



Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 04:09 PM JST

PDB ID : 7VMM
EMDB ID : EMD-33936
Title : Structure of recombinant RyR2 (EGTA dataset, class 1, closed state)
Authors : Kobayashi, T.; Tsutsumi, A.; Kurebayashi, N.; Kodama, M.; Kikkawa, M.;
Murayama, T.; Ogawa, H.
Deposited on : 2021-10-09
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

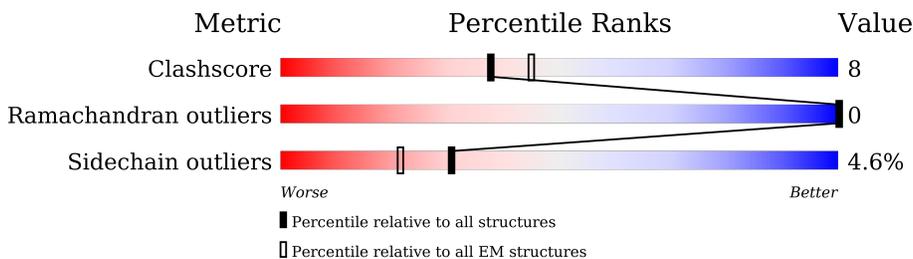
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	26% 65% 15% 19%
1	B	4966	26% 65% 15% 19%
1	C	4966	26% 65% 15% 19%
1	D	4966	26% 65% 15% 19%
2	G	176	44% 16% 39%
2	H	176	45% 15% 39%
2	I	176	43% 18% 39%
2	J	176	45% 16% 39%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 123564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

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

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

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

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-67	MET	-	initiating methionine	UNP P68106
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
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J	-14	HIS	-	expression tag	UNP P68106

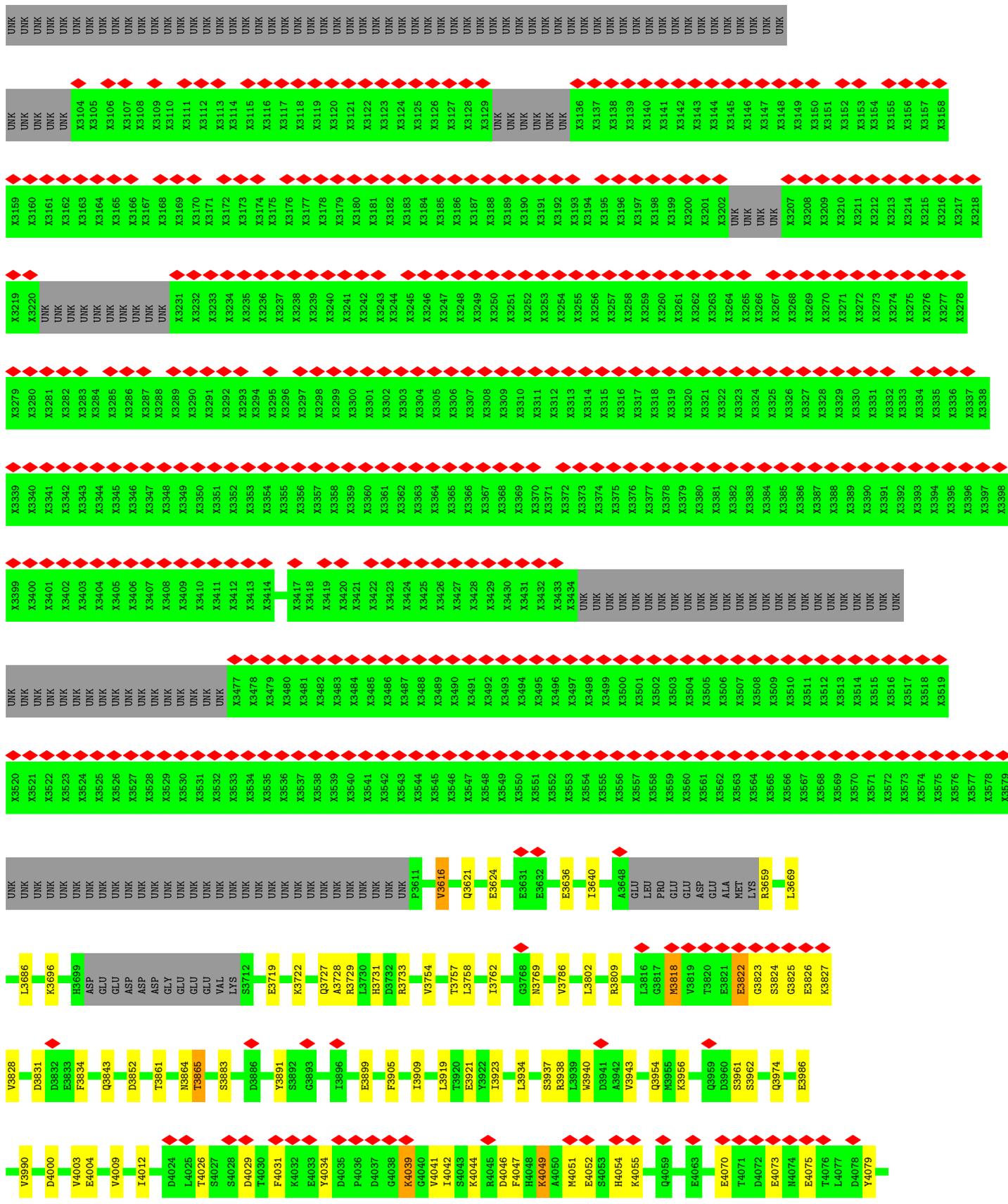
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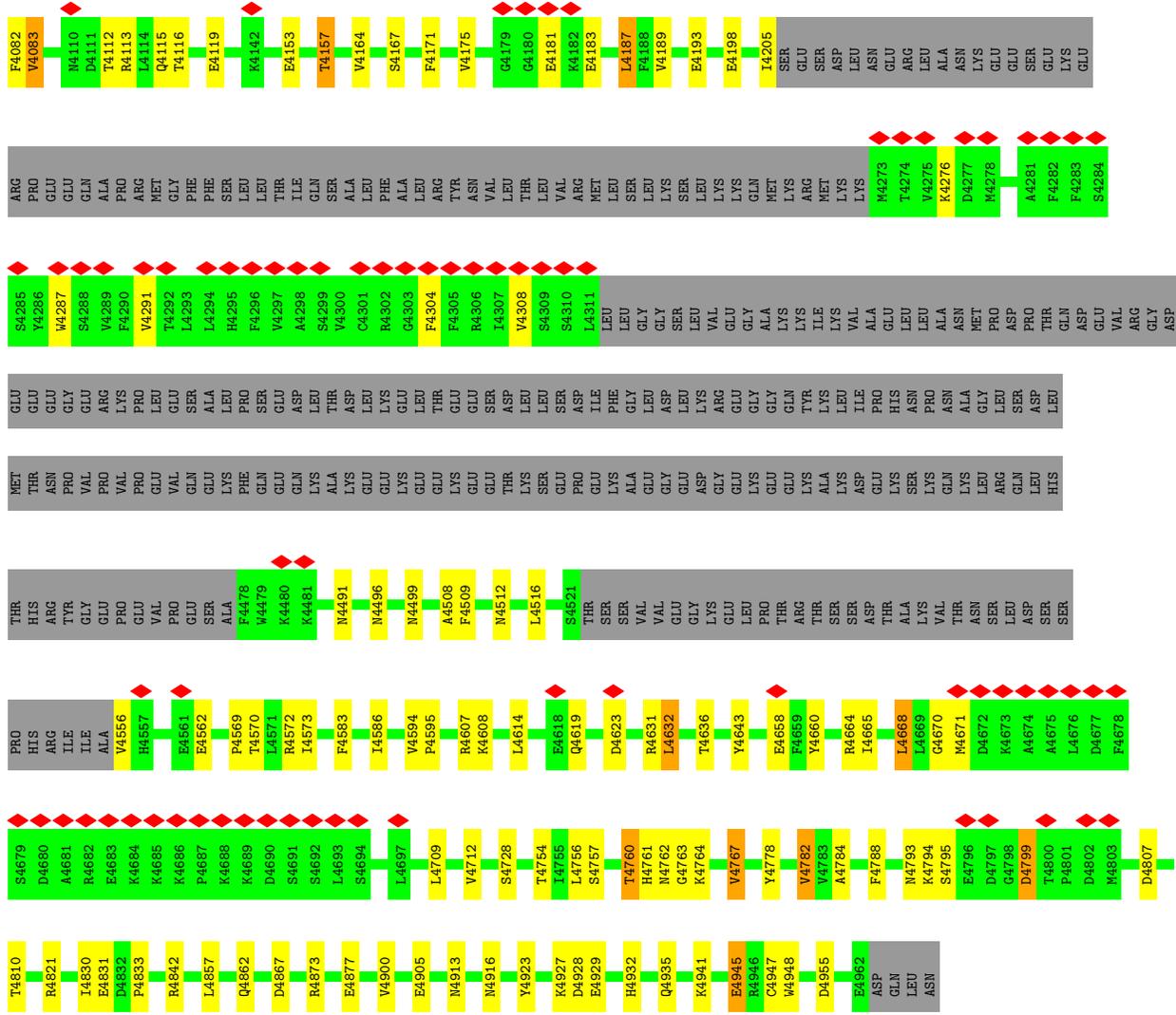
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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	PRO	-	expression tag	UNP P68106
J	-12	GLN	-	expression tag	UNP P68106
J	-11	GLY	-	expression tag	UNP P68106
J	-10	GLN	-	expression tag	UNP P68106
J	-9	ARG	-	expression tag	UNP P68106
J	-8	GLU	-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

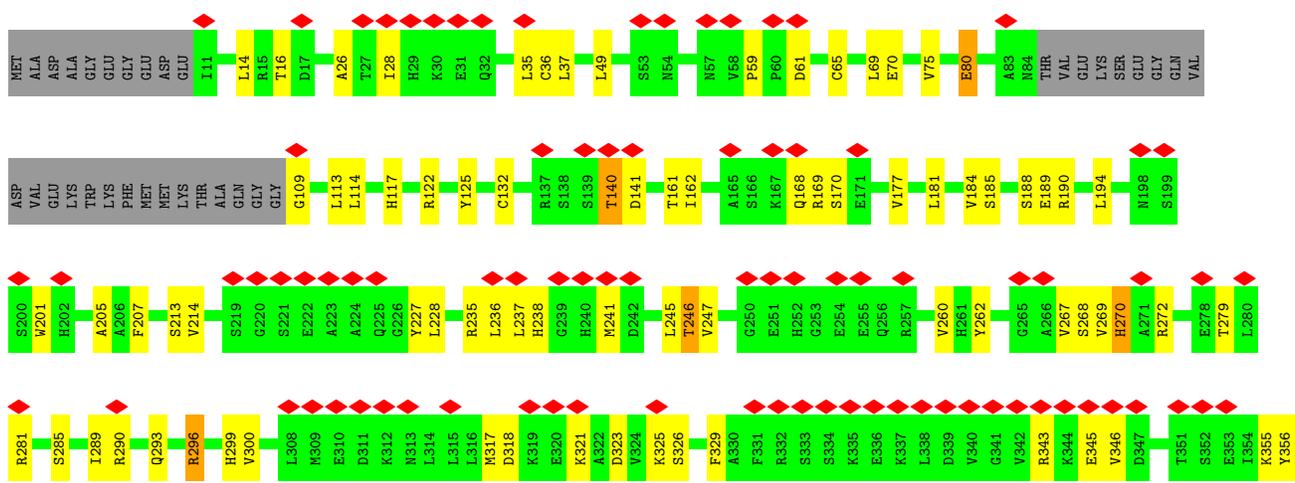
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

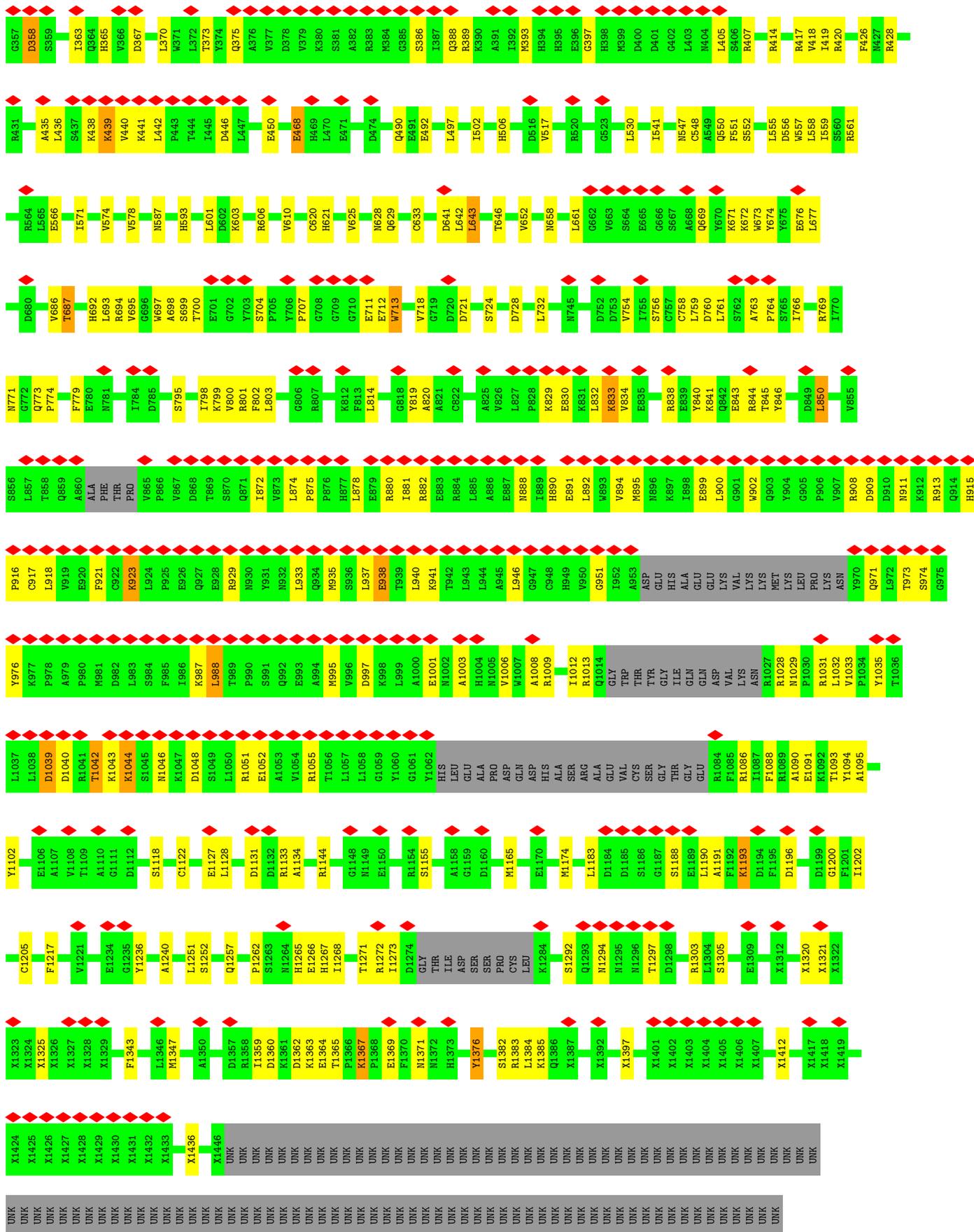
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0

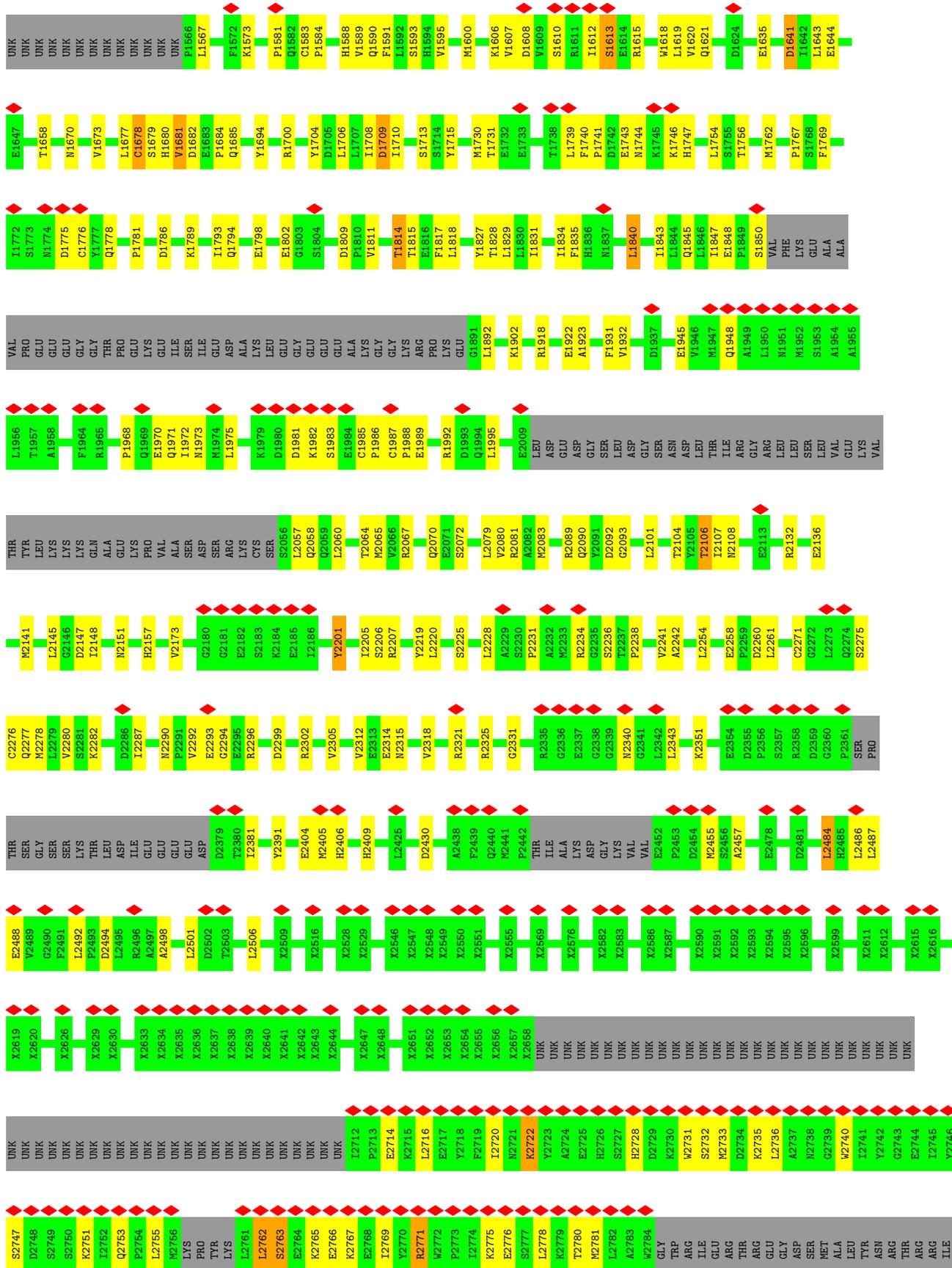




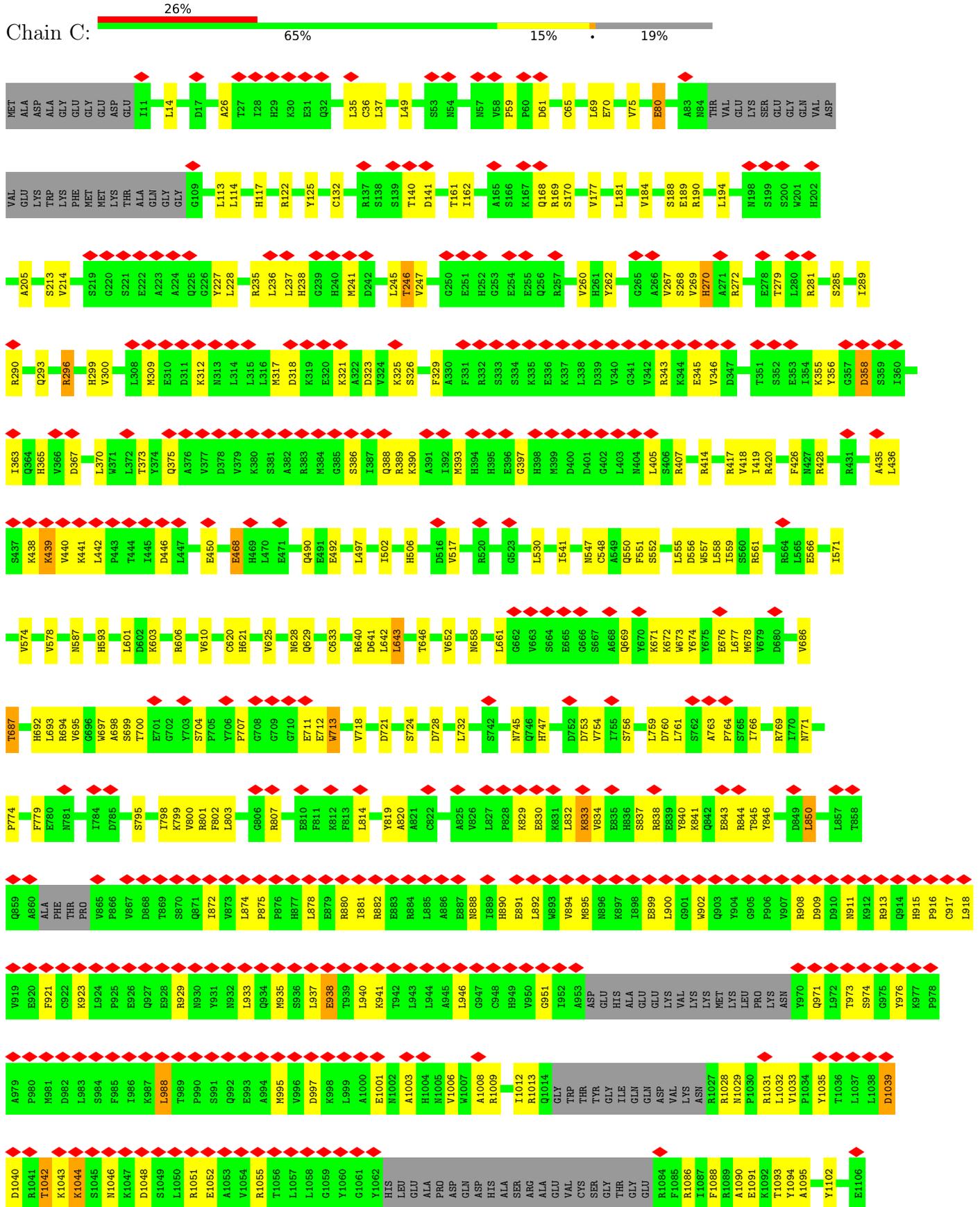
• Molecule 1: Ryanodine receptor 2

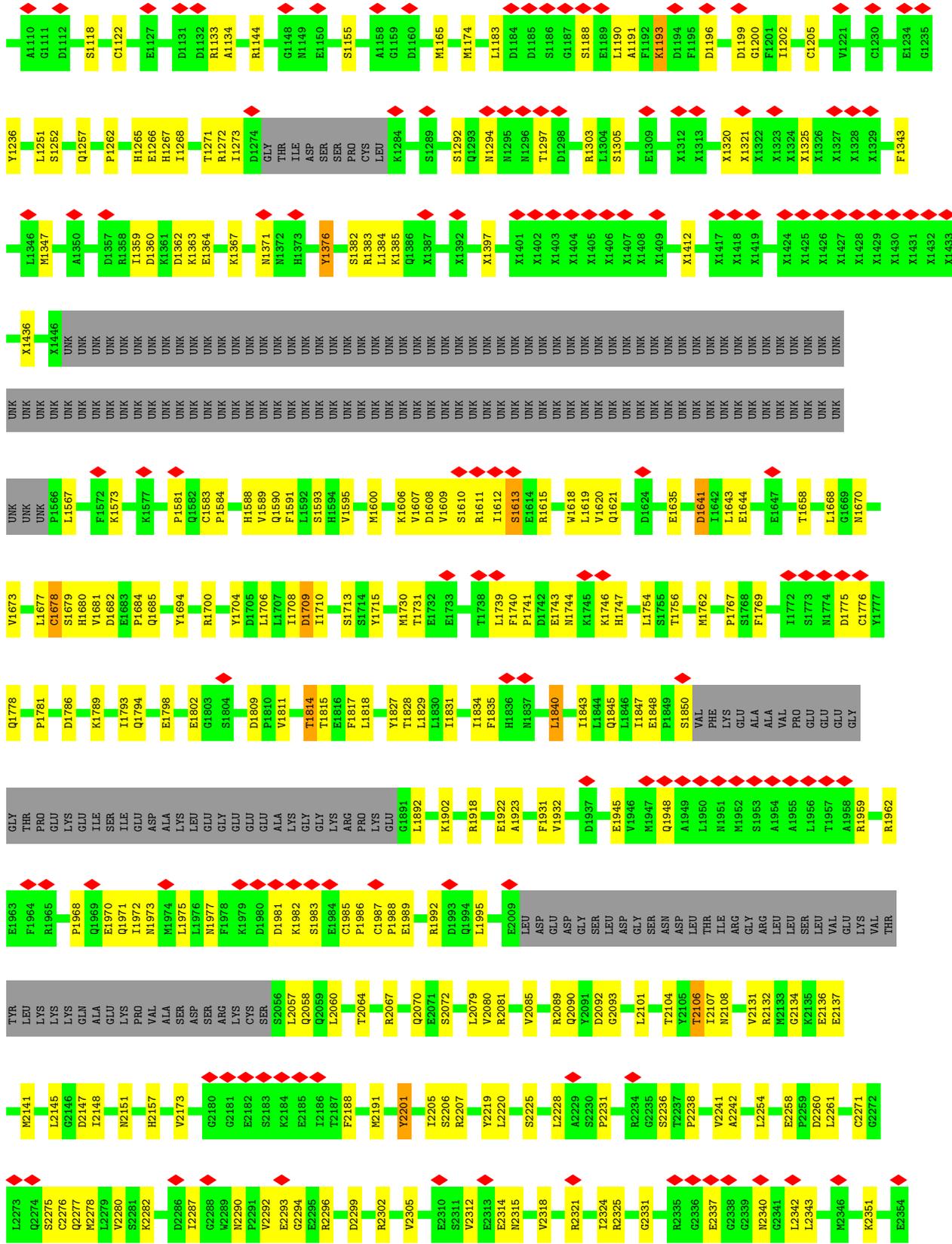


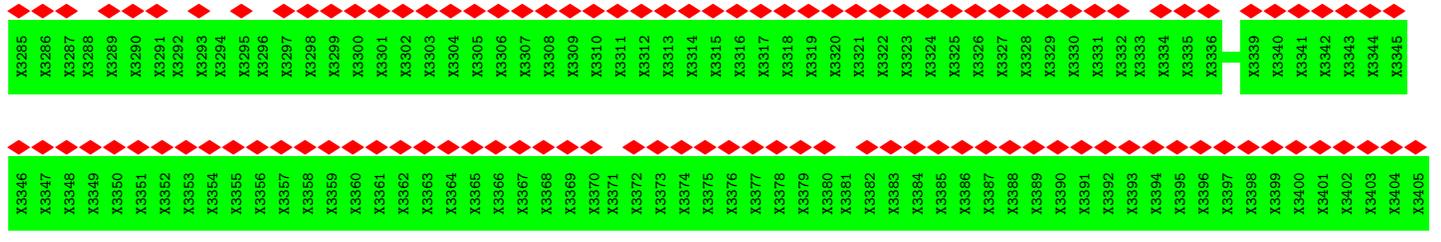




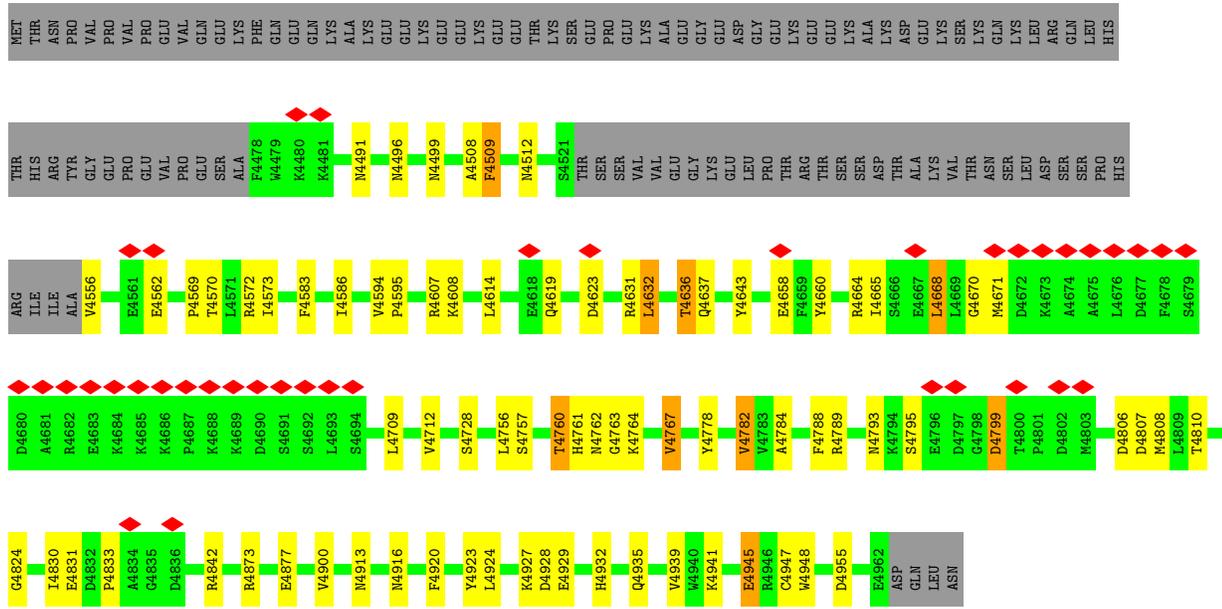
X3536	X3477	UNK	X3413	X3583	X3293	X3173	X3112	X2990	X2929	SER
X3537	X3478	UNK	X3414	X3354	X3294	X3174	X3115	X2991	X2930	GLN
X3538	X3479	UNK	X3419	X3355	X3295	X3175	X3116	X2992	X2931	THR
X3539	X3480	UNK	X3420	X3356	X3296	X3176	X3117	X2993	X2932	SER
X3540	X3481	UNK	X3421	X3357	X3297	X3177	X3118	X2994	X2933	GLN
X3541	X3482	UNK	X3422	X3358	X3298	X3178	X3119	X2995	X2934	VAL
X3542	X3483	UNK	X3423	X3359	X3299	X3179	X3120	X2996	X2935	SER
X3543	X3484	UNK	X3424	X3360	X3300	X3180	X3121	X3000	X2936	ILE
X3544	X3485	UNK	X3425	X3361	X3301	X3181	X3122	X3001	X2937	ASP
X3545	X3486	UNK	X3426	X3362	X3302	X3182	X3123	X3002	D2874	ALA
X3546	X3487	UNK	X3427	X3363	X3303	X3183	X3124	X3003	T2875	ALA
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X3550	X3490	UNK	X3430	X3366	X3306	X3186	X3127	X3006	A2878	GLY
X3551	X3491	UNK	X3431	X3367	X3307	X3187	X3128	X3007	K2879	THR
X3552	X3492	UNK	X3432	X3368	X3308	X3188	X3129	X3008	E2880	PRO
X3553	X3493	UNK	X3433	X3369	X3309	X3189	UNK	X3009	K2881	ARG
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X3557	X3497	UNK	UNK	X3373	X3313	X3193	UNK	X3013	E2886	SER
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X3559	X3499	UNK	UNK	X3375	X3315	X3195	UNK	X3015	A2888	LEU
X3560	X3500	UNK	UNK	X3376	X3316	X3196	UNK	X3016	Q2889	SER
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X3565	X3505	UNK	UNK	X3381	X3321	X3201	UNK	X3021	F2894	
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X3534	X3534	UNK	UNK	X3410	X3350	UNK	UNK	UNK	X2916	
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						UNK	UNK	UNK	X2919	
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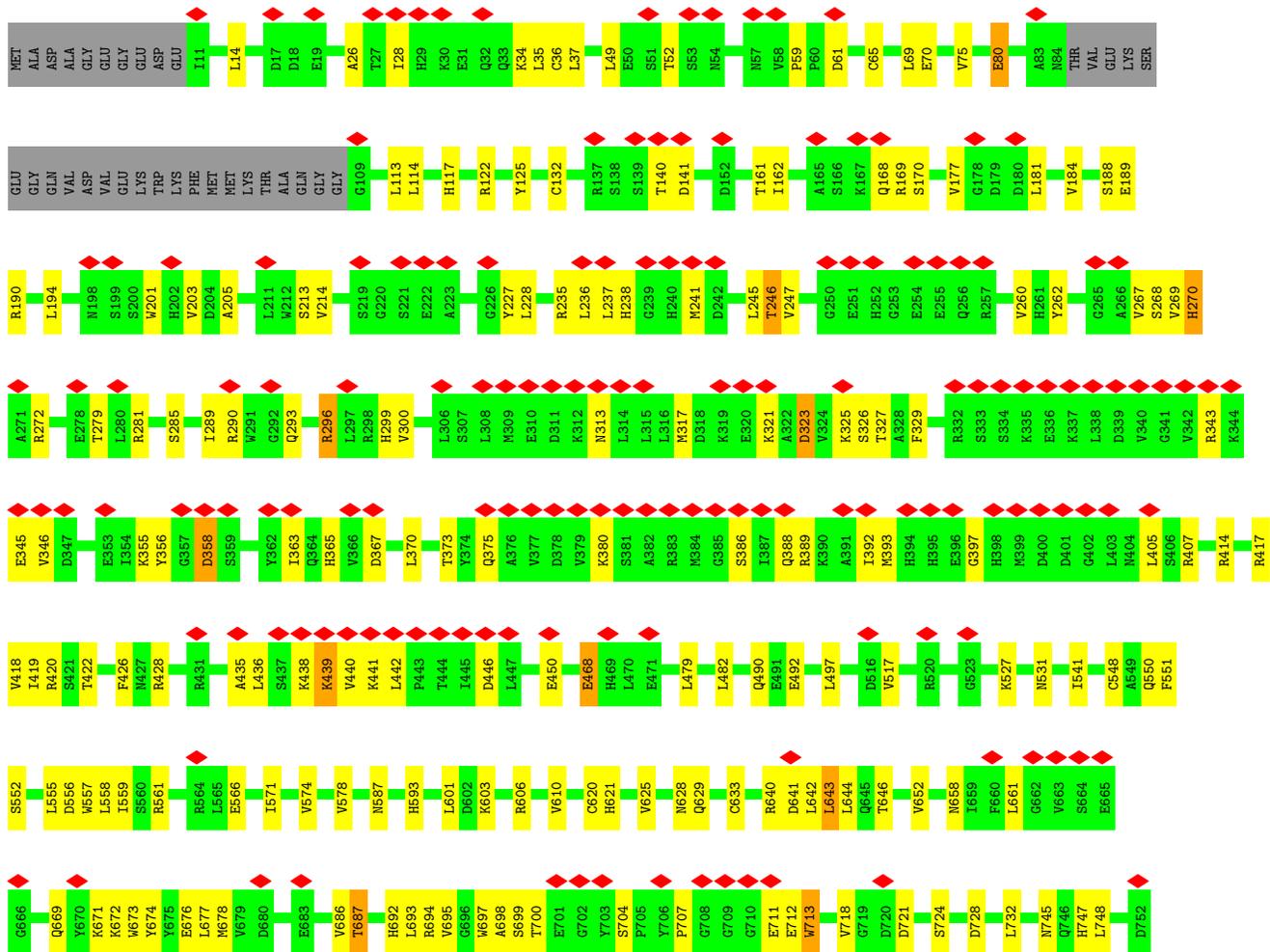


