



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:32 AM UTC

PDB ID : 7VMO / pdb_00007vmo
EMDB ID : EMD-33938
Title : Structure of recombinant RyR2 (Ca²⁺ dataset, class 1, open 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:

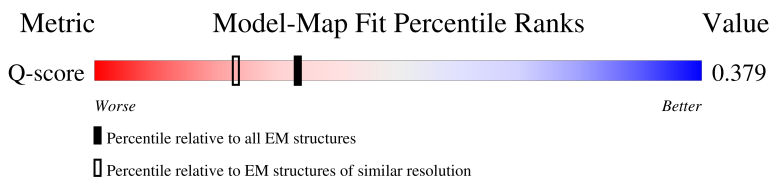
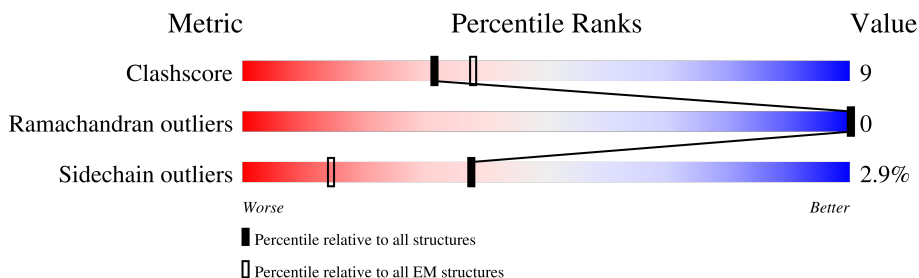
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.



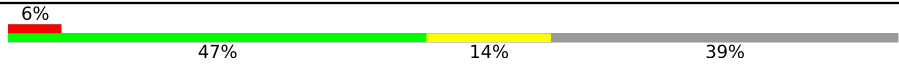
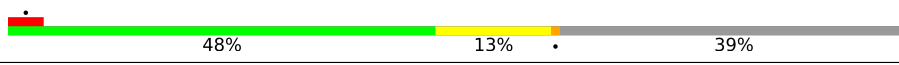
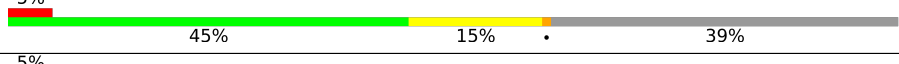
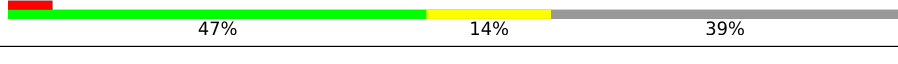
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13836 (2.95 - 3.95)

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	<p>26% (red), 64% (green), 16% (yellow), 20% (grey)</p>
1	B	4966	<p>26% (red), 64% (green), 15% (yellow), 20% (grey)</p>
1	C	4966	<p>26% (red), 64% (green), 16% (yellow), 20% (grey)</p>
1	D	4966	<p>26% (red), 64% (green), 15% (yellow), 20% (grey)</p>

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 122036 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	3991	29688	18782	5180	5553	173	0	0
1	B	3991	29688	18782	5180	5553	173	0	0
1	C	3991	29688	18782	5180	5553	173	0	0
1	D	3991	29688	18782	5180	5553	173	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
J	-15	HIS	-	expression tag	UNP P68106
J	-14	HIS	-	expression tag	UNP P68106

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

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

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

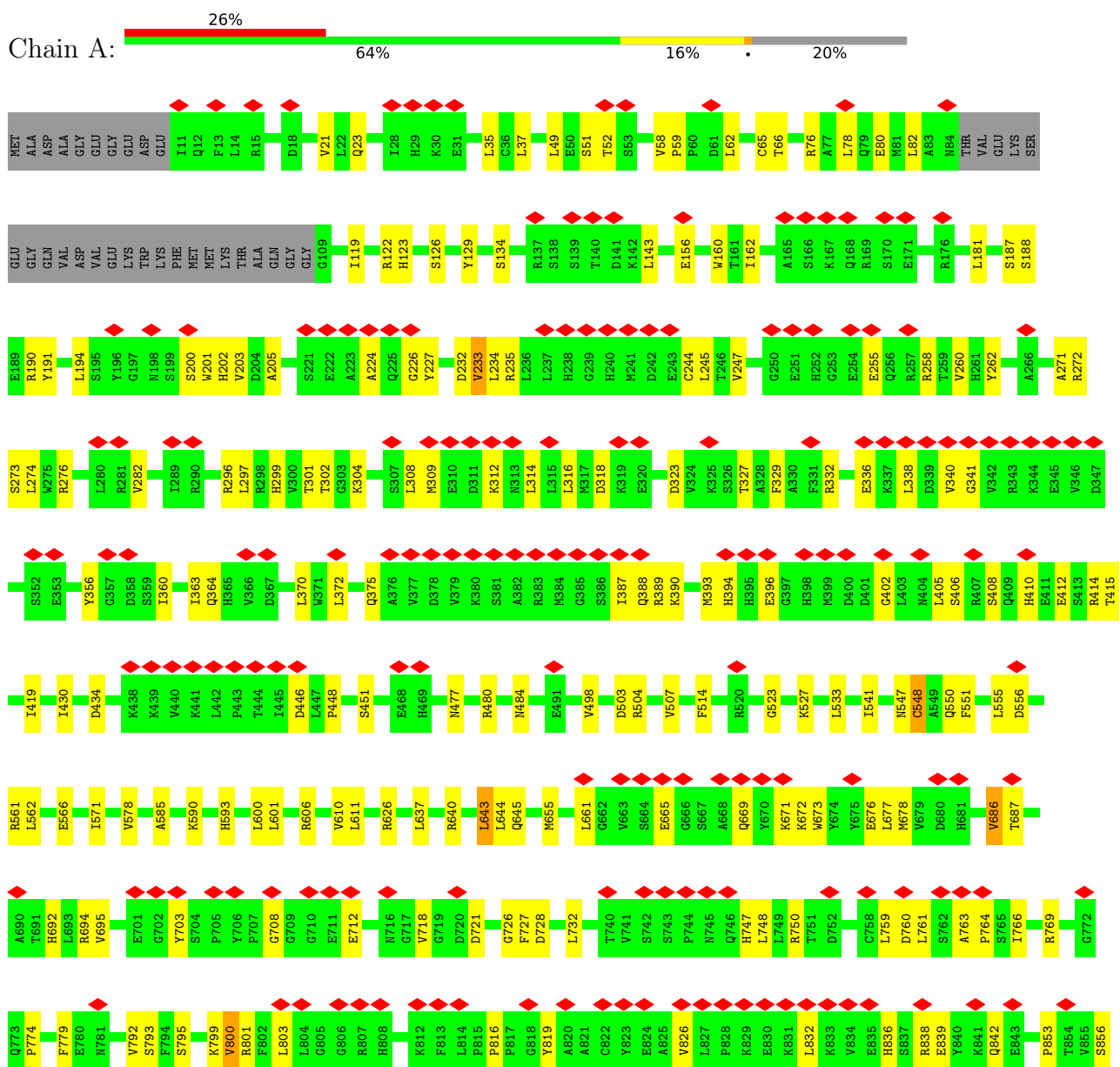
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

