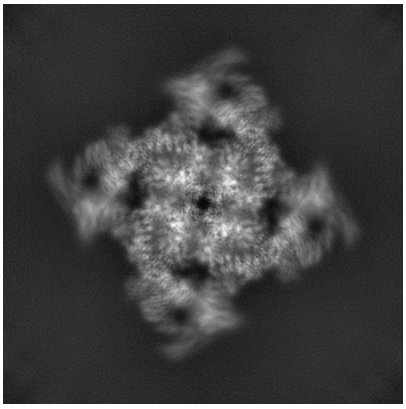
6.1.2 Raw map



X



Y

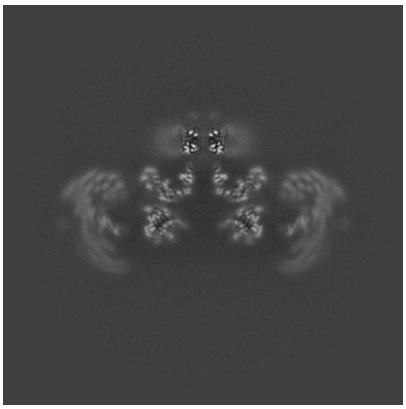


Z

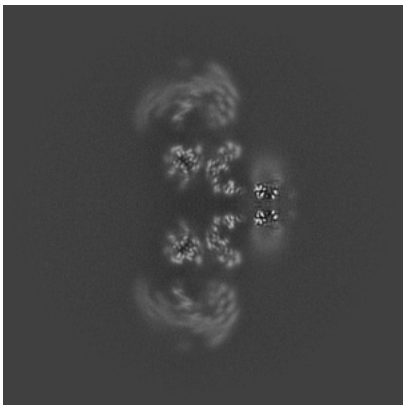
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