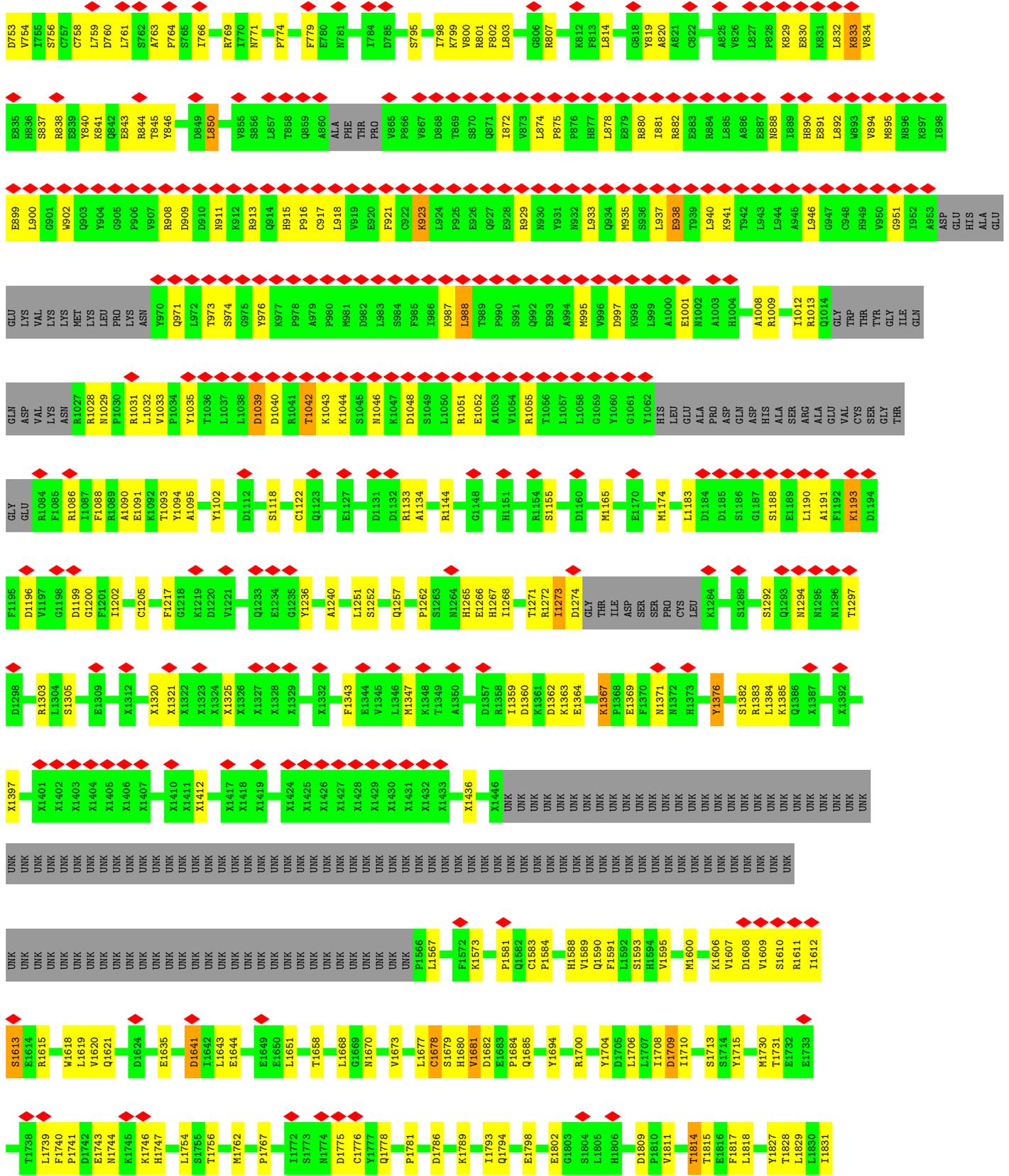


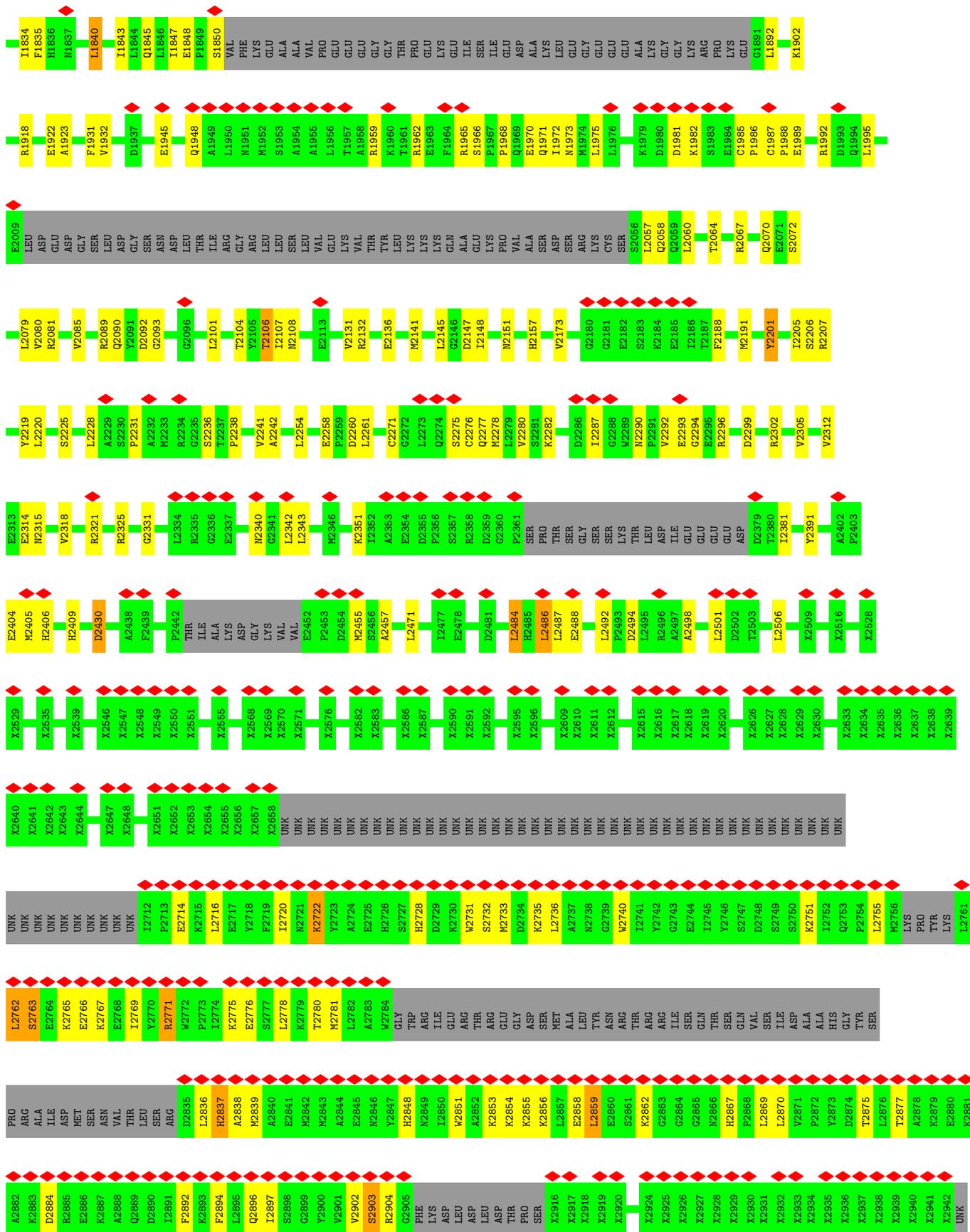
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GLY	W4287	GLU	H4110	K4023	T3861	ASP	UNK	X3529	UNK	X3408	X3348	X3287
GLU	S4288	GLN	H4110	D4024	N3864	ASP	UNK	X3530	UNK	X3409	X3349	X3288
ARG	W4289	ALA	D4112	D4024	T3865	GLY	UNK	X3531	UNK	X3410	X3350	X3289
PRO	F4290	PRO	R4113	L4025	L3865	GLU	UNK	X3532	UNK	X3411	X3351	X3290
PRO	V4291	ARG	L4114	L4025	V3874	GLU	UNK	X3533	UNK	X3412	X3352	X3291
LEU	T4292	MET	Q4115	S4027	S3883	VAL	UNK	X3534	UNK	X3413	X3353	X3292
GLY	L4293	PHE	T4116	S4027	S3883	LYS	UNK	X3535	UNK	X3414	X3354	X3293
SER	L4294	PHE	T4116	S4028	Y3891	LYS	UNK	X3536	UNK	X3415	X3355	X3294
ALA	H4295	SER	E4119	D4029	Y3891	LYS	UNK	X3537	UNK	X3416	X3356	X3295
LEU	F4296	LEU	K4142	T4030	S3892	VAL	UNK	X3538	UNK	X3419	X3357	X3297
PRO	W4297	LEU	F4031	T4030	S3892	LYS	UNK	X3539	UNK	X3420	X3358	X3298
SER	W4297	THR	K4032	K4032	G3893	UNK	UNK	X3540	UNK	X3421	X3359	X3299
GLU	A4298	ILE	E4153	E4033	G3893	UNK	UNK	X3541	UNK	X3422	X3360	X3300
ASP	A4298	GLN	E4153	E4033	D3895	UNK	UNK	X3542	UNK	X3423	X3361	X3301
LEU	S4299	THR	T4157	Y4034	I3896	UNK	UNK	X3543	UNK	X3424	X3362	X3302
THR	V4300	SER	T4157	D4035	I3897	UNK	UNK	X3544	UNK	X3425	X3363	X3303
ASP	V4300	ALA	V4164	P4036	D3898	UNK	UNK	X3545	UNK	X3426	X3364	X3304
LEU	C4301	ALA	S4167	D4037	E3899	UNK	UNK	X3546	UNK	X3427	X3365	X3305
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GLU	G4303	ALA	F4171	G4038	I3809	UNK	UNK	X3548	UNK	X3429	X3367	X3307
LEU	F4304	ARG	F4171	G4038	L3809	UNK	UNK	X3549	UNK	X3430	X3368	X3308
THR	F4305	THR	V4175	G4040	L3809	UNK	UNK	X3550	UNK	X3431	X3369	X3309
GLU	R4306	ASN	V4175	V4041	L3919	UNK	UNK	X3551	UNK	X3432	X3370	X3310
GLU	I4307	VAL	V4175	V4042	T3920	UNK	UNK	X3552	UNK	X3433	X3371	X3311
SER	I4307	VAL	V4175	V4042	R3921	UNK	UNK	X3553	UNK	X3434	X3372	X3312
ASP	V4308	LEU	G4180	S4043	E3921	UNK	UNK	X3554	UNK	UNK	UNK	X3313
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ASP	S4310	VAL	E4183	D4046	I3923	UNK	UNK	X3558	UNK	UNK	UNK	X3317
ASP	L4311	ARG	E4183	F4047	L3923	UNK	UNK	X3559	UNK	UNK	UNK	X3318
ILE	LEU	MET	L4187	H4049	L3934	UNK	UNK	X3560	UNK	UNK	UNK	X3319
LEU	LEU	LEU	L4187	K4049	L3934	UNK	UNK	X3561	UNK	UNK	UNK	X3320
GLY	GLY	SER	F4188	R4050	S3937	UNK	UNK	X3562	UNK	UNK	UNK	X3321
LEU	GLY	LEU	V4189	A4050	R3938	UNK	UNK	X3563	UNK	UNK	UNK	X3322
SER	SER	LYS	E4193	M4051	I3939	UNK	UNK	X3564	UNK	UNK	UNK	X3323
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VAL	VAL	LEU	E4193	S4053	W3940	UNK	UNK	X3566	UNK	UNK	UNK	X3325
ARG	GLU	LEU	E4198	H4054	V3943	UNK	UNK	X3567	UNK	UNK	UNK	X3326
GLY	ALA	GLN	I4205	K4055	Q3954	UNK	UNK	X3568	UNK	UNK	UNK	X3327
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LYS	LYS	LYS	SER	E4063	K3956	UNK	UNK	X3571	UNK	UNK	UNK	X3330
ILE	ILE	LYS	ASP	E4063	S3961	UNK	UNK	X3572	UNK	UNK	UNK	X3331
VAL	VAL	LYS	LEU	E4070	S3962	UNK	UNK	X3573	UNK	UNK	UNK	X3332
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GLU	GLU	ARG	GLU	T4071	Q3974	UNK	UNK	X3575	UNK	UNK	UNK	X3334
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ALA	ALA	ASN	ASN	M4074	V3990	UNK	UNK	X3578	UNK	UNK	UNK	X3337
MET	MET	ASP	LYS	E4075	V3990	UNK	UNK	X3579	UNK	UNK	UNK	X3338
PRO	PRO	GLU	GLU	T4076	D4000	UNK	UNK	X3580	UNK	UNK	UNK	X3339
ASP	ASP	GLU	GLU	L4077	V4003	UNK	UNK	X3581	UNK	UNK	UNK	X3340
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GLU	GLU	VAL	VAL	E4081	E4081	UNK	UNK	X3585	UNK	UNK	UNK	X3344
VAL	VAL	ARG	ARG	F4082	F4082	UNK	UNK	X3586	UNK	UNK	UNK	X3345
ARG	ARG	GLY	GLY	V4083	V4083	UNK	UNK	X3587	UNK	UNK	UNK	X3346
ASP	ASP	ASP	ASP	H4087	H4087	UNK	UNK	X3588	UNK	UNK	UNK	X3347



• Molecule 1: Ryanodine receptor 2







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I3896	UNK	X3266	UNK
E3891	UNK	X3267	UNK
E3892	UNK	X3268	UNK
E3893	UNK	X3269	UNK
K3894	UNK	X3270	UNK
D3895	UNK	X3271	UNK
I3896	UNK	X3272	UNK
E3891	UNK	X3273	UNK
E3892	UNK	X3274	UNK
E3893	UNK	X3275	UNK
K3894	UNK	X3276	UNK
D3895	UNK	X3277	UNK
I3896	UNK	X3278	UNK
E3891	UNK	X3279	UNK
E3892	UNK	X3280	UNK
E3893	UNK	X3281	UNK
K3894	UNK	X3282	UNK
D3895	UNK	X3283	UNK
I3896	UNK	X3284	UNK
E3891	UNK	X3285	UNK
E3892	UNK	X3286	UNK
E3893	UNK	X3287	UNK
K3894	UNK	X3288	UNK
D3895	UNK	X3289	UNK
I3896	UNK	X3290	UNK
E3891	UNK	X3291	UNK
E3892	UNK	X3292	UNK
E3893	UNK	X3293	UNK
K3894	UNK	X3294	UNK
D3895	UNK	X3295	UNK
I3896	UNK	X3296	UNK
E3891	UNK	X3297	UNK
E3892	UNK	X3298	UNK
E3893	UNK	X3299	UNK
K3894	UNK	X3300	UNK
D3895	UNK	X3301	UNK
I3896	UNK	X3302	UNK
E3891	UNK	X3303	UNK
E3892	UNK	X3304	UNK
E3893	UNK	X3305	UNK
K3894	UNK	X3306	UNK
D3895	UNK	X3307	UNK
I3896	UNK	X3308	UNK
E3891	UNK	X3309	UNK
E3892	UNK	X3310	UNK
E3893	UNK	X3311	UNK
K3894	UNK	X3312	UNK
D3895	UNK	X3313	UNK
I3896	UNK	X3314	UNK
E3891	UNK	X3315	UNK
E3892	UNK	X3316	UNK
E3893	UNK	X3317	UNK
K3894	UNK	X3318	UNK
D3895	UNK	X3319	UNK
I3896	UNK	X3320	UNK
E3891	UNK	X3321	UNK
E3892	UNK	X3322	UNK
E3893	UNK	X3323	UNK
K3894	UNK	X3324	UNK
D3895	UNK	X3325	UNK
I3896	UNK	X3326	UNK
E3891	UNK	X3327	UNK
E3892	UNK	X3328	UNK
E3893	UNK	X3329	UNK
K3894	UNK	X3330	UNK
D3895	UNK	X3331	UNK
I3896	UNK	X3332	UNK
E3891	UNK	X3333	UNK
E3892	UNK	X3334	UNK
E3893	UNK	X3335	UNK
K3894	UNK	X3336	UNK
D3895	UNK	X3337	UNK
I3896	UNK	X3338	UNK
E3891	UNK	X3339	UNK
E3892	UNK	X3340	UNK
E3893	UNK	X3341	UNK
K3894	UNK	X3342	UNK
D3895	UNK	X3343	UNK
I3896	UNK	X3344	UNK
E3891	UNK	X3345	UNK
E3892	UNK	X3346	UNK
E3893	UNK	X3347	UNK
K3894	UNK	X3348	UNK
D3895	UNK	X3349	UNK
I3896	UNK	X3350	UNK
E3891	UNK	X3351	UNK
E3892	UNK	X3352	UNK
E3893	UNK	X3353	UNK
K3894	UNK	X3354	UNK
D3895	UNK	X3355	UNK
I3896	UNK	X3356	UNK
E3891	UNK	X3357	UNK
E3892	UNK	X3358	UNK
E3893	UNK	X3359	UNK
K3894	UNK	X3360	UNK
D3895	UNK	X3361	UNK
I3896	UNK	X3362	UNK
E3891	UNK	X3363	UNK
E3892	UNK	X3364	UNK
E3893	UNK	X3365	UNK
K3894	UNK	X3366	UNK
D3895	UNK	X3367	UNK
I3896	UNK	X3368	UNK
E3891	UNK	X3369	UNK
E3892	UNK	X3370	UNK
E3893	UNK	X3371	UNK
K3894	UNK	X3372	UNK
D3895	UNK	X3373	UNK
I3896	UNK	X3374	UNK
E3891	UNK	X3375	UNK
E3892	UNK	X3376	UNK
E3893	UNK	X3377	UNK
K3894	UNK	X3378	UNK
D3895	UNK	X3379	UNK
I3896	UNK	X3380	UNK
E3891	UNK	X3381	UNK
E3892	UNK	X3382	UNK
E3893	UNK	X3383	UNK
K3894	UNK	X3384	UNK
D3895	UNK	X3385	UNK
I3896	UNK	X3386	UNK
E3891	UNK	X3387	UNK
E3892	UNK	X3388	UNK
E3893	UNK	X3389	UNK
K3894	UNK	X3390	UNK
D3895	UNK	X3391	UNK
I3896	UNK	X3392	UNK
E3891	UNK	X3393	UNK
E3892	UNK	X3394	UNK
E3893	UNK	X3395	UNK
K3894	UNK	X3396	UNK
D3895	UNK	X3397	UNK
I3896	UNK	X3398	UNK
E3891	UNK	X3399	UNK
E3892	UNK	X3400	UNK
E3893	UNK	X3401	UNK
K3894	UNK	X3402	UNK
D3895	UNK	X3403	UNK
I3896	UNK	X3404	UNK
E3891	UNK	X3405	UNK
E3892	UNK	X3406	UNK
E3893	UNK	X3407	UNK
K3894	UNK	X3408	UNK
D3895	UNK	X3409	UNK
I3896	UNK	X3410	UNK
E389			



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



MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	ALA	SER	SER	MET	ASP	GLU	LYS	THR	THR	THR	GLY	GLY	TRP	ARG	GLY	GLY	VAL	VAL	GLU	GLY	LEU	LEU	GLN	LEU	LEU	ARG	ALA	ALA	ARG	ARG	LEU	GLU	HIS	HIS	HIS	PRO	PRO	GLN	GLY	GLN	ARG	GLU
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PRO	GLY	SER	GLY	GLY	SER	GLY	THR	G2	S9	D12	K19	C23	V24	Y27	Q32	D38	S39	S40	R41	D42	R43	K48	F49	R50	I51	E55	K58	E61	L69	R72	T78	P79	D80	V81	Y83	H88	I92	T97	D101
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• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	ALA	SER	SER	MET	ASP	GLU	LYS	THR	THR	THR	GLY	GLY	TRP	ARG	GLY	GLY	VAL	VAL	GLU	GLY	LEU	LEU	GLN	LEU	LEU	ARG	ALA	ALA	ARG	ARG	LEU	GLU	HIS	HIS	HIS	PRO	PRO	GLN	GLY	GLN	ARG	GLU
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PRO	GLY	SER	GLY	GLY	SER	GLY	THR	G2	S9	D12	K19	C23	V24	V25	H26	T27	T28	Q32	D38	S39	S40	R41	D42	R43	K48	F49	I51	E55	K58	E61	L69	R72	T78	P79	D80	V81	A82	Y83	H88	V91
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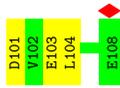


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	ALA	SER	SER	MET	ASP	GLU	LYS	THR	THR	THR	GLY	GLY	TRP	ARG	GLY	GLY	VAL	VAL	GLU	GLY	LEU	LEU	GLN	LEU	LEU	ARG	ALA	ALA	ARG	ARG	LEU	GLU	HIS	HIS	HIS	PRO	PRO	GLN	GLY	GLN	ARG	GLU
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PRO	GLY	SER	GLY	GLY	SER	GLY	THR	G2	S9	D12	K19	C23	V24	Y27	Q32	K35	D38	S39	S40	R43	R43	K48	F49	R50	I51	G52	K53	O54	E55	K58	E61	L69	R72	T78	P79	D80	V81	H88	I92	T97
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45120	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.069	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.284, 1.284, 1.284	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/26895	0.42	0/36316
1	B	0.25	0/26895	0.42	0/36316
1	C	0.25	0/26895	0.42	0/36316
1	D	0.25	0/26895	0.42	0/36316
2	G	0.26	0/835	0.47	0/1123
2	H	0.26	0/835	0.47	0/1123
2	I	0.26	0/835	0.47	0/1123
2	J	0.26	0/835	0.47	0/1123
All	All	0.25	0/110920	0.42	0/149756

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	468	GLU	Peptide
1	C	468	GLU	Peptide
1	D	468	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30071	0	26714	459	0
1	B	30071	0	26714	452	0
1	C	30071	0	26714	462	0
1	D	30071	0	26714	466	0
2	G	819	0	821	18	0
2	H	819	0	821	17	0
2	I	819	0	821	20	0
2	J	819	0	821	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	123564	0	110140	1884	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 8.