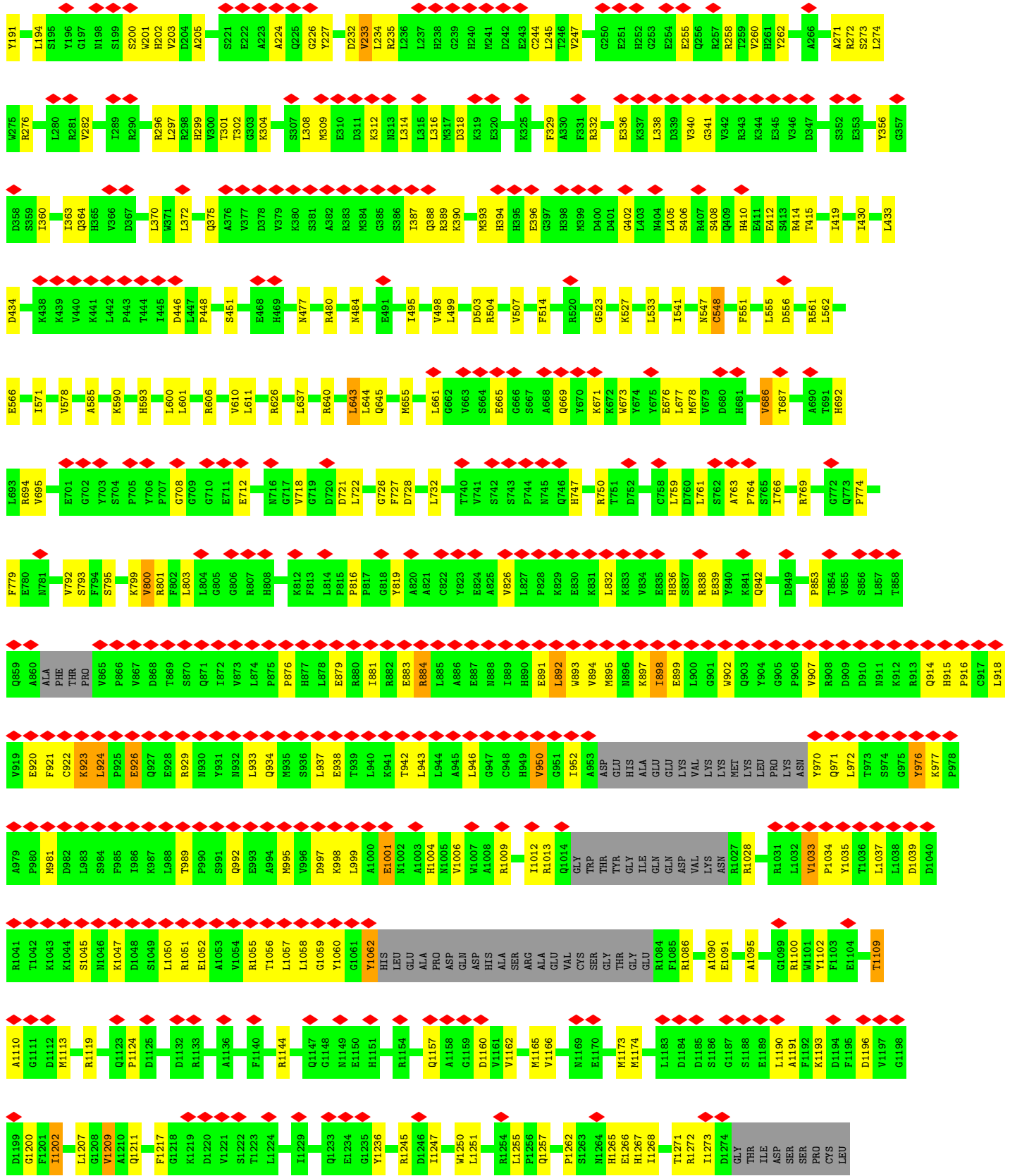
3 Residue-property plots

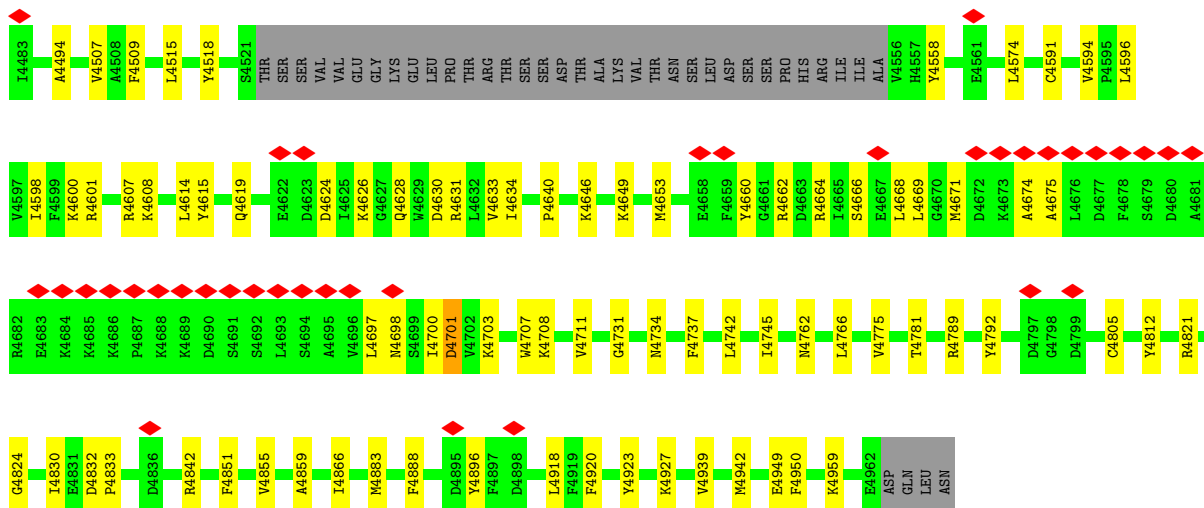
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 2