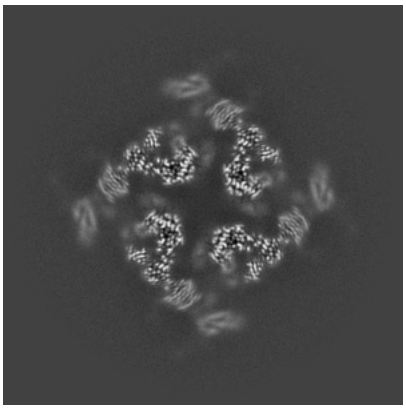
6.2.1 Primary map



X Index: 256

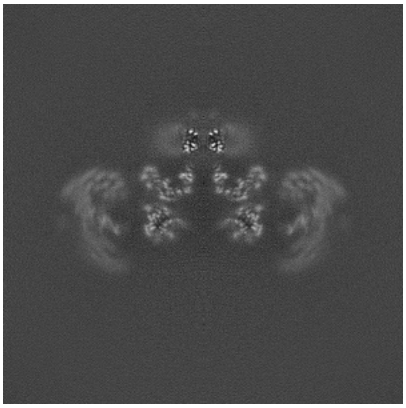


Y Index: 256

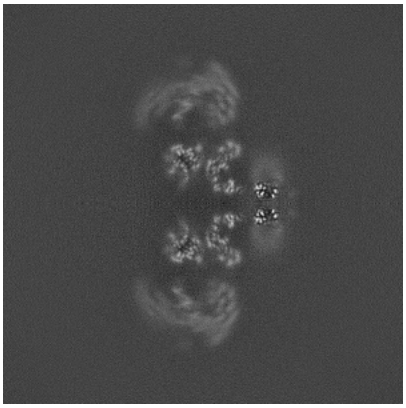


Z Index: 256

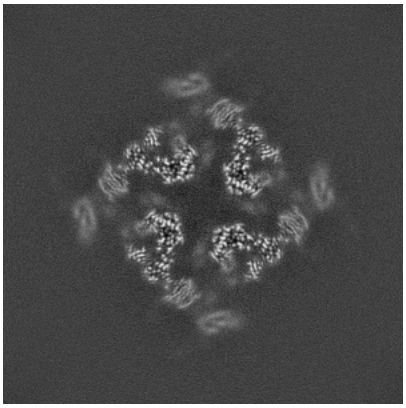
6.2.2 Raw map



X Index: 256



Y Index: 256

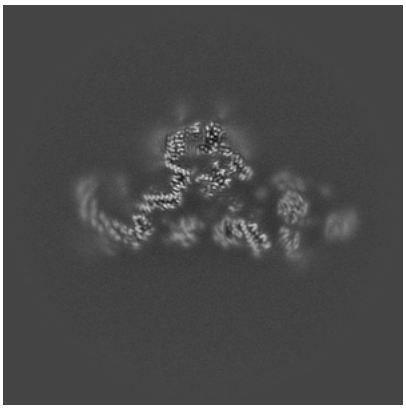


Z Index: 256

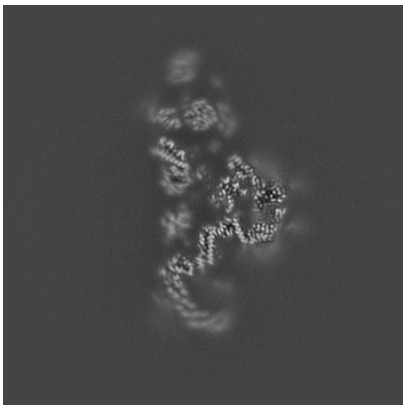
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

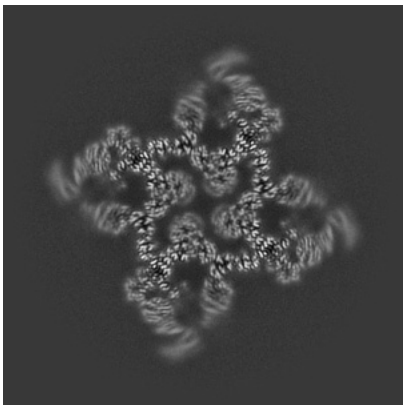
6.3.1 Primary map



X Index: 281

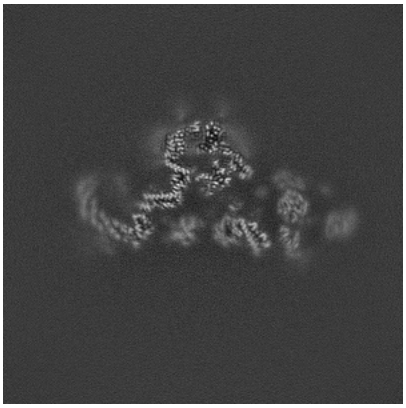


Y Index: 231

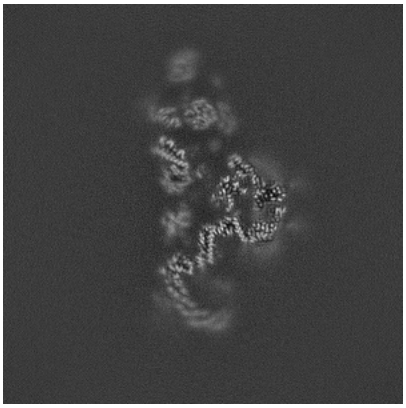


Z Index: 226

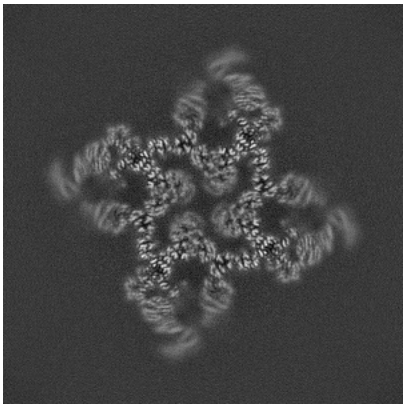
6.3.2 Raw map



X Index: 281



Y Index: 231

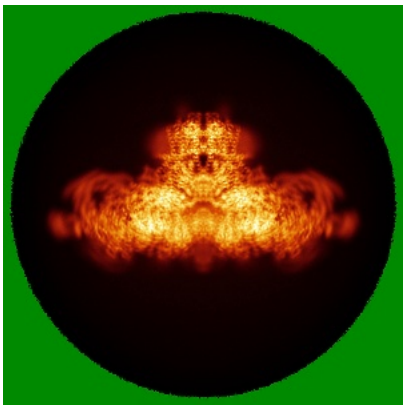


Z Index: 226

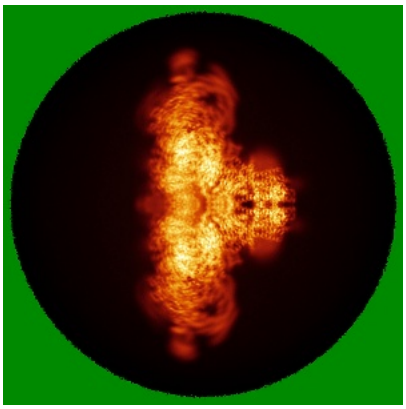
The images above show the largest variance slices of the map in three orthogonal directions.