All (1884) 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:A:2404:GLU:HG3	1:A:2405:MET:H	1.38	0.89
1:B:2404:GLU:HG3	1:B:2405:MET:H	1.38	0.89
1:D:2404:GLU:HG3	1:D:2405:MET:H	1.38	0.88
1:C:2404:GLU:HG3	1:C:2405:MET:H	1.38	0.87
1:A:4821:ARG:NH2	1:D:4824:GLY:O	2.08	0.86
1:D:1190:LEU:HD21	1:D:1193:LYS:HB3	1.58	0.85
1:A:1190:LEU:HD21	1:A:1193:LYS:HB3	1.59	0.85
1:C:1190:LEU:HD21	1:C:1193:LYS:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1190:LEU:HD21	1:B:1193:LYS:HB3	1.59	0.85
1:A:2406:HIS:HA	1:A:2409:HIS:HB3	1.62	0.82
1:B:2406:HIS:HA	1:B:2409:HIS:HB3	1.61	0.82
1:C:2406:HIS:HA	1:C:2409:HIS:HB3	1.62	0.81
1:C:4789:ARG:NH2	1:D:4558:TYR:OH	2.14	0.80
1:A:358:ASP:OD1	1:A:358:ASP:N	2.15	0.80
1:D:2406:HIS:HA	1:D:2409:HIS:HB3	1.62	0.80
1:C:358:ASP:OD1	1:C:358:ASP:N	2.15	0.79
1:D:358:ASP:N	1:D:358:ASP:OD1	2.15	0.78
1:B:358:ASP:N	1:B:358:ASP:OD1	2.15	0.77
1:C:4833:PRO:HB3	1:C:4842:ARG:HD3	1.66	0.77
2:J:58:LYS:HA	2:J:61:GLU:HG2	1.66	0.77
2:G:58:LYS:HA	2:G:61:GLU:HG2	1.66	0.77
1:B:4833:PRO:HB3	1:B:4842:ARG:HD3	1.66	0.76
2:H:58:LYS:HA	2:H:61:GLU:HG2	1.66	0.76
1:C:1741:PRO:HB3	1:C:1746:LYS:HE3	1.67	0.76
1:A:4833:PRO:HB3	1:A:4842:ARG:HD3	1.66	0.76
1:D:4833:PRO:HB3	1:D:4842:ARG:HD3	1.66	0.76
2:I:58:LYS:HA	2:I:61:GLU:HG2	1.66	0.76
1:B:1741:PRO:HB3	1:B:1746:LYS:HE3	1.67	0.75
1:D:1741:PRO:HB3	1:D:1746:LYS:HE3	1.67	0.75
1:A:4867:ASP:OD1	1:B:4873:ARG:NH1	2.19	0.74
1:A:1741:PRO:HB3	1:A:1746:LYS:HE3	1.67	0.74
1:C:760:ASP:HB3	1:C:764:PRO:HG2	1.70	0.74
1:A:760:ASP:HB3	1:A:764:PRO:HG2	1.70	0.74
1:C:4042:ILE:HG22	1:C:4044:LYS:H	1.53	0.73
1:B:4042:ILE:HG22	1:B:4044:LYS:H	1.53	0.73
1:D:4042:ILE:HG22	1:D:4044:LYS:H	1.53	0.73
1:A:4042:ILE:HG22	1:A:4044:LYS:H	1.53	0.73
1:C:558:LEU:HB3	1:C:571:ILE:HD11	1.71	0.73
1:A:558:LEU:HB3	1:A:571:ILE:HD11	1.71	0.72
1:B:760:ASP:HB3	1:B:764:PRO:HG2	1.70	0.72
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.72	0.72
1:B:694:ARG:HG2	1:B:728:ASP:HB3	1.71	0.72
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.72	0.72
1:B:558:LEU:HB3	1:B:571:ILE:HD11	1.71	0.72
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.72	0.72
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.72	0.72
1:A:694:ARG:HG2	1:A:728:ASP:HB3	1.72	0.72
1:A:162:ILE:HD11	1:A:181:LEU:HD22	1.72	0.72
1:D:760:ASP:HB3	1:D:764:PRO:HG2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ILE:HD11	1:D:181:LEU:HD22	1.72	0.71
1:D:558:LEU:HB3	1:D:571:ILE:HD11	1.71	0.71
1:C:2853:LYS:HA	1:C:2856:LYS:HE2	1.74	0.70
1:A:4873:ARG:NH1	1:D:4867:ASP:OD1	2.25	0.70
1:C:162:ILE:HD11	1:C:181:LEU:HD22	1.72	0.70
1:B:2853:LYS:HA	1:B:2856:LYS:HE2	1.74	0.70
1:B:162:ILE:HD11	1:B:181:LEU:HD22	1.72	0.70
1:C:694:ARG:HG2	1:C:728:ASP:HB3	1.71	0.70
1:D:694:ARG:HG2	1:D:728:ASP:HB3	1.72	0.70
1:B:1989:GLU:HG2	1:B:1992:ARG:HD3	1.74	0.69
1:D:2853:LYS:HA	1:D:2856:LYS:HE2	1.74	0.69
1:A:2853:LYS:HA	1:A:2856:LYS:HE2	1.74	0.69
1:C:1272:ARG:NH2	1:C:1584:PRO:O	2.26	0.69
1:A:1989:GLU:HG2	1:A:1992:ARG:HD3	1.74	0.69
1:D:1613:SER:O	1:D:1615:ARG:NH2	2.26	0.69
1:A:1613:SER:O	1:A:1615:ARG:NH2	2.26	0.69
1:A:1730:MET:SD	1:A:2106:THR:OG1	2.52	0.68
1:A:1682:ASP:HB2	1:A:1685:GLN:HB3	1.76	0.68
1:C:1682:ASP:HB2	1:C:1685:GLN:HB3	1.76	0.68
1:A:1272:ARG:NH2	1:A:1584:PRO:O	2.26	0.68
1:B:1682:ASP:HB2	1:B:1685:GLN:HB3	1.75	0.68
1:B:1272:ARG:NH2	1:B:1584:PRO:O	2.26	0.68
1:C:671:LYS:HB3	1:C:761:LEU:HB2	1.76	0.68
1:D:1272:ARG:NH2	1:D:1584:PRO:O	2.26	0.68
1:C:1613:SER:O	1:C:1615:ARG:NH2	2.26	0.68
1:C:1989:GLU:HG2	1:C:1992:ARG:HD3	1.74	0.68
1:D:1989:GLU:HG2	1:D:1992:ARG:HD3	1.74	0.67
1:B:1613:SER:O	1:B:1615:ARG:NH2	2.26	0.67
1:A:1262:PRO:HG2	1:A:1265:HIS:HB2	1.77	0.67
1:C:1262:PRO:HG2	1:C:1265:HIS:HB2	1.77	0.67
1:D:900:LEU:HD22	1:D:902:TRP:HE1	1.59	0.67
1:D:1682:ASP:HB2	1:D:1685:GLN:HB3	1.75	0.67
1:C:1730:MET:SD	1:C:2106:THR:OG1	2.52	0.67
1:D:1744:ASN:HD21	1:D:1746:LYS:HE2	1.60	0.67
1:A:671:LYS:HB3	1:A:761:LEU:HB2	1.76	0.67
1:C:1769:PHE:O	2:I:83:TYR:OH	2.12	0.67
1:B:671:LYS:HB3	1:B:761:LEU:HB2	1.76	0.67
1:D:1262:PRO:HG2	1:D:1265:HIS:HB2	1.77	0.67
1:B:1262:PRO:HG2	1:B:1265:HIS:HB2	1.77	0.66
1:D:1730:MET:SD	1:D:2106:THR:OG1	2.52	0.66
1:D:1775:ASP:OD1	1:D:1776:CYS:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:LEU:HD22	1:A:902:TRP:HE1	1.59	0.66
1:C:900:LEU:HD22	1:C:902:TRP:HE1	1.59	0.66
1:C:1775:ASP:OD1	1:C:1776:CYS:N	2.26	0.66
1:D:671:LYS:HB3	1:D:761:LEU:HB2	1.76	0.66
1:C:2731:TRP:HE1	1:C:2735:LYS:HZ2	1.42	0.66
1:D:4619:GLN:HE22	1:D:4631:ARG:HH12	1.44	0.66
1:A:1744:ASN:HD21	1:A:1746:LYS:HE2	1.60	0.66
1:B:900:LEU:HD22	1:B:902:TRP:HE1	1.60	0.66
1:B:1730:MET:SD	1:B:2106:THR:OG1	2.52	0.66
1:C:4115:GLN:O	1:C:4119:GLU:HG2	1.96	0.66
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.29	0.65
1:B:1744:ASN:HD21	1:B:1746:LYS:HE2	1.60	0.65
1:A:759:LEU:HD13	1:A:766:ILE:HG12	1.79	0.65
1:C:4619:GLN:HE22	1:C:4631:ARG:HH12	1.44	0.65
1:B:4115:GLN:O	1:B:4119:GLU:HG2	1.96	0.65
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.29	0.65
1:A:2731:TRP:HE1	1:A:2735:LYS:HZ2	1.44	0.65
1:D:759:LEU:HD13	1:D:766:ILE:HG12	1.79	0.65
1:D:4115:GLN:O	1:D:4119:GLU:HG2	1.96	0.65
1:B:1775:ASP:OD1	1:B:1776:CYS:N	2.26	0.65
1:C:4042:ILE:HG21	1:C:4047:PHE:HB2	1.79	0.65
1:B:2731:TRP:HE1	1:B:2735:LYS:HZ2	1.43	0.65
1:C:759:LEU:HD13	1:C:766:ILE:HG12	1.79	0.65
1:A:1266:GLU:O	1:A:1267:HIS:ND1	2.30	0.65
1:C:1744:ASN:HD21	1:C:1746:LYS:HE2	1.60	0.65
1:A:1267:HIS:O	1:A:1292:SER:OG	2.15	0.65
1:B:1267:HIS:O	1:B:1292:SER:OG	2.15	0.65
1:B:4003:VAL:HG11	1:B:4113:ARG:HG2	1.80	0.64
1:D:4003:VAL:HG11	1:D:4113:ARG:HG2	1.80	0.64
1:C:1266:GLU:O	1:C:1267:HIS:ND1	2.30	0.64
1:A:4115:GLN:O	1:A:4119:GLU:HG2	1.96	0.64
1:A:4619:GLN:HE22	1:A:4631:ARG:HH12	1.44	0.64
1:B:1266:GLU:O	1:B:1267:HIS:ND1	2.30	0.64
1:B:1359:ILE:HG12	1:B:1363:LYS:HD2	1.79	0.64
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.29	0.64
1:D:1266:GLU:O	1:D:1267:HIS:ND1	2.30	0.64
1:D:3818:MET:SD	1:D:3818:MET:N	2.68	0.64
1:C:3818:MET:SD	1:C:3818:MET:N	2.68	0.64
1:B:4619:GLN:HE22	1:B:4631:ARG:HH12	1.44	0.64
1:A:4003:VAL:HG11	1:A:4113:ARG:HG2	1.80	0.64
1:B:426:PHE:HB3	1:B:497:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:LEU:HD13	1:B:766:ILE:HG12	1.79	0.64
1:B:3822:GLU:HB3	1:B:3826:GLU:HA	1.80	0.64
1:C:1265:HIS:HD2	1:C:1268:ILE:HB	1.63	0.64
1:C:4003:VAL:HG11	1:C:4113:ARG:HG2	1.80	0.64
1:A:426:PHE:HB3	1:A:497:LEU:HD21	1.80	0.64
1:A:1775:ASP:OD1	1:A:1776:CYS:N	2.26	0.63
1:D:2731:TRP:HE1	1:D:2735:LYS:HZ2	1.44	0.63
1:D:3822:GLU:HB3	1:D:3826:GLU:HA	1.80	0.63
1:A:3822:GLU:HB3	1:A:3826:GLU:HA	1.80	0.63
1:A:4042:ILE:HG21	1:A:4047:PHE:HB2	1.79	0.63
1:B:4042:ILE:HG21	1:B:4047:PHE:HB2	1.79	0.63
1:C:3822:GLU:HB3	1:C:3826:GLU:HA	1.80	0.63
1:D:1267:HIS:O	1:D:1292:SER:OG	2.15	0.63
1:A:1265:HIS:HD2	1:A:1268:ILE:HB	1.63	0.63
1:A:3954:GLN:NE2	1:A:3974:GLN:OE1	2.32	0.63
1:D:1359:ILE:HG12	1:D:1363:LYS:HD2	1.79	0.63
1:C:1267:HIS:O	1:C:1292:SER:OG	2.15	0.63
1:C:3954:GLN:NE2	1:C:3974:GLN:OE1	2.32	0.63
1:C:426:PHE:HB3	1:C:497:LEU:HD21	1.80	0.63
1:B:36:CYS:SG	1:B:37:LEU:N	2.72	0.63
1:B:1847:ILE:HG23	1:B:1892:LEU:HB3	1.81	0.63
1:A:14:LEU:HD11	1:A:214:VAL:HG11	1.81	0.62
1:B:1265:HIS:HD2	1:B:1268:ILE:HB	1.63	0.62
1:B:2735:LYS:HD2	1:B:2740:TRP:CD1	2.34	0.62
1:C:14:LEU:HD11	1:C:214:VAL:HG11	1.81	0.62
1:A:36:CYS:SG	1:A:37:LEU:N	2.72	0.62
1:A:1359:ILE:HG12	1:A:1363:LYS:HD2	1.79	0.62
1:A:4055:LYS:NZ	1:D:4659:PHE:O	2.26	0.62
1:C:2735:LYS:HD2	1:C:2740:TRP:CD1	2.34	0.62
1:B:3954:GLN:NE2	1:B:3974:GLN:OE1	2.32	0.62
1:C:3822:GLU:OE2	1:C:3824:SER:N	2.32	0.62
1:D:36:CYS:SG	1:D:37:LEU:N	2.72	0.62
1:D:1265:HIS:HD2	1:D:1268:ILE:HB	1.63	0.62
1:D:1847:ILE:HG23	1:D:1892:LEU:HB3	1.81	0.62
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.29	0.62
1:D:4042:ILE:HG21	1:D:4047:PHE:HB2	1.79	0.62
1:C:36:CYS:SG	1:C:37:LEU:N	2.72	0.62
1:D:325:LYS:HG3	1:D:367:ASP:OD1	2.00	0.62
1:D:3954:GLN:NE2	1:D:3974:GLN:OE1	2.32	0.62
1:A:2735:LYS:HD2	1:A:2740:TRP:CD1	2.34	0.62
1:D:426:PHE:HB3	1:D:497:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:HG3	1:A:367:ASP:OD1	2.00	0.62
1:C:325:LYS:HG3	1:C:367:ASP:OD1	2.00	0.62
1:C:1359:ILE:HG12	1:C:1363:LYS:HD2	1.79	0.62
1:C:3754:VAL:HA	1:C:3757:THR:HG22	1.82	0.62
1:A:3822:GLU:OE2	1:A:3824:SER:N	2.32	0.62
1:B:14:LEU:HD11	1:B:214:VAL:HG11	1.81	0.62
1:D:2735:LYS:HD2	1:D:2740:TRP:CD1	2.34	0.61
1:D:3754:VAL:HA	1:D:3757:THR:HG22	1.82	0.61
1:A:1847:ILE:HG23	1:A:1892:LEU:HB3	1.81	0.61
1:A:3754:VAL:HA	1:A:3757:THR:HG22	1.82	0.61
2:H:69:LEU:HA	2:H:104:LEU:HD22	1.82	0.61
1:C:872:ILE:HD11	1:C:941:LYS:HA	1.83	0.61
1:C:1847:ILE:HG23	1:C:1892:LEU:HB3	1.81	0.61
1:A:281:ARG:NH1	1:A:345:GLU:OE2	2.33	0.61
2:I:69:LEU:HA	2:I:104:LEU:HD22	1.83	0.61
1:D:1052:GLU:HA	1:D:1055:ARG:HB2	1.82	0.61
1:B:325:LYS:HG3	1:B:367:ASP:OD1	2.00	0.61
1:B:4079:TYR:O	1:B:4083:VAL:HG13	2.01	0.61
1:D:14:LEU:HD11	1:D:214:VAL:HG11	1.81	0.61
1:B:3754:VAL:HA	1:B:3757:THR:HG22	1.82	0.61
2:H:79:PRO:HD3	2:H:97:THR:HG22	1.83	0.61
1:C:880:ARG:HG3	1:C:881:ILE:HD12	1.82	0.61
1:D:872:ILE:HD11	1:D:941:LYS:HA	1.82	0.61
1:A:4079:TYR:O	1:A:4083:VAL:HG13	2.01	0.61
1:B:1829:LEU:HB3	1:B:1834:ILE:HD11	1.83	0.61
1:A:880:ARG:HG3	1:A:881:ILE:HD12	1.82	0.61
1:D:281:ARG:NH1	1:D:345:GLU:OE2	2.33	0.61
2:J:69:LEU:HA	2:J:104:LEU:HD22	1.83	0.61
1:A:1829:LEU:HB3	1:A:1834:ILE:HD11	1.83	0.60
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.83	0.60
2:G:79:PRO:HD3	2:G:97:THR:HG22	1.83	0.60
1:B:373:THR:HG22	1:B:397:GLY:HA2	1.82	0.60
1:B:872:ILE:HD11	1:B:941:LYS:HA	1.83	0.60
2:I:24:VAL:HG22	2:I:48:LYS:HG2	1.83	0.60
1:A:3822:GLU:HG3	1:A:3827:LYS:HG3	1.83	0.60
1:C:1829:LEU:HB3	1:C:1834:ILE:HD11	1.83	0.60
1:C:4079:TYR:O	1:C:4083:VAL:HG13	2.01	0.60
2:I:79:PRO:HD3	2:I:97:THR:HG22	1.83	0.60
1:D:4079:TYR:O	1:D:4083:VAL:HG13	2.01	0.60
1:B:3822:GLU:HG3	1:B:3827:LYS:HG3	1.84	0.60
1:B:4044:LYS:HB2	1:B:4075:GLU:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.67	0.60
1:D:1829:LEU:HB3	1:D:1834:ILE:HD11	1.83	0.60
1:D:2275:SER:OG	1:D:2287:ILE:O	2.17	0.60
1:D:3891:TYR:O	1:D:3956:LYS:NZ	2.35	0.60
1:C:281:ARG:NH1	1:C:345:GLU:OE2	2.33	0.60
1:C:373:THR:HG22	1:C:397:GLY:HA2	1.82	0.60
1:C:1052:GLU:HA	1:C:1055:ARG:HB2	1.82	0.60
1:C:2275:SER:OG	1:C:2287:ILE:O	2.17	0.60
1:B:880:ARG:HG3	1:B:881:ILE:HD12	1.82	0.60
1:A:373:THR:HG22	1:A:397:GLY:HA2	1.82	0.60
2:G:69:LEU:HA	2:G:104:LEU:HD22	1.82	0.60
1:B:2855:LYS:HA	1:B:2855:LYS:HE3	1.84	0.60
1:C:1681:VAL:HG23	1:C:1682:ASP:H	1.67	0.60
1:D:4153:GLU:O	1:D:4157:THR:OG1	2.19	0.60
1:A:4044:LYS:HB2	1:A:4075:GLU:HG2	1.83	0.60
1:A:2855:LYS:HE3	1:A:2855:LYS:HA	1.84	0.60
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.84	0.60
2:J:79:PRO:HD3	2:J:97:THR:HG22	1.83	0.60
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.67	0.60
1:B:3822:GLU:OE2	1:B:3824:SER:N	2.32	0.60
1:B:4153:GLU:O	1:B:4157:THR:OG1	2.19	0.60
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.67	0.60
1:C:1684:PRO:HD3	2:I:42:ASP:HB3	1.83	0.60
1:A:872:ILE:HD11	1:A:941:LYS:HA	1.83	0.60
1:A:4153:GLU:O	1:A:4157:THR:OG1	2.19	0.60
1:C:69:LEU:HD22	1:C:113:LEU:HD11	1.84	0.60
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.67	0.59
1:B:1052:GLU:HA	1:B:1055:ARG:HB2	1.82	0.59
1:D:69:LEU:HD22	1:D:113:LEU:HD11	1.84	0.59
1:D:279:THR:HG22	1:D:281:ARG:H	1.67	0.59
1:C:279:THR:HG22	1:C:281:ARG:H	1.67	0.59
1:C:4044:LYS:HB2	1:C:4075:GLU:HG2	1.83	0.59
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.67	0.59
1:A:365:HIS:NE2	1:A:367:ASP:OD2	2.35	0.59
1:A:2275:SER:OG	1:A:2287:ILE:O	2.17	0.59
1:B:69:LEU:HD22	1:B:113:LEU:HD11	1.84	0.59
1:B:1681:VAL:HG23	1:B:1682:ASP:H	1.67	0.59
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.84	0.59
1:A:900:LEU:HD22	1:A:902:TRP:NE1	2.18	0.59
1:C:3831:ASP:HB3	1:C:3834:PHE:HB3	1.85	0.59
1:D:373:THR:HG22	1:D:397:GLY:HA2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1681:VAL:HG23	1:D:1682:ASP:H	1.67	0.59
1:B:365:HIS:NE2	1:B:367:ASP:OD2	2.35	0.59
1:B:386:SER:HB3	1:B:388:GLN:HE22	1.67	0.59
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.83	0.59
1:D:4044:LYS:HB2	1:D:4075:GLU:HG2	1.83	0.59
1:A:69:LEU:HD22	1:A:113:LEU:HD11	1.84	0.59
1:A:1052:GLU:HA	1:A:1055:ARG:HB2	1.82	0.59
1:B:279:THR:HG22	1:B:281:ARG:H	1.67	0.59
1:C:4153:GLU:O	1:C:4157:THR:OG1	2.19	0.59
1:C:4778:TYR:O	1:C:4782:VAL:HG12	2.03	0.59
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.67	0.59
1:D:880:ARG:HG3	1:D:881:ILE:HD12	1.82	0.59
1:D:3831:ASP:HB3	1:D:3834:PHE:HB3	1.85	0.59
1:D:4778:TYR:O	1:D:4782:VAL:HG12	2.03	0.59
1:B:2148:ILE:HA	1:B:2151:ASN:HD22	1.68	0.59
1:D:386:SER:HB3	1:D:388:GLN:HE22	1.67	0.59
1:D:2148:ILE:HA	1:D:2151:ASN:HD22	1.68	0.59
1:D:2855:LYS:HA	1:D:2855:LYS:HE3	1.84	0.59
1:C:386:SER:HB3	1:C:388:GLN:HE22	1.67	0.59
1:D:3822:GLU:HG3	1:D:3827:LYS:HG3	1.84	0.59
2:J:24:VAL:HG22	2:J:48:LYS:HG2	1.83	0.59
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.84	0.59
1:C:2148:ILE:HA	1:C:2151:ASN:HD22	1.68	0.59
1:C:3822:GLU:HG3	1:C:3827:LYS:HG3	1.84	0.59
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.67	0.59
1:D:900:LEU:HD22	1:D:902:TRP:NE1	2.18	0.59
1:C:365:HIS:NE2	1:C:367:ASP:OD2	2.35	0.58
1:A:279:THR:HG22	1:A:281:ARG:H	1.67	0.58
1:B:281:ARG:NH1	1:B:345:GLU:OE2	2.33	0.58
1:C:2855:LYS:HA	1:C:2855:LYS:HE3	1.84	0.58
1:A:3831:ASP:HB3	1:A:3834:PHE:HB3	1.85	0.58
1:B:3818:MET:SD	1:B:3818:MET:N	2.68	0.58
1:B:3937:SER:OG	1:B:3938:ARG:N	2.37	0.58
1:A:3937:SER:OG	1:A:3938:ARG:N	2.37	0.58
1:B:290:ARG:H	1:B:293:GLN:HE21	1.51	0.58
1:B:900:LEU:HD22	1:B:902:TRP:NE1	2.18	0.58
1:A:2148:ILE:HA	1:A:2151:ASN:HD22	1.68	0.58
1:B:676:GLU:HB2	1:B:803:LEU:HB2	1.84	0.58
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.67	0.58
1:C:2312:VAL:HG23	1:C:2315:ASN:HB2	1.86	0.58
1:D:365:HIS:NE2	1:D:367:ASP:OD2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2312:VAL:HG23	1:D:2315:ASN:HB2	1.86	0.58
1:D:4756:LEU:O	1:D:4760:THR:OG1	2.21	0.58
1:A:4756:LEU:O	1:A:4760:THR:OG1	2.21	0.58
1:C:900:LEU:HD22	1:C:902:TRP:NE1	2.18	0.58
1:B:2275:SER:OG	1:B:2287:ILE:O	2.17	0.58
1:C:3937:SER:OG	1:C:3938:ARG:N	2.37	0.58
1:A:290:ARG:H	1:A:293:GLN:HE21	1.51	0.58
1:A:1814:THR:OG1	1:A:1815:THR:N	2.36	0.58
1:A:1681:VAL:HG23	1:A:1682:ASP:H	1.67	0.58
1:B:3891:TYR:O	1:B:3956:LYS:NZ	2.35	0.58
1:B:4778:TYR:O	1:B:4782:VAL:HG12	2.03	0.58
1:C:1814:THR:OG1	1:C:1815:THR:N	2.36	0.58
1:D:769:ARG:HA	1:D:774:PRO:HA	1.86	0.57
1:D:908:ARG:HG2	1:D:916:PRO:HG3	1.86	0.57
1:A:2325:ARG:NH2	1:D:189:GLU:O	2.36	0.57
1:B:3831:ASP:HB3	1:B:3834:PHE:HB3	1.85	0.57
1:D:3937:SER:OG	1:D:3938:ARG:N	2.37	0.57
1:A:2312:VAL:HG23	1:A:2315:ASN:HB2	1.86	0.57
1:A:4778:TYR:O	1:A:4782:VAL:HG12	2.03	0.57
1:C:769:ARG:HA	1:C:774:PRO:HA	1.87	0.57
1:C:2404:GLU:HG3	1:C:2405:MET:N	2.16	0.57
1:C:4756:LEU:O	1:C:4760:THR:OG1	2.21	0.57
1:D:933:LEU:O	1:D:937:LEU:HG	2.05	0.57
1:A:908:ARG:HG2	1:A:916:PRO:HG3	1.86	0.57
1:A:1918:ARG:O	1:A:1922:GLU:HG2	2.04	0.57
1:B:2141:MET:SD	1:B:2173:VAL:HG11	2.45	0.57
1:A:386:SER:HB3	1:A:388:GLN:HE22	1.67	0.57
1:D:1918:ARG:O	1:D:1922:GLU:HG2	2.04	0.57
1:A:2276:CYS:SG	1:A:2290:ASN:ND2	2.78	0.57
1:B:1814:THR:OG1	1:B:1815:THR:N	2.36	0.57
1:B:2312:VAL:HG23	1:B:2315:ASN:HB2	1.86	0.57
1:C:908:ARG:HG2	1:C:916:PRO:HG3	1.86	0.57
1:C:3891:TYR:O	1:C:3956:LYS:NZ	2.35	0.57
1:A:933:LEU:O	1:A:937:LEU:HG	2.05	0.57
1:A:2141:MET:SD	1:A:2173:VAL:HG11	2.45	0.57
1:A:3818:MET:SD	1:A:3818:MET:N	2.68	0.57
1:B:1009:ARG:O	1:B:1013:ARG:NH1	2.38	0.57
1:C:933:LEU:O	1:C:937:LEU:HG	2.05	0.57
1:D:2276:CYS:SG	1:D:2290:ASN:ND2	2.78	0.57
1:C:2716:LEU:O	1:C:2720:ILE:HG12	2.05	0.57
1:D:1814:THR:OG1	1:D:1815:THR:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ARG:HA	1:A:774:PRO:HA	1.86	0.57
1:A:2716:LEU:O	1:A:2720:ILE:HG12	2.05	0.57
1:B:1267:HIS:HB2	1:B:1294:ASN:HB2	1.87	0.57
1:B:1918:ARG:O	1:B:1922:GLU:HG2	2.04	0.57
1:B:4756:LEU:O	1:B:4760:THR:OG1	2.21	0.57
1:C:548:CYS:HB3	1:C:578:VAL:HG23	1.86	0.57
1:A:1684:PRO:HD3	2:G:42:ASP:HB3	1.87	0.57
1:A:2228:LEU:HD22	1:A:2296:ARG:HG3	1.87	0.57
1:B:548:CYS:HB3	1:B:578:VAL:HG23	1.86	0.57
1:B:2716:LEU:O	1:B:2720:ILE:HG12	2.05	0.57
1:C:1009:ARG:O	1:C:1013:ARG:NH1	2.38	0.57
1:C:2145:LEU:HD23	1:C:2148:ILE:HD11	1.87	0.57
1:D:290:ARG:H	1:D:293:GLN:HE21	1.51	0.57
1:D:2228:LEU:HD22	1:D:2296:ARG:HG3	1.87	0.57
1:B:769:ARG:HA	1:B:774:PRO:HA	1.86	0.56
1:C:2141:MET:SD	1:C:2173:VAL:HG11	2.45	0.56
1:D:1009:ARG:O	1:D:1013:ARG:NH1	2.38	0.56
1:A:548:CYS:HB3	1:A:578:VAL:HG23	1.86	0.56
1:B:2145:LEU:HD23	1:B:2148:ILE:HD11	1.87	0.56
1:C:290:ARG:H	1:C:293:GLN:HE21	1.51	0.56
1:D:2145:LEU:HD23	1:D:2148:ILE:HD11	1.87	0.56
1:A:2145:LEU:HD23	1:A:2148:ILE:HD11	1.87	0.56
1:B:908:ARG:HG2	1:B:916:PRO:HG3	1.86	0.56
1:B:933:LEU:O	1:B:937:LEU:HG	2.05	0.56
1:B:1383:ARG:HE	1:B:1385:LYS:HE2	1.71	0.56
1:B:2070:GLN:O	1:B:3659:ARG:NH1	2.38	0.56
1:C:1918:ARG:O	1:C:1922:GLU:HG2	2.04	0.56
1:D:3822:GLU:OE2	1:D:3824:SER:N	2.32	0.56
1:A:1267:HIS:HB2	1:A:1294:ASN:HB2	1.87	0.56
1:A:1383:ARG:HE	1:A:1385:LYS:HE2	1.71	0.56
1:A:2404:GLU:HG3	1:A:2405:MET:N	2.16	0.56
2:G:88:HIS:H	2:G:92:ILE:HB	1.71	0.56
1:B:606:ARG:NH2	1:B:1635:GLU:OE1	2.34	0.56
1:C:587:ASN:OD1	1:C:2132:ARG:NH1	2.38	0.56
1:C:1383:ARG:HE	1:C:1385:LYS:HE2	1.71	0.56
1:C:2228:LEU:HD22	1:C:2296:ARG:HG3	1.87	0.56
1:C:2276:CYS:SG	1:C:2290:ASN:ND2	2.78	0.56
1:C:2836:LEU:HA	1:C:2839:MET:HE3	1.86	0.56
1:D:548:CYS:HB3	1:D:578:VAL:HG23	1.86	0.56
1:D:1383:ARG:HE	1:D:1385:LYS:HE2	1.71	0.56
1:D:2716:LEU:O	1:D:2720:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:88:HIS:H	2:J:92:ILE:HB	1.71	0.56
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.88	0.56
1:A:1122:CYS:HA	1:A:1133:ARG:HD3	1.88	0.56
1:B:1684:PRO:HD3	2:H:42:ASP:HB3	1.86	0.56
1:B:2276:CYS:SG	1:B:2290:ASN:ND2	2.78	0.56
1:B:2277:GLN:HA	1:B:2280:VAL:HG22	1.87	0.56
2:H:32:GLN:NE2	2:H:97:THR:OG1	2.34	0.56
1:D:2141:MET:SD	1:D:2173:VAL:HG11	2.45	0.56
1:A:677:LEU:HD12	1:A:802:PHE:HA	1.87	0.56
1:A:1678:CYS:SG	1:A:1679:SER:N	2.78	0.56
1:A:2314:GLU:O	1:A:2318:VAL:HG13	2.06	0.56
1:B:2228:LEU:HD22	1:B:2296:ARG:HG3	1.87	0.56
1:C:4824:GLY:O	1:D:4821:ARG:NH2	2.39	0.56
1:A:587:ASN:OD1	1:A:2132:ARG:NH1	2.38	0.56
1:A:1009:ARG:O	1:A:1013:ARG:NH1	2.38	0.56
1:B:973:THR:OG1	1:B:976:TYR:O	2.18	0.56
1:B:1122:CYS:HA	1:B:1133:ARG:HD3	1.88	0.56
1:C:2314:GLU:O	1:C:2318:VAL:HG13	2.06	0.56
2:I:88:HIS:H	2:I:92:ILE:HB	1.71	0.56
1:D:1678:CYS:SG	1:D:1679:SER:N	2.78	0.56
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.88	0.56
1:B:168:GLN:HG3	1:B:169:ARG:HG3	1.88	0.56
2:H:88:HIS:H	2:H:92:ILE:HB	1.71	0.56
1:C:606:ARG:NH2	1:C:1635:GLU:OE1	2.34	0.56
1:C:1267:HIS:HB2	1:C:1294:ASN:HB2	1.87	0.56
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.88	0.56
1:C:2070:GLN:O	1:C:3659:ARG:NH1	2.38	0.56
1:C:3728:ALA:HA	1:C:3731:HIS:ND1	2.21	0.56
1:A:3891:TYR:O	1:A:3956:LYS:NZ	2.35	0.56
1:D:677:LEU:HD12	1:D:802:PHE:HA	1.87	0.56
1:B:2731:TRP:NE1	1:B:2762:LEU:HD13	2.21	0.55
1:D:3728:ALA:HA	1:D:3731:HIS:ND1	2.21	0.55
1:B:1678:CYS:SG	1:B:1679:SER:N	2.78	0.55
1:C:1678:CYS:SG	1:C:1679:SER:N	2.78	0.55
1:C:2064:THR:HG22	1:C:2067:ARG:HH12	1.72	0.55
1:D:1267:HIS:HB2	1:D:1294:ASN:HB2	1.87	0.55
1:B:677:LEU:HD12	1:B:802:PHE:HA	1.87	0.55
1:B:2314:GLU:O	1:B:2318:VAL:HG13	2.06	0.55
1:B:3728:ALA:HA	1:B:3731:HIS:ND1	2.21	0.55
1:C:677:LEU:HD12	1:C:802:PHE:HA	1.87	0.55
1:A:168:GLN:HG3	1:A:169:ARG:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2731:TRP:NE1	1:A:2762:LEU:HD13	2.22	0.55
1:B:235:ARG:NH1	1:B:268:SER:O	2.40	0.55
1:D:2314:GLU:O	1:D:2318:VAL:HG13	2.06	0.55
1:A:732:LEU:HB3	1:A:779:PHE:CZ	2.42	0.55
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.88	0.55
1:C:1122:CYS:HA	1:C:1133:ARG:HD3	1.88	0.55
1:D:2064:THR:HG22	1:D:2067:ARG:HH12	1.72	0.55
1:D:2147:ASP:O	1:D:2151:ASN:ND2	2.40	0.55
1:D:2858:GLU:HG3	1:D:2859:LEU:HD23	1.88	0.55
1:A:2064:THR:HG22	1:A:2067:ARG:HH12	1.72	0.55
1:A:2766:GLU:HA	1:A:2769:ILE:HG23	1.89	0.55
1:B:732:LEU:HB3	1:B:779:PHE:CZ	2.42	0.55
1:B:2220:LEU:HD11	1:B:2242:ALA:HB2	1.89	0.55
1:C:168:GLN:HG3	1:C:169:ARG:HG3	1.87	0.55
1:C:2220:LEU:HD11	1:C:2242:ALA:HB2	1.89	0.55
1:D:1122:CYS:HA	1:D:1133:ARG:HD3	1.88	0.55
1:A:2147:ASP:O	1:A:2151:ASN:ND2	2.40	0.55
1:C:2731:TRP:NE1	1:C:2762:LEU:HD13	2.22	0.55
1:C:2851:TRP:HA	1:C:2854:LYS:HE2	1.88	0.55
2:I:32:GLN:NE2	2:I:97:THR:OG1	2.34	0.55
1:D:235:ARG:NH1	1:D:268:SER:O	2.40	0.55
1:D:1042:THR:O	1:D:1046:ASN:ND2	2.40	0.55
1:A:1794:GLN:O	1:A:1798:GLU:HG2	2.06	0.55
1:A:2070:GLN:O	1:A:3659:ARG:NH1	2.38	0.55
1:B:587:ASN:OD1	1:B:2132:ARG:NH1	2.38	0.55
1:D:2277:GLN:HA	1:D:2280:VAL:HG22	1.88	0.55
1:C:1265:HIS:CD2	1:C:1268:ILE:HB	2.43	0.55
1:D:1794:GLN:O	1:D:1798:GLU:HG2	2.06	0.55
1:D:2731:TRP:NE1	1:D:2762:LEU:HD13	2.22	0.55
1:A:1042:THR:O	1:A:1046:ASN:ND2	2.40	0.54
1:A:2220:LEU:HD11	1:A:2242:ALA:HB2	1.89	0.54
1:A:2851:TRP:HA	1:A:2854:LYS:HE2	1.89	0.54
1:A:3728:ALA:HA	1:A:3731:HIS:ND1	2.21	0.54
1:B:2064:THR:HG22	1:B:2067:ARG:HH12	1.72	0.54
1:B:2766:GLU:HA	1:B:2769:ILE:HG23	1.89	0.54
1:C:732:LEU:HB3	1:C:779:PHE:CZ	2.42	0.54
1:C:1794:GLN:O	1:C:1798:GLU:HG2	2.06	0.54
1:A:235:ARG:NH1	1:A:268:SER:O	2.40	0.54
1:B:1794:GLN:O	1:B:1798:GLU:HG2	2.06	0.54
2:H:39:SER:O	2:H:43:ARG:NH1	2.41	0.54
1:C:235:ARG:NH1	1:C:268:SER:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2277:GLN:HA	1:C:2280:VAL:HG22	1.88	0.54
2:H:78:THR:O	2:H:81:VAL:HG12	2.08	0.54
1:D:168:GLN:HG3	1:D:169:ARG:HG3	1.88	0.54
1:A:2858:GLU:HG3	1:A:2859:LEU:HD23	1.88	0.54
2:I:23:CYS:SG	2:I:51:ILE:HD11	2.48	0.54
1:D:587:ASN:OD1	1:D:2132:ARG:NH1	2.38	0.54
1:D:2404:GLU:HG3	1:D:2405:MET:N	2.16	0.54
1:A:2277:GLN:HA	1:A:2280:VAL:HG22	1.88	0.54
1:B:2147:ASP:O	1:B:2151:ASN:ND2	2.40	0.54
2:H:23:CYS:SG	2:H:51:ILE:HD11	2.48	0.54
1:D:1265:HIS:CD2	1:D:1268:ILE:HB	2.42	0.54
1:D:2070:GLN:O	1:D:3659:ARG:NH1	2.38	0.54
1:D:2851:TRP:HA	1:D:2854:LYS:HE2	1.88	0.54
1:A:59:PRO:HB3	1:A:296:ARG:HH12	1.73	0.54
1:B:356:TYR:HA	1:B:405:LEU:HB2	1.90	0.54
1:B:838:ARG:H	1:B:841:LYS:HZ3	1.55	0.54
1:C:1397:UNK:HA	1:C:1412:UNK:HA	1.90	0.54
1:A:4049:LYS:HA	1:A:4052:GLU:HG2	1.90	0.54
1:B:1610:SER:HB3	1:B:1619:LEU:HB3	1.89	0.54
1:B:2762:LEU:HD23	1:B:2767:LYS:HA	1.90	0.54
1:C:2858:GLU:HG3	1:C:2859:LEU:HD23	1.88	0.54
1:D:2220:LEU:HD11	1:D:2242:ALA:HB2	1.89	0.54
1:B:2404:GLU:HG3	1:B:2405:MET:N	2.16	0.54
1:B:4049:LYS:HA	1:B:4052:GLU:HG2	1.90	0.54
1:C:2147:ASP:O	1:C:2151:ASN:ND2	2.40	0.54
1:C:4164:VAL:HG22	1:C:4198:GLU:OE2	2.08	0.54
1:D:2766:GLU:HA	1:D:2769:ILE:HG23	1.89	0.54
1:A:2762:LEU:HD23	1:A:2767:LYS:HA	1.90	0.54
1:B:2851:TRP:HA	1:B:2854:LYS:HE2	1.89	0.54
1:C:1042:THR:O	1:C:1046:ASN:ND2	2.40	0.54
1:D:356:TYR:HA	1:D:405:LEU:HB2	1.90	0.54
1:A:902:TRP:HA	1:A:913:ARG:O	2.08	0.54
1:A:1610:SER:HB3	1:A:1619:LEU:HB3	1.89	0.54
1:B:1767:PRO:HG3	1:B:1781:PRO:HB3	1.90	0.54
2:I:78:THR:O	2:I:81:VAL:HG12	2.08	0.54
1:A:1767:PRO:HG3	1:A:1781:PRO:HB3	1.90	0.53
1:A:1845:GLN:NE2	1:A:1848:GLU:OE2	2.41	0.53
2:G:23:CYS:SG	2:G:51:ILE:HD11	2.48	0.53
1:B:59:PRO:HB3	1:B:296:ARG:HH12	1.73	0.53
1:B:228:LEU:HD13	1:B:405:LEU:HD13	1.90	0.53
1:B:902:TRP:HA	1:B:913:ARG:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:PRO:HB3	1:C:296:ARG:HH12	1.73	0.53
1:C:902:TRP:HA	1:C:913:ARG:O	2.08	0.53
2:I:39:SER:O	2:I:43:ARG:NH1	2.41	0.53
2:J:78:THR:O	2:J:81:VAL:HG12	2.08	0.53
1:A:973:THR:OG1	1:A:976:TYR:O	2.18	0.53
1:B:1265:HIS:CD2	1:B:1268:ILE:HB	2.42	0.53
1:B:2858:GLU:HG3	1:B:2859:LEU:HD23	1.88	0.53
1:C:1845:GLN:NE2	1:C:1848:GLU:OE2	2.41	0.53
1:D:921:PHE:O	1:D:929:ARG:NH1	2.37	0.53
2:J:23:CYS:SG	2:J:51:ILE:HD11	2.48	0.53
2:G:78:THR:O	2:G:81:VAL:HG12	2.08	0.53
1:B:1042:THR:O	1:B:1046:ASN:ND2	2.40	0.53
2:H:58:LYS:HG3	2:H:81:VAL:HG22	1.91	0.53
1:C:356:TYR:HA	1:C:405:LEU:HB2	1.90	0.53
1:D:1397:UNK:HA	1:D:1412:UNK:HA	1.90	0.53
1:C:1199:ASP:OD1	1:C:1199:ASP:N	2.40	0.53
1:D:1767:PRO:HG3	1:D:1781:PRO:HB3	1.91	0.53
1:B:1397:UNK:HA	1:B:1412:UNK:HA	1.90	0.53
2:I:58:LYS:HG3	2:I:81:VAL:HG22	1.91	0.53
1:D:732:LEU:HB3	1:D:779:PHE:CZ	2.42	0.53
1:A:228:LEU:HD13	1:A:405:LEU:HD13	1.90	0.53
1:C:2766:GLU:HA	1:C:2769:ILE:HG23	1.89	0.53
1:B:1845:GLN:NE2	1:B:1848:GLU:OE2	2.41	0.53
1:B:4183:GLU:O	1:B:4187:LEU:HG	2.09	0.53
1:C:61:ASP:OD2	1:C:417:ARG:NH2	2.42	0.53
1:C:1610:SER:HB3	1:C:1619:LEU:HB3	1.89	0.53
1:D:228:LEU:HD13	1:D:405:LEU:HD13	1.90	0.53
1:D:902:TRP:HA	1:D:913:ARG:O	2.08	0.53
1:D:4046:ASP:OD1	1:D:4046:ASP:N	2.42	0.53
1:D:4049:LYS:HA	1:D:4052:GLU:HG2	1.89	0.53
2:J:39:SER:O	2:J:43:ARG:NH1	2.41	0.53
2:G:39:SER:O	2:G:43:ARG:NH1	2.41	0.53
1:B:246:THR:OG1	1:B:247:VAL:N	2.42	0.53
1:C:189:GLU:O	1:D:2325:ARG:NH2	2.41	0.53
1:C:228:LEU:HD13	1:C:405:LEU:HD13	1.90	0.53
1:C:1767:PRO:HG3	1:C:1781:PRO:HB3	1.91	0.53
1:D:61:ASP:OD2	1:D:417:ARG:NH2	2.42	0.53
1:D:1588:HIS:HE1	1:D:1590:GLN:HE21	1.57	0.53
1:A:1588:HIS:HE1	1:A:1590:GLN:HE21	1.57	0.53
1:A:4046:ASP:OD1	1:A:4046:ASP:N	2.42	0.53
1:B:61:ASP:OD2	1:B:417:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2404:GLU:HG3	1:B:2405:MET:HG3	1.91	0.53
1:C:2762:LEU:HD23	1:C:2767:LYS:HA	1.90	0.53
1:D:246:THR:OG1	1:D:247:VAL:N	2.42	0.53
1:D:2762:LEU:HD23	1:D:2767:LYS:HA	1.90	0.53
1:A:356:TYR:HA	1:A:405:LEU:HB2	1.90	0.53
1:A:3899:GLU:N	1:A:3899:GLU:OE2	2.42	0.53
1:B:1588:HIS:HE1	1:B:1590:GLN:HE21	1.57	0.53
1:D:1610:SER:HB3	1:D:1619:LEU:HB3	1.89	0.53
1:D:4183:GLU:O	1:D:4187:LEU:HG	2.09	0.53
1:A:629:GLN:HE21	1:A:1670:ASN:HD22	1.57	0.52
1:C:973:THR:OG1	1:C:976:TYR:O	2.18	0.52
1:D:59:PRO:HB3	1:D:296:ARG:HH12	1.73	0.52
1:A:606:ARG:NH2	1:A:1635:GLU:OE1	2.34	0.52
1:A:1397:UNK:HA	1:A:1412:UNK:HA	1.90	0.52
2:G:58:LYS:HG3	2:G:81:VAL:HG22	1.91	0.52
1:C:833:LYS:HE3	1:C:834:VAL:H	1.75	0.52
1:A:246:THR:OG1	1:A:247:VAL:N	2.42	0.52
1:A:707:PRO:O	1:A:838:ARG:NH1	2.43	0.52
1:A:4183:GLU:O	1:A:4187:LEU:HG	2.09	0.52
1:B:674:TYR:HD2	1:B:758:CYS:HG	1.57	0.52
1:B:707:PRO:O	1:B:838:ARG:NH1	2.43	0.52
1:C:246:THR:OG1	1:C:247:VAL:N	2.42	0.52
1:D:707:PRO:O	1:D:838:ARG:NH1	2.43	0.52
1:C:707:PRO:O	1:C:838:ARG:NH1	2.43	0.52
1:C:4183:GLU:O	1:C:4187:LEU:HG	2.09	0.52
1:B:3729:ARG:O	1:B:3733:ARG:NH1	2.43	0.52
1:C:238:HIS:HB2	1:C:241:MET:HB2	1.92	0.52
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.92	0.52
1:C:844:ARG:HE	1:C:845:THR:H	1.57	0.52
1:A:238:HIS:HB2	1:A:241:MET:HB2	1.92	0.52
1:A:4754:THR:OG1	1:D:4765:GLN:OE1	2.28	0.52
1:C:3729:ARG:O	1:C:3733:ARG:NH1	2.43	0.52
1:C:3899:GLU:N	1:C:3899:GLU:OE2	2.42	0.52
1:C:4049:LYS:HA	1:C:4052:GLU:HG2	1.90	0.52
1:D:3729:ARG:O	1:D:3733:ARG:NH1	2.43	0.52
1:D:3961:SER:OG	1:D:3962:SER:N	2.43	0.52
1:A:61:ASP:OD2	1:A:417:ARG:NH2	2.42	0.52
1:A:1265:HIS:CD2	1:A:1268:ILE:HB	2.43	0.52
1:A:1567:LEU:HD22	1:A:1581:PRO:HB3	1.92	0.52
1:A:2404:GLU:HG3	1:A:2405:MET:HG3	1.91	0.52
1:A:3729:ARG:O	1:A:3733:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4784:ALA:HA	1:A:4788:PHE:HD2	1.75	0.52
1:D:238:HIS:HB2	1:D:241:MET:HB2	1.92	0.52
1:D:2254:LEU:O	1:D:3809:ARG:HD3	2.10	0.52
1:D:2404:GLU:HG3	1:D:2405:MET:HG3	1.91	0.52
2:G:9:SER:HB2	2:G:72:ARG:HB2	1.91	0.52
1:B:629:GLN:HE21	1:B:1670:ASN:HD22	1.57	0.52
1:B:643:LEU:HD13	1:B:1658:THR:HG23	1.92	0.52
1:B:3899:GLU:OE2	1:B:3899:GLU:N	2.42	0.52
1:C:629:GLN:HE21	1:C:1670:ASN:HD22	1.57	0.52
1:C:2254:LEU:O	1:C:3809:ARG:HD3	2.10	0.52
1:D:3899:GLU:N	1:D:3899:GLU:OE2	2.42	0.52
1:A:1048:ASP:HA	1:A:1051:ARG:HD2	1.92	0.52
1:B:1567:LEU:HD22	1:B:1581:PRO:HB3	1.92	0.52
1:C:1029:ASN:HB2	1:C:1032:LEU:HD13	1.92	0.52
1:C:1588:HIS:HE1	1:C:1590:GLN:HE21	1.57	0.52
1:D:1845:GLN:NE2	1:D:1848:GLU:OE2	2.41	0.52
1:A:833:LYS:HE3	1:A:834:VAL:H	1.75	0.52
2:H:9:SER:HB2	2:H:72:ARG:HB2	1.91	0.52
1:D:606:ARG:NH2	1:D:1635:GLU:OE1	2.35	0.52
2:J:58:LYS:HG3	2:J:81:VAL:HG22	1.91	0.52
1:A:4164:VAL:HG22	1:A:4198:GLU:OE2	2.10	0.51
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.92	0.51
1:B:2728:HIS:O	1:B:2732:SER:OG	2.24	0.51
1:C:343:ARG:HH21	1:C:345:GLU:H	1.58	0.51
1:C:890:HIS:O	1:C:894:VAL:HG23	2.10	0.51
1:D:1199:ASP:OD1	1:D:1199:ASP:N	2.40	0.51
2:J:9:SER:HB2	2:J:72:ARG:HB2	1.91	0.51
1:A:844:ARG:HE	1:A:845:THR:H	1.57	0.51
1:A:2254:LEU:O	1:A:3809:ARG:HD3	2.10	0.51
1:B:343:ARG:HH21	1:B:345:GLU:H	1.58	0.51
1:B:833:LYS:HE3	1:B:834:VAL:H	1.75	0.51
1:B:1754:LEU:HG	1:B:1756:THR:HG23	1.93	0.51
1:B:4112:THR:O	1:B:4116:THR:HG23	2.10	0.51
1:D:643:LEU:HD13	1:D:1658:THR:HG23	1.92	0.51
1:D:911:ASN:OD1	1:D:911:ASN:N	2.41	0.51
1:D:4164:VAL:HG22	1:D:4198:GLU:OE2	2.10	0.51
1:A:643:LEU:HD13	1:A:1658:THR:HG23	1.92	0.51
1:B:1048:ASP:HA	1:B:1051:ARG:HD2	1.92	0.51
1:B:4763:GLY:O	1:B:4767:VAL:HG22	2.11	0.51
1:B:4784:ALA:HA	1:B:4788:PHE:HD2	1.75	0.51
1:C:4112:THR:O	1:C:4116:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:ASP:N	1:D:721:ASP:OD1	2.43	0.51
1:C:1257:GLN:HA	1:C:1384:LEU:HD22	1.92	0.51
1:C:2271:CYS:SG	1:C:2294:GLY:N	2.84	0.51
1:C:2404:GLU:HG3	1:C:2405:MET:HG3	1.91	0.51
1:C:4763:GLY:O	1:C:4767:VAL:HG22	2.11	0.51
1:D:343:ARG:HH21	1:D:345:GLU:H	1.58	0.51
1:D:1932:VAL:HG21	1:D:3616:VAL:HA	1.92	0.51