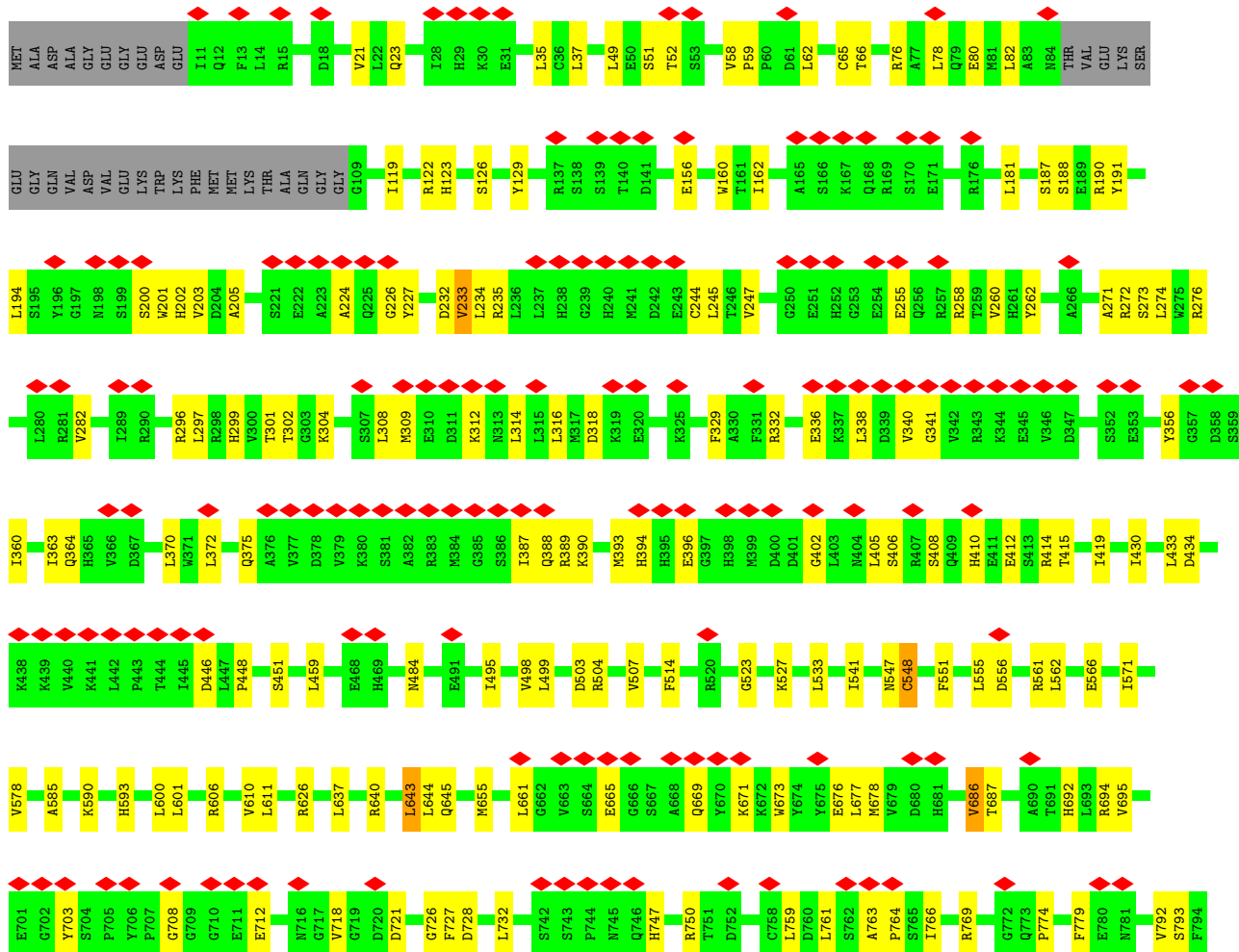


ALA	L1983	SER	R2162	V2318	E2404	A2505	X2613	UNK	K2735	K2855	SER	X2929
LYS	F1984	ARG	A2163	V2319	M2405	A2506	X2614	UNK	L2736	K2856	MET	X2930
GLY	C1985	LYS	L2164	R2320	H2406	S2507	X2615	UNK	A2737	L2857	ALA	X2931
LYS	P1986	CYS	M2171	R2321	H2409	X2508	X2616	UNK	M2738	E2858	LEU	X2919
ARG	C1987	SER	M2175	R2325	H2425	X2509	X2617	UNK	G2739	L2859	ASN	X2921
PRO	P1988	L2057	V2175	R2326	L2428	X2522	X2618	UNK	W2740	E2860	ARG	X2922
LYS	E1989	Q2058	G2179	F2330	L2428	X2523	X2619	UNK	I2741	S2861	THR	X2923
GLU	G1891	D1992	G2180	F2330	G2429	X2524	X2620	UNK	Y2742	K2862	ARG	X2924
L1892	L1892	S2062	G2181	A2333	D2430	X2525	X2621	UNK	G2743	G2863	ARG	X2924
L1893	L1893	E2063	E2182	R2335	L2431	X2526	X2622	UNK	E2744	G2864	ILE	X2925
K1896	L1986	M2065	S2183	R2335	V2432	X2527	X2623	UNK	G2745	G2865	SER	X2926
R1918	E2000	V2066	K2184	G2336	I2434	X2528	X2624	UNK	I2745	G2866	GLN	X2926
A1926	M2003	E2075	E2185	E2337	V2435	X2529	X2625	UNK	Y2746	M2866	THR	X2929
F1927	M2003	D2076	R2197	E2340	S2436	X2530	X2626	UNK	S2747	H2867	SER	X2930
S1928	L2008	D2076	I2205	G2341	I2437	X2531	X2627	UNK	D2748	P2868	GLN	X2930
D1929	E2009	L2079	S2206	G2341	A2438	X2532	X2628	UNK	S2749	L2869	VAL	X2931
V1932	ASP	V2080	R2207	L2342	M2441	X2533	X2629	UNK	S2750	L2870	SER	X2932
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Q1948	ASP	L2086	H2216	A2345	ILE	X2543	X2632	UNK	P2754	Q2753	HIS	X2935
A1949	GLY	L2087	H2217	K2351	ALA	X2544	X2633	UNK	L2755	P2754	GLY	X2936
L1950	GLY	Y2091	L2220	L2352	LYS	X2545	X2634	UNK	L2756	L2755	THR	X2937
M1951	SER	D2092	L2228	A2353	VAL	X2546	X2635	UNK	M2756	L2756	SER	X2938
M1952	ASN	G2095	L2228	E2354	VAL	X2547	X2636	UNK	LYS	PRO	PRO	X2939
S1953	ASP	C2095	P2231	E2355	E2452	X2548	X2637	UNK	TYR	ALA	ALA	X2940
A1954	LEU	V2098	R2231	D2355	P2453	X2549	X2638	UNK	L2761	L2761	HIS	X2941