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

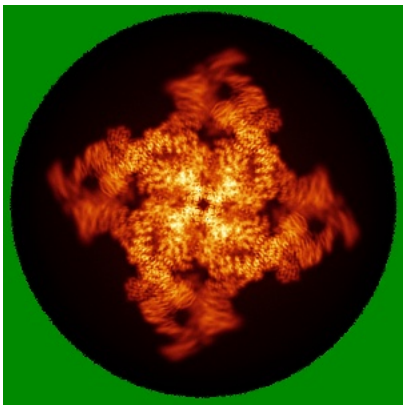
6.4.1 Primary map



X

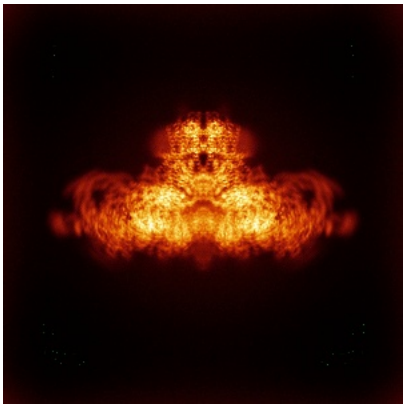


Y

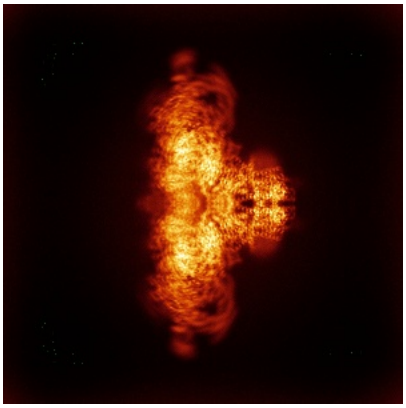


Z

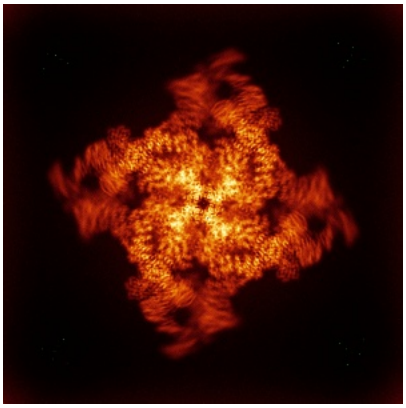
6.4.2 Raw map



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.

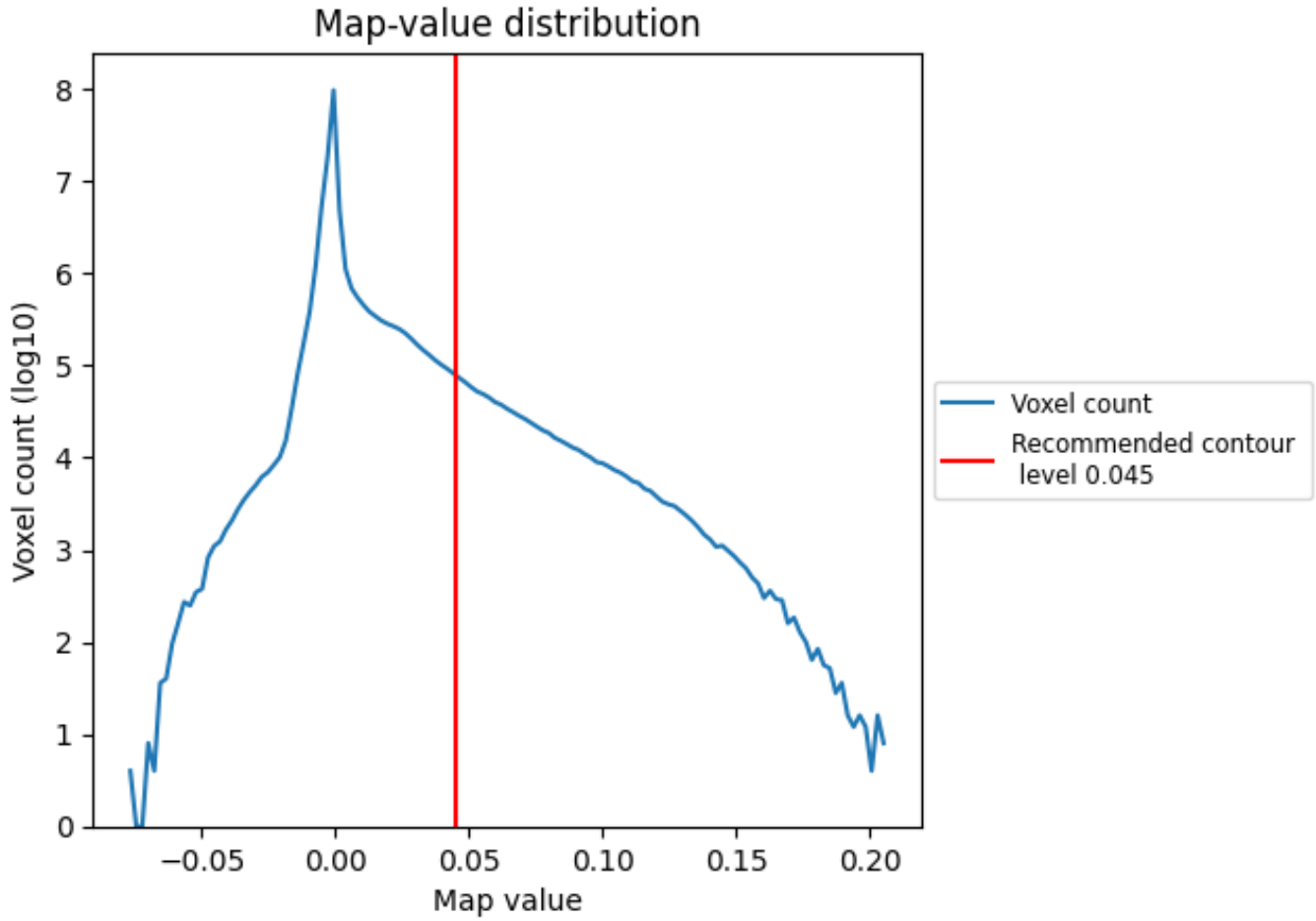
6.6 Mask visualisation (i)