1:D:2271:CYS:SG	1:D:2294:GLY:N	2.84	0.51
1:D:3940:TRP:HA	1:D:3943:VAL:HG22	1.93	0.51
1:B:238:HIS:HB2	1:B:241:MET:HB2	1.92	0.51
1:B:2254:LEU:O	1:B:3809:ARG:HD3	2.10	0.51
1:D:1029:ASN:HB2	1:D:1032:LEU:HD13	1.92	0.51
1:B:699:SER:OG	1:B:700:THR:N	2.44	0.51
1:B:1932:VAL:HG21	1:B:3616:VAL:HA	1.92	0.51
1:C:1932:VAL:HG21	1:C:3616:VAL:HA	1.92	0.51
1:C:3961:SER:OG	1:C:3962:SER:N	2.43	0.51
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.93	0.51
1:C:921:PHE:O	1:C:929:ARG:NH1	2.37	0.51
1:C:2206:SER:OG	1:C:2207:ARG:N	2.44	0.51
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.92	0.51
1:D:4784:ALA:HA	1:D:4788:PHE:HD2	1.75	0.51
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.92	0.51
1:A:721:ASP:N	1:A:721:ASP:OD1	2.43	0.51
1:A:1095:ALA:HB1	1:A:1200:GLY:HA3	1.92	0.51
1:A:4763:GLY:O	1:A:4767:VAL:HG22	2.11	0.51
1:D:633:CYS:SG	1:D:1673:VAL:HG13	2.51	0.51
1:D:844:ARG:HE	1:D:845:THR:H	1.57	0.51
1:D:1095:ALA:HB1	1:D:1200:GLY:HA3	1.92	0.51
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.14	0.51
1:A:4762:ASN:O	1:A:4764:LYS:N	2.44	0.51
1:B:1095:ALA:HB1	1:B:1200:GLY:HA3	1.92	0.51
1:B:1257:GLN:HA	1:B:1384:LEU:HD22	1.93	0.51
1:C:1321:UNK:HA	1:C:1436:UNK:HA	1.93	0.51
1:C:1567:LEU:HD22	1:C:1581:PRO:HB3	1.92	0.51
1:C:4046:ASP:OD1	1:C:4046:ASP:N	2.42	0.51
1:D:629:GLN:HE21	1:D:1670:ASN:HD22	1.57	0.51
1:D:833:LYS:HE3	1:D:834:VAL:H	1.75	0.51
1:D:890:HIS:O	1:D:894:VAL:HG23	2.10	0.51
1:D:1257:GLN:HA	1:D:1384:LEU:HD22	1.93	0.51
1:D:4762:ASN:O	1:D:4764:LYS:N	2.44	0.51
1:A:633:CYS:SG	1:A:1673:VAL:HG13	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2271:CYS:SG	1:A:2294:GLY:N	2.84	0.51
1:B:844:ARG:HE	1:B:845:THR:H	1.57	0.51
1:B:2455:MET:HG3	1:B:2457:ALA:H	1.76	0.51
1:B:3961:SER:OG	1:B:3962:SER:N	2.43	0.51
1:B:3986:GLU:O	1:B:4935:GLN:NE2	2.44	0.51
1:B:4164:VAL:HG22	1:B:4198:GLU:OE2	2.11	0.51
1:B:4665:ILE:O	1:B:4668:LEU:HD23	2.11	0.51
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.93	0.51
1:D:4763:GLY:O	1:D:4767:VAL:HG22	2.11	0.51
2:J:50:ARG:N	2:J:55:GLU:OE2	2.41	0.51
1:A:699:SER:OG	1:A:700:THR:N	2.44	0.50
1:A:3986:GLU:O	1:A:4935:GLN:NE2	2.44	0.50
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.14	0.50
1:B:2080:VAL:HG13	1:B:3669:LEU:HD22	1.93	0.50
1:C:1095:ALA:HB1	1:C:1200:GLY:HA3	1.92	0.50
1:C:2231:PRO:HD3	1:C:2381:ILE:HD11	1.93	0.50
1:C:3940:TRP:HA	1:C:3943:VAL:HG22	1.93	0.50
1:D:1567:LEU:HD22	1:D:1581:PRO:HB3	1.92	0.50
1:D:2206:SER:OG	1:D:2207:ARG:N	2.44	0.50
1:A:1932:VAL:HG21	1:A:3616:VAL:HA	1.92	0.50
1:A:2836:LEU:HA	1:A:2839:MET:HE3	1.92	0.50
1:B:407:ARG:HH21	1:B:3864:ASN:HB3	1.77	0.50
1:B:890:HIS:O	1:B:894:VAL:HG23	2.10	0.50
1:B:2231:PRO:HD3	1:B:2381:ILE:HD11	1.93	0.50
1:B:2271:CYS:SG	1:B:2294:GLY:N	2.84	0.50
1:C:643:LEU:HD13	1:C:1658:THR:HG23	1.92	0.50
1:C:4665:ILE:O	1:C:4668:LEU:HD23	2.11	0.50
2:I:9:SER:HB2	2:I:72:ARG:HB2	1.91	0.50
1:D:4665:ILE:O	1:D:4668:LEU:HD23	2.11	0.50
1:A:4665:ILE:O	1:A:4668:LEU:HD23	2.11	0.50
1:B:1029:ASN:HB2	1:B:1032:LEU:HD13	1.92	0.50
1:B:1321:UNK:HA	1:B:1436:UNK:HA	1.93	0.50
1:C:1754:LEU:HG	1:C:1756:THR:HG23	1.92	0.50
1:C:2080:VAL:HG13	1:C:3669:LEU:HD22	1.93	0.50
1:C:2776:GLU:O	1:C:2780:THR:HG23	2.12	0.50
1:C:4784:ALA:HA	1:C:4788:PHE:HD2	1.75	0.50
1:D:1048:ASP:HA	1:D:1051:ARG:HD2	1.92	0.50
1:A:189:GLU:O	1:B:2325:ARG:NH2	2.44	0.50
1:A:436:LEU:HD21	1:A:517:VAL:HG12	1.94	0.50
1:A:890:HIS:O	1:A:894:VAL:HG23	2.10	0.50
1:A:1029:ASN:HB2	1:A:1032:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2278:MET:N	1:A:2278:MET:SD	2.85	0.50
1:A:3961:SER:OG	1:A:3962:SER:N	2.43	0.50
1:A:4112:THR:O	1:A:4116:THR:HG23	2.10	0.50
1:B:2776:GLU:O	1:B:2780:THR:HG23	2.12	0.50
1:D:407:ARG:HH21	1:D:3864:ASN:HB3	1.77	0.50
1:D:3986:GLU:O	1:D:4935:GLN:NE2	2.44	0.50
1:D:4112:THR:O	1:D:4116:THR:HG23	2.10	0.50
1:D:4276:LYS:HZ1	1:D:4562:GLU:HG3	1.76	0.50
1:A:4607:ARG:NE	1:A:4643:TYR:OH	2.45	0.50
1:B:692:HIS:HB3	1:B:795:SER:HB3	1.94	0.50
1:B:4607:ARG:NE	1:B:4643:TYR:OH	2.45	0.50
1:C:2278:MET:N	1:C:2278:MET:SD	2.85	0.50
1:D:1321:UNK:HA	1:D:1436:UNK:HA	1.93	0.50
1:A:407:ARG:HH21	1:A:3864:ASN:HB3	1.77	0.50
1:B:3940:TRP:HA	1:B:3943:VAL:HG22	1.93	0.50
1:C:1048:ASP:HA	1:C:1051:ARG:HD2	1.92	0.50
1:D:436:LEU:HD21	1:D:517:VAL:HG12	1.94	0.50
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.93	0.50
1:D:1754:LEU:HG	1:D:1756:THR:HG23	1.92	0.50
1:A:343:ARG:HH21	1:A:345:GLU:H	1.58	0.50
1:A:1257:GLN:HA	1:A:1384:LEU:HD22	1.92	0.50
1:A:2776:GLU:O	1:A:2780:THR:HG23	2.12	0.50
1:B:756:SER:OG	1:B:769:ARG:HB2	2.12	0.50
1:B:1001:GLU:HG2	1:B:1035:TYR:CD2	2.47	0.50
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.94	0.50
1:A:2455:MET:HG3	1:A:2457:ALA:H	1.77	0.50
1:B:2206:SER:OG	1:B:2207:ARG:N	2.44	0.50
1:C:633:CYS:SG	1:C:1673:VAL:HG13	2.51	0.50
1:C:2455:MET:HG3	1:C:2457:ALA:H	1.77	0.50
1:D:1677:LEU:HA	1:D:1680:HIS:HB2	1.94	0.50
1:D:2776:GLU:O	1:D:2780:THR:HG23	2.12	0.50
1:A:80:GLU:OE1	1:A:80:GLU:HA	2.12	0.50
1:A:756:SER:OG	1:A:769:ARG:HB2	2.12	0.50
1:A:1199:ASP:OD1	1:A:1199:ASP:N	2.40	0.50
1:C:114:LEU:HB2	1:C:117:HIS:CD2	2.47	0.50
1:D:2836:LEU:HA	1:D:2839:MET:HE3	1.93	0.50
1:A:686:VAL:HG13	1:A:687:THR:HG22	1.93	0.49
1:B:721:ASP:OD1	1:B:721:ASP:N	2.43	0.49
1:B:4070:GLU:OE1	1:B:4070:GLU:N	2.43	0.49
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.14	0.49
1:A:1001:GLU:HG2	1:A:1035:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1677:LEU:HA	1:A:1680:HIS:HB2	1.94	0.49
1:A:2080:VAL:HG13	1:A:3669:LEU:HD22	1.93	0.49
1:A:2206:SER:OG	1:A:2207:ARG:N	2.44	0.49
1:A:4029:ASP:OD1	1:A:4029:ASP:N	2.45	0.49
1:B:2278:MET:N	1:B:2278:MET:SD	2.85	0.49
1:C:3986:GLU:O	1:C:4935:GLN:NE2	2.44	0.49
1:D:80:GLU:OE1	1:D:80:GLU:HA	2.12	0.49
1:D:2080:VAL:HG13	1:D:3669:LEU:HD22	1.93	0.49
1:D:2278:MET:SD	1:D:2278:MET:N	2.85	0.49
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.94	0.49
1:B:763:ALA:HB3	1:B:764:PRO:HD3	1.95	0.49
1:C:692:HIS:HB3	1:C:795:SER:HB3	1.94	0.49
1:C:1986:PRO:HB2	1:C:1988:PRO:HD2	1.95	0.49
1:C:4029:ASP:OD2	1:C:4054:HIS:NE2	2.43	0.49
1:D:227:TYR:HA	1:D:355:LYS:HA	1.95	0.49
1:D:4029:ASP:OD2	1:D:4054:HIS:NE2	2.43	0.49
1:A:4029:ASP:OD2	1:A:4054:HIS:NE2	2.43	0.49
2:G:50:ARG:N	2:G:55:GLU:OE2	2.41	0.49
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.14	0.49
1:C:878:LEU:HD11	1:C:951:GLY:HA2	1.95	0.49
1:C:1001:GLU:HG2	1:C:1035:TYR:CD2	2.47	0.49
1:C:1677:LEU:HA	1:C:1680:HIS:HB2	1.94	0.49
1:C:4029:ASP:OD1	1:C:4029:ASP:N	2.45	0.49
1:D:756:SER:OG	1:D:769:ARG:HB2	2.12	0.49
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.94	0.49
1:A:1321:UNK:HA	1:A:1436:UNK:HA	1.93	0.49
1:A:2231:PRO:HD3	1:A:2381:ILE:HD11	1.93	0.49
1:A:4508:ALA:O	1:A:4512:ASN:ND2	2.45	0.49
1:B:633:CYS:SG	1:B:1673:VAL:HG13	2.51	0.49
1:B:4046:ASP:N	1:B:4046:ASP:OD1	2.42	0.49
1:C:672:LYS:HB3	1:C:819:TYR:HA	1.94	0.49
1:C:699:SER:OG	1:C:700:THR:N	2.44	0.49
1:C:721:ASP:OD1	1:C:721:ASP:N	2.43	0.49
1:D:674:TYR:HD2	1:D:758:CYS:HG	1.61	0.49
1:D:4607:ARG:NE	1:D:4643:TYR:OH	2.45	0.49
1:A:428:ARG:HG3	1:A:446:ASP:OD2	2.13	0.49
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.45	0.49
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.93	0.49
1:A:1754:LEU:HG	1:A:1756:THR:HG23	1.92	0.49
1:B:1362:ASP:N	1:B:1362:ASP:OD1	2.45	0.49
1:B:1986:PRO:HB2	1:B:1988:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3898:ASP:OD1	1:B:3898:ASP:N	2.44	0.49
1:C:435:ALA:HA	1:C:438:LYS:HE3	1.95	0.49
1:C:686:VAL:HG13	1:C:687:THR:HG22	1.93	0.49
1:D:672:LYS:HB3	1:D:819:TYR:HA	1.94	0.49
1:D:699:SER:OG	1:D:700:THR:N	2.44	0.49
1:D:1362:ASP:OD1	1:D:1362:ASP:N	2.45	0.49
1:B:80:GLU:OE1	1:B:80:GLU:HA	2.12	0.49
1:B:686:VAL:HG13	1:B:687:THR:HG22	1.93	0.49
1:C:407:ARG:HH21	1:C:3864:ASN:HB3	1.77	0.49
1:D:692:HIS:HB3	1:D:795:SER:HB3	1.94	0.49
1:D:878:LEU:HD11	1:D:951:GLY:HA2	1.95	0.49
1:D:1001:GLU:HG2	1:D:1035:TYR:CD2	2.47	0.49
1:D:2455:MET:HG3	1:D:2457:ALA:H	1.77	0.49
1:A:1008:ALA:O	1:A:1012:ILE:HG23	2.13	0.49
1:A:2101:LEU:O	1:A:2104:THR:HG22	2.13	0.49
1:A:2340:ASN:OD1	1:A:2340:ASN:N	2.46	0.49
1:B:114:LEU:HB2	1:B:117:HIS:CD2	2.47	0.49
1:C:436:LEU:HD21	1:C:517:VAL:HG12	1.94	0.49
1:C:756:SER:OG	1:C:769:ARG:HB2	2.12	0.49
1:C:763:ALA:HB3	1:C:764:PRO:HD3	1.95	0.49
1:C:1359:ILE:HG13	1:C:1360:ASP:H	1.78	0.49
1:C:1362:ASP:N	1:C:1362:ASP:OD1	2.45	0.49
1:C:1985:CYS:SG	1:C:1992:ARG:HD2	2.53	0.49
1:C:4607:ARG:NE	1:C:4643:TYR:OH	2.45	0.49
1:D:686:VAL:HG13	1:D:687:THR:HG22	1.93	0.49
1:D:2231:PRO:HD3	1:D:2381:ILE:HD11	1.93	0.49
1:A:227:TYR:HA	1:A:355:LYS:HA	1.94	0.49
1:A:692:HIS:HB3	1:A:795:SER:HB3	1.94	0.49
1:A:878:LEU:HD11	1:A:951:GLY:HA2	1.95	0.49
1:A:1359:ILE:HG13	1:A:1360:ASP:H	1.78	0.49
1:A:1715:TYR:CZ	1:A:1762:MET:HB3	2.48	0.49
1:C:428:ARG:HG3	1:C:446:ASP:OD2	2.13	0.49
1:C:3898:ASP:OD1	1:C:3898:ASP:N	2.44	0.49
1:D:1986:PRO:HB2	1:D:1988:PRO:HD2	1.95	0.49
1:A:114:LEU:HB2	1:A:117:HIS:CD2	2.47	0.49
1:B:672:LYS:HB3	1:B:819:TYR:HA	1.94	0.49
1:B:1677:LEU:HA	1:B:1680:HIS:HB2	1.94	0.49
1:B:4762:ASN:O	1:B:4764:LYS:N	2.44	0.49
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.94	0.49
1:A:3940:TRP:HA	1:A:3943:VAL:HG22	1.93	0.48
1:A:4928:ASP:O	1:A:4932:HIS:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4709:LEU:HA	1:C:4712:VAL:HG22	1.95	0.48
1:D:370:LEU:HB2	1:D:393:MET:HB2	1.95	0.48
1:D:2484:LEU:O	1:D:2488:GLU:HG2	2.13	0.48
1:A:300:VAL:O	1:A:420:ARG:NH1	2.40	0.48
1:A:921:PHE:O	1:A:929:ARG:NH1	2.37	0.48
1:B:428:ARG:HG3	1:B:446:ASP:OD2	2.13	0.48
1:B:435:ALA:HA	1:B:438:LYS:HE3	1.95	0.48
1:B:436:LEU:HD21	1:B:517:VAL:HG12	1.94	0.48
1:B:878:LEU:HD11	1:B:951:GLY:HA2	1.95	0.48
1:C:80:GLU:OE1	1:C:80:GLU:HA	2.12	0.48
1:C:1715:TYR:CZ	1:C:1762:MET:HB3	2.48	0.48
1:C:2484:LEU:O	1:C:2488:GLU:HG2	2.13	0.48
1:D:114:LEU:HB2	1:D:117:HIS:CD2	2.47	0.48
1:D:1008:ALA:O	1:D:1012:ILE:HG23	2.13	0.48
1:D:1985:CYS:SG	1:D:1992:ARG:HD2	2.53	0.48
1:A:672:LYS:HB3	1:A:819:TYR:HA	1.94	0.48
1:B:4029:ASP:OD1	1:B:4029:ASP:N	2.45	0.48
1:C:370:LEU:HB2	1:C:393:MET:HB2	1.95	0.48
1:C:1008:ALA:O	1:C:1012:ILE:HG23	2.13	0.48
1:A:1985:CYS:SG	1:A:1992:ARG:HD2	2.53	0.48
1:A:1986:PRO:HB2	1:A:1988:PRO:HD2	1.94	0.48
1:B:370:LEU:HB2	1:B:393:MET:HB2	1.95	0.48
1:B:1008:ALA:O	1:B:1012:ILE:HG23	2.13	0.48
1:B:2836:LEU:HA	1:B:2839:MET:HE3	1.95	0.48
1:C:227:TYR:HA	1:C:355:LYS:HA	1.94	0.48
1:D:1359:ILE:HG13	1:D:1360:ASP:H	1.78	0.48
1:A:490:GLN:O	1:A:490:GLN:NE2	2.45	0.48
1:A:658:ASN:HD22	1:A:833:LYS:H	1.61	0.48
1:C:2331:GLY:HA3	1:C:2391:TYR:HE1	1.79	0.48
1:C:4570:THR:HA	1:C:4573:ILE:HG12	1.96	0.48
1:C:4757:SER:O	1:C:4761:HIS:HB2	2.14	0.48
1:C:4928:ASP:O	1:C:4932:HIS:NE2	2.46	0.48
1:C:4947:CYS:SG	1:C:4948:TRP:N	2.87	0.48
1:D:763:ALA:HB3	1:D:764:PRO:HD3	1.95	0.48
1:A:2484:LEU:O	1:A:2488:GLU:HG2	2.13	0.48
1:A:4709:LEU:HA	1:A:4712:VAL:HG22	1.95	0.48
1:B:1359:ILE:HG13	1:B:1360:ASP:H	1.78	0.48
1:B:1769:PHE:O	2:H:83:TYR:OH	2.28	0.48
1:B:1985:CYS:SG	1:B:1992:ARG:HD2	2.53	0.48
1:B:2101:LEU:O	1:B:2104:THR:HG22	2.13	0.48
1:C:4808:MET:HB2	1:D:4518:TYR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.94	0.48
1:B:2331:GLY:HA3	1:B:2391:TYR:HE1	1.79	0.48
1:D:2101:LEU:O	1:D:2104:THR:HG22	2.13	0.48
1:B:4709:LEU:HA	1:B:4712:VAL:HG22	1.95	0.48
1:C:2728:HIS:O	1:C:2732:SER:OG	2.24	0.48
1:D:70:GLU:OE1	1:D:122:ARG:NE	2.44	0.48
1:A:718:VAL:HG23	1:A:724:SER:HB3	1.96	0.48
1:B:4757:SER:O	1:B:4761:HIS:HB2	2.14	0.48
1:C:2722:LYS:HD2	1:C:2722:LYS:HA	1.63	0.48
1:D:428:ARG:HG3	1:D:446:ASP:OD2	2.13	0.48
1:D:435:ALA:HA	1:D:438:LYS:HE3	1.95	0.48
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.47	0.48
1:A:2296:ARG:NH1	1:A:2299:ASP:OD2	2.47	0.48
1:A:4947:CYS:SG	1:A:4948:TRP:N	2.87	0.48
1:B:552:SER:HA	1:B:555:LEU:HD13	1.96	0.48
1:B:712:GLU:HB3	1:B:713:TRP:CD2	2.49	0.48
1:B:718:VAL:HG23	1:B:724:SER:HB3	1.96	0.48
1:B:1715:TYR:CZ	1:B:1762:MET:HB3	2.48	0.48
1:B:3923:ILE:HD13	1:B:3934:LEU:HD12	1.96	0.48
1:B:4029:ASP:OD2	1:B:4054:HIS:NE2	2.43	0.48
1:B:4928:ASP:O	1:B:4932:HIS:NE2	2.46	0.48
1:B:4947:CYS:SG	1:B:4948:TRP:N	2.87	0.48
1:C:552:SER:HA	1:C:555:LEU:HD13	1.96	0.48
1:C:658:ASN:HD22	1:C:833:LYS:H	1.61	0.48
1:D:4709:LEU:HA	1:D:4712:VAL:HG22	1.95	0.48
1:D:4757:SER:O	1:D:4761:HIS:HB2	2.14	0.48
1:D:4928:ASP:O	1:D:4932:HIS:NE2	2.46	0.48
1:A:435:ALA:HA	1:A:438:LYS:HE3	1.95	0.47
1:A:674:TYR:HD2	1:A:758:CYS:HG	1.62	0.47
1:B:227:TYR:HA	1:B:355:LYS:HA	1.94	0.47
1:B:620:CYS:SG	1:B:621:HIS:N	2.87	0.47
1:B:658:ASN:HD22	1:B:833:LYS:H	1.61	0.47
1:B:1709:ASP:HA	1:B:1713:SER:HB3	1.96	0.47
1:C:712:GLU:HB3	1:C:713:TRP:CD2	2.49	0.47
1:A:641:ASP:OD1	1:A:642:LEU:N	2.47	0.47
1:B:441:LYS:HG2	1:B:442:LEU:HD23	1.95	0.47
1:B:875:PRO:O	1:B:882:ARG:NH2	2.46	0.47
1:B:2484:LEU:O	1:B:2488:GLU:HG2	2.13	0.47
1:B:2892:PHE:O	1:B:2896:GLN:HG2	2.14	0.47
1:C:620:CYS:SG	1:C:621:HIS:N	2.87	0.47
1:C:1090:ALA:HB3	1:C:1202:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1700:ARG:NH1	1:C:1817:PHE:O	2.47	0.47
1:C:2892:PHE:O	1:C:2896:GLN:HG2	2.14	0.47
1:D:1715:TYR:CZ	1:D:1762:MET:HB3	2.48	0.47
1:D:2296:ARG:NH1	1:D:2299:ASP:OD2	2.47	0.47
1:A:1343:PHE:HB2	1:A:1376:TYR:HD2	1.80	0.47
2:G:32:GLN:NE2	2:G:97:THR:OG1	2.34	0.47
1:B:4570:THR:HA	1:B:4573:ILE:HG12	1.96	0.47
1:C:3923:ILE:HD13	1:C:3934:LEU:HD12	1.96	0.47
1:A:620:CYS:SG	1:A:621:HIS:N	2.87	0.47
1:A:2331:GLY:HA3	1:A:2391:TYR:HE1	1.79	0.47
1:A:2903:SER:OG	1:A:2904:ARG:N	2.48	0.47
1:A:4570:THR:HA	1:A:4573:ILE:HG12	1.96	0.47
1:B:641:ASP:OD1	1:B:642:LEU:N	2.47	0.47
1:B:1343:PHE:HB2	1:B:1376:TYR:HD2	1.80	0.47
1:B:1700:ARG:NH1	1:B:1817:PHE:O	2.47	0.47
2:H:50:ARG:N	2:H:55:GLU:OE2	2.41	0.47
1:C:718:VAL:HG23	1:C:724:SER:HB3	1.96	0.47
2:I:50:ARG:N	2:I:55:GLU:OE2	2.41	0.47
1:D:603:LYS:HG2	1:D:1573:LYS:HZ1	1.80	0.47
1:D:718:VAL:HG23	1:D:724:SER:HB3	1.96	0.47
1:A:712:GLU:HB3	1:A:713:TRP:CD2	2.49	0.47
1:A:844:ARG:HE	1:A:845:THR:HG22	1.80	0.47
1:A:3923:ILE:HD13	1:A:3934:LEU:HD12	1.96	0.47
1:A:4757:SER:O	1:A:4761:HIS:HB2	2.14	0.47
1:B:4608:LYS:HG3	1:B:4614:LEU:HB2	1.97	0.47
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.47	0.47
1:C:1343:PHE:HB2	1:C:1376:TYR:HD2	1.80	0.47
1:D:267:VAL:HA	1:D:270:HIS:ND1	2.29	0.47
1:D:844:ARG:HE	1:D:845:THR:HG22	1.80	0.47
1:D:2331:GLY:HA3	1:D:2391:TYR:HE1	1.79	0.47
1:D:2340:ASN:OD1	1:D:2340:ASN:N	2.46	0.47
1:D:4947:CYS:SG	1:D:4948:TRP:N	2.87	0.47
1:A:370:LEU:HB2	1:A:393:MET:HB2	1.95	0.47
1:A:4905:GLU:OE2	1:D:4182:LYS:HD3	2.15	0.47
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.47	0.47
1:C:267:VAL:HA	1:C:270:HIS:ND1	2.30	0.47
1:C:441:LYS:HG2	1:C:442:LEU:HD23	1.96	0.47
1:C:911:ASN:OD1	1:C:911:ASN:N	2.41	0.47
1:C:1709:ASP:HA	1:C:1713:SER:HB3	1.96	0.47
1:D:441:LYS:HG2	1:D:442:LEU:HD23	1.96	0.47
1:D:712:GLU:HB3	1:D:713:TRP:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:HIS:CE1	1:A:917:CYS:HB2	2.50	0.47
1:A:1700:ARG:NH1	1:A:1817:PHE:O	2.47	0.47
1:A:1981:ASP:OD1	1:A:1982:LYS:N	2.48	0.47
1:A:2728:HIS:O	1:A:2732:SER:OG	2.24	0.47
1:A:2765:LYS:O	1:A:2769:ILE:HG23	2.15	0.47
1:B:228:LEU:HD23	1:B:289:ILE:HB	1.96	0.47
1:B:2092:ASP:OD1	1:B:2093:GLY:N	2.48	0.47
1:B:2271:CYS:SG	1:B:2293:GLU:HB2	2.55	0.47
1:B:2296:ARG:NH1	1:B:2299:ASP:OD2	2.47	0.47
1:B:2903:SER:OG	1:B:2904:ARG:N	2.48	0.47
1:B:3640:ILE:HG22	1:B:3729:ARG:HH11	1.80	0.47
1:C:70:GLU:OE1	1:C:122:ARG:NE	2.44	0.47
1:C:671:LYS:HA	1:C:761:LEU:HD12	1.97	0.47
1:C:844:ARG:HE	1:C:845:THR:HG22	1.80	0.47
1:C:875:PRO:O	1:C:882:ARG:NH2	2.46	0.47
1:C:1704:TYR:O	1:C:1708:ILE:HG12	2.15	0.47
1:C:1981:ASP:OD1	1:C:1982:LYS:N	2.48	0.47
1:C:2296:ARG:NH1	1:C:2299:ASP:OD2	2.47	0.47
1:C:4608:LYS:HG3	1:C:4614:LEU:HB2	1.97	0.47
1:C:4762:ASN:O	1:C:4764:LYS:N	2.44	0.47
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.47	0.47
1:D:1700:ARG:NH1	1:D:1817:PHE:O	2.47	0.47
1:D:1981:ASP:OD1	1:D:1982:LYS:N	2.48	0.47
1:D:2092:ASP:OD1	1:D:2093:GLY:N	2.48	0.47
1:D:2728:HIS:O	1:D:2732:SER:OG	2.24	0.47
1:A:441:LYS:HG2	1:A:442:LEU:HD23	1.95	0.47
1:A:2081:ARG:HG3	1:A:3686:LEU:HD22	1.97	0.47
1:A:3640:ILE:HG22	1:A:3729:ARG:HH11	1.80	0.47
1:A:4070:GLU:OE1	1:A:4070:GLU:N	2.43	0.47
1:B:439:LYS:HD2	1:B:440:VAL:O	2.15	0.47
1:C:2716:LEU:HD22	1:C:2778:LEU:HD21	1.97	0.47
1:D:228:LEU:HD23	1:D:289:ILE:HB	1.96	0.47
1:D:2892:PHE:O	1:D:2896:GLN:HG2	2.14	0.47
1:D:2903:SER:OG	1:D:2904:ARG:N	2.48	0.47
2:J:32:GLN:NE2	2:J:97:THR:OG1	2.34	0.47
1:A:267:VAL:HA	1:A:270:HIS:ND1	2.30	0.47
1:A:2716:LEU:HD22	1:A:2778:LEU:HD21	1.97	0.47
1:B:1981:ASP:OD1	1:B:1982:LYS:N	2.48	0.47
1:C:2101:LEU:O	1:C:2104:THR:HG22	2.13	0.47
1:C:2765:LYS:O	1:C:2769:ILE:HG23	2.15	0.47
1:C:4830:ILE:HB	1:C:4842:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:SER:HA	1:D:555:LEU:HD13	1.96	0.47
1:D:658:ASN:HD22	1:D:833:LYS:H	1.61	0.47
1:D:1793:ILE:HG12	1:D:1843:ILE:HD11	1.97	0.47
1:D:4070:GLU:OE1	1:D:4070:GLU:N	2.43	0.47
1:A:228:LEU:HD23	1:A:289:ILE:HB	1.96	0.47
1:A:552:SER:HA	1:A:555:LEU:HD13	1.96	0.47
1:A:646:THR:HG21	1:A:1685:GLN:HE22	1.80	0.47
1:A:1090:ALA:HB3	1:A:1202:ILE:HD11	1.96	0.47
1:A:1704:TYR:O	1:A:1708:ILE:HG12	2.15	0.47
1:B:1902:LYS:HG3	1:B:2079:LEU:HD11	1.97	0.47
1:B:2716:LEU:HD22	1:B:2778:LEU:HD21	1.97	0.47
1:B:2765:LYS:O	1:B:2769:ILE:HG23	2.15	0.47
1:B:4830:ILE:HB	1:B:4842:ARG:HH21	1.80	0.47
1:C:1902:LYS:HG3	1:C:2079:LEU:HD11	1.97	0.47
1:C:4070:GLU:OE1	1:C:4070:GLU:N	2.43	0.47
1:D:620:CYS:SG	1:D:621:HIS:N	2.87	0.47
1:D:646:THR:HG21	1:D:1685:GLN:HE22	1.80	0.47
1:D:671:LYS:HA	1:D:761:LEU:HD12	1.96	0.47
1:D:2081:ARG:HG3	1:D:3686:LEU:HD22	1.97	0.47
1:D:2765:LYS:O	1:D:2769:ILE:HG23	2.15	0.47
1:A:439:LYS:HD2	1:A:440:VAL:O	2.15	0.46
1:A:923:LYS:HB2	1:A:923:LYS:HE3	1.71	0.46
1:A:2271:CYS:SG	1:A:2293:GLU:HB2	2.55	0.46
1:B:915:HIS:CE1	1:B:917:CYS:HB2	2.50	0.46
1:B:1090:ALA:HB3	1:B:1202:ILE:HD11	1.96	0.46
1:B:1793:ILE:HG12	1:B:1843:ILE:HD11	1.97	0.46
1:B:3822:GLU:OE2	1:B:3823:GLY:N	2.49	0.46
1:C:603:LYS:HG2	1:C:1573:LYS:HZ1	1.80	0.46
1:C:874:LEU:HD11	1:C:941:LYS:HD3	1.97	0.46
1:C:915:HIS:CE1	1:C:917:CYS:HB2	2.50	0.46
1:C:2903:SER:OG	1:C:2904:ARG:N	2.48	0.46
1:C:3640:ILE:HG22	1:C:3729:ARG:HH11	1.80	0.46
1:D:754:VAL:HG23	1:D:771:ASN:HA	1.97	0.46
1:D:997:ASP:O	1:D:1001:GLU:HG3	2.16	0.46
1:D:4570:THR:HA	1:D:4573:ILE:HG12	1.96	0.46
1:A:671:LYS:HA	1:A:761:LEU:HD12	1.96	0.46
1:A:997:ASP:O	1:A:1001:GLU:HG3	2.16	0.46
1:A:2892:PHE:O	1:A:2896:GLN:HG2	2.14	0.46
1:A:3786:VAL:HG11	1:A:3865:THR:HG23	1.98	0.46
1:A:4830:ILE:HB	1:A:4842:ARG:HH21	1.80	0.46
1:B:267:VAL:HA	1:B:270:HIS:ND1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1793:ILE:HG12	1:C:1843:ILE:HD11	1.97	0.46
1:D:1343:PHE:HB2	1:D:1376:TYR:HD2	1.80	0.46
1:D:2716:LEU:HD22	1:D:2778:LEU:HD21	1.97	0.46
1:D:2848:HIS:HE1	1:D:2869:LEU:HD13	1.80	0.46
1:D:4830:ILE:HG22	1:D:4831:GLU:H	1.80	0.46
1:A:603:LYS:HG2	1:A:1573:LYS:HZ1	1.80	0.46
1:A:874:LEU:HD11	1:A:941:LYS:HD3	1.97	0.46
1:B:1102:TYR:HB2	1:B:1165:MET:HG3	1.97	0.46
1:B:3786:VAL:HG11	1:B:3865:THR:HG23	1.98	0.46
1:C:300:VAL:O	1:C:420:ARG:NH1	2.40	0.46
1:C:641:ASP:OD1	1:C:642:LEU:N	2.47	0.46
1:C:2271:CYS:SG	1:C:2293:GLU:HB2	2.55	0.46
1:D:641:ASP:OD1	1:D:642:LEU:N	2.48	0.46
1:D:1709:ASP:HA	1:D:1713:SER:HB3	1.96	0.46
1:D:4508:ALA:O	1:D:4512:ASN:ND2	2.45	0.46
1:A:1709:ASP:HA	1:A:1713:SER:HB3	1.96	0.46
1:A:1793:ILE:HG12	1:A:1843:ILE:HD11	1.97	0.46
1:B:844:ARG:HE	1:B:845:THR:HG22	1.80	0.46
1:B:921:PHE:O	1:B:929:ARG:NH1	2.37	0.46
1:C:309:MET:HB2	1:C:312:LYS:HZ3	1.81	0.46
1:C:1677:LEU:O	1:C:1681:VAL:HG22	2.16	0.46
1:D:1102:TYR:HB2	1:D:1165:MET:HG3	1.97	0.46
1:D:1305:SER:OG	1:D:1588:HIS:O	2.34	0.46
1:A:892:LEU:HA	1:A:895:MET:HB2	1.98	0.46
1:A:4608:LYS:HG3	1:A:4614:LEU:HB2	1.97	0.46
1:B:671:LYS:HA	1:B:761:LEU:HD12	1.96	0.46
1:B:2081:ARG:HG3	1:B:3686:LEU:HD22	1.97	0.46
1:C:892:LEU:HA	1:C:895:MET:HB2	1.98	0.46
1:C:4276:LYS:HZ1	1:C:4562:GLU:HG3	1.80	0.46
1:D:915:HIS:CE1	1:D:917:CYS:HB2	2.50	0.46
1:D:1090:ALA:HB3	1:D:1202:ILE:HD11	1.96	0.46
1:D:3923:ILE:HD13	1:D:3934:LEU:HD12	1.96	0.46
1:B:603:LYS:HG2	1:B:1573:LYS:HZ1	1.80	0.46
1:B:2848:HIS:HE1	1:B:2869:LEU:HD13	1.80	0.46
1:C:228:LEU:HD23	1:C:289:ILE:HB	1.96	0.46
1:C:417:ARG:NH1	1:C:420:ARG:HH22	2.14	0.46
1:C:2340:ASN:OD1	1:C:2340:ASN:N	2.46	0.46
1:D:442:LEU:HD23	1:D:442:LEU:H	1.81	0.46
1:D:1902:LYS:HG3	1:D:2079:LEU:HD11	1.97	0.46
1:D:2271:CYS:SG	1:D:2293:GLU:HB2	2.55	0.46
1:A:1305:SER:OG	1:A:1588:HIS:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2092:ASP:OD1	1:A:2093:GLY:N	2.48	0.46
1:A:4830:ILE:HG22	1:A:4831:GLU:H	1.80	0.46
1:B:799:LYS:HG2	1:B:1621:GLN:NE2	2.31	0.46
1:B:800:VAL:HB	1:B:1620:VAL:HG23	1.98	0.46
1:B:892:LEU:HA	1:B:895:MET:HB2	1.98	0.46
1:B:1677:LEU:O	1:B:1681:VAL:HG22	2.16	0.46
1:B:3621:GLN:O	1:B:3624:GLU:HG3	2.16	0.46
1:C:2092:ASP:OD1	1:C:2093:GLY:N	2.48	0.46
1:D:1704:TYR:O	1:D:1708:ILE:HG12	2.15	0.46
1:D:2201:TYR:O	1:D:2205:ILE:HG22	2.16	0.46
1:D:4608:LYS:HG3	1:D:4614:LEU:HB2	1.97	0.46
1:A:442:LEU:HD23	1:A:442:LEU:H	1.81	0.46
1:A:1902:LYS:HG3	1:A:2079:LEU:HD11	1.97	0.46
1:B:247:VAL:O	1:B:272:ARG:NH1	2.44	0.46
1:C:3822:GLU:OE2	1:C:3823:GLY:N	2.49	0.46
1:D:629:GLN:NE2	1:D:1670:ASN:HD22	2.13	0.46
1:D:3640:ILE:HG22	1:D:3729:ARG:HH11	1.80	0.46
1:D:3822:GLU:OE2	1:D:3823:GLY:N	2.49	0.46
1:A:1747:HIS:O	1:A:1747:HIS:ND1	2.47	0.46
1:A:2201:TYR:O	1:A:2205:ILE:HG22	2.16	0.46
1:B:801:ARG:HA	1:B:1618:TRP:O	2.16	0.46
1:B:2107:ILE:HG13	1:B:2108:ASN:H	1.81	0.46
2:H:72:ARG:HG2	2:H:103:GLU:HB2	1.98	0.46
1:C:2081:ARG:HG3	1:C:3686:LEU:HD22	1.97	0.46
1:C:2771:ARG:HH22	1:C:2775:LYS:HD3	1.81	0.46
1:C:2848:HIS:HE1	1:C:2869:LEU:HD13	1.80	0.46
1:C:4830:ILE:HG22	1:C:4831:GLU:H	1.80	0.46
1:D:380:LYS:HD3	1:D:380:LYS:HA	1.71	0.46
1:D:417:ARG:NH1	1:D:420:ARG:HH22	2.14	0.46
1:A:629:GLN:NE2	1:A:1670:ASN:HD22	2.13	0.46
1:A:754:VAL:HG23	1:A:771:ASN:HA	1.97	0.46
1:A:800:VAL:HB	1:A:1620:VAL:HG23	1.98	0.46
1:A:2848:HIS:HE1	1:A:2869:LEU:HD13	1.80	0.46
1:A:3822:GLU:OE2	1:A:3823:GLY:N	2.48	0.46
1:B:442:LEU:HD23	1:B:442:LEU:H	1.81	0.46
1:B:646:THR:HG21	1:B:1685:GLN:HE22	1.80	0.46
1:C:629:GLN:NE2	1:C:1670:ASN:HD22	2.13	0.46
1:C:799:LYS:HG2	1:C:1621:GLN:NE2	2.31	0.46
1:C:801:ARG:HA	1:C:1618:TRP:O	2.16	0.46
1:C:997:ASP:O	1:C:1001:GLU:HG3	2.16	0.46
1:C:1747:HIS:O	1:C:1747:HIS:ND1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:THR:O	1:D:375:GLN:NE2	2.43	0.46
1:D:439:LYS:HD2	1:D:440:VAL:O	2.15	0.46
1:A:799:LYS:HG2	1:A:1621:GLN:NE2	2.31	0.45
1:B:2238:PRO:O	1:B:2241:VAL:HG12	2.17	0.45
1:C:754:VAL:HG23	1:C:771:ASN:HA	1.97	0.45
1:C:2201:TYR:O	1:C:2205:ILE:HG22	2.16	0.45
1:C:2238:PRO:O	1:C:2241:VAL:HG12	2.17	0.45
1:C:4508:ALA:O	1:C:4512:ASN:ND2	2.45	0.45
2:I:72:ARG:HG2	2:I:103:GLU:HB2	1.98	0.45
1:D:799:LYS:HG2	1:D:1621:GLN:NE2	2.31	0.45
1:D:946:LEU:HD13	1:D:995:MET:SD	2.56	0.45
1:D:2771:ARG:HH22	1:D:2775:LYS:HD3	1.81	0.45
1:A:875:PRO:O	1:A:882:ARG:NH2	2.46	0.45
1:A:1102:TYR:HB2	1:A:1165:MET:HG3	1.97	0.45
1:A:1677:LEU:O	1:A:1681:VAL:HG22	2.16	0.45
1:A:2771:ARG:HH22	1:A:2775:LYS:HD3	1.81	0.45
1:B:417:ARG:NH1	1:B:420:ARG:HH22	2.14	0.45
1:B:629:GLN:NE2	1:B:1670:ASN:HD22	2.13	0.45
1:B:4793:ASN:O	1:B:4795:SER:N	2.49	0.45
1:C:439:LYS:HD2	1:C:440:VAL:O	2.15	0.45
1:C:646:THR:HG21	1:C:1685:GLN:HE22	1.80	0.45
1:D:1677:LEU:O	1:D:1681:VAL:HG22	2.16	0.45
1:A:946:LEU:HD13	1:A:995:MET:SD	2.56	0.45
2:G:72:ARG:HG2	2:G:103:GLU:HB2	1.98	0.45
1:B:874:LEU:HD11	1:B:941:LYS:HD3	1.97	0.45
1:B:997:ASP:O	1:B:1001:GLU:HG3	2.16	0.45
1:B:2201:TYR:O	1:B:2205:ILE:HG22	2.16	0.45
1:D:490:GLN:O	1:D:490:GLN:NE2	2.44	0.45
1:D:2057:LEU:O	1:D:2060:LEU:HD23	2.17	0.45
1:D:3621:GLN:O	1:D:3624:GLU:HG3	2.16	0.45
2:J:72:ARG:HG2	2:J:103:GLU:HB2	1.98	0.45
1:B:1747:HIS:O	1:B:1747:HIS:ND1	2.47	0.45
1:C:1591:PHE:CZ	1:C:1593:SER:HB2	2.52	0.45
1:C:3621:GLN:O	1:C:3624:GLU:HG3	2.16	0.45
1:D:874:LEU:HD11	1:D:941:LYS:HD3	1.97	0.45
1:A:4044:LYS:HE2	1:A:4044:LYS:HB3	1.82	0.45
1:A:4873:ARG:O	1:A:4877:GLU:HG2	2.17	0.45
1:B:207:PHE:CE1	1:C:2324:ILE:HB	2.52	0.45
1:B:373:THR:O	1:B:375:GLN:NE2	2.43	0.45
1:B:490:GLN:O	1:B:490:GLN:NE2	2.44	0.45
1:B:4830:ILE:HG22	1:B:4831:GLU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:973:THR:OG1	1:D:976:TYR:O	2.18	0.45
1:D:2238:PRO:O	1:D:2241:VAL:HG12	2.16	0.45
1:D:4830:ILE:HB	1:D:4842:ARG:HH21	1.80	0.45
1:A:2057:LEU:O	1:A:2060:LEU:HD23	2.17	0.45
1:A:4793:ASN:O	1:A:4795:SER:N	2.49	0.45
1:B:1704:TYR:O	1:B:1708:ILE:HG12	2.15	0.45
1:C:442:LEU:HD23	1:C:442:LEU:H	1.81	0.45
1:C:800:VAL:HB	1:C:1620:VAL:HG23	1.98	0.45
1:C:2107:ILE:HG13	1:C:2108:ASN:H	1.81	0.45
1:C:3786:VAL:HG11	1:C:3865:THR:HG23	1.98	0.45
1:D:1591:PHE:CZ	1:D:1593:SER:HB2	2.52	0.45
1:A:2107:ILE:HG22	1:A:2157:HIS:CD2	2.52	0.45
1:A:2107:ILE:HG13	1:A:2108:ASN:H	1.81	0.45
1:A:3621:GLN:O	1:A:3624:GLU:HG3	2.16	0.45
1:B:754:VAL:HG23	1:B:771:ASN:HA	1.97	0.45
1:B:1367:LYS:NZ	1:B:1369:GLU:OE2	2.35	0.45
1:B:2107:ILE:HG22	1:B:2157:HIS:CD2	2.52	0.45
1:C:1102:TYR:HB2	1:C:1165:MET:HG3	1.97	0.45
1:D:3786:VAL:HG11	1:D:3865:THR:HG23	1.98	0.45
1:A:625:VAL:HG23	1:A:628:ASN:HB2	1.99	0.45
1:A:4187:LEU:HG	1:A:4187:LEU:H	1.68	0.45
2:G:38:ASP:OD1	2:G:39:SER:N	2.50	0.45
1:B:946:LEU:HD13	1:B:995:MET:SD	2.56	0.45
1:B:1305:SER:OG	1:B:1588:HIS:O	2.34	0.45
1:C:2057:LEU:O	1:C:2060:LEU:HD23	2.17	0.45
1:C:2498:ALA:O	1:C:2501:LEU:HD23	2.16	0.45
1:D:892:LEU:HA	1:D:895:MET:HB2	1.98	0.45
1:D:2848:HIS:CE1	1:D:2869:LEU:HD13	2.52	0.45
1:D:4873:ARG:O	1:D:4877:GLU:HG2	2.17	0.45
1:A:417:ARG:NH1	1:A:420:ARG:HH22	2.14	0.45
1:C:2107:ILE:HG22	1:C:2157:HIS:CD2	2.52	0.45
1:D:290:ARG:H	1:D:293:GLN:NE2	2.15	0.45
1:D:2107:ILE:HG13	1:D:2108:ASN:H	1.81	0.45
1:D:4583:PHE:O	1:D:4586:ILE:HG22	2.17	0.45
1:A:70:GLU:OE1	1:A:122:ARG:NE	2.45	0.45
1:A:801:ARG:HA	1:A:1618:TRP:O	2.16	0.45
1:A:2238:PRO:O	1:A:2241:VAL:HG12	2.17	0.45
1:B:2771:ARG:HH22	1:B:2775:LYS:HD3	1.81	0.45
1:B:4508:ALA:O	1:B:4512:ASN:ND2	2.45	0.45
1:C:2848:HIS:CE1	1:C:2869:LEU:HD13	2.52	0.45
1:C:4026:THR:O	1:C:4031:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ILE:HD13	1:D:492:GLU:HG3	1.99	0.45
2:J:38:ASP:OD1	2:J:39:SER:N	2.50	0.45
1:A:419:ILE:HD13	1:A:492:GLU:HG3	1.99	0.44
1:A:2720:ILE:HD11	1:A:2778:LEU:HD22	1.99	0.44
1:A:4583:PHE:O	1:A:4586:ILE:HG22	2.17	0.44
1:B:14:LEU:HB3	1:B:113:LEU:HD12	2.00	0.44
1:B:1591:PHE:CZ	1:B:1593:SER:HB2	2.52	0.44
1:B:1970:GLU:HA	1:B:1973:ASN:HB2	1.99	0.44
1:C:1968:PRO:HA	1:C:1971:GLN:HB3	1.99	0.44
1:C:1970:GLU:HA	1:C:1973:ASN:HB2	1.99	0.44
1:C:2058:GLN:HG3	1:C:2090:GLN:NE2	2.32	0.44
1:D:625:VAL:HG23	1:D:628:ASN:HB2	1.99	0.44
1:D:2058:GLN:HG3	1:D:2090:GLN:NE2	2.32	0.44
1:B:300:VAL:O	1:B:420:ARG:NH1	2.40	0.44
1:B:923:LYS:HB2	1:B:923:LYS:HE3	1.71	0.44
1:C:1305:SER:OG	1:C:1588:HIS:O	2.34	0.44
1:C:2763:SER:H	1:C:2766:GLU:HB2	1.82	0.44
1:D:923:LYS:HB2	1:D:923:LYS:HE3	1.71	0.44
1:D:2498:ALA:O	1:D:2501:LEU:HD23	2.16	0.44
1:D:3919:LEU:O	1:D:3923:ILE:HG12	2.18	0.44
1:D:4026:THR:O	1:D:4031:PHE:HB3	2.18	0.44
1:A:833:LYS:HE3	1:A:834:VAL:N	2.33	0.44
1:B:414:ARG:O	1:B:418:VAL:HG12	2.18	0.44
1:B:2058:GLN:HG3	1:B:2090:GLN:NE2	2.32	0.44
1:B:4873:ARG:O	1:B:4877:GLU:HG2	2.17	0.44
1:C:14:LEU:HB3	1:C:113:LEU:HD12	2.00	0.44
1:C:946:LEU:HD13	1:C:995:MET:SD	2.56	0.44
1:C:4793:ASN:O	1:C:4795:SER:N	2.49	0.44
1:D:801:ARG:HA	1:D:1618:TRP:O	2.16	0.44
1:D:1798:GLU:O	1:D:1802:GLU:HG2	2.18	0.44
1:D:2107:ILE:HG22	1:D:2157:HIS:CD2	2.52	0.44
1:B:189:GLU:O	1:C:2325:ARG:NH2	2.49	0.44
1:B:2836:LEU:HD22	1:B:2839:MET:HE1	1.99	0.44
1:B:3919:LEU:O	1:B:3923:ILE:HG12	2.18	0.44
1:C:36:CYS:SG	1:C:65:CYS:HB3	2.58	0.44
1:C:1320:UNK:HA	1:C:1325:UNK:HA	2.00	0.44
1:C:3919:LEU:O	1:C:3923:ILE:HG12	2.18	0.44
1:C:4039:LYS:O	1:C:4041:VAL:HG23	2.17	0.44
1:D:317:MET:HB2	1:D:321:LYS:HE3	2.00	0.44
1:D:800:VAL:HB	1:D:1620:VAL:HG23	1.98	0.44
1:D:4799:ASP:N	1:D:4799:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:GLN:HG3	1:A:2090:GLN:NE2	2.32	0.44
1:A:2763:SER:H	1:A:2766:GLU:HB2	1.83	0.44
1:A:4039:LYS:O	1:A:4041:VAL:HG23	2.18	0.44
1:B:1251:LEU:HD23	1:B:1600:MET:HE2	1.99	0.44
1:B:1972:ILE:HA	1:B:1975:LEU:HG	1.99	0.44
1:B:2498:ALA:O	1:B:2501:LEU:HD23	2.16	0.44
1:C:317:MET:HB2	1:C:321:LYS:HE3	2.00	0.44
1:C:2720:ILE:HD11	1:C:2778:LEU:HD22	1.99	0.44
1:C:2858:GLU:O	1:C:2862:LYS:HG2	2.17	0.44
1:C:4583:PHE:O	1:C:4586:ILE:HG22	2.17	0.44
1:D:36:CYS:SG	1:D:65:CYS:HB3	2.58	0.44
1:D:1970:GLU:HA	1:D:1973:ASN:HB2	1.99	0.44
1:A:2498:ALA:O	1:A:2501:LEU:HD23	2.16	0.44
1:B:833:LYS:HE3	1:B:834:VAL:N	2.33	0.44
1:B:4039:LYS:O	1:B:4041:VAL:HG23	2.18	0.44
1:C:414:ARG:O	1:C:418:VAL:HG12	2.18	0.44
1:C:2342:LEU:N	1:C:2430:ASP:OD2	2.47	0.44
1:C:4873:ARG:O	1:C:4877:GLU:HG2	2.17	0.44
1:D:2471:LEU:HD23	1:D:2471:LEU:HA	1.80	0.44
1:D:2858:GLU:O	1:D:2862:LYS:HG2	2.17	0.44
1:A:14:LEU:HB3	1:A:113:LEU:HD12	2.00	0.44
1:A:36:CYS:SG	1:A:65:CYS:HB3	2.58	0.44
1:A:935:MET:O	1:A:938:GLU:HG3	2.18	0.44
1:A:1591:PHE:CZ	1:A:1593:SER:HB2	2.52	0.44
1:A:1972:ILE:HA	1:A:1975:LEU:HG	2.00	0.44
1:A:3919:LEU:O	1:A:3923:ILE:HG12	2.18	0.44
1:B:419:ILE:HD13	1:B:492:GLU:HG3	1.99	0.44
1:B:625:VAL:HG23	1:B:628:ASN:HB2	1.99	0.44
1:C:799:LYS:HG2	1:C:1621:GLN:HE22	1.83	0.44