A1955	THR	V2098	R2231	S2357	P2453	X2550	X2639	UNK	L2762	L2762	GLY	X2942
L1956	THR	R2099	G2234	R2358	D2454	X2551	X2640	UNK	S2763	S2763	THR	X2942
T1957	ARG	A2100	R2234	R2358	M2455	X2552	X2641	UNK	K2765	K2765	LEU	X2942
A1958	GLY	L2101	G2235	S2357	H2463	X2553	X2642	UNK	E2766	E2766	SER	X2942
F1964	LEU	P2102	S2236	R2358	M2467	X2554	X2643	UNK	K2767	K2767	ARG	X2942
S1966	LEU	K2103	T2237	P2358	L2471	X2555	X2644	UNK	E2768	E2768	ARG	X2942
F1967	LEU	T2104	P2238	P2358	L2475	X2556	X2645	UNK	I2769	I2769	ARG	X2942
P1968	LEU	T2104	V2241	S2357	Y2475	X2557	X2646	UNK	Y2770	Y2770	ARG	X2942
G1972	LEU	T2107	P2259	R2358	E2478	X2558	X2647	UNK	R2771	R2771	ARG	X2942
M1973	LEU	L2118	V2259	SER	V2479	X2559	X2648	UNK	W2772	W2772	ARG	X2942
M1975	LEU	L2119	V2265	LYS	V2479	X2560	X2649	UNK	P2773	P2773	ARG	X2942
L1976	LEU	L2119	C2271	THR	Q2480	X2561	X2650	UNK	I2774	I2774	ARG	X2942
L1977	LEU	L2128	C2276	ASP	D2481	X2562	X2651	UNK	K2775	K2775	ARG	X2942
M1977	LEU	V2131	C2276	GLU	F2482	X2563	X2652	UNK	E2776	E2776	ARG	X2942
F1978	LEU	L2145	L2279	GLU	L2486	X2564	X2653	UNK	S2777	S2777	ARG	X2942
K1979	LEU	L2148	Y2284	GLU	V2489	X2565	X2654	UNK	L2778	L2778	ARG	X2942
D1980	LEU	T2148	P2285	ASP	D2494	X2566	X2655	UNK	K2779	K2779	ARG	X2942
D1981	LEU	F2154	D2286	ASP	L2495	X2567	X2656	UNK	T2780	T2780	ARG	X2942
K1982	LEU	M2159	R2296	ASP	L2495	X2568	X2657	UNK	M2781	M2781	ARG	X2942
						X2569	X2658	UNK	L2782	L2782	ARG	X2942
						X2590	X2659	UNK	A2783	A2783	ARG	X2942
						X2591	X2660	UNK	W2784	W2784	ARG	X2942
						X2592	X2661	UNK	S2785	S2785	ARG	X2942
						X2593	X2662	UNK	TRP	TRP	ARG	X2942
						X2594	X2663	UNK	ILE	ILE	ARG	X2942
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						X2597	X2666	UNK	GLY	GLY	ARG	X2942
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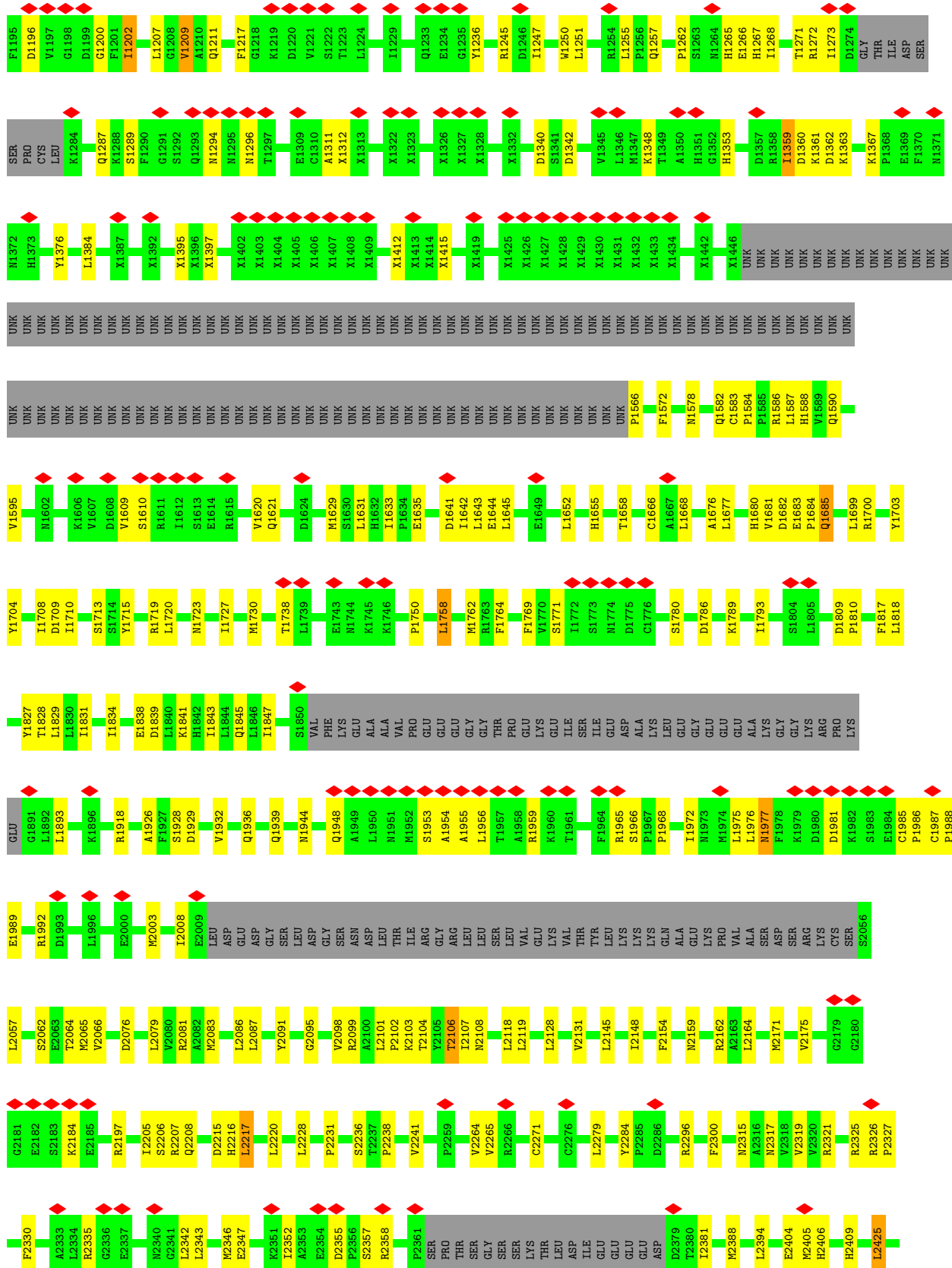