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

7 Map analysis

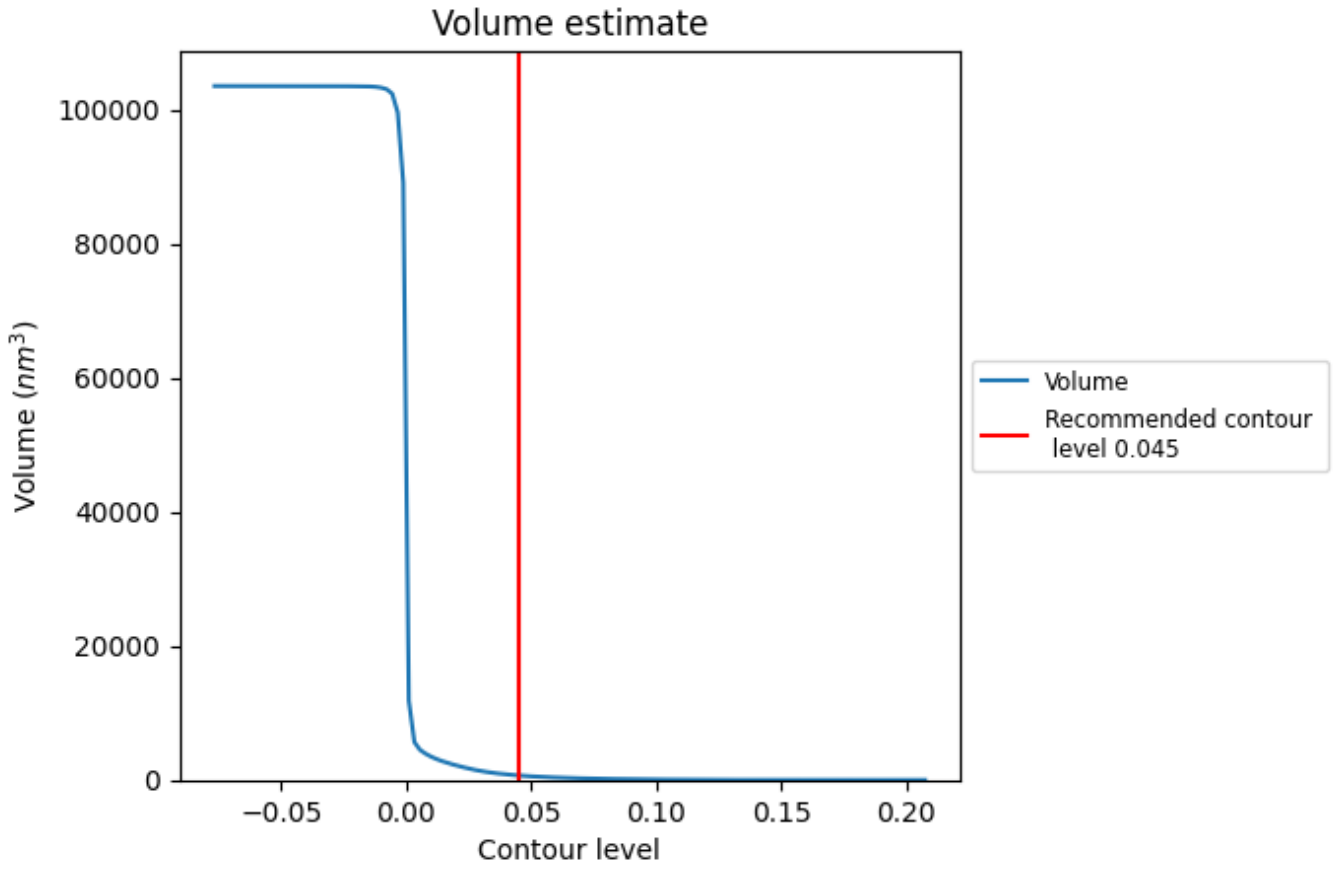
This section contains the results of statistical analysis of the map.