1:C:1347:MET:HG2	1:C:1371:ASN:HD22	1.83	0.44
1:C:2282:LYS:HA	1:C:2282:LYS:HD2	1.90	0.44
1:C:4799:ASP:N	1:C:4799:ASP:OD1	2.51	0.44
1:D:4009:VAL:HA	1:D:4012:ILE:HG12	2.00	0.44
1:A:2867:HIS:HB2	1:A:2870:LEU:HG	2.00	0.44
1:B:36:CYS:SG	1:B:65:CYS:HB3	2.58	0.44
1:B:674:TYR:N	1:B:820:ALA:O	2.51	0.44
1:B:1811:VAL:HB	1:B:1818:LEU:HD13	2.00	0.44
1:B:2057:LEU:O	1:B:2060:LEU:HD23	2.17	0.44
1:B:4496:ASN:HD22	1:B:4499:ASN:HD22	1.66	0.44
1:C:329:PHE:HB3	1:C:363:ILE:HD11	2.00	0.44
1:C:674:TYR:N	1:C:820:ALA:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:ARG:HG2	1:C:940:LEU:HD12	2.00	0.44
1:C:935:MET:O	1:C:938:GLU:HG3	2.18	0.44
1:D:14:LEU:HB3	1:D:113:LEU:HD12	2.00	0.44
1:D:329:PHE:HB3	1:D:363:ILE:HD11	2.00	0.44
1:D:1347:MET:HG2	1:D:1371:ASN:HD22	1.83	0.44
1:D:2894:PHE:HA	1:D:2897:ILE:HG12	2.00	0.44
1:A:26:ALA:HB2	1:A:194:LEU:HD21	2.00	0.44
1:A:799:LYS:HG2	1:A:1621:GLN:HE22	1.83	0.44
1:A:2258:GLU:HG3	1:A:2261:LEU:HB2	2.00	0.44
1:B:1347:MET:HG2	1:B:1371:ASN:HD22	1.83	0.44
1:B:1968:PRO:HA	1:B:1971:GLN:HB3	1.99	0.44
1:B:2720:ILE:HD11	1:B:2778:LEU:HD22	1.99	0.44
1:C:625:VAL:HG23	1:C:628:ASN:HB2	1.99	0.44
1:C:1798:GLU:O	1:C:1802:GLU:HG2	2.18	0.44
1:C:2867:HIS:HB2	1:C:2870:LEU:HG	2.00	0.44
1:D:833:LYS:HE3	1:D:834:VAL:N	2.33	0.44
1:D:2342:LEU:N	1:D:2430:ASP:OD2	2.47	0.44
1:A:1798:GLU:O	1:A:1802:GLU:HG2	2.18	0.43
1:A:1970:GLU:HA	1:A:1973:ASN:HB2	1.99	0.43
1:B:70:GLU:OE1	1:B:122:ARG:NE	2.45	0.43
1:B:2258:GLU:HG3	1:B:2261:LEU:HB2	2.00	0.43
1:B:2763:SER:H	1:B:2766:GLU:HB2	1.83	0.43
1:D:414:ARG:O	1:D:418:VAL:HG12	2.18	0.43
1:D:1320:UNK:HA	1:D:1325:UNK:HA	2.00	0.43
1:D:4039:LYS:O	1:D:4041:VAL:HG23	2.17	0.43
1:A:1165:MET:HB3	1:A:1236:TYR:CE2	2.53	0.43
1:A:1347:MET:HG2	1:A:1371:ASN:HD22	1.83	0.43
1:A:4496:ASN:HD22	1:A:4499:ASN:HD22	1.66	0.43
1:B:329:PHE:HB3	1:B:363:ILE:HD11	2.00	0.43
1:B:1040:ASP:HA	1:B:1043:LYS:HG3	2.01	0.43
1:B:1798:GLU:O	1:B:1802:GLU:HG2	2.18	0.43
1:C:490:GLN:O	1:C:490:GLN:NE2	2.45	0.43
2:I:38:ASP:OD1	2:I:39:SER:N	2.50	0.43
1:D:300:VAL:O	1:D:420:ARG:NH1	2.40	0.43
1:D:1811:VAL:HB	1:D:1818:LEU:HD13	2.00	0.43
1:A:317:MET:HB2	1:A:321:LYS:HE3	2.00	0.43
1:A:595:LYS:HE2	1:A:595:LYS:HB3	1.89	0.43
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.99	0.43
1:C:1165:MET:HB3	1:C:1236:TYR:CE2	2.53	0.43
1:C:1972:ILE:HA	1:C:1975:LEU:HG	2.00	0.43
1:D:674:TYR:N	1:D:820:ALA:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:935:MET:O	1:D:938:GLU:HG3	2.18	0.43
1:D:1747:HIS:O	1:D:1747:HIS:ND1	2.47	0.43
1:D:2720:ILE:HD11	1:D:2778:LEU:HD22	1.99	0.43
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.99	0.43
1:A:674:TYR:N	1:A:820:ALA:O	2.51	0.43
1:A:1786:ASP:O	1:A:1789:LYS:HG2	2.18	0.43
1:A:2722:LYS:HD2	1:A:2722:LYS:HA	1.63	0.43
1:B:850:LEU:H	1:B:850:LEU:HG	1.57	0.43
1:B:1031:ARG:NH1	1:B:1039:ASP:OD2	2.52	0.43
1:B:4026:THR:O	1:B:4031:PHE:HB3	2.18	0.43
1:C:419:ILE:HD13	1:C:492:GLU:HG3	1.99	0.43
1:C:837:SER:H	1:C:841:LYS:HZ1	1.65	0.43
1:C:1786:ASP:O	1:C:1789:LYS:HG2	2.18	0.43
1:D:640:ARG:HD3	2:J:35:LYS:HD3	2.00	0.43
1:D:799:LYS:HG2	1:D:1621:GLN:HE22	1.83	0.43
1:D:1972:ILE:HA	1:D:1975:LEU:HG	2.00	0.43
1:D:2278:MET:O	1:D:2282:LYS:HG2	2.19	0.43
1:D:2867:HIS:HB2	1:D:2870:LEU:HG	2.00	0.43
1:A:1968:PRO:HA	1:A:1971:GLN:HB3	1.99	0.43
1:A:2848:HIS:CE1	1:A:2869:LEU:HD13	2.52	0.43
1:A:2894:PHE:HA	1:A:2897:ILE:HG12	2.00	0.43
1:A:4009:VAL:HA	1:A:4012:ILE:HG12	2.00	0.43
1:B:317:MET:HB2	1:B:321:LYS:HE3	2.00	0.43
1:B:911:ASN:OD1	1:B:911:ASN:N	2.41	0.43
1:B:2848:HIS:CE1	1:B:2869:LEU:HD13	2.52	0.43
1:B:4009:VAL:HA	1:B:4012:ILE:HG12	2.00	0.43
1:C:807:ARG:O	1:C:1615:ARG:NE	2.48	0.43
1:C:1776:CYS:SG	1:C:1778:GLN:HB2	2.59	0.43
1:C:1811:VAL:HB	1:C:1818:LEU:HD13	2.00	0.43
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.99	0.43
1:D:882:ARG:HG2	1:D:940:LEU:HD12	2.00	0.43
1:D:1165:MET:HB3	1:D:1236:TYR:CE2	2.53	0.43
1:D:1776:CYS:SG	1:D:1778:GLN:HB2	2.59	0.43
1:D:2763:SER:H	1:D:2766:GLU:HB2	1.83	0.43
1:D:4205:ILE:HG23	1:D:4491:ASN:HB3	2.01	0.43
1:D:4807:ASP:HB3	1:D:4810:THR:HB	2.00	0.43
1:A:414:ARG:O	1:A:418:VAL:HG12	2.18	0.43
1:A:2278:MET:O	1:A:2282:LYS:HG2	2.19	0.43
1:B:1320:UNK:HA	1:B:1325:UNK:HA	1.99	0.43
1:B:4670:GLY:O	1:B:4671:MET:HG2	2.19	0.43
1:B:4799:ASP:OD1	1:B:4799:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ASP:OD1	2:H:39:SER:N	2.50	0.43
1:C:838:ARG:H	1:C:841:LYS:NZ	2.17	0.43
1:C:894:VAL:HG13	1:C:918:LEU:HB3	2.01	0.43
1:D:190:ARG:HD3	1:D:205:ALA:O	2.19	0.43
1:D:1091:GLU:HB3	1:D:1094:TYR:CD2	2.52	0.43
1:D:1118:SER:HA	1:D:1134:ALA:HA	2.01	0.43
1:D:1786:ASP:O	1:D:1789:LYS:HG2	2.18	0.43
1:D:1945:GLU:O	1:D:1948:GLN:HG3	2.19	0.43
1:D:4000:ASP:O	1:D:4004:GLU:HG3	2.19	0.43
1:D:4496:ASN:HD22	1:D:4499:ASN:HD22	1.66	0.43
1:A:290:ARG:H	1:A:293:GLN:NE2	2.15	0.43
1:A:329:PHE:HB3	1:A:363:ILE:HD11	2.00	0.43
1:A:838:ARG:H	1:A:841:LYS:HZ3	1.65	0.43
1:A:1091:GLU:HB3	1:A:1094:TYR:CD2	2.52	0.43
1:A:2858:GLU:O	1:A:2862:LYS:HG2	2.17	0.43
1:A:4287:TRP:O	1:A:4291:VAL:HG13	2.19	0.43
1:A:4799:ASP:N	1:A:4799:ASP:OD1	2.51	0.43
1:B:140:THR:OG1	1:C:2337:GLU:HG3	2.19	0.43
1:B:799:LYS:HG2	1:B:1621:GLN:HE22	1.83	0.43
1:B:2858:GLU:O	1:B:2862:LYS:HG2	2.17	0.43
1:C:4009:VAL:HA	1:C:4012:ILE:HG12	2.00	0.43
1:C:4205:ILE:HG23	1:C:4491:ASN:HB3	2.01	0.43
1:D:1968:PRO:HA	1:D:1971:GLN:HB3	1.99	0.43
1:A:1945:GLU:O	1:A:1948:GLN:HG3	2.19	0.43
1:A:4026:THR:O	1:A:4031:PHE:HB3	2.17	0.43
1:A:4670:GLY:O	1:A:4671:MET:HG2	2.19	0.43
1:B:882:ARG:HG2	1:B:940:LEU:HD12	2.00	0.43
1:B:935:MET:O	1:B:938:GLU:HG3	2.18	0.43
1:B:4583:PHE:O	1:B:4586:ILE:HG22	2.18	0.43
1:C:161:THR:HG23	1:C:184:VAL:HB	2.01	0.43
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.99	0.43
1:C:829:LYS:O	1:C:830:GLU:HG3	2.19	0.43
1:C:988:LEU:HD11	1:C:1055:ARG:HG2	2.00	0.43
1:C:1271:THR:OG1	1:C:1272:ARG:N	2.52	0.43
1:C:2258:GLU:HG3	1:C:2261:LEU:HB2	2.00	0.43
1:C:2894:PHE:HA	1:C:2897:ILE:HG12	2.00	0.43
1:D:26:ALA:HB2	1:D:194:LEU:HD21	2.00	0.43
1:D:829:LYS:O	1:D:830:GLU:HG3	2.19	0.43
1:D:838:ARG:H	1:D:841:LYS:NZ	2.17	0.43
1:D:4029:ASP:OD1	1:D:4029:ASP:N	2.45	0.43
1:A:882:ARG:HG2	1:A:940:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLU:HG2	1:A:971:GLN:HE22	1.84	0.43
1:A:988:LEU:HD11	1:A:1055:ARG:HG2	2.00	0.43
1:A:1811:VAL:HB	1:A:1818:LEU:HD13	2.00	0.43
1:A:2342:LEU:N	1:A:2430:ASP:OD2	2.47	0.43
1:A:4807:ASP:HB3	1:A:4810:THR:HB	2.00	0.43
1:B:698:ALA:HA	1:B:724:SER:HA	2.00	0.43
1:B:1786:ASP:O	1:B:1789:LYS:HG2	2.18	0.43
1:B:2278:MET:O	1:B:2282:LYS:HG2	2.19	0.43
1:B:4205:ILE:HG23	1:B:4491:ASN:HB3	2.01	0.43
1:C:373:THR:O	1:C:375:GLN:NE2	2.43	0.43
1:C:698:ALA:HA	1:C:724:SER:HA	2.00	0.43
1:C:1040:ASP:HA	1:C:1043:LYS:HG3	2.01	0.43
1:C:3758:LEU:O	1:C:3762:ILE:HG12	2.19	0.43
1:D:899:GLU:HG2	1:D:971:GLN:HE22	1.84	0.43
1:D:2837:HIS:ND1	1:D:2838:ALA:N	2.67	0.43
1:D:4287:TRP:O	1:D:4291:VAL:HG13	2.19	0.43
1:D:4793:ASN:O	1:D:4795:SER:N	2.49	0.43
1:A:829:LYS:O	1:A:830:GLU:HG3	2.19	0.43
1:A:911:ASN:OD1	1:A:911:ASN:N	2.41	0.43
1:A:1031:ARG:HA	1:A:1031:ARG:HD3	1.84	0.43
1:A:1217:PHE:O	1:A:1240:ALA:N	2.52	0.43
1:B:1165:MET:HB3	1:B:1236:TYR:CE2	2.53	0.43
1:B:1945:GLU:O	1:B:1948:GLN:HG3	2.19	0.43
1:B:2867:HIS:HB2	1:B:2870:LEU:HG	2.00	0.43
1:B:4287:TRP:O	1:B:4291:VAL:HG13	2.19	0.43
1:C:26:ALA:HB2	1:C:194:LEU:HD21	2.00	0.43
1:C:697:TRP:HB2	1:C:766:ILE:HD13	2.01	0.43
1:C:845:THR:OG1	1:C:846:TYR:N	2.51	0.43
1:C:1031:ARG:NH1	1:C:1039:ASP:OD2	2.52	0.43
1:C:1945:GLU:O	1:C:1948:GLN:HG3	2.19	0.43
1:C:4806:ASP:HA	1:D:4520:VAL:HG12	2.01	0.43
2:I:53:LYS:HD3	2:I:53:LYS:HA	1.92	0.43
1:D:3758:LEU:O	1:D:3762:ILE:HG12	2.19	0.43
1:A:661:LEU:HD13	1:A:673:TRP:CD1	2.54	0.42
1:A:843:GLU:HB3	1:A:1606:LYS:HD3	2.01	0.42
1:A:1031:ARG:NH1	1:A:1039:ASP:OD2	2.52	0.42
1:A:1608:ASP:OD1	1:A:1608:ASP:N	2.52	0.42
1:A:4516:LEU:HD23	1:D:4809:LEU:HD13	2.01	0.42
1:B:26:ALA:HB2	1:B:194:LEU:HD21	2.00	0.42
1:B:894:VAL:HG13	1:B:918:LEU:HB3	2.01	0.42
1:B:1776:CYS:SG	1:B:1778:GLN:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ASN:HB2	1:C:832:LEU:HD12	2.01	0.42
1:C:1987:CYS:N	1:C:1988:PRO:HD2	2.34	0.42
1:D:798:ILE:HD12	1:D:798:ILE:HA	1.91	0.42
1:D:807:ARG:O	1:D:1615:ARG:NE	2.48	0.42
1:D:1743:GLU:CD	1:D:1744:ASN:HD22	2.22	0.42
2:J:27:TYR:N	2:J:40:SER:OG	2.51	0.42
1:A:1251:LEU:HD23	1:A:1600:MET:HE2	2.01	0.42
1:A:4205:ILE:HG23	1:A:4491:ASN:HB3	2.01	0.42
1:B:190:ARG:HD3	1:B:205:ALA:O	2.19	0.42
1:B:674:TYR:CE2	1:B:756:SER:HB2	2.54	0.42
1:B:843:GLU:HB3	1:B:1606:LYS:HD3	2.01	0.42
1:B:988:LEU:HD11	1:B:1055:ARG:HG2	2.00	0.42
1:B:1743:GLU:CD	1:B:1744:ASN:HD22	2.22	0.42
1:B:1987:CYS:N	1:B:1988:PRO:HD2	2.34	0.42
1:C:850:LEU:H	1:C:850:LEU:HG	1.57	0.42
1:D:247:VAL:O	1:D:272:ARG:NH1	2.44	0.42
1:D:661:LEU:HD13	1:D:673:TRP:CD1	2.54	0.42
1:D:674:TYR:CE2	1:D:756:SER:HB2	2.54	0.42
1:D:1031:ARG:NH1	1:D:1039:ASP:OD2	2.52	0.42
1:D:2258:GLU:HG3	1:D:2261:LEU:HB2	2.00	0.42
1:A:161:THR:HG23	1:A:184:VAL:HB	2.01	0.42
1:A:1320:UNK:HA	1:A:1325:UNK:HA	2.00	0.42
1:A:1776:CYS:SG	1:A:1778:GLN:HB2	2.59	0.42
1:B:838:ARG:H	1:B:841:LYS:NZ	2.17	0.42
1:B:845:THR:OG1	1:B:846:TYR:N	2.51	0.42
1:B:1827:TYR:CZ	1:B:1831:ILE:HD11	2.54	0.42
1:B:3758:LEU:O	1:B:3762:ILE:HG12	2.19	0.42
1:C:1118:SER:HA	1:C:1134:ALA:HA	2.01	0.42
1:C:1641:ASP:HB2	1:C:1644:GLU:HG3	2.00	0.42
1:C:2278:MET:O	1:C:2282:LYS:HG2	2.19	0.42
1:C:4670:GLY:O	1:C:4671:MET:HG2	2.19	0.42
1:C:4923:TYR:CZ	1:C:4927:LYS:HD2	2.55	0.42
1:D:245:LEU:HD11	1:D:260:VAL:HG12	2.01	0.42
1:D:658:ASN:HB2	1:D:832:LEU:HD12	2.01	0.42
1:D:875:PRO:O	1:D:882:ARG:NH2	2.46	0.42
1:D:894:VAL:HG13	1:D:918:LEU:HB3	2.01	0.42
1:D:988:LEU:HD11	1:D:1055:ARG:HG2	2.00	0.42
1:D:1271:THR:OG1	1:D:1272:ARG:N	2.52	0.42
1:D:1641:ASP:HB2	1:D:1644:GLU:HG3	2.01	0.42
1:D:3905:PHE:O	1:D:3909:ILE:HG12	2.20	0.42
1:D:4189:VAL:HG21	1:D:4948:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1743:GLU:CD	1:A:1744:ASN:HD22	2.22	0.42
1:A:1827:TYR:CZ	1:A:1831:ILE:HD11	2.54	0.42
1:A:3719:GLU:HA	1:A:3722:LYS:HG2	2.01	0.42
1:B:661:LEU:HD13	1:B:673:TRP:CD1	2.54	0.42
1:B:802:PHE:HB2	1:B:1618:TRP:HB2	2.01	0.42
1:B:2282:LYS:HA	1:B:2282:LYS:HD2	1.90	0.42
1:B:2894:PHE:HA	1:B:2897:ILE:HG12	2.00	0.42
1:C:1743:GLU:CD	1:C:1744:ASN:HD22	2.22	0.42
1:C:4509:PHE:HD1	1:C:4509:PHE:HA	1.78	0.42
1:D:3719:GLU:HA	1:D:3722:LYS:HG2	2.01	0.42
1:D:4857:LEU:HD23	1:D:4857:LEU:HA	1.91	0.42
1:A:190:ARG:HD3	1:A:205:ALA:O	2.19	0.42
1:A:838:ARG:H	1:A:841:LYS:NZ	2.17	0.42
1:A:1088:PHE:HB2	1:A:1205:CYS:SG	2.60	0.42
1:A:1271:THR:OG1	1:A:1272:ARG:N	2.52	0.42
1:A:4000:ASP:O	1:A:4004:GLU:HG3	2.19	0.42
1:B:697:TRP:HB2	1:B:766:ILE:HD13	2.01	0.42
1:B:829:LYS:O	1:B:830:GLU:HG3	2.19	0.42
1:B:1706:LEU:O	1:B:1710:ILE:HG13	2.20	0.42
1:B:1789:LYS:HB2	1:B:1835:PHE:CE1	2.55	0.42
1:B:2722:LYS:HD2	1:B:2722:LYS:HA	1.63	0.42
1:B:4000:ASP:O	1:B:4004:GLU:HG3	2.19	0.42
1:C:2305:VAL:O	1:C:2312:VAL:HG22	2.20	0.42
1:C:4182:LYS:HA	1:C:4182:LYS:HD2	1.89	0.42
1:D:697:TRP:HB2	1:D:766:ILE:HD13	2.01	0.42
1:D:1827:TYR:CZ	1:D:1831:ILE:HD11	2.54	0.42
1:A:698:ALA:HA	1:A:724:SER:HA	2.00	0.42
1:A:1118:SER:HA	1:A:1134:ALA:HA	2.01	0.42
1:A:1233:GLN:HG3	1:B:3493:UNK:CB	2.49	0.42
1:A:1595:VAL:O	1:A:1595:VAL:HG23	2.20	0.42
1:A:2487:LEU:O	1:A:2492:LEU:HG	2.20	0.42
1:B:557:TRP:CE3	1:B:558:LEU:HD23	2.55	0.42
1:B:1608:ASP:OD1	1:B:1608:ASP:N	2.52	0.42
1:B:4913:ASN:HB3	1:B:4916:ASN:HB2	2.02	0.42
1:C:1251:LEU:HD23	1:C:1600:MET:HE2	2.00	0.42
1:C:1706:LEU:O	1:C:1710:ILE:HG13	2.20	0.42
1:C:1789:LYS:HB2	1:C:1835:PHE:CE1	2.55	0.42
1:C:2471:LEU:HD23	1:C:2471:LEU:HA	1.80	0.42
1:C:4000:ASP:O	1:C:4004:GLU:HG3	2.19	0.42
1:C:4496:ASN:HD22	1:C:4499:ASN:HD22	1.66	0.42
1:D:843:GLU:HB3	1:D:1606:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1744:ASN:ND2	1:D:1746:LYS:HE2	2.31	0.42
1:D:1789:LYS:HB2	1:D:1835:PHE:CE1	2.55	0.42
1:D:1959:ARG:HH21	1:D:1962:ARG:HH12	1.68	0.42
1:D:4923:TYR:CZ	1:D:4927:LYS:HD2	2.55	0.42
2:J:53:LYS:HD3	2:J:53:LYS:HA	1.92	0.42
1:A:674:TYR:CE2	1:A:756:SER:HB2	2.54	0.42
1:A:1643:LEU:HD22	1:A:1694:TYR:O	2.20	0.42
1:A:4923:TYR:CZ	1:A:4927:LYS:HD2	2.54	0.42
1:B:1044:LYS:HD2	1:B:1044:LYS:HA	1.78	0.42
1:B:2837:HIS:ND1	1:B:2838:ALA:N	2.67	0.42
1:B:3905:PHE:O	1:B:3909:ILE:HG12	2.20	0.42
1:B:4189:VAL:HG21	1:B:4948:TRP:CZ2	2.55	0.42
2:H:27:TYR:N	2:H:40:SER:OG	2.51	0.42
1:C:557:TRP:CE3	1:C:558:LEU:HD23	2.55	0.42
1:C:2837:HIS:ND1	1:C:2838:ALA:N	2.67	0.42
1:C:4287:TRP:O	1:C:4291:VAL:HG13	2.19	0.42
1:D:698:ALA:HA	1:D:724:SER:HA	2.00	0.42
1:D:1643:LEU:HD22	1:D:1694:TYR:O	2.20	0.42
1:A:697:TRP:HB2	1:A:766:ILE:HD13	2.01	0.42
1:A:1835:PHE:O	1:A:1840:LEU:HD12	2.20	0.42
1:A:3905:PHE:O	1:A:3909:ILE:HG12	2.20	0.42
1:B:245:LEU:HD11	1:B:260:VAL:HG12	2.01	0.42
1:B:987:LYS:HE2	1:B:987:LYS:HB3	1.92	0.42
1:B:1303:ARG:NH2	1:B:1590:GLN:OE1	2.53	0.42
1:B:1595:VAL:HG23	1:B:1595:VAL:O	2.20	0.42
1:B:1835:PHE:O	1:B:1840:LEU:HD12	2.20	0.42
1:B:4660:TYR:HB3	1:B:4664:ARG:HH21	1.85	0.42
1:B:4807:ASP:HB3	1:B:4810:THR:HB	2.00	0.42
1:C:247:VAL:O	1:C:272:ARG:NH1	2.44	0.42
1:C:661:LEU:HD13	1:C:673:TRP:CD1	2.54	0.42
1:C:693:LEU:HD13	1:C:798:ILE:HG12	2.02	0.42
1:C:899:GLU:HG2	1:C:971:GLN:HE22	1.84	0.42
1:C:1088:PHE:HB2	1:C:1205:CYS:SG	2.60	0.42
1:C:1668:LEU:HD23	1:C:2131:VAL:HG22	2.02	0.42
1:C:4807:ASP:HB3	1:C:4810:THR:HB	2.00	0.42
2:I:28:THR:O	2:I:28:THR:OG1	2.36	0.42
1:D:34:LYS:O	1:D:52:THR:OG1	2.37	0.42
1:D:1367:LYS:NZ	1:D:1369:GLU:OE2	2.35	0.42
1:D:1608:ASP:OD1	1:D:1608:ASP:N	2.52	0.42
1:D:1682:ASP:HB3	1:D:1684:PRO:HD2	2.01	0.42
1:D:2305:VAL:O	1:D:2312:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4569:PRO:HB3	1:D:4572:ARG:HH21	1.85	0.42
1:D:4670:GLY:O	1:D:4671:MET:HG2	2.19	0.42
1:A:547:ASN:OD1	1:A:547:ASN:N	2.53	0.42
1:A:1641:ASP:HB2	1:A:1644:GLU:HG3	2.00	0.42
1:A:1668:LEU:HD23	1:A:2131:VAL:HG22	2.02	0.42
1:A:1789:LYS:HB2	1:A:1835:PHE:CE1	2.55	0.42
2:G:27:TYR:N	2:G:40:SER:OG	2.51	0.42
1:B:161:THR:HG23	1:B:184:VAL:HB	2.01	0.42
1:B:1217:PHE:O	1:B:1240:ALA:N	2.52	0.42
1:B:1271:THR:OG1	1:B:1272:ARG:N	2.52	0.42
1:B:2755:LEU:HD12	1:B:2767:LYS:CD	2.50	0.42
1:B:3636:GLU:HG2	1:B:3696:LYS:HE3	2.01	0.42
1:B:4923:TYR:CZ	1:B:4927:LYS:HD2	2.54	0.42
1:C:833:LYS:HE3	1:C:834:VAL:N	2.33	0.42
1:C:840:TYR:CE2	1:C:850:LEU:HA	2.55	0.42
1:C:1608:ASP:OD1	1:C:1608:ASP:N	2.52	0.42
1:C:4913:ASN:HB3	1:C:4916:ASN:HB2	2.02	0.42
1:D:161:THR:HG23	1:D:184:VAL:HB	2.01	0.42
1:D:674:TYR:HB2	1:D:819:TYR:HB3	2.02	0.42
1:D:1088:PHE:HB2	1:D:1205:CYS:SG	2.60	0.42
1:D:1273:ILE:HG13	1:D:1274:ASP:N	2.32	0.42
1:D:3636:GLU:HG2	1:D:3696:LYS:HE3	2.01	0.42
1:D:4913:ASN:HB3	1:D:4916:ASN:HB2	2.02	0.42
1:A:28:ILE:HG21	1:A:201:TRP:HH2	1.85	0.42
1:A:658:ASN:HB2	1:A:832:LEU:HD12	2.01	0.42
1:A:4632:LEU:H	1:A:4632:LEU:HD23	1.85	0.42
1:B:2487:LEU:O	1:B:2492:LEU:HG	2.20	0.42
1:B:4079:TYR:HA	1:B:4082:PHE:HB3	2.02	0.42
1:C:245:LEU:HD11	1:C:260:VAL:HG12	2.01	0.42
1:C:674:TYR:CE2	1:C:756:SER:HB2	2.54	0.42
1:C:745:ASN:O	1:C:747:HIS:ND1	2.49	0.42
1:C:802:PHE:HB2	1:C:1618:TRP:HB2	2.01	0.42
1:C:1044:LYS:HD2	1:C:1044:LYS:HA	1.78	0.42
1:C:3905:PHE:O	1:C:3909:ILE:HG12	2.20	0.42
1:C:4189:VAL:HG21	1:C:4948:TRP:CZ2	2.55	0.42
1:D:557:TRP:CZ2	1:D:561:ARG:HG3	2.55	0.42
1:D:837:SER:H	1:D:841:LYS:HZ1	1.67	0.42
1:D:840:TYR:CE2	1:D:850:LEU:HA	2.55	0.42
1:D:1040:ASP:HA	1:D:1043:LYS:HG3	2.01	0.42
1:D:1217:PHE:O	1:D:1240:ALA:N	2.52	0.42
1:D:1303:ARG:NH2	1:D:1590:GLN:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1595:VAL:O	1:D:1595:VAL:HG23	2.20	0.42
1:D:1987:CYS:N	1:D:1988:PRO:HD2	2.34	0.42
1:D:4047:PHE:O	1:D:4051:MET:HG2	2.20	0.42
1:A:557:TRP:CZ2	1:A:561:ARG:HG3	2.55	0.41
1:A:894:VAL:HG13	1:A:918:LEU:HB3	2.01	0.41
1:A:1303:ARG:NH2	1:A:1590:GLN:OE1	2.53	0.41
1:A:1977:ASN:OD1	1:A:1977:ASN:N	2.53	0.41
1:A:4569:PRO:HB3	1:A:4572:ARG:HH21	1.85	0.41
1:B:290:ARG:H	1:B:293:GLN:NE2	2.15	0.41
1:B:899:GLU:HG2	1:B:971:GLN:HE22	1.84	0.41
1:B:1643:LEU:HD22	1:B:1694:TYR:O	2.20	0.41
1:B:1744:ASN:ND2	1:B:1746:LYS:HE2	2.30	0.41
1:B:3802:LEU:HB2	1:B:3883:SER:OG	2.20	0.41
1:C:190:ARG:HD3	1:C:205:ALA:O	2.19	0.41
1:C:375:GLN:NE2	1:C:390:LYS:O	2.53	0.41
1:C:557:TRP:CZ2	1:C:561:ARG:HG3	2.55	0.41
1:C:2487:LEU:O	1:C:2492:LEU:HG	2.20	0.41
1:C:3636:GLU:HG2	1:C:3696:LYS:HE3	2.01	0.41
1:C:3825:GLY:O	1:C:3828:VAL:HG12	2.20	0.41
1:D:669:GLN:HB3	1:D:673:TRP:HZ2	1.85	0.41
1:D:845:THR:OG1	1:D:846:TYR:N	2.51	0.41
1:D:1251:LEU:HD23	1:D:1600:MET:HE2	2.02	0.41
1:D:2486:LEU:HD13	1:D:2486:LEU:HA	1.87	0.41
1:D:4079:TYR:HA	1:D:4082:PHE:HB3	2.02	0.41
1:A:125:TYR:CE1	1:A:417:ARG:HD3	2.55	0.41
1:A:2837:HIS:ND1	1:A:2838:ALA:N	2.67	0.41
1:A:4913:ASN:HB3	1:A:4916:ASN:HB2	2.02	0.41
1:B:557:TRP:CZ2	1:B:561:ARG:HG3	2.55	0.41
1:B:3825:GLY:O	1:B:3828:VAL:HG12	2.20	0.41
1:C:843:GLU:HB3	1:C:1606:LYS:HD3	2.01	0.41
1:C:1744:ASN:ND2	1:C:1746:LYS:HE2	2.30	0.41
1:C:1977:ASN:OD1	1:C:1977:ASN:N	2.53	0.41
1:C:4175:VAL:HG22	1:C:4187:LEU:HD13	2.02	0.41
1:D:125:TYR:CE1	1:D:417:ARG:HD3	2.56	0.41
1:D:1706:LEU:O	1:D:1710:ILE:HG13	2.20	0.41
1:D:2487:LEU:O	1:D:2492:LEU:HG	2.20	0.41
1:D:2755:LEU:HD12	1:D:2767:LYS:CD	2.50	0.41
1:D:2836:LEU:HD22	1:D:2839:MET:HE1	2.01	0.41
1:A:557:TRP:CE3	1:A:558:LEU:HD23	2.55	0.41
1:A:745:ASN:O	1:A:747:HIS:ND1	2.49	0.41
1:A:1040:ASP:HA	1:A:1043:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1706:LEU:O	1:A:1710:ILE:HG13	2.20	0.41
1:A:1744:ASN:ND2	1:A:1746:LYS:HE2	2.30	0.41
1:A:1931:PHE:CE1	1:A:1995:LEU:HB2	2.55	0.41
1:A:4928:ASP:OD1	1:A:4929:GLU:N	2.46	0.41
2:G:53:LYS:HD3	2:G:53:LYS:HA	1.92	0.41
1:B:541:ILE:HD11	1:B:574:VAL:HG13	2.02	0.41
1:B:547:ASN:OD1	1:B:547:ASN:N	2.53	0.41
1:B:658:ASN:HB2	1:B:832:LEU:HD12	2.01	0.41
1:B:1682:ASP:HB3	1:B:1684:PRO:HD2	2.01	0.41
1:B:4574:LEU:HD12	1:B:4574:LEU:HA	1.90	0.41
1:C:125:TYR:CE1	1:C:417:ARG:HD3	2.56	0.41
1:C:1303:ARG:NH2	1:C:1590:GLN:OE1	2.53	0.41
1:D:28:ILE:HG21	1:D:201:TRP:HH2	1.85	0.41
1:D:557:TRP:CE3	1:D:558:LEU:HD23	2.55	0.41
1:D:1682:ASP:CB	1:D:1685:GLN:HB3	2.48	0.41
1:D:4608:LYS:HG2	1:D:4614:LEU:HD22	2.03	0.41
1:D:4941:LYS:O	1:D:4945:GLU:HG3	2.21	0.41
1:A:669:GLN:HB3	1:A:673:TRP:HZ2	1.86	0.41
1:A:802:PHE:HB2	1:A:1618:TRP:HB2	2.01	0.41
1:A:1682:ASP:HB3	1:A:1684:PRO:HD2	2.01	0.41
1:A:2836:LEU:HD22	1:A:2839:MET:HE1	2.02	0.41
1:A:3758:LEU:O	1:A:3762:ILE:HG12	2.19	0.41
1:A:4189:VAL:HG21	1:A:4948:TRP:CZ2	2.55	0.41
1:B:185:SER:HG	1:B:190:ARG:H	1.68	0.41
1:B:1118:SER:HA	1:B:1134:ALA:HA	2.01	0.41
1:B:3719:GLU:HA	1:B:3722:LYS:HG2	2.02	0.41
1:B:3870:ILE:H	1:B:3870:ILE:HG12	1.67	0.41
1:B:4175:VAL:HG22	1:B:4187:LEU:HD13	2.02	0.41
1:B:4569:PRO:HB3	1:B:4572:ARG:HH21	1.85	0.41
1:C:318:ASP:OD1	1:C:318:ASP:N	2.54	0.41
1:C:3719:GLU:HA	1:C:3722:LYS:HG2	2.02	0.41
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.85	0.41
1:D:2282:LYS:HA	1:D:2282:LYS:HD2	1.90	0.41
1:D:4171:PHE:CE1	1:D:4175:VAL:HG21	2.56	0.41
1:D:4660:TYR:HB3	1:D:4664:ARG:HH21	1.85	0.41
1:A:1091:GLU:HG2	1:A:1093:THR:H	1.85	0.41
1:A:1987:CYS:N	1:A:1988:PRO:HD2	2.34	0.41
1:A:4941:LYS:O	1:A:4945:GLU:HG3	2.21	0.41
1:C:1091:GLU:HG2	1:C:1093:THR:H	1.85	0.41
1:C:1740:PHE:CD1	1:C:1923:ALA:HB1	2.56	0.41
1:C:2755:LEU:HD12	1:C:2767:LYS:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1809:ASP:N	1:D:1809:ASP:OD1	2.54	0.41
1:D:2722:LYS:HD2	1:D:2722:LYS:HA	1.63	0.41
1:A:16:THR:OG1	1:A:109:GLY:O	2.35	0.41
1:A:693:LEU:HD13	1:A:798:ILE:HG12	2.01	0.41
1:A:840:TYR:CE2	1:A:850:LEU:HA	2.55	0.41
1:A:1086:ARG:HH21	1:A:1251:LEU:HD13	1.86	0.41
1:A:1829:LEU:O	1:A:1834:ILE:HG12	2.21	0.41
1:A:2733:MET:O	1:A:2736:LEU:HG	2.21	0.41
1:A:2755:LEU:HD12	1:A:2767:LYS:CD	2.50	0.41
1:A:4171:PHE:CE1	1:A:4175:VAL:HG21	2.56	0.41
1:B:888:ASN:O	1:B:891:GLU:HG2	2.21	0.41
1:B:1641:ASP:HB2	1:B:1644:GLU:HG3	2.00	0.41
1:B:1931:PHE:CE1	1:B:1995:LEU:HB2	2.55	0.41
1:B:4171:PHE:CE1	1:B:4175:VAL:HG21	2.56	0.41
1:C:1643:LEU:HD22	1:C:1694:TYR:O	2.20	0.41
1:C:1809:ASP:N	1:C:1809:ASP:OD1	2.54	0.41
1:C:1827:TYR:CZ	1:C:1831:ILE:HD11	2.54	0.41
1:C:1829:LEU:O	1:C:1834:ILE:HG12	2.21	0.41
1:C:1835:PHE:O	1:C:1840:LEU:HD12	2.20	0.41
1:C:1959:ARG:HH21	1:C:1962:ARG:HH12	1.68	0.41
1:C:3802:LEU:HB2	1:C:3883:SER:OG	2.20	0.41
1:C:4047:PHE:O	1:C:4051:MET:HG2	2.20	0.41
1:C:4569:PRO:HB3	1:C:4572:ARG:HH21	1.85	0.41
1:C:4632:LEU:HD23	1:C:4632:LEU:H	1.85	0.41
1:D:323:ASP:O	1:D:327:THR:OG1	2.27	0.41
1:D:748:LEU:HD23	1:D:748:LEU:HA	1.91	0.41
1:D:1740:PHE:CD1	1:D:1923:ALA:HB1	2.56	0.41
1:D:1931:PHE:CE1	1:D:1995:LEU:HB2	2.56	0.41
1:D:4044:LYS:HE2	1:D:4044:LYS:HB3	1.82	0.41
1:A:245:LEU:HD11	1:A:260:VAL:HG12	2.01	0.41
1:A:674:TYR:HB2	1:A:819:TYR:HB3	2.02	0.41
1:A:773:GLN:H	1:A:773:GLN:HG2	1.70	0.41
1:A:3636:GLU:HG2	1:A:3696:LYS:HE3	2.02	0.41
1:A:3802:LEU:HB2	1:A:3883:SER:OG	2.21	0.41
1:B:318:ASP:OD1	1:B:318:ASP:N	2.54	0.41
1:B:1088:PHE:HB2	1:B:1205:CYS:SG	2.60	0.41
1:B:2340:ASN:OD1	1:B:2340:ASN:N	2.46	0.41
1:C:669:GLN:HB3	1:C:673:TRP:HZ2	1.85	0.41
1:C:888:ASN:O	1:C:891:GLU:HG2	2.21	0.41
1:C:1609:VAL:HG12	1:C:1611:ARG:H	1.86	0.41
1:C:1931:PHE:CE1	1:C:1995:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4928:ASP:OD1	1:C:4929:GLU:N	2.46	0.41
1:D:557:TRP:CE2	1:D:561:ARG:HG3	2.56	0.41
1:D:1829:LEU:O	1:D:1834:ILE:HG12	2.21	0.41
1:D:1835:PHE:O	1:D:1840:LEU:HD12	2.20	0.41
1:D:2188:PHE:HB3	1:D:2191:MET:HB3	2.03	0.41
1:D:2733:MET:O	1:D:2736:LEU:HG	2.21	0.41
1:A:987:LYS:HE2	1:A:987:LYS:HB3	1.92	0.41
1:A:1682:ASP:CB	1:A:1685:GLN:HB3	2.48	0.41
1:A:4079:TYR:HA	1:A:4082:PHE:HB3	2.02	0.41
1:B:125:TYR:CE1	1:B:417:ARG:HD3	2.56	0.41
1:B:557:TRP:CE2	1:B:561:ARG:HG3	2.56	0.41
1:B:1809:ASP:N	1:B:1809:ASP:OD1	2.54	0.41
1:B:2733:MET:O	1:B:2736:LEU:HG	2.21	0.41
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.85	0.41
1:C:290:ARG:H	1:C:293:GLN:NE2	2.15	0.41
1:C:557:TRP:CE2	1:C:561:ARG:HG3	2.56	0.41
1:C:674:TYR:HB2	1:C:819:TYR:HB3	2.02	0.41
1:C:1031:ARG:HA	1:C:1031:ARG:HD3	1.84	0.41
1:C:1682:ASP:HB3	1:C:1684:PRO:HD2	2.01	0.41
1:C:4660:TYR:HB3	1:C:4664:ARG:HH21	1.85	0.41
1:D:541:ILE:HD11	1:D:574:VAL:HG13	2.02	0.41
1:D:802:PHE:HB2	1:D:1618:TRP:HB2	2.01	0.41
1:D:1086:ARG:HH21	1:D:1251:LEU:HD13	1.86	0.41
1:A:527:LYS:NZ	1:A:531:ASN:OD1	2.38	0.41
1:A:845:THR:OG1	1:A:846:TYR:N	2.51	0.41
1:A:1959:ARG:HH21	1:A:1962:ARG:HH12	1.68	0.41
1:A:2305:VAL:O	1:A:2312:VAL:HG22	2.20	0.41
1:A:4608:LYS:HG2	1:A:4614:LEU:HD22	2.03	0.41
1:A:4660:TYR:HB3	1:A:4664:ARG:HH21	1.85	0.41
1:A:4794:LYS:HE3	1:A:4794:LYS:HB3	1.95	0.41
2:G:28:THR:O	2:G:28:THR:OG1	2.36	0.41
1:B:16:THR:OG1	1:B:109:GLY:O	2.35	0.41
1:B:530:LEU:HD23	1:B:530:LEU:HA	1.87	0.41
1:B:840:TYR:CE2	1:B:850:LEU:HA	2.55	0.41
1:B:1086:ARG:HH21	1:B:1251:LEU:HD13	1.86	0.41
1:B:1091:GLU:HG2	1:B:1093:THR:H	1.85	0.41
1:B:1829:LEU:O	1:B:1834:ILE:HG12	2.21	0.41
1:B:2234:ARG:HD2	1:B:2234:ARG:HA	1.94	0.41
1:B:2260:ASP:N	1:B:2260:ASP:OD1	2.54	0.41
1:B:2305:VAL:O	1:B:2312:VAL:HG22	2.20	0.41
1:B:2887:LYS:O	1:B:2891:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4047:PHE:O	1:B:4051:MET:HG2	2.20	0.41
1:B:4608:LYS:HG2	1:B:4614:LEU:HD22	2.03	0.41
1:B:4632:LEU:HD23	1:B:4632:LEU:H	1.85	0.41
1:B:4867:ASP:OD1	1:C:4873:ARG:NH1	2.54	0.41
1:C:640:ARG:HH22	2:I:91:VAL:HG13	1.86	0.41
1:C:1086:ARG:HH21	1:C:1251:LEU:HD13	1.86	0.41
1:C:1091:GLU:HB3	1:C:1094:TYR:CD2	2.52	0.41
1:C:1595:VAL:HG23	1:C:1595:VAL:O	2.20	0.41
1:C:4171:PHE:CE1	1:C:4175:VAL:HG21	2.56	0.41
1:C:4636:THR:OG1	1:C:4637:GLN:N	2.54	0.41
1:C:4941:LYS:O	1:C:4945:GLU:HG3	2.21	0.41
1:D:987:LYS:HE2	1:D:987:LYS:HB3	1.92	0.41
1:D:1091:GLU:HG2	1:D:1093:THR:H	1.85	0.41
1:D:1965:ARG:O	1:D:1966:SER:OG	2.37	0.41
1:D:3802:LEU:HB2	1:D:3883:SER:OG	2.21	0.41
1:D:4304:PHE:O	1:D:4308:VAL:HG22	2.21	0.41
1:D:4594:VAL:N	1:D:4595:PRO:HD2	2.36	0.41
1:D:4794:LYS:HE3	1:D:4794:LYS:HB3	1.96	0.41
1:A:850:LEU:H	1:A:850:LEU:HG	1.57	0.41
1:A:1740:PHE:CD1	1:A:1923:ALA:HB1	2.56	0.41
1:A:3825:GLY:O	1:A:3828:VAL:HG12	2.20	0.41
1:B:28:ILE:HG21	1:B:201:TRP:HH2	1.85	0.41
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.93	0.41
1:B:693:LEU:HD13	1:B:798:ILE:HG12	2.02	0.41
1:B:1363:LYS:HE2	1:B:1365:THR:HG22	2.03	0.41
1:B:3612:ARG:O	1:B:3612:ARG:NH1	2.54	0.41
1:C:541:ILE:HD11	1:C:574:VAL:HG13	2.02	0.41
1:C:4079:TYR:HA	1:C:4082:PHE:HB3	2.02	0.41
1:C:4594:VAL:N	1:C:4595:PRO:HD2	2.36	0.41
1:D:1668:LEU:HD23	1:D:2131:VAL:HG22	2.02	0.41
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.85	0.41
1:A:318:ASP:OD1	1:A:318:ASP:N	2.54	0.40
1:A:380:LYS:HA	1:A:380:LYS:HD3	1.71	0.40
1:A:4304:PHE:O	1:A:4308:VAL:HG22	2.21	0.40
1:B:1740:PHE:CD1	1:B:1923:ALA:HB1	2.56	0.40
1:C:2260:ASP:OD1	1:C:2260:ASP:N	2.54	0.40
1:C:2331:GLY:HA3	1:C:2391:TYR:CE1	2.56	0.40
1:C:4924:LEU:HD23	1:C:4924:LEU:HA	1.92	0.40
1:D:644:LEU:HD11	1:D:1651:LEU:HD22	2.03	0.40
1:D:3870:ILE:H	1:D:3870:ILE:HG12	1.67	0.40
1:D:4164:VAL:HA	1:D:4167:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:ASN:O	1:A:891:GLU:HG2	2.21	0.40
1:A:1003:ALA:O	1:A:1006:VAL:HG22	2.22	0.40
1:A:1363:LYS:HE2	1:A:1365:THR:HG22	2.03	0.40
1:A:4047:PHE:O	1:A:4051:MET:HG2	2.20	0.40
1:A:4276:LYS:NZ	1:A:4562:GLU:HG3	2.36	0.40
1:A:4862:GLN:HG2	1:D:4859:ALA:HB2	2.03	0.40
1:B:674:TYR:HB2	1:B:819:TYR:HB3	2.02	0.40
1:B:2747:SER:O	1:B:2753:GLN:NE2	2.49	0.40
1:C:4276:LYS:NZ	1:C:4562:GLU:HG3	2.36	0.40
1:D:527:LYS:NZ	1:D:531:ASN:OD1	2.38	0.40
1:D:693:LEU:HD13	1:D:798:ILE:HG12	2.02	0.40
1:D:3825:GLY:O	1:D:3828:VAL:HG12	2.20	0.40
1:D:4830:ILE:HB	1:D:4842:ARG:NH2	2.36	0.40
1:A:313:ASN:HD21	1:A:392:ILE:HA	1.87	0.40
1:A:373:THR:O	1:A:375:GLN:NE2	2.43	0.40
1:A:541:ILE:HD11	1:A:574:VAL:HG13	2.02	0.40
1:A:557:TRP:CE2	1:A:561:ARG:HG3	2.56	0.40
1:A:1131:ASP:HB3	1:A:1133:ARG:HG2	2.04	0.40
1:A:1809:ASP:N	1:A:1809:ASP:OD1	2.54	0.40
1:A:2260:ASP:N	1:A:2260:ASP:OD1	2.54	0.40
1:A:2331:GLY:HA3	1:A:2391:TYR:CE1	2.56	0.40
1:A:2887:LYS:O	1:A:2891:ILE:HG23	2.21	0.40
1:A:4164:VAL:HA	1:A:4167:SER:OG	2.22	0.40
1:A:4276:LYS:HZ1	1:A:4562:GLU:HG3	1.86	0.40
1:A:4594:VAL:N	1:A:4595:PRO:HD2	2.36	0.40
1:A:4857:LEU:HD23	1:A:4857:LEU:HA	1.91	0.40
1:B:669:GLN:HB3	1:B:673:TRP:HZ2	1.85	0.40
1:B:1131:ASP:HB3	1:B:1133:ARG:HG2	2.04	0.40
1:B:2065:MET:SD	1:B:2083:MET:HG3	2.62	0.40
1:B:4276:LYS:HZ1	1:B:4562:GLU:HG3	1.87	0.40
1:C:502:ILE:HG22	1:C:506:HIS:CD2	2.56	0.40
1:C:530:LEU:HD23	1:C:530:LEU:HA	1.87	0.40
1:C:1682:ASP:CB	1:C:1685:GLN:HB3	2.48	0.40
1:C:2733:MET:O	1:C:2736:LEU:HG	2.21	0.40
1:C:3954:GLN:NE2	1:C:3971:MET:SD	2.95	0.40
1:D:313:ASN:HD21	1:D:392:ILE:HA	1.87	0.40
1:D:1609:VAL:HG12	1:D:1611:ARG:H	1.86	0.40
1:D:4632:LEU:HD23	1:D:4632:LEU:H	1.85	0.40
1:A:1609:VAL:HG12	1:A:1611:ARG:H	1.86	0.40
1:A:1731:THR:O	1:A:1735:LYS:HG3	2.21	0.40
1:B:773:GLN:H	1:B:773:GLN:HG2	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:ALA:O	1:B:1006:VAL:HG22	2.22	0.40
1:B:4010:GLU:HG2	1:B:4120:LEU:HD13	2.03	0.40
1:C:547:ASN:OD1	1:C:547:ASN:N	2.53	0.40
1:C:678:MET:HA	1:C:753:ASP:O	2.22	0.40
1:C:1982:LYS:HD2	1:C:1983:SER:H	1.86	0.40
1:C:2085:VAL:HG12	1:C:3686:LEU:HD13	2.03	0.40
1:C:2134:GLY:H	1:C:2137:GLU:HB2	1.87	0.40
1:C:2188:PHE:HB3	1:C:2191:MET:HB3	2.03	0.40
1:C:2859:LEU:HD22	1:C:2859:LEU:HA	1.93	0.40
1:C:3874:VAL:HG11	1:C:3937:SER:OG	2.22	0.40
1:C:4083:VAL:O	1:C:4087:HIS:HB3	2.22	0.40
1:C:4093:ILE:O	1:C:4097:VAL:HG23	2.22	0.40
1:C:4164:VAL:HA	1:C:4167:SER:OG	2.21	0.40
1:D:418:VAL:O	1:D:422:THR:HG23	2.22	0.40
1:D:888:ASN:O	1:D:891:GLU:HG2	2.21	0.40
1:D:2085:VAL:HG12	1:D:3686:LEU:HD13	2.03	0.40
1:D:2260:ASP:OD1	1:D:2260:ASP:N	2.54	0.40
1:D:3762:ILE:HD12	1:D:3840:ARG:HG3	2.03	0.40
1:A:1289:SER:HA	1:A:1353:HIS:HB3	2.04	0.40
1:B:502:ILE:HG22	1:B:506:HIS:CD2	2.56	0.40
1:B:1127:GLU:HG3	1:B:1128:LEU:N	2.37	0.40
1:B:1982:LYS:HD2	1:B:1983:SER:H	1.86	0.40
1:B:4589:TYR:OH	1:B:4715:ASP:OD2	2.38	0.40
1:B:4594:VAL:N	1:B:4595:PRO:HD2	2.36	0.40
1:B:4603:LYS:HD2	1:B:4607:ARG:NH1	2.37	0.40
1:C:1003:ALA:O	1:C:1006:VAL:HG22	2.22	0.40
2:I:26:HIS:HD2	2:I:40:SER:OG	2.05	0.40
1:D:37:LEU:HD13	1:D:203:VAL:HG21	2.04	0.40
1:D:479:LEU:HD23	1:D:482:LEU:HD21	2.04	0.40
1:D:678:MET:HA	1:D:753:ASP:O	2.22	0.40
1:D:745:ASN:O	1:D:747:HIS:ND1	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3255/4966 (66%)	3051 (94%)	204 (6%)	0	100	100
1	B	3255/4966 (66%)	3050 (94%)	205 (6%)	0	100	100
1	C	3255/4966 (66%)	3050 (94%)	205 (6%)	0	100	100
1	D	3255/4966 (66%)	3049 (94%)	206 (6%)	0	100	100
2	G	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	H	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	I	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	J	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
All	All	13440/20568 (65%)	12608 (94%)	832 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2862/3387 (84%)	2726 (95%)	136 (5%)	25	60
1	B	2862/3387 (84%)	2726 (95%)	136 (5%)	25	60
1	C	2862/3387 (84%)	2727 (95%)	135 (5%)	26	60
1	D	2862/3387 (84%)	2726 (95%)	136 (5%)	25	60
2	G	88/140 (63%)	87 (99%)	1 (1%)	73	88
2	H	88/140 (63%)	86 (98%)	2 (2%)	50	77
2	I	88/140 (63%)	87 (99%)	1 (1%)	73	88
2	J	88/140 (63%)	87 (99%)	1 (1%)	73	88
All	All	11800/14108 (84%)	11252 (95%)	548 (5%)	31	61