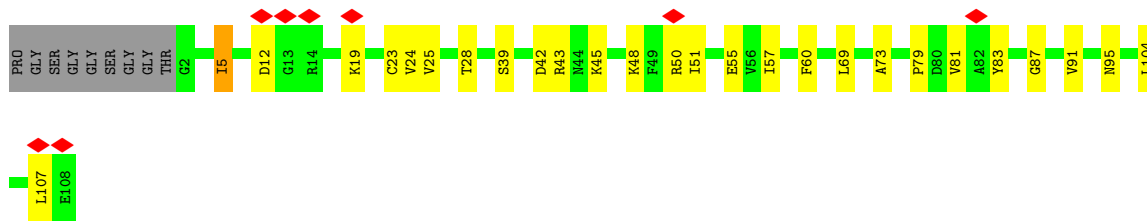


• Molecule 1: Ryanodine receptor 2

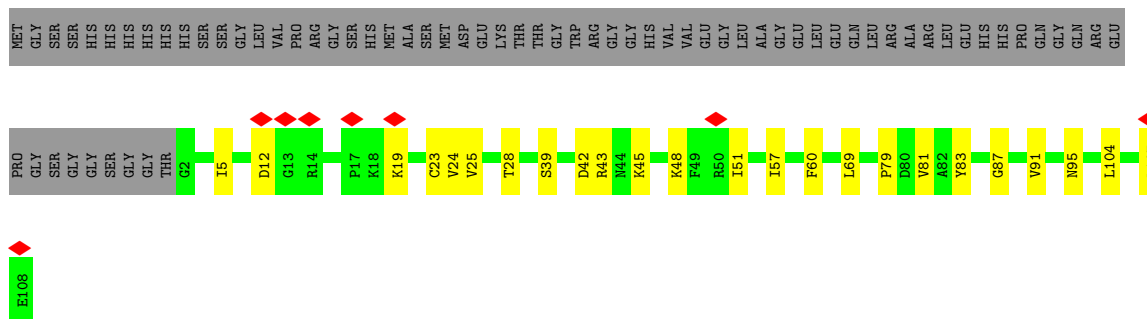


S795	P866	E926	T986	D1048	Q1123	L1207	K1288	X1392	UNK	UNK	V1609	S1713	P1750
K799	V867	Q927	K987	S1049	P1124	G1208	S1289	X1395	UNK	UNK	S1610	S1714	P1758
V800	V868	E928	L988	L1050	D1125	V1209	G1291	X1396	UNK	UNK	R1611	S1715	L1758
R801	D868	R929	T989	R1051	D1132	A1210	S1292	X1397	UNK	UNK	I1612	R1719	M1762
F802	T969	R930	P990	A1052	R1133	Q1211	Q1293	X1402	UNK	UNK	S1613	L1720	R1763
L803	S870	Y931	S991	V1054	D1136	E1247	M1294	X1403	UNK	UNK	E1614	M1723	F1764
L804	Q871	N930	Q992	R1055	R1138	G1218	M1296	X1404	UNK	UNK	V1620	I1727	F1769
G805	I872	N932	E993	R1056	D1137	K1219	T1297	X1405	UNK	UNK	Q1621	M1730	V1770
G806	V873	L933	F993	L1057	G1138	D1220	A1311	X1406	UNK	UNK	D1624	M1738	S1771
R807	L874	Q934	A994	L1057	G1139	V1221	X1312	X1407	UNK	UNK	M1629	L1739	I1772
H808	P875	M935	M995	L1058	F1140	S1222	X1313	X1408	UNK	UNK	L1630	E1743	S1773
	P876	S936	V996	G1059	R1144	L1224	X1313	X1409	UNK	UNK	H1631	M1744	M1774
	H877	L937	D987	Y1060	R1144	I1229	X1322	X1412	UNK	UNK	H1632	K1745	D1775
	F813	E938	K998	Y1061	Q1147	I1233	X1323	X1413	UNK	UNK	L1633	K1746	C1776
	L814	L940	A1000	HIS	G1148	E1234	X1326	X1414	UNK	UNK	E1641	P1750	S1780
	P816	L943	E1001	LEU	M1149	G1235	X1327	X1415	UNK	UNK	L1643	L1758	D1786
	P817	T942	M1002	GLU	E1150	Y1236	X1328	X1419	UNK	UNK	E1644	M1762	K1789
	G818	L943	A1003	ALA	H1151	Y1236	X1328	X1419	UNK	UNK	L1645	R1763	T1792
	Y819	L944	H1004	PRD	H1151	Y1236	X1328	X1419	UNK	UNK	E1649	F1764	I1793
	A820	L944	H1005	ASP	R1154	A1240	X1332	X1425	UNK	UNK	L1652	P1769	S1804
	A821	A945	V1006	GLN	R1157	R1245	X1332	X1426	UNK	UNK	H1655	V1769	L1805
	C822	L946	W1007	ASP	Q1157	I1246	D1340	X1427	UNK	UNK	L1658	I1770	D1809
	Y823	G947	A1008	HIS	A1158	I1247	S1341	X1428	UNK	UNK	H1663	S1771	P1810
	E824	C948	R1009	ALA	G1159	I1247	D1342	X1428	UNK	UNK	C1666	I1772	F1817
	A825	R949	R1009	SER	G1160	W1250	V1345	X1429	UNK	UNK	A1687	S1773	L1818
	V826	V950	I1012	ARG	L1251	L1251	M1346	X1430	UNK	UNK	L1668	I1774	Y1804
	L827	G951	R1013	ALA	V1162	R1254	L1347	X1431	UNK	UNK	L1676	D1775	I1805
	P828	L952	R1014	VAL	V1166	L1255	M1348	X1432	UNK	UNK	L1677	C1776	L1805
	E830	A953	GLY	SER	M1165	P1256	T1349	X1432	UNK	UNK	A1676	C1666	D1809
	K831	W893	TRP	THR	V1166	Q1257	H1351	X1433	UNK	UNK	L1677	C1666	P1810
	L832	V894	THR	GLY	M1169	Q1257	G1352	X1433	UNK	UNK	H1680	T1792	F1817
	K833	M895	TYR	GLY	E1170	P1262	H1352	X1434	UNK	UNK	D1682	I1793	L1818
	V834	M896	ILE	GLY	M1173	S1263	H1353	X1442	UNK	UNK	E1683	S1804	Y1827
	E835	M896	GLN	GLU	M1174	N1264	H1353	X1446	UNK	UNK	P1684	L1805	L1828
	E836	M899	GLN	GLU	D1184	H1265	D1357	UNK	UNK	UNK	Q1685	D1809	L1829
	S837	M900	ASP	VAL	D1185	H1266	R1358	UNK	UNK	UNK	L1699	P1810	
	R838	L900	VAL	VAL	D1185	I1268	I1359	UNK	UNK	UNK	R1700		
	E839	G901	LYS	LYS	D1185	I1268	K1360	UNK	UNK	UNK	Y1703		
	Y840	W902	LYS	ASN	D1185	D1271	K1361	UNK	UNK	UNK	Y1704		
	K841	Q903	LYS	ASN	D1185	D1271	D1362	UNK	UNK	UNK	I1708		
	Q842	Q904	LEU	MET	D1185	D1271	E1364	UNK	UNK	UNK	D1709		
	D849	G905	PRD	ASN	D1185	D1271	E1364	UNK	UNK	UNK	I1710		
	P853	V907	ASN	R1027	D1185	D1271	K1367	UNK	UNK	UNK			
	T854	R908	LYS	R1031	D1185	D1271	P1368	UNK	UNK	UNK			
	V855	L872	LYS	L1032	D1185	D1271	E1369	UNK	UNK	UNK			
	S856	T973	LYS	P1034	D1185	D1271	F1370	UNK	UNK	UNK			
	L857	T973	LYS	Y1035	D1185	D1271	SER	UNK	UNK	UNK			
	T858	S974	LYS	T1036	D1185	D1271	N1371	UNK	UNK	UNK			
	Q859	G975	LYS	L1037	D1185	D1271	M1372	UNK	UNK	UNK			
	A860	Y876	LYS	L1039	D1185	D1271	H1373	UNK	UNK	UNK			
	ALA	K977	LYS	D1040	D1185	D1271	Y1376	UNK	UNK	UNK			
	THR	P978	LYS	R1041	D1185	D1271	L1384	UNK	UNK	UNK			
	THR	A979	LYS	T1042	D1185	D1271	X1387	UNK	UNK	UNK			
	PRD	P980	LYS	K1043	D1185	D1271		UNK	UNK	UNK			
		M981	LYS	K1044	D1185	D1271		UNK	UNK	UNK			
		D982	LYS	S1045	D1185	D1271		UNK	UNK	UNK			
		L983	LYS	M1046	D1185	D1271		UNK	UNK	UNK			
		S984	LYS	K1047	D1185	D1271		UNK	UNK	UNK			
		F985	LYS		D1185	D1271		UNK	UNK	UNK			





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45432	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.110	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	421.25998, 421.25998, 421.25998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.239, 1.239, 1.239	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, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/26573	0.31	2/35881 (0.0%)
1	B	0.11	0/26573	0.31	2/35881 (0.0%)
1	C	0.11	0/26573	0.31	2/35881 (0.0%)
1	D	0.11	0/26573	0.31	2/35881 (0.0%)
2	G	0.12	0/835	0.36	0/1123
2	H	0.12	0/835	0.35	0/1123
2	I	0.12	0/835	0.36	0/1123
2	J	0.12	0/835	0.35	0/1123
All	All	0.11	0/109632	0.31	8/148016 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	923	LYS	CA-C-N	5.58	128.15	120.67
1	A	923	LYS	C-N-CA	5.58	128.15	120.67
1	D	923	LYS	CA-C-N	5.58	128.15	120.67
1	D	923	LYS	C-N-CA	5.58	128.15	120.67
1	B	923	LYS	CA-C-N	5.56	128.12	120.67
1	B	923	LYS	C-N-CA	5.56	128.12	120.67
1	C	923	LYS	CA-C-N	5.55	128.10	120.67
1	C	923	LYS	C-N-CA	5.55	128.10	120.67

There are no chirality outliers.

There are no planarity outliers.

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	29688	0	26383	497	0
1	B	29688	0	26383	496	0
1	C	29688	0	26383	503	0
1	D	29688	0	26383	491	0
2	G	819	0	821	14	0
2	H	819	0	821	16	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
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	122036	0	108816	2013	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 9.