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.

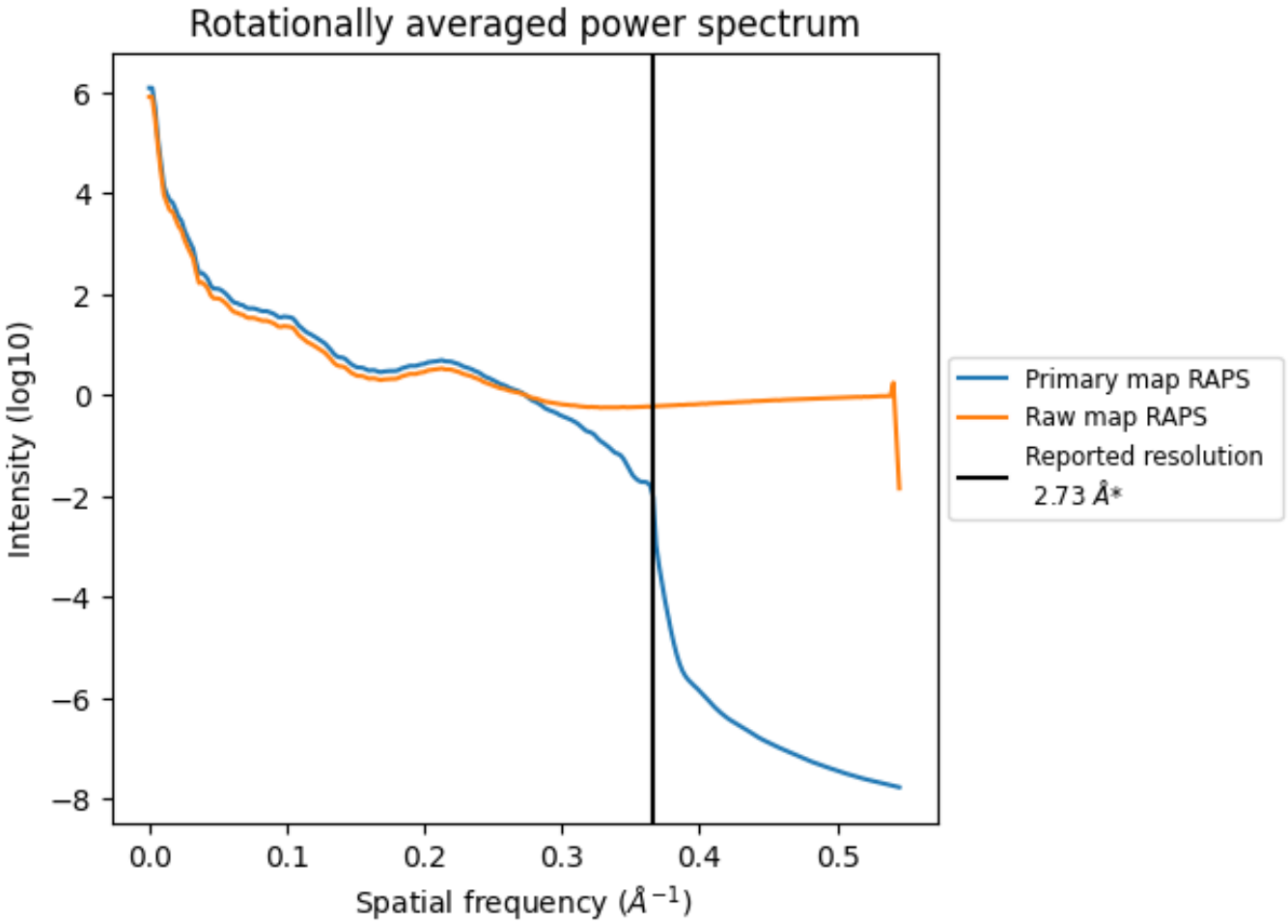
7.2 Volume estimate



The volume at the recommended contour level is 670 nm^3; this corresponds to an approximate mass of 605 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)