All (548) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	80	GLU
1	A	132	CYS
1	A	140	THR
1	A	141	ASP
1	A	170	SER
1	A	177	VAL
1	A	213	SER
1	A	236	LEU
1	A	237	LEU
1	A	246	THR
1	A	269	VAL
1	A	270	HIS
1	A	285	SER
1	A	296	ARG
1	A	299	HIS
1	A	323	ASP
1	A	326	SER
1	A	346	VAL
1	A	358	ASP
1	A	439	LYS
1	A	450	GLU
1	A	468	GLU
1	A	550	GLN
1	A	551	PHE
1	A	556	ASP
1	A	566	GLU
1	A	643	LEU
1	A	652	VAL
1	A	687	THR
1	A	695	VAL
1	A	704	SER
1	A	711	GLU
1	A	713	TRP
1	A	814	LEU
1	A	833	LYS
1	A	850	LEU
1	A	909	ASP
1	A	923	LYS
1	A	938	GLU
1	A	974	SER
1	A	988	LEU
1	A	1028	ARG

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Mol	Chain	Res	Type
1	A	1033	VAL
1	A	1039	ASP
1	A	1042	THR
1	A	1044	LYS
1	A	1155	SER
1	A	1174	MET
1	A	1183	LEU
1	A	1188	SER
1	A	1193	LYS
1	A	1196	ASP
1	A	1252	SER
1	A	1273	ILE
1	A	1297	THR
1	A	1364	GLU
1	A	1367	LYS
1	A	1376	TYR
1	A	1382	SER
1	A	1583	CYS
1	A	1589	VAL
1	A	1607	VAL
1	A	1612	ILE
1	A	1613	SER
1	A	1641	ASP
1	A	1678	CYS
1	A	1681	VAL
1	A	1709	ASP
1	A	1731	THR
1	A	1739	LEU
1	A	1814	THR
1	A	1840	LEU
1	A	1850	SER
1	A	2072	SER
1	A	2089	ARG
1	A	2106	THR
1	A	2136	GLU
1	A	2201	TYR
1	A	2219	TYR
1	A	2225	SER
1	A	2236	SER
1	A	2292	VAL
1	A	2302	ARG
1	A	2321	ARG