All (2013) 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:1682:ASP:HB2	1:A:1685:GLN:HB3	1.60	0.82
1:C:1682:ASP:HB2	1:C:1685:GLN:HB3	1.60	0.82
1:B:1682:ASP:HB2	1:B:1685:GLN:HB3	1.60	0.82
1:D:1682:ASP:HB2	1:D:1685:GLN:HB3	1.60	0.81
1:D:4105:SER:HB2	1:D:4118:LEU:HD21	1.64	0.80
1:C:4105:SER:HB2	1:C:4118:LEU:HD21	1.64	0.80
1:A:4105:SER:HB2	1:A:4118:LEU:HD21	1.64	0.79
1:B:4105:SER:HB2	1:B:4118:LEU:HD21	1.64	0.78
1:C:1052:GLU:HA	1:C:1055:ARG:HD2	1.65	0.78
1:D:1052:GLU:HA	1:D:1055:ARG:HD2	1.65	0.77
1:B:1052:GLU:HA	1:B:1055:ARG:HD2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.67	0.76
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.67	0.76
1:A:2406:HIS:HA	1:A:2409:HIS:HB3	1.69	0.76
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.67	0.76
1:A:1052:GLU:HA	1:A:1055:ARG:HD2	1.65	0.75
1:B:2406:HIS:HA	1:B:2409:HIS:HB3	1.68	0.75
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.67	0.75
1:C:2406:HIS:HA	1:C:2409:HIS:HB3	1.69	0.75
1:D:2406:HIS:HA	1:D:2409:HIS:HB3	1.68	0.74
1:C:2342:LEU:HG	1:C:2434:VAL:HG21	1.71	0.72
1:B:2342:LEU:HG	1:B:2434:VAL:HG21	1.71	0.71
1:A:2342:LEU:HG	1:A:2434:VAL:HG21	1.71	0.71
1:A:1700:ARG:NH1	1:A:1817:PHE:O	2.24	0.71
1:D:2342:LEU:HG	1:D:2434:VAL:HG21	1.71	0.71
1:B:1700:ARG:NH1	1:B:1817:PHE:O	2.24	0.71
1:B:759:LEU:HD13	1:B:766:ILE:HG22	1.73	0.70
1:B:981:MET:HE1	1:B:1059:GLY:HA3	1.74	0.69
1:C:1700:ARG:NH1	1:C:1817:PHE:O	2.24	0.69
1:A:644:LEU:HD13	1:A:1631:LEU:HD21	1.75	0.69
1:D:1700:ARG:NH1	1:D:1817:PHE:O	2.24	0.69
1:A:981:MET:HE1	1:A:1059:GLY:HA3	1.74	0.69
1:C:759:LEU:HD13	1:C:766:ILE:HG22	1.73	0.69
1:D:644:LEU:HD13	1:D:1631:LEU:HD21	1.75	0.69
1:C:992:GLN:HG3	1:C:1058:LEU:HD11	1.75	0.69
1:B:644:LEU:HD13	1:B:1631:LEU:HD21	1.74	0.68
1:D:759:LEU:HD13	1:D:766:ILE:HG22	1.73	0.68
1:D:981:MET:HE1	1:D:1059:GLY:HA3	1.75	0.68
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.76	0.68
1:D:156:GLU:HG2	1:D:187:SER:HB3	1.76	0.68
1:D:992:GLN:HG3	1:D:1058:LEU:HD11	1.75	0.68
1:A:759:LEU:HD13	1:A:766:ILE:HG22	1.73	0.68
1:B:992:GLN:HG3	1:B:1058:LEU:HD11	1.75	0.68
1:C:981:MET:HE1	1:C:1059:GLY:HA3	1.75	0.68
1:C:644:LEU:HD13	1:C:1631:LEU:HD21	1.74	0.68
1:A:1262:PRO:HG2	1:A:1265:HIS:HB2	1.75	0.67
1:A:1684:PRO:HD3	2:G:42:ASP:HB3	1.75	0.67
1:D:1262:PRO:HG2	1:D:1265:HIS:HB2	1.75	0.67
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.76	0.67
1:A:992:GLN:HG3	1:A:1058:LEU:HD11	1.75	0.67
1:A:1680:HIS:CE1	2:G:91:VAL:HG22	2.28	0.67
1:B:676:GLU:HB2	1:B:803:LEU:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1262:PRO:HG2	1:C:1265:HIS:HB2	1.75	0.67
1:A:156:GLU:HG2	1:A:187:SER:HB3	1.76	0.67
1:A:1255:LEU:HD21	1:A:1384:LEU:HD13	1.78	0.67
1:C:4824:GLY:O	1:D:4821:ARG:NH2	2.28	0.67
1:D:2735:LYS:HA	1:D:2740:TRP:HE3	1.60	0.66
1:C:2735:LYS:HA	1:C:2740:TRP:HE3	1.60	0.66
1:B:1262:PRO:HG2	1:B:1265:HIS:HB2	1.75	0.66
1:B:1266:GLU:O	1:B:1267:HIS:ND1	2.29	0.66
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.28	0.66
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.76	0.66
1:B:1255:LEU:HD21	1:B:1384:LEU:HD13	1.78	0.66
1:D:1266:GLU:O	1:D:1267:HIS:ND1	2.29	0.66
1:B:156:GLU:HG2	1:B:187:SER:HB3	1.76	0.66
1:B:2735:LYS:HA	1:B:2740:TRP:HE3	1.60	0.66
1:A:1266:GLU:O	1:A:1267:HIS:ND1	2.29	0.65
1:A:2735:LYS:HA	1:A:2740:TRP:HE3	1.60	0.65
1:B:943:LEU:HA	1:B:946:LEU:HD12	1.78	0.65
1:D:590:LYS:H	1:D:593:HIS:HD2	1.44	0.65
1:C:1255:LEU:HD21	1:C:1384:LEU:HD13	1.77	0.65
1:C:1266:GLU:O	1:C:1267:HIS:ND1	2.29	0.65
1:D:943:LEU:HA	1:D:946:LEU:HD12	1.78	0.65
1:A:943:LEU:HA	1:A:946:LEU:HD12	1.78	0.65
1:C:943:LEU:HA	1:C:946:LEU:HD12	1.78	0.65
1:C:1124:PRO:HD2	1:C:1595:VAL:HG23	1.78	0.65
2:I:24:VAL:HG22	2:I:48:LYS:HG2	1.78	0.65
1:B:1124:PRO:HD2	1:B:1595:VAL:HG23	1.78	0.65
1:A:590:LYS:H	1:A:593:HIS:HD2	1.44	0.65
1:C:156:GLU:HG2	1:C:187:SER:HB3	1.76	0.65
1:C:590:LYS:H	1:C:593:HIS:HD2	1.44	0.65
1:A:1102:TYR:HD1	1:A:1165:MET:HG2	1.62	0.65
1:D:1255:LEU:HD21	1:D:1384:LEU:HD13	1.78	0.65
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.78	0.64
1:D:1723:ASN:O	1:D:1918:ARG:NH2	2.31	0.64
1:A:1359:ILE:HG12	1:A:1363:LYS:HD2	1.79	0.64
1:C:1723:ASN:O	1:C:1918:ARG:NH2	2.31	0.64
1:B:62:LEU:HA	1:B:65:CYS:HB3	1.80	0.64
1:C:1359:ILE:HG12	1:C:1363:LYS:HD2	1.79	0.64
1:D:671:LYS:HA	1:D:761:LEU:HD12	1.79	0.64
1:D:1102:TYR:HD1	1:D:1165:MET:HG2	1.62	0.64
1:D:1124:PRO:HD2	1:D:1595:VAL:HG23	1.79	0.64
1:A:671:LYS:HA	1:A:761:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2171:MET:HE2	1:D:2216:HIS:HB3	1.80	0.64
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.78	0.64
1:C:62:LEU:HA	1:C:65:CYS:HB3	1.80	0.64
1:C:2850:ILE:O	1:C:2854:LYS:HG3	1.98	0.64
1:A:1124:PRO:HD2	1:A:1595:VAL:HG23	1.78	0.64