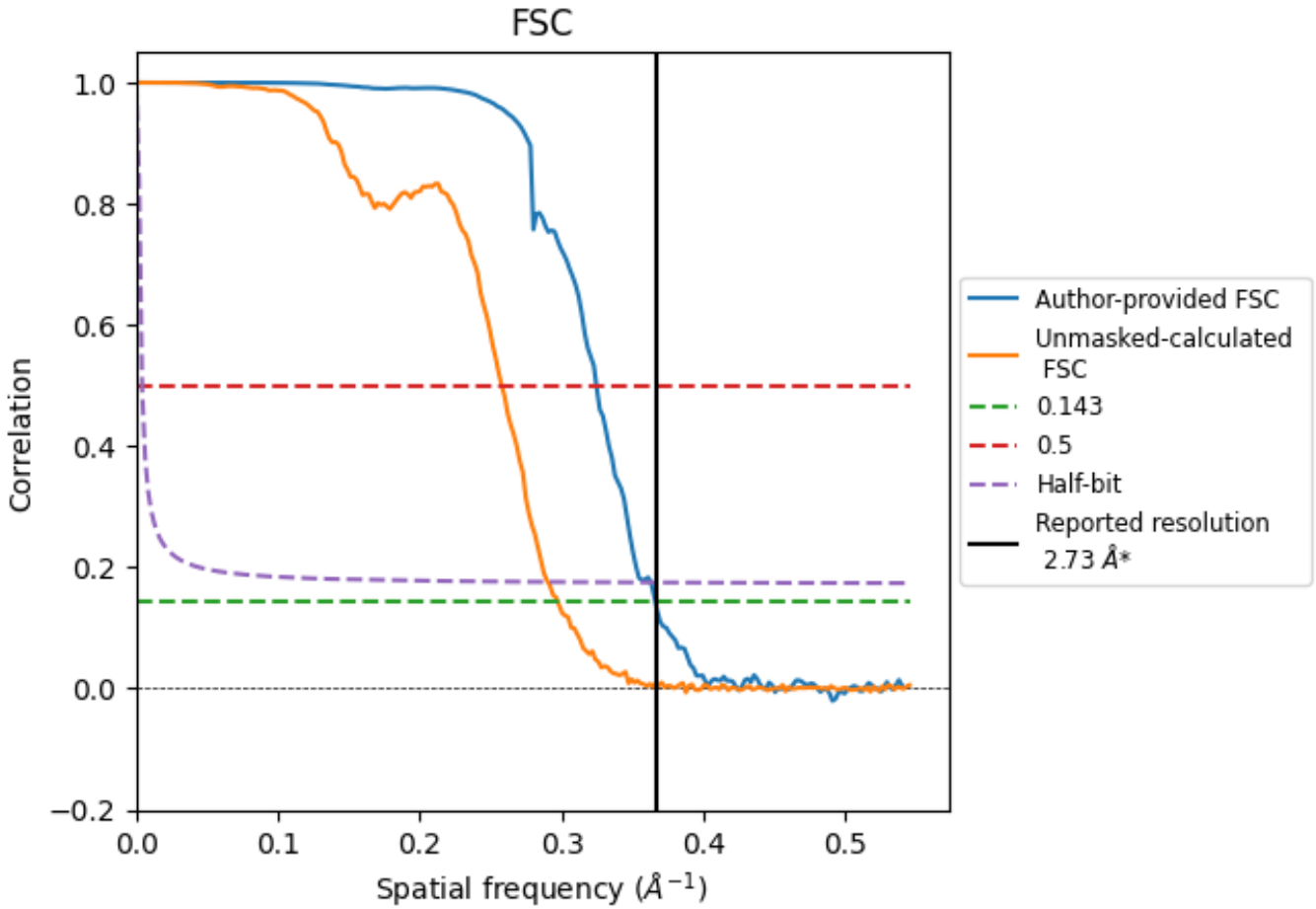


*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

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 0.366 Å^{-1}

8.2 Resolution estimates (i)

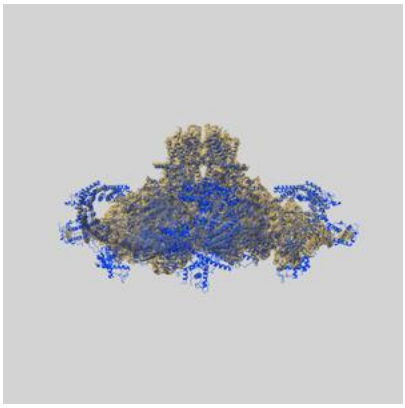
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.08	2.75
Unmasked-calculated*	3.36	3.88	3.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.73 by more than 10 %