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Mol	Chain	Res	Type
1	A	2343	LEU
1	A	2351	LYS
1	A	2430	ASP
1	A	2484	LEU
1	A	2486	LEU
1	A	2494	ASP
1	A	2506	LEU
1	A	2714	GLU
1	A	2722	LYS
1	A	2751	LYS
1	A	2762	LEU
1	A	2763	SER
1	A	2771	ARG
1	A	2781	MET
1	A	2837	HIS
1	A	2859	LEU
1	A	2875	THR
1	A	2877	THR
1	A	2884	ASP
1	A	2902	VAL
1	A	2903	SER
1	A	3616	VAL
1	A	3818	MET
1	A	3822	GLU
1	A	3852	ASP
1	A	3861	THR
1	A	3865	THR
1	A	3990	VAL
1	A	4034	TYR
1	A	4039	LYS
1	A	4049	LYS
1	A	4073	GLU
1	A	4083	VAL
1	A	4157	THR
1	A	4181	GLU
1	A	4187	LEU
1	A	4509	PHE
1	A	4556	VAL
1	A	4623	ASP
1	A	4632	LEU
1	A	4636	THR
1	A	4658	GLU

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Mol	Chain	Res	Type
1	A	4668	LEU
1	A	4728	SER
1	A	4760	THR
1	A	4767	VAL
1	A	4782	VAL
1	A	4799	ASP
1	A	4900	VAL
1	A	4945	GLU
1	A	4955	ASP
2	G	101	ASP
1	B	75	VAL
1	B	80	GLU
1	B	132	CYS
1	B	140	THR
1	B	141	ASP
1	B	170	SER
1	B	177	VAL
1	B	213	SER
1	B	236	LEU
1	B	237	LEU
1	B	246	THR
1	B	269	VAL
1	B	270	HIS
1	B	285	SER
1	B	296	ARG
1	B	299	HIS
1	B	323	ASP
1	B	326	SER
1	B	346	VAL
1	B	358	ASP
1	B	439	LYS
1	B	450	GLU
1	B	468	GLU
1	B	550	GLN
1	B	551	PHE
1	B	556	ASP
1	B	566	GLU
1	B	643	LEU
1	B	652	VAL
1	B	687	THR
1	B	695	VAL
1	B	704	SER

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Mol	Chain	Res	Type
1	B	711	GLU
1	B	713	TRP
1	B	814	LEU
1	B	833	LYS
1	B	850	LEU
1	B	909	ASP
1	B	923	LYS
1	B	938	GLU
1	B	974	SER
1	B	988	LEU
1	B	1028	ARG
1	B	1033	VAL
1	B	1039	ASP
1	B	1042	THR
1	B	1044	LYS
1	B	1155	SER
1	B	1174	MET
1	B	1183	LEU
1	B	1188	SER
1	B	1193	LYS
1	B	1196	ASP
1	B	1252	SER
1	B	1273	ILE
1	B	1297	THR
1	B	1364	GLU
1	B	1367	LYS
1	B	1376	TYR
1	B	1382	SER
1	B	1583	CYS
1	B	1589	VAL
1	B	1607	VAL
1	B	1612	ILE
1	B	1613	SER
1	B	1641	ASP
1	B	1678	CYS
1	B	1681	VAL
1	B	1709	ASP
1	B	1731	THR
1	B	1739	LEU
1	B	1814	THR
1	B	1840	LEU
1	B	1850	SER

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Mol	Chain	Res	Type
1	B	2072	SER
1	B	2089	ARG
1	B	2106	THR
1	B	2136	GLU
1	B	2201	TYR
1	B	2219	TYR
1	B	2225	SER
1	B	2236	SER
1	B	2292	VAL
1	B	2302	ARG
1	B	2321	ARG
1	B	2343	LEU
1	B	2351	LYS
1	B	2430	ASP
1	B	2484	LEU
1	B	2486	LEU
1	B	2494	ASP
1	B	2506	LEU
1	B	2714	GLU
1	B	2722	LYS
1	B	2751	LYS
1	B	2762	LEU
1	B	2763	SER
1	B	2771	ARG
1	B	2781	MET
1	B	2837	HIS
1	B	2859	LEU
1	B	2875	THR
1	B	2877	THR
1	B	2884	ASP
1	B	2902	VAL
1	B	2903	SER
1	B	3616	VAL
1	B	3818	MET
1	B	3822	GLU
1	B	3852	ASP
1	B	3861	THR
1	B	3865	THR
1	B	3990	VAL
1	B	4034	TYR
1	B	4039	LYS
1	B	4049	LYS

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Mol	Chain	Res	Type
1	B	4073	GLU
1	B	4083	VAL
1	B	4157	THR
1	B	4181	GLU
1	B	4187	LEU
1	B	4509	PHE
1	B	4556	VAL
1	B	4623	ASP
1	B	4632	LEU
1	B	4636	THR
1	B	4658	GLU
1	B	4668	LEU
1	B	4728	SER
1	B	4760	THR
1	B	4767	VAL
1	B	4782	VAL
1	B	4799	ASP
1	B	4900	VAL
1	B	4945	GLU
1	B	4955	ASP
2	H	42	ASP
2	H	101	ASP
1	C	75	VAL
1	C	80	GLU
1	C	132	CYS
1	C	140	THR
1	C	141	ASP
1	C	170	SER
1	C	177	VAL
1	C	213	SER
1	C	236	LEU
1	C	237	LEU
1	C	246	THR
1	C	269	VAL
1	C	270	HIS
1	C	285	SER
1	C	296	ARG
1	C	299	HIS
1	C	323	ASP
1	C	326	SER
1	C	346	VAL
1	C	358	ASP

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Mol	Chain	Res	Type
1	C	439	LYS
1	C	450	GLU
1	C	468	GLU
1	C	550	GLN
1	C	551	PHE
1	C	556	ASP
1	C	566	GLU
1	C	643	LEU
1	C	652	VAL
1	C	687	THR
1	C	695	VAL
1	C	704	SER
1	C	711	GLU
1	C	713	TRP
1	C	814	LEU
1	C	833	LYS
1	C	850	LEU
1	C	909	ASP
1	C	923	LYS
1	C	938	GLU
1	C	974	SER
1	C	988	LEU
1	C	1028	ARG
1	C	1033	VAL
1	C	1039	ASP
1	C	1042	THR
1	C	1044	LYS
1	C	1155	SER
1	C	1174	MET
1	C	1183	LEU
1	C	1188	SER
1	C	1193	LYS
1	C	1196	ASP
1	C	1252	SER
1	C	1273	ILE
1	C	1297	THR
1	C	1364	GLU
1	C	1367	LYS
1	C	1376	TYR
1	C	1382	SER
1	C	1583	CYS
1	C	1589	VAL

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Mol	Chain	Res	Type
1	C	1607	VAL
1	C	1612	ILE
1	C	1613	SER
1	C	1641	ASP
1	C	1678	CYS
1	C	1709	ASP
1	C	1731	THR
1	C	1739	LEU
1	C	1814	THR
1	C	1840	LEU
1	C	1850	SER
1	C	2072	SER
1	C	2089	ARG
1	C	2106	THR
1	C	2136	GLU
1	C	2201	TYR
1	C	2219	TYR
1	C	2225	SER
1	C	2236	SER
1	C	2292	VAL
1	C	2302	ARG
1	C	2321	ARG
1	C	2343	LEU
1	C	2351	LYS
1	C	2430	ASP
1	C	2484	LEU
1	C	2486	LEU
1	C	2494	ASP
1	C	2506	LEU
1	C	2714	GLU
1	C	2722	LYS
1	C	2751	LYS
1	C	2762	LEU
1	C	2763	SER
1	C	2771	ARG
1	C	2781	MET
1	C	2837	HIS
1	C	2859	LEU
1	C	2875	THR
1	C	2877	THR
1	C	2884	ASP
1	C	2902	VAL

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Mol	Chain	Res	Type
1	C	2903	SER
1	C	3616	VAL
1	C	3818	MET
1	C	3822	GLU
1	C	3852	ASP
1	C	3861	THR
1	C	3865	THR
1	C	3990	VAL
1	C	4034	TYR
1	C	4039	LYS
1	C	4049	LYS
1	C	4073	GLU
1	C	4083	VAL
1	C	4157	THR
1	C	4181	GLU
1	C	4187	LEU
1	C	4509	PHE
1	C	4556	VAL
1	C	4623	ASP
1	C	4632	LEU
1	C	4636	THR
1	C	4658	GLU
1	C	4668	LEU
1	C	4728	SER
1	C	4760	THR
1	C	4767	VAL
1	C	4782	VAL
1	C	4799	ASP
1	C	4900	VAL
1	C	4945	GLU
1	C	4955	ASP
2	I	101	ASP
1	D	75	VAL
1	D	80	GLU
1	D	132	CYS
1	D	140	THR
1	D	141	ASP
1	D	170	SER
1	D	177	VAL
1	D	213	SER
1	D	236	LEU
1	D	237	LEU

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Mol	Chain	Res	Type
1	D	246	THR
1	D	269	VAL
1	D	270	HIS
1	D	285	SER
1	D	296	ARG
1	D	299	HIS
1	D	323	ASP
1	D	326	SER
1	D	346	VAL
1	D	358	ASP
1	D	439	LYS
1	D	450	GLU
1	D	468	GLU
1	D	550	GLN
1	D	551	PHE
1	D	556	ASP
1	D	566	GLU
1	D	643	LEU
1	D	652	VAL
1	D	687	THR
1	D	695	VAL
1	D	704	SER
1	D	711	GLU
1	D	713	TRP
1	D	814	LEU
1	D	833	LYS
1	D	850	LEU
1	D	909	ASP
1	D	923	LYS
1	D	938	GLU
1	D	974	SER
1	D	988	LEU
1	D	1028	ARG
1	D	1033	VAL
1	D	1039	ASP
1	D	1042	THR
1	D	1044	LYS
1	D	1155	SER
1	D	1174	MET
1	D	1183	LEU
1	D	1188	SER
1	D	1193	LYS

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Mol	Chain	Res	Type
1	D	1196	ASP
1	D	1252	SER
1	D	1273	ILE
1	D	1297	THR
1	D	1364	GLU
1	D	1367	LYS
1	D	1376	TYR
1	D	1382	SER
1	D	1583	CYS
1	D	1589	VAL
1	D	1607	VAL
1	D	1612	ILE
1	D	1613	SER
1	D	1641	ASP
1	D	1678	CYS
1	D	1681	VAL
1	D	1709	ASP
1	D	1731	THR
1	D	1739	LEU
1	D	1814	THR
1	D	1840	LEU
1	D	1850	SER
1	D	2072	SER
1	D	2089	ARG
1	D	2106	THR
1	D	2136	GLU
1	D	2201	TYR
1	D	2219	TYR
1	D	2225	SER
1	D	2236	SER
1	D	2292	VAL
1	D	2302	ARG
1	D	2321	ARG
1	D	2343	LEU
1	D	2351	LYS
1	D	2430	ASP
1	D	2484	LEU
1	D	2486	LEU
1	D	2494	ASP
1	D	2506	LEU
1	D	2714	GLU
1	D	2722	LYS

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Mol	Chain	Res	Type
1	D	2751	LYS
1	D	2762	LEU
1	D	2763	SER
1	D	2771	ARG
1	D	2781	MET
1	D	2837	HIS
1	D	2859	LEU
1	D	2875	THR
1	D	2877	THR
1	D	2884	ASP
1	D	2902	VAL
1	D	2903	SER
1	D	3616	VAL
1	D	3818	MET
1	D	3822	GLU
1	D	3852	ASP
1	D	3861	THR
1	D	3865	THR
1	D	3990	VAL
1	D	4034	TYR
1	D	4039	LYS
1	D	4049	LYS
1	D	4073	GLU
1	D	4083	VAL
1	D	4157	THR
1	D	4181	GLU
1	D	4187	LEU
1	D	4509	PHE
1	D	4556	VAL
1	D	4623	ASP
1	D	4632	LEU
1	D	4636	THR
1	D	4658	GLU
1	D	4668	LEU
1	D	4728	SER
1	D	4760	THR
1	D	4767	VAL
1	D	4782	VAL
1	D	4799	ASP
1	D	4900	VAL
1	D	4945	GLU
1	D	4955	ASP

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Mol	Chain	Res	Type
2	J	101	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	202	HIS
1	A	293	GLN
1	A	544	ASN
1	A	550	GLN
1	A	593	HIS
1	A	629	GLN
1	A	658	ASN
1	A	669	GLN
1	A	808	HIS
1	A	888	ASN
1	A	934	GLN
1	A	971	GLN
1	A	1046	ASN
1	A	1178	ASN
1	A	1233	GLN
1	A	1265	HIS
1	A	1371	ASN
1	A	1588	HIS
1	A	1616	GLN
1	A	1655	HIS
1	A	1685	GLN
1	A	1744	ASN
1	A	1944	ASN
1	A	2090	GLN
1	A	2150	ASN
1	A	2151	ASN
1	A	2274	GLN
1	A	2290	ASN
1	A	2317	ASN
1	A	2385	ASN
1	A	2480	GLN
1	A	2726	HIS
1	A	3952	HIS
1	A	3954	GLN
1	A	3974	GLN
1	A	4008	ASN

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Mol	Chain	Res	Type
1	A	4200	GLN
1	A	4491	ASN
1	A	4496	ASN
1	A	4619	GLN
2	G	26	HIS
2	G	32	GLN
2	G	88	HIS
1	B	123	HIS
1	B	202	HIS
1	B	293	GLN
1	B	544	ASN
1	B	550	GLN
1	B	593	HIS
1	B	629	GLN
1	B	658	ASN
1	B	669	GLN
1	B	808	HIS
1	B	888	ASN
1	B	934	GLN
1	B	971	GLN
1	B	1046	ASN
1	B	1178	ASN
1	B	1233	GLN
1	B	1265	HIS
1	B	1371	ASN
1	B	1588	HIS
1	B	1616	GLN
1	B	1655	HIS
1	B	1685	GLN
1	B	1744	ASN
1	B	1944	ASN
1	B	2090	GLN
1	B	2150	ASN
1	B	2151	ASN
1	B	2274	GLN
1	B	2290	ASN
1	B	2317	ASN
1	B	2385	ASN
1	B	2480	GLN
1	B	2726	HIS
1	B	3952	HIS
1	B	3954	GLN

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Mol	Chain	Res	Type
1	B	3974	GLN
1	B	4008	ASN
1	B	4200	GLN
1	B	4491	ASN
1	B	4496	ASN
1	B	4619	GLN
2	H	26	HIS
2	H	32	GLN
2	H	88	HIS
1	C	123	HIS
1	C	202	HIS
1	C	293	GLN
1	C	544	ASN
1	C	550	GLN
1	C	593	HIS
1	C	629	GLN
1	C	658	ASN
1	C	669	GLN
1	C	808	HIS
1	C	888	ASN
1	C	934	GLN
1	C	971	GLN
1	C	1046	ASN
1	C	1178	ASN
1	C	1233	GLN
1	C	1265	HIS
1	C	1371	ASN
1	C	1588	HIS
1	C	1616	GLN
1	C	1655	HIS
1	C	1685	GLN
1	C	1744	ASN
1	C	1944	ASN
1	C	2090	GLN
1	C	2150	ASN
1	C	2151	ASN
1	C	2274	GLN
1	C	2290	ASN
1	C	2317	ASN
1	C	2385	ASN
1	C	2480	GLN
1	C	2726	HIS

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Mol	Chain	Res	Type
1	C	3952	HIS
1	C	3954	GLN
1	C	3974	GLN
1	C	4008	ASN
1	C	4200	GLN
1	C	4491	ASN
1	C	4496	ASN
1	C	4619	GLN
1	C	4786	ASN
2	I	26	HIS
2	I	32	GLN
2	I	88	HIS
1	D	123	HIS
1	D	202	HIS
1	D	293	GLN
1	D	544	ASN
1	D	550	GLN
1	D	593	HIS
1	D	629	GLN
1	D	658	ASN
1	D	669	GLN
1	D	808	HIS
1	D	888	ASN
1	D	934	GLN
1	D	971	GLN
1	D	1046	ASN
1	D	1178	ASN
1	D	1233	GLN
1	D	1265	HIS
1	D	1371	ASN
1	D	1588	HIS
1	D	1616	GLN
1	D	1655	HIS
1	D	1685	GLN
1	D	1744	ASN
1	D	1944	ASN
1	D	2090	GLN
1	D	2150	ASN
1	D	2151	ASN
1	D	2274	GLN
1	D	2290	ASN
1	D	2317	ASN

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Mol	Chain	Res	Type
1	D	2385	ASN
1	D	2480	GLN
1	D	2726	HIS
1	D	3952	HIS
1	D	3954	GLN
1	D	3974	GLN
1	D	4008	ASN
1	D	4200	GLN
1	D	4491	ASN
1	D	4496	ASN
1	D	4619	GLN
2	J	26	HIS
2	J	32	GLN
2	J	88	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

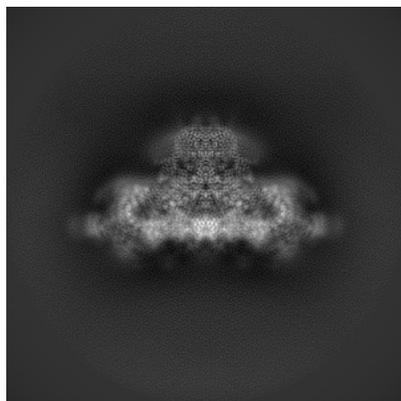
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33936. These allow visual inspection of the internal detail of the map and identification of artifacts.