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.28	0.64
1:B:1001:GLU:OE2	1:B:1047:LYS:NZ	2.31	0.64
1:C:2171:MET:HE2	1:C:2216:HIS:HB3	1.80	0.64
1:A:1723:ASN:O	1:A:1918:ARG:NH2	2.31	0.64
1:B:671:LYS:HA	1:B:761:LEU:HD12	1.79	0.63
1:B:1102:TYR:HD1	1:B:1165:MET:HG2	1.62	0.63
1:B:2850:ILE:O	1:B:2854:LYS:HG3	1.98	0.63
2:J:24:VAL:HG22	2:J:48:LYS:HG2	1.78	0.63
1:A:62:LEU:HA	1:A:65:CYS:HB3	1.80	0.63
1:A:1001:GLU:OE2	1:A:1047:LYS:NZ	2.31	0.63
1:A:2850:ILE:O	1:A:2854:LYS:HG3	1.98	0.63
1:C:1001:GLU:OE2	1:C:1047:LYS:NZ	2.31	0.63
1:C:4111:ASP:O	1:C:4115:GLN:N	2.32	0.63
1:D:4111:ASP:O	1:D:4115:GLN:N	2.32	0.63
1:B:590:LYS:H	1:B:593:HIS:HD2	1.44	0.63
1:B:1359:ILE:HG12	1:B:1363:LYS:HD2	1.79	0.63
1:C:4018:MET:HB3	1:C:4065:LEU:HD21	1.80	0.63
1:D:62:LEU:HA	1:D:65:CYS:HB3	1.80	0.63
1:D:2850:ILE:O	1:D:2854:LYS:HG3	1.98	0.63
1:D:4018:MET:HB3	1:D:4065:LEU:HD21	1.80	0.63
1:C:671:LYS:HA	1:C:761:LEU:HD12	1.79	0.63
1:A:2171:MET:HE2	1:A:2216:HIS:HB3	1.80	0.63
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.28	0.63
1:C:548:CYS:HB3	1:C:578:VAL:HG23	1.81	0.63
1:B:1723:ASN:O	1:B:1918:ARG:NH2	2.31	0.63
1:C:1102:TYR:HD1	1:C:1165:MET:HG2	1.62	0.63
1:B:2171:MET:HE2	1:B:2216:HIS:HB3	1.80	0.63
1:A:548:CYS:HB3	1:A:578:VAL:HG23	1.81	0.62
1:B:4018:MET:HB3	1:B:4065:LEU:HD21	1.80	0.62
1:A:894:VAL:O	1:A:898:ILE:HG13	2.00	0.62
1:C:2107:ILE:HG13	1:C:2108:ASN:H	1.64	0.62
1:D:258:ARG:NH1	1:D:316:LEU:O	2.33	0.62
1:A:4111:ASP:O	1:A:4115:GLN:N	2.32	0.62
1:D:1001:GLU:OE2	1:D:1047:LYS:NZ	2.31	0.62
1:D:1359:ILE:HG12	1:D:1363:LYS:HD2	1.79	0.62
1:D:2107:ILE:HG13	1:D:2108:ASN:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:548:CYS:HB3	1:D:578:VAL:HG23	1.81	0.62
1:D:415:THR:O	1:D:419:ILE:HG13	2.00	0.62
1:D:894:VAL:O	1:D:898:ILE:HG13	2.00	0.62
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.82	0.62
1:C:894:VAL:O	1:C:898:ILE:HG13	2.00	0.62
1:A:4018:MET:HB3	1:A:4065:LEU:HD21	1.80	0.62
1:B:2107:ILE:HG13	1:B:2108:ASN:H	1.64	0.62
1:B:415:THR:O	1:B:419:ILE:HG13	2.00	0.62
1:A:258:ARG:NH1	1:A:316:LEU:O	2.33	0.62
1:A:2107:ILE:HG13	1:A:2108:ASN:H	1.64	0.62
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.33	0.62
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.82	0.62
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.82	0.62
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.82	0.61
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.33	0.61
1:B:548:CYS:HB3	1:B:578:VAL:HG23	1.81	0.61
1:B:894:VAL:O	1:B:898:ILE:HG13	2.00	0.61
1:C:258:ARG:NH1	1:C:316:LEU:O	2.33	0.61
1:A:415:THR:O	1:A:419:ILE:HG13	2.00	0.61
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.33	0.61
1:B:4111:ASP:O	1:B:4115:GLN:N	2.32	0.61
1:C:2081:ARG:HG3	1:C:3686:LEU:HD22	1.82	0.61
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.33	0.61
1:C:4697:LEU:O	1:C:4698:ASN:ND2	2.34	0.61
1:D:4478:PHE:HA	1:D:4481:LYS:HE2	1.82	0.61
1:A:3613:HIS:O	1:A:3617:ASN:ND2	2.34	0.61
1:A:4824:GLY:O	1:B:4821:ARG:NH2	2.33	0.61
1:B:258:ARG:NH1	1:B:316:LEU:O	2.33	0.61
2:G:39:SER:O	2:G:43:ARG:NH1	2.33	0.61
1:C:1681:VAL:HG23	1:C:1682:ASP:H	1.66	0.61
1:A:4478:PHE:HA	1:A:4481:LYS:HE2	1.82	0.61
2:H:39:SER:O	2:H:43:ARG:NH1	2.34	0.61
1:C:308:LEU:HD13	1:C:314:LEU:HG	1.83	0.61
1:C:4478:PHE:HA	1:C:4481:LYS:HE2	1.82	0.61
1:A:123:HIS:HD2	1:A:126:SER:H	1.49	0.61
1:A:708:GLY:O	1:A:838:ARG:NH1	2.34	0.61
1:B:4697:LEU:O	1:B:4698:ASN:ND2	2.34	0.61
1:C:415:THR:O	1:C:419:ILE:HG13	2.00	0.61
1:C:853:PRO:HG2	1:C:1209:VAL:HA	1.83	0.61
1:C:3613:HIS:O	1:C:3617:ASN:ND2	2.34	0.61
1:D:3613:HIS:O	1:D:3617:ASN:ND2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:HIS:HD2	1:B:126:SER:H	1.49	0.60
1:B:4137:ILE:HG23	1:B:4950:PHE:HB2	1.83	0.60
1:D:4697:LEU:O	1:D:4698:ASN:ND2	2.34	0.60
2:J:39:SER:O	2:J:43:ARG:NH1	2.34	0.60
1:C:247:VAL:O	1:C:272:ARG:NH1	2.35	0.60
1:A:2081:ARG:HG3	1:A:3686:LEU:HD22	1.82	0.60
1:B:708:GLY:O	1:B:838:ARG:NH1	2.34	0.60
1:B:2145:LEU:HD23	1:B:2148:ILE:HD11	1.83	0.60
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.28	0.60
1:D:308:LEU:HD13	1:D:314:LEU:HG	1.83	0.60
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.82	0.60
1:A:2145:LEU:HD23	1:A:2148:ILE:HD11	1.83	0.60
1:A:4701:ASP:OD1	1:A:4701:ASP:N	2.31	0.60
1:B:360:ILE:HG23	1:B:402:GLY:HA2	1.83	0.60
1:C:4137:ILE:HG23	1:C:4950:PHE:HB2	1.84	0.60
1:D:247:VAL:O	1:D:272:ARG:NH1	2.35	0.60
1:A:360:ILE:HG23	1:A:402:GLY:HA2	1.83	0.60
1:B:1681:VAL:HG23	1:B:1682:ASP:H	1.66	0.60
1:C:708:GLY:O	1:C:838:ARG:NH1	2.34	0.60
2:I:39:SER:O	2:I:43:ARG:NH1	2.33	0.60
1:A:1681:VAL:HG23	1:A:1682:ASP:H	1.66	0.60
1:A:4697:LEU:O	1:A:4698:ASN:ND2	2.34	0.60
1:B:853:PRO:HG2	1:B:1209:VAL:HA	1.83	0.60