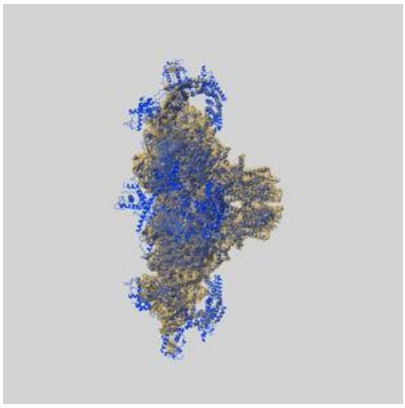
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-80683 and PDB model 26IO. Per-residue inclusion information can be found in section 3 on page 12.

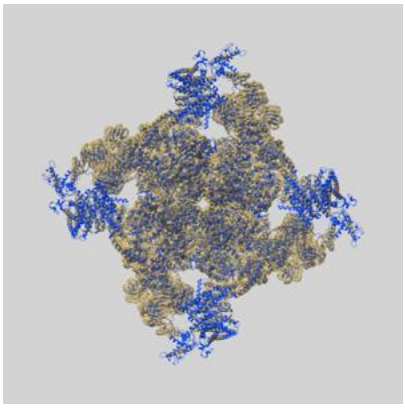
9.1 Map-model overlay



X



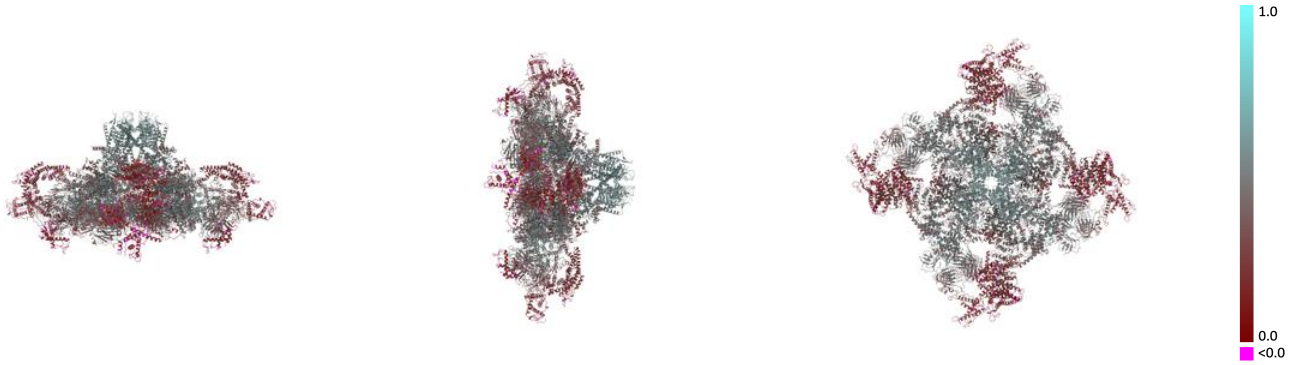
Y



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.

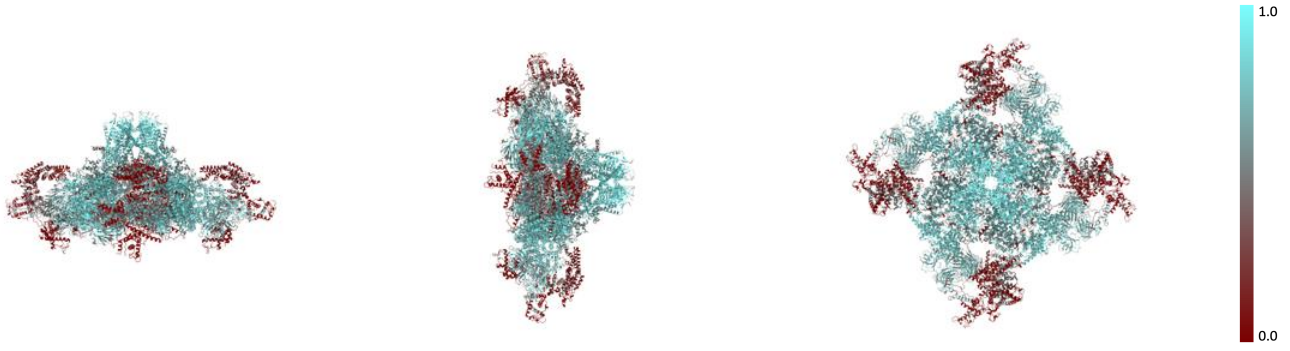
9.2 Q-score mapped to coordinate model (i)



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.