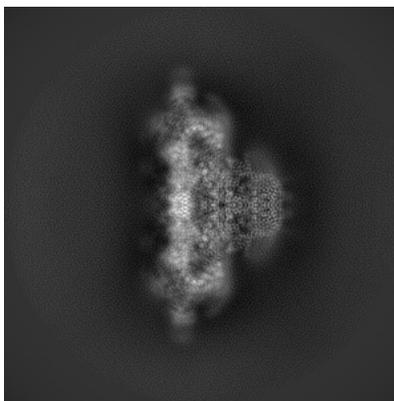
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

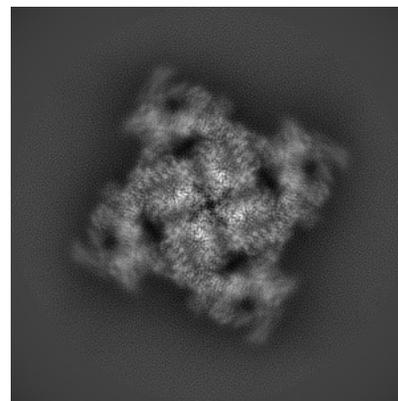
6.1.1 Primary map



X

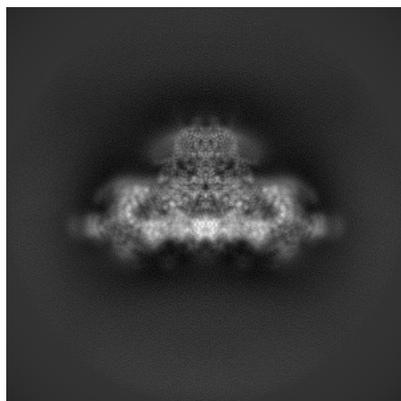


Y

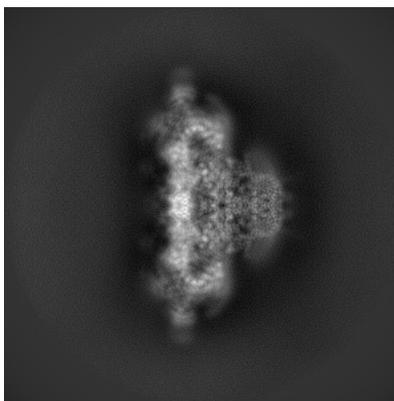


Z

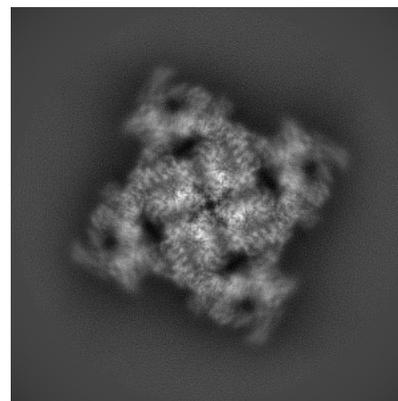
6.1.2 Raw map



X



Y

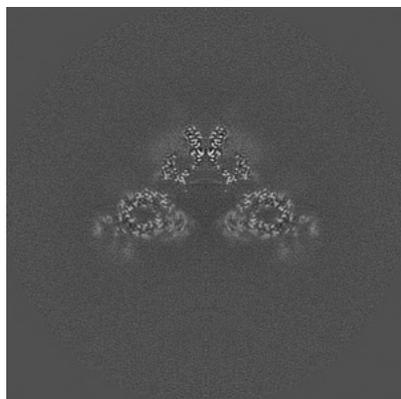


Z

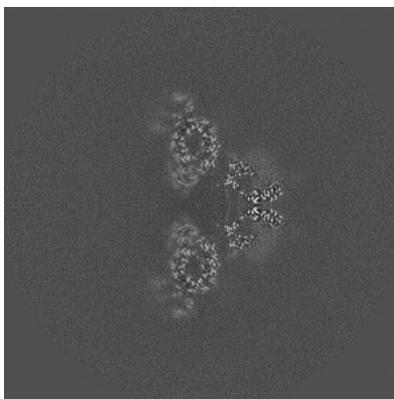
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

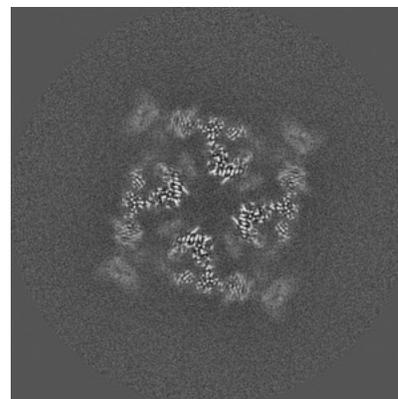
6.2.1 Primary map



X Index: 200

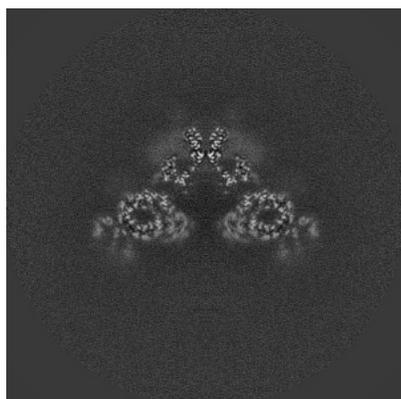


Y Index: 200

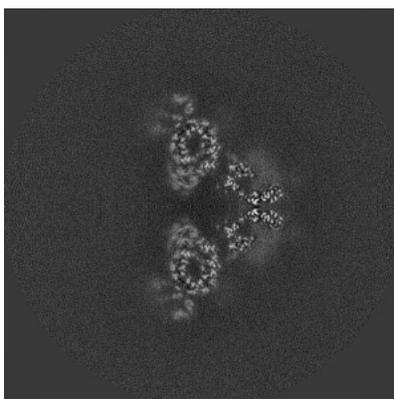


Z Index: 200

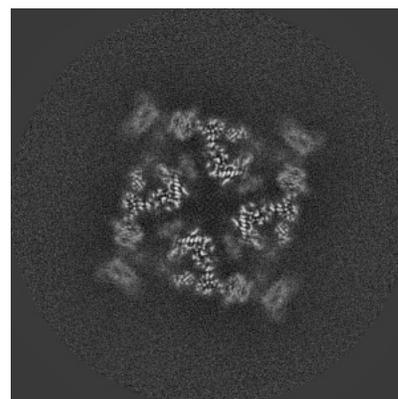
6.2.2 Raw map



X Index: 200



Y Index: 200

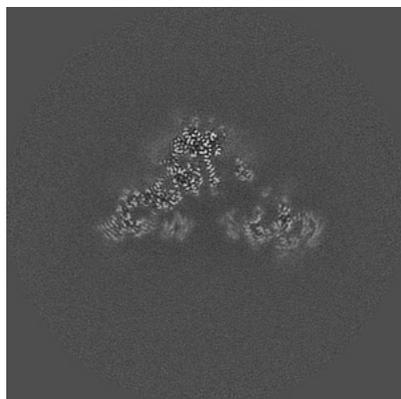


Z Index: 200

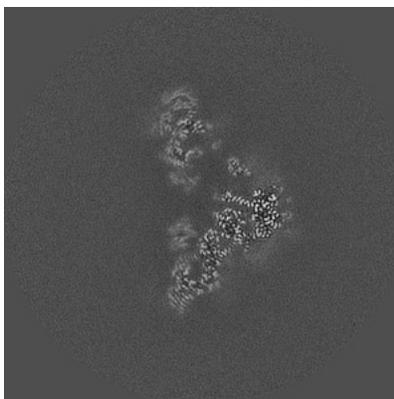
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

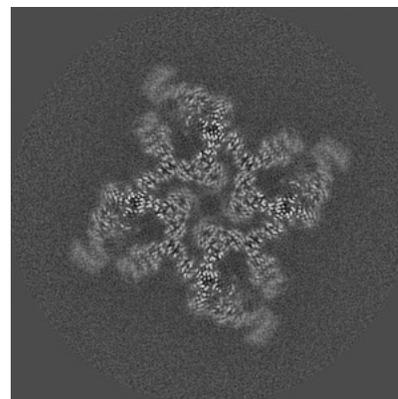
6.3.1 Primary map



X Index: 193

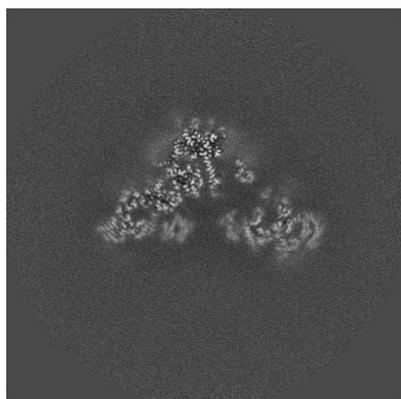


Y Index: 207

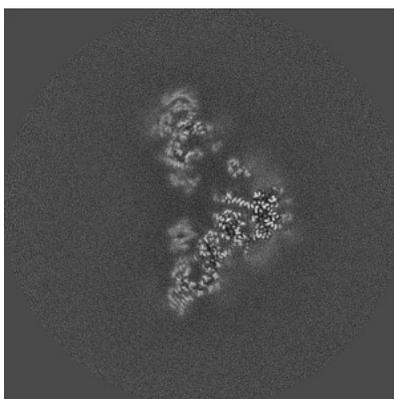


Z Index: 180

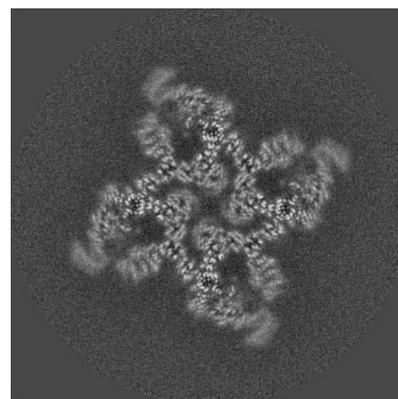
6.3.2 Raw map



X Index: 193



Y Index: 207

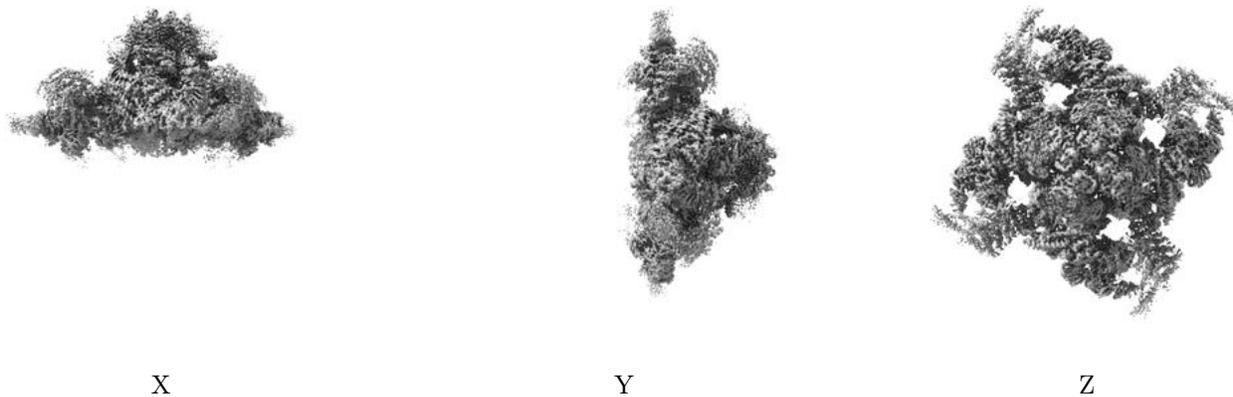


Z Index: 180

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

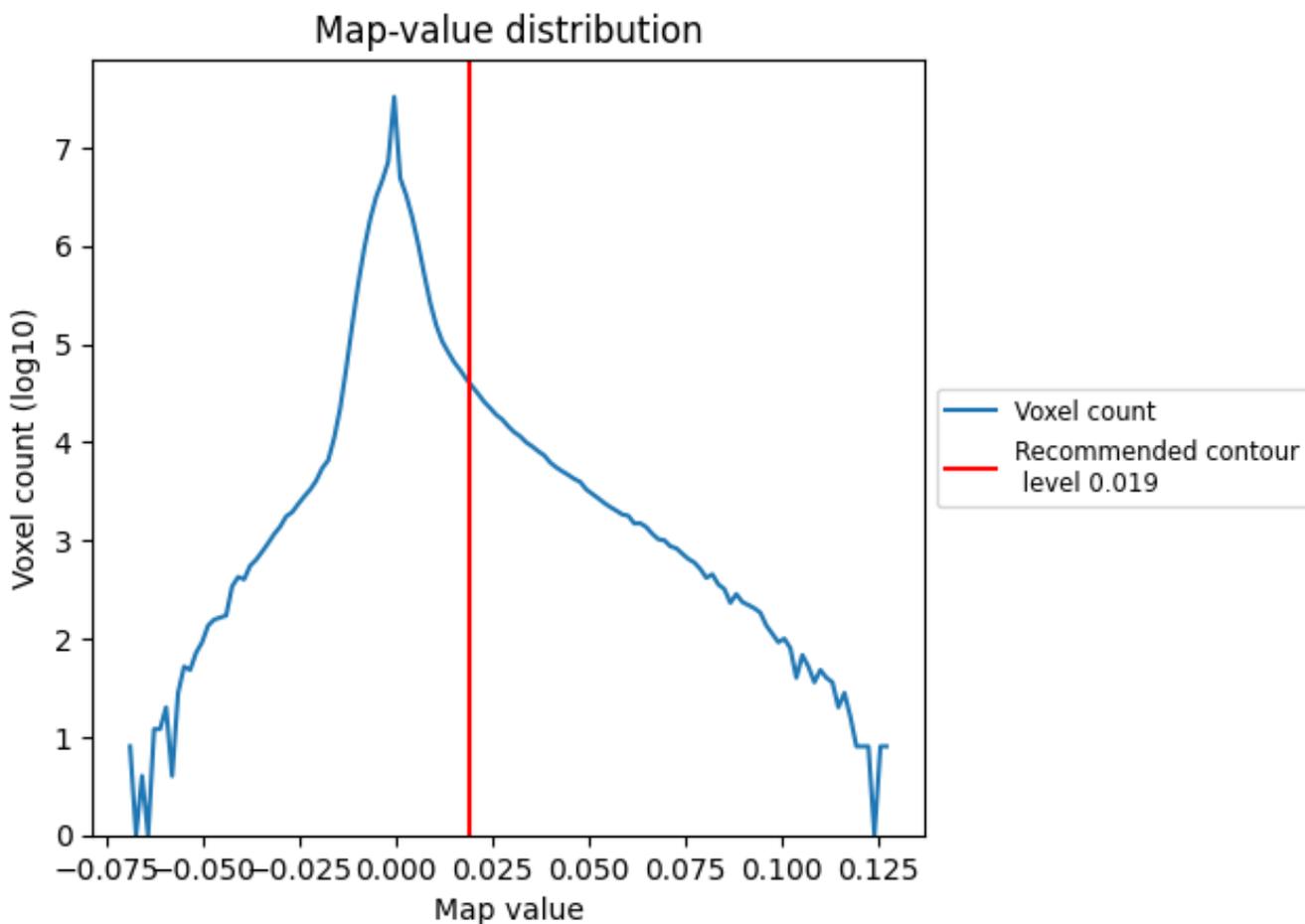
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

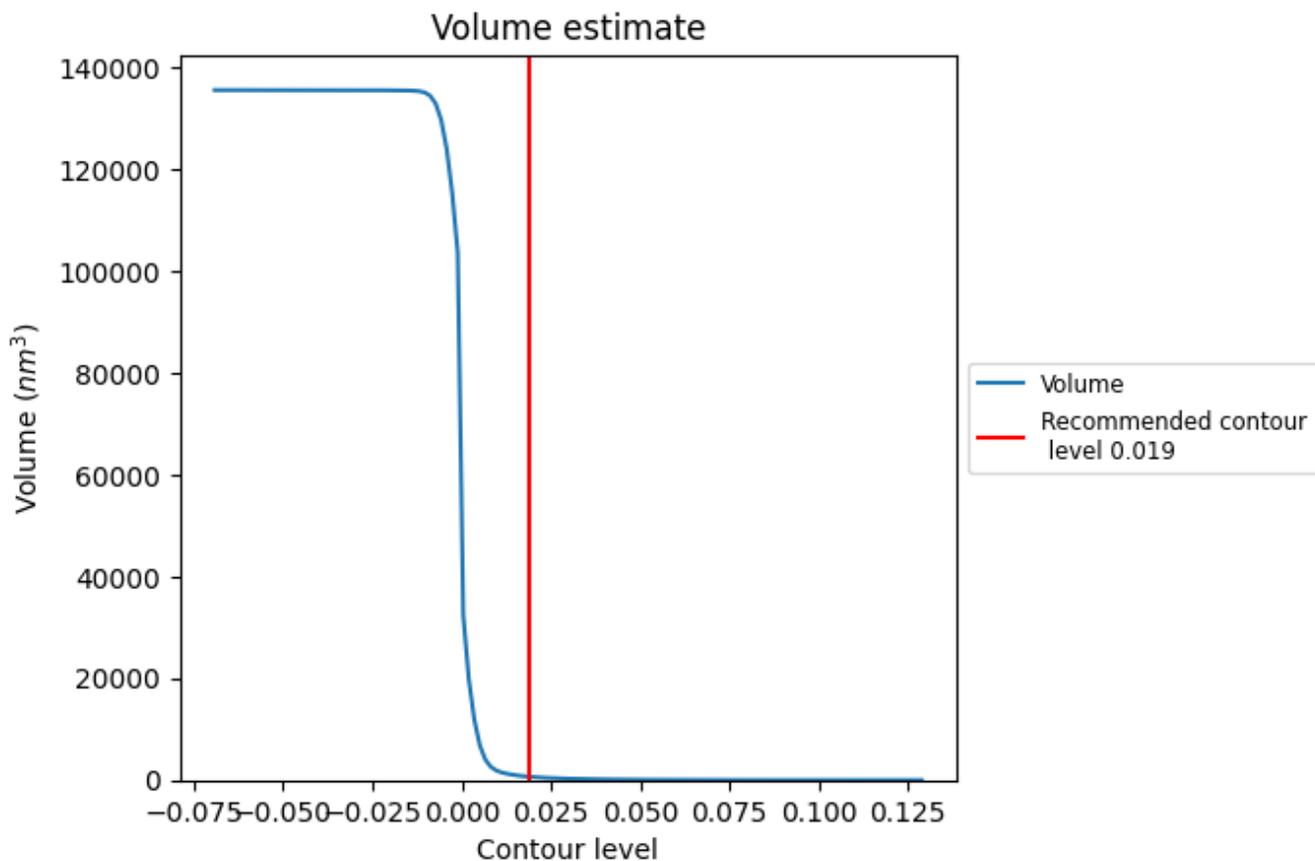
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

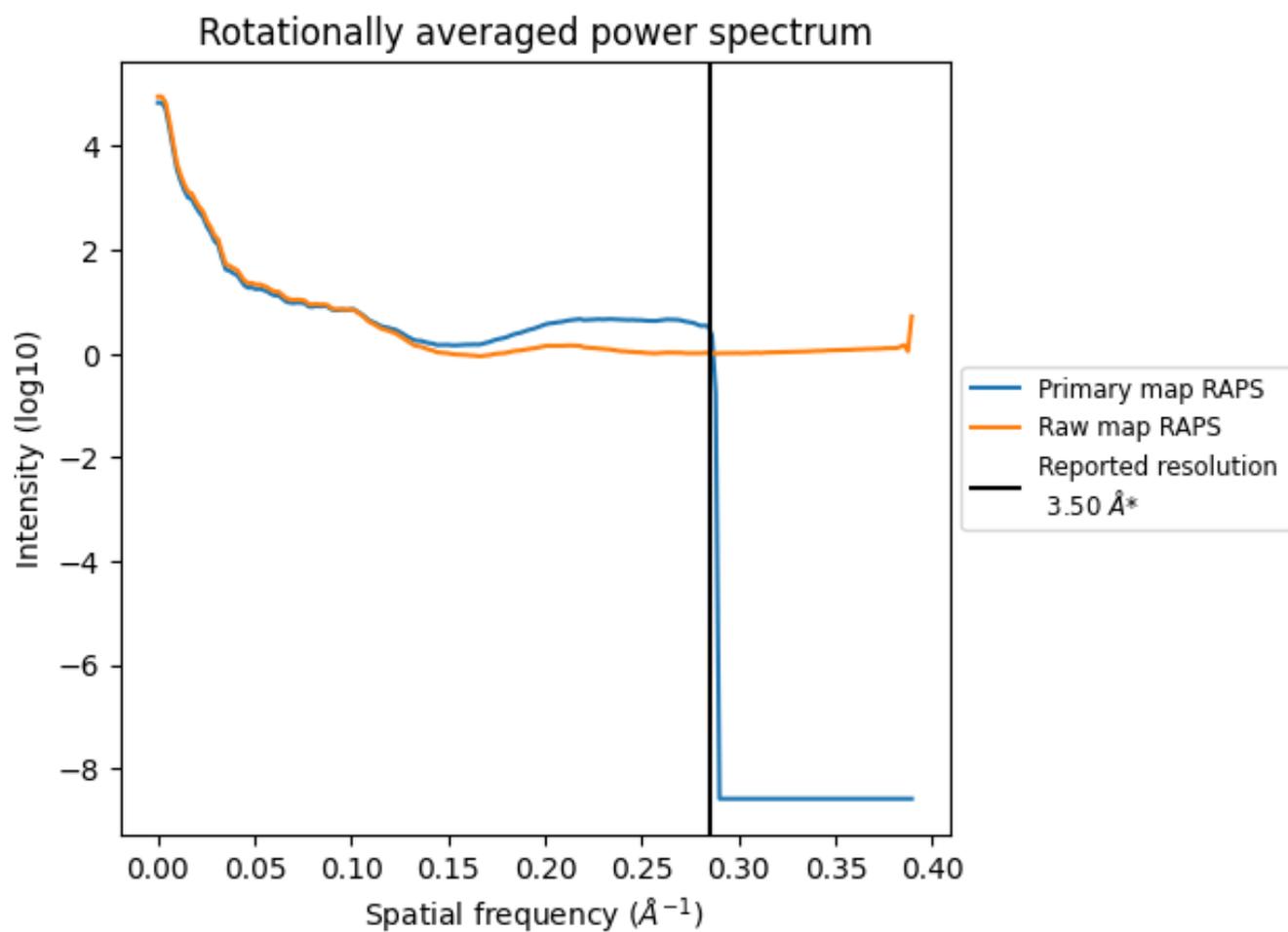
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 653 nm^3 ; this corresponds to an approximate mass of 590 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

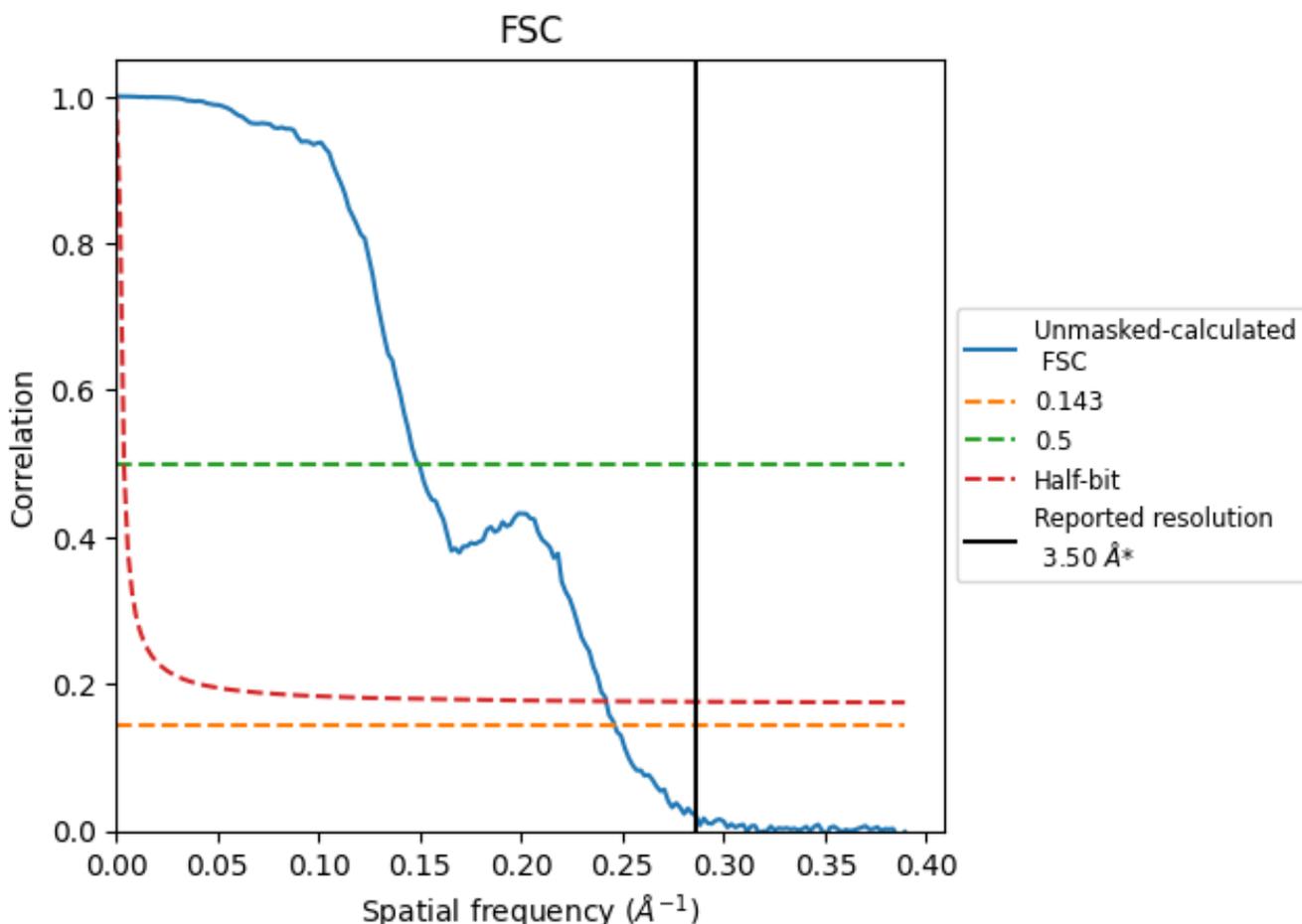


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

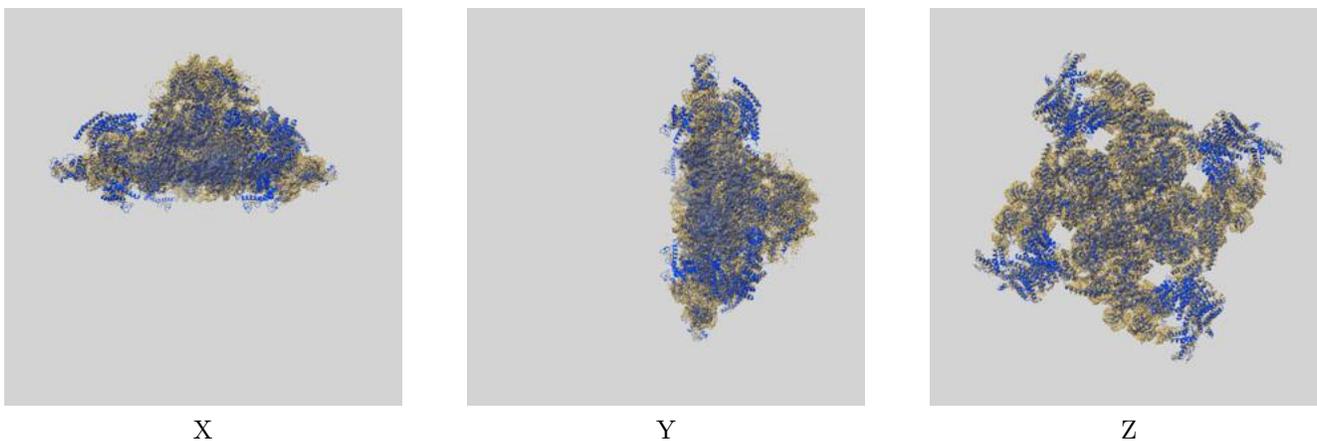
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	6.71	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

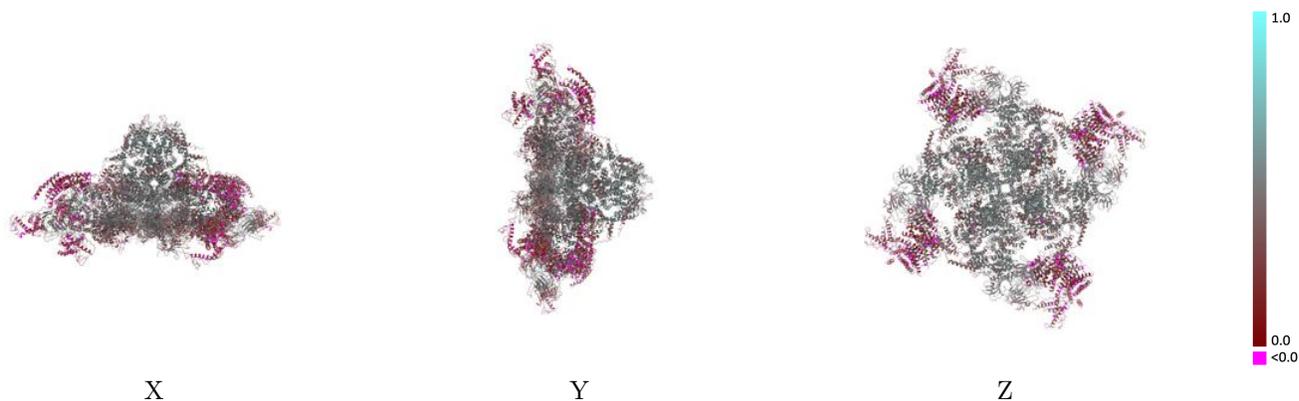
This section contains information regarding the fit between EMDB map EMD-33936 and PDB model 7VMM. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



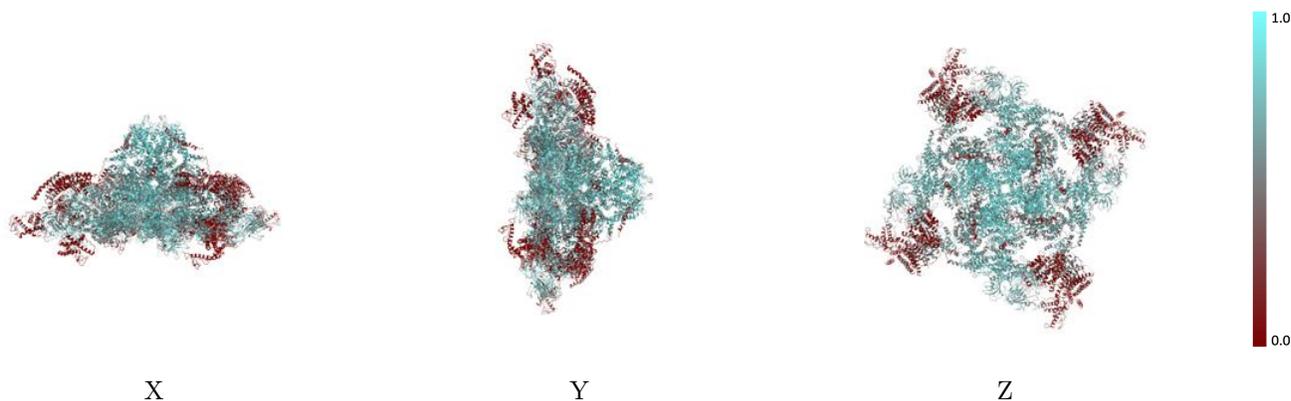
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



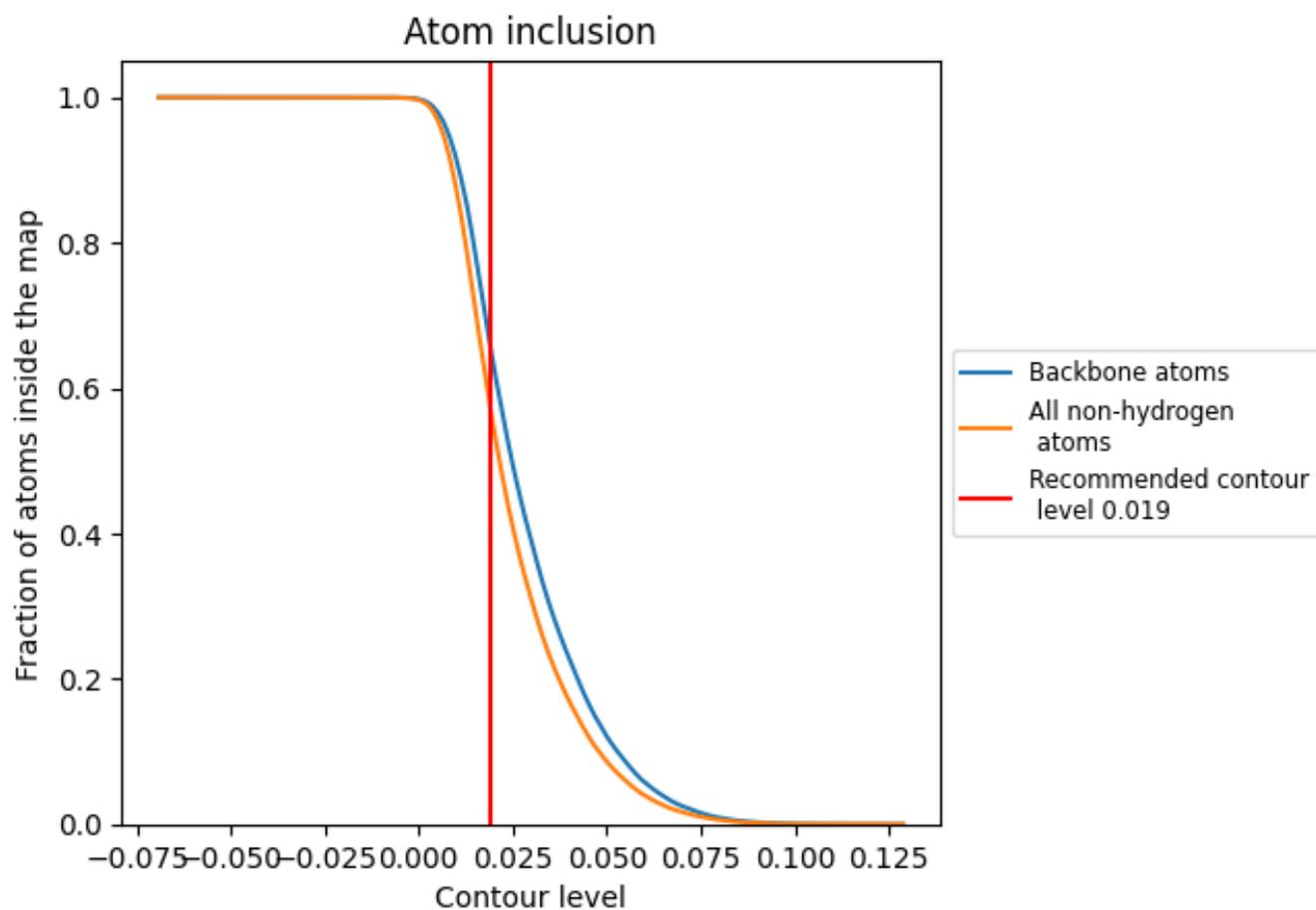
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5732	 0.3810
A	 0.5696	 0.3790
B	 0.5715	 0.3820
C	 0.5706	 0.3780
D	 0.5686	 0.3760
G	 0.6853	 0.4520
H	 0.6914	 0.4520
I	 0.6815	 0.4520
J	 0.6877	 0.4520