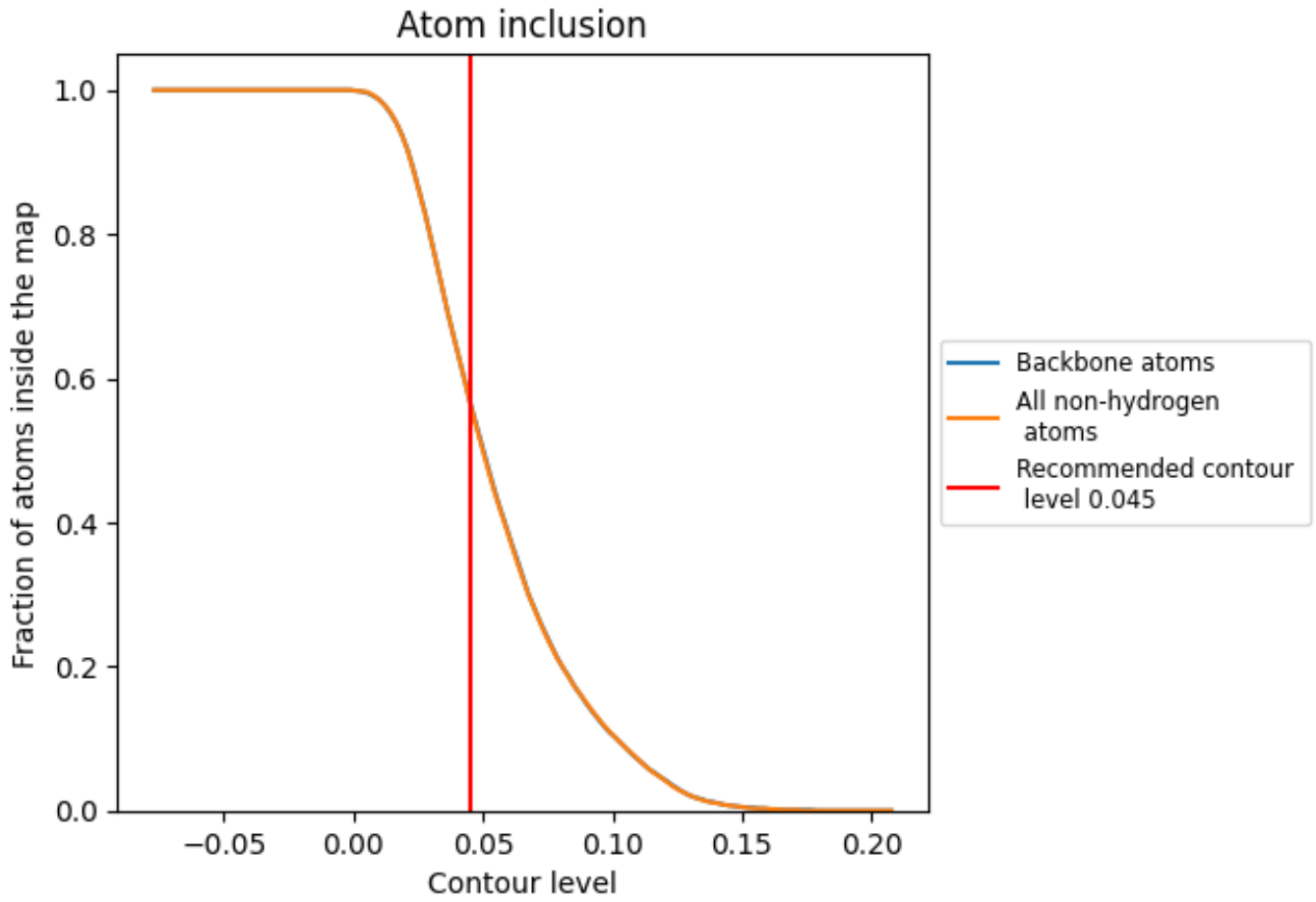
9.3 Atom inclusion mapped to coordinate model (i)



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, 57% of all backbone atoms, 57% 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	0.5680	0.3820
A	0.5720	0.3800
B	0.5720	0.3810
C	0.5720	0.3800
D	0.5720	0.3800
G	0.7150	0.4370
H	0.7150	0.4410
I	0.7160	0.4390
J	0.7150	0.4380