1:B:2081:ARG:HG3	1:B:3686:LEU:HD22	1.82	0.60
1:B:4478:PHE:HA	1:B:4481:LYS:HE2	1.82	0.60
1:D:363:ILE:HG22	1:D:372:LEU:HD22	1.84	0.60
1:D:708:GLY:O	1:D:838:ARG:NH1	2.34	0.60
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.83	0.60
1:D:1682:ASP:HB3	1:D:1684:PRO:HD2	1.84	0.60
1:D:1719:ARG:O	1:D:1723:ASN:HB2	2.02	0.60
1:C:4789:ARG:NH1	1:D:4558:TYR:OH	2.35	0.60
1:D:1681:VAL:HG23	1:D:1682:ASP:H	1.66	0.60
1:B:4624:ASP:O	1:B:4628:GLN:NE2	2.35	0.60
1:A:363:ILE:HG22	1:A:372:LEU:HD22	1.84	0.60
1:A:4624:ASP:O	1:A:4628:GLN:NE2	2.35	0.60
1:B:4824:GLY:O	1:C:4821:ARG:NH2	2.34	0.60
1:C:1682:ASP:HB3	1:C:1684:PRO:HD2	1.84	0.60
1:A:247:VAL:O	1:A:272:ARG:NH1	2.35	0.59
1:B:1682:ASP:HB3	1:B:1684:PRO:HD2	1.84	0.59
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.83	0.59
1:D:4624:ASP:O	1:D:4628:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TYR:OH	1:B:2325:ARG:NH1	2.34	0.59
1:A:412:GLU:OE2	1:A:484:ASN:ND2	2.36	0.59
1:B:247:VAL:O	1:B:272:ARG:NH1	2.35	0.59
1:C:123:HIS:HD2	1:C:126:SER:H	1.49	0.59
1:C:1719:ARG:O	1:C:1723:ASN:HB2	2.02	0.59
1:C:4624:ASP:O	1:C:4628:GLN:NE2	2.35	0.59
1:D:1680:HIS:CE1	2:J:91:VAL:HG22	2.37	0.59
1:A:308:LEU:HD13	1:A:314:LEU:HG	1.83	0.59
1:A:1051:ARG:HG2	1:A:1055:ARG:HE	1.67	0.59
1:A:853:PRO:HG2	1:A:1209:VAL:HA	1.83	0.59
1:A:4042:ILE:HG22	1:A:4044:LYS:H	1.68	0.59
1:C:2145:LEU:HD23	1:C:2148:ILE:HD11	1.83	0.59
1:A:4821:ARG:NH2	1:D:4824:GLY:O	2.35	0.59
1:B:412:GLU:OE2	1:B:484:ASN:ND2	2.36	0.59
1:C:1006:VAL:HG23	1:C:1009:ARG:HH12	1.68	0.59
1:D:853:PRO:HG2	1:D:1209:VAL:HA	1.83	0.59
1:D:2081:ARG:HG3	1:D:3686:LEU:HD22	1.82	0.59
1:C:1051:ARG:HG2	1:C:1055:ARG:HE	1.68	0.59
1:D:1051:ARG:HG2	1:D:1055:ARG:HE	1.67	0.59
1:B:191:TYR:OH	1:C:2325:ARG:NH1	2.35	0.59
1:C:360:ILE:HG23	1:C:402:GLY:HA2	1.83	0.59
1:C:412:GLU:OE2	1:C:484:ASN:ND2	2.35	0.59
1:D:2145:LEU:HD23	1:D:2148:ILE:HD11	1.83	0.59
1:A:1682:ASP:HB3	1:A:1684:PRO:HD2	1.84	0.59
1:A:4137:ILE:HG23	1:A:4950:PHE:HB2	1.83	0.59
1:A:4923:TYR:O	1:A:4927:LYS:HB2	2.02	0.59
1:B:1719:ARG:O	1:B:1723:ASN:HB2	2.02	0.59
1:C:1609:VAL:HG23	1:C:1610:SER:H	1.68	0.59
1:D:123:HIS:HD2	1:D:126:SER:H	1.49	0.59
1:D:360:ILE:HG23	1:D:402:GLY:HA2	1.83	0.59
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.83	0.59
1:B:308:LEU:HD13	1:B:314:LEU:HG	1.83	0.59
1:B:4789:ARG:NH1	1:C:4558:TYR:OH	2.36	0.59
1:B:4923:TYR:O	1:B:4927:LYS:HB2	2.02	0.59
1:C:4923:TYR:O	1:C:4927:LYS:HB2	2.02	0.58
1:D:412:GLU:OE2	1:D:484:ASN:ND2	2.35	0.58
1:D:4137:ILE:HG23	1:D:4950:PHE:HB2	1.84	0.58
1:B:2855:LYS:HD3	1:B:2867:HIS:HD2	1.68	0.58
1:B:2887:LYS:O	1:B:2891:ILE:HG22	2.03	0.58
1:B:3773:GLN:OE1	1:B:3850:ASN:ND2	2.36	0.58
1:B:4121:ALA:O	1:B:4125:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ILE:HG22	1:C:372:LEU:HD22	1.84	0.58
1:C:1641:ASP:HB3	1:C:1644:GLU:HG3	1.85	0.58
1:C:2887:LYS:O	1:C:2891:ILE:HG22	2.03	0.58
1:C:3773:GLN:OE1	1:C:3850:ASN:ND2	2.36	0.58
1:D:1641:ASP:HB3	1:D:1644:GLU:HG3	1.85	0.58
1:D:2887:LYS:O	1:D:2891:ILE:HG22	2.03	0.58
1:A:2855:LYS:HD3	1:A:2867:HIS:HD2	1.68	0.58
1:D:1272:ARG:NH2	1:D:1584:PRO:O	2.35	0.58
1:A:1006:VAL:HG23	1:A:1009:ARG:HH12	1.68	0.58
1:A:1641:ASP:HB3	1:A:1644:GLU:HG3	1.85	0.58
1:A:1719:ARG:O	1:A:1723:ASN:HB2	2.02	0.58
1:B:1641:ASP:HB3	1:B:1644:GLU:HG3	1.85	0.58
1:C:4042:ILE:HG22	1:C:4044:LYS:H	1.68	0.58
1:D:3773:GLN:OE1	1:D:3850:ASN:ND2	2.36	0.58
1:D:4042:ILE:HG22	1:D:4044:LYS:H	1.68	0.58
1:D:4923:TYR:O	1:D:4927:LYS:HB2	2.02	0.58
1:A:1989:GLU:HA	1:A:1992:ARG:HD3	1.85	0.58
1:B:4042:ILE:HG22	1:B:4044:LYS:H	1.68	0.58
1:A:3773:GLN:OE1	1:A:3850:ASN:ND2	2.36	0.58
1:A:4121:ALA:O	1:A:4125:LEU:HG	2.04	0.58
1:B:329:PHE:HB3	1:B:363:ILE:HD11	1.85	0.58
1:B:921:PHE:HA	1:B:924:LEU:HD23	1.86	0.58
1:B:1684:PRO:HD3	2:H:42:ASP:HB3	1.84	0.58
1:C:4121:ALA:O	1:C:4125:LEU:HG	2.04	0.58
1:B:363:ILE:HG22	1:B:372:LEU:HD22	1.84	0.58
1:B:3613:HIS:O	1:B:3617:ASN:ND2	2.34	0.58
1:A:836:HIS:NE2	1:A:842:GLN:OE1	2.35	0.58
1:A:4106:GLU:OE1	1:A:4134:ARG:NH1	2.37	0.58
1:A:4789:ARG:NH1	1:B:4558:TYR:OH	2.37	0.58
1:B:1006:VAL:HG23	1:B:1009:ARG:HH12	1.68	0.58
1:B:2065:MET:HE3	1:B:2086:LEU:HD23	1.86	0.58
1:C:188:SER:HB3	1:C:190:ARG:HD2	1.86	0.58
1:D:1609:VAL:HG23	1:D:1610:SER:H	1.68	0.58
1:B:226:GLY:O	1:B:356:TYR:N	2.33	0.58
1:B:1989:GLU:HA	1:B:1992:ARG:HD3	1.85	0.58
1:C:2855:LYS:HD3	1:C:2867:HIS:HD2	1.68	0.58
1:D:188:SER:HB3	1:D:190:ARG:HD2	1.86	0.58
1:D:4106:GLU:OE1	1:D:4134:ARG:NH1	2.37	0.58
1:A:329:PHE:HB3	1:A:363:ILE:HD11	1.85	0.58
1:B:1051:ARG:HG2	1:B:1055:ARG:HE	1.68	0.58
1:C:1272:ARG:NH2	1:C:1584:PRO:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1684:PRO:HD3	2:J:42:ASP:HB3	1.85	0.58
1:D:2855:LYS:HD3	1:D:2867:HIS:HD2	1.68	0.58
1:A:1986:PRO:HB2	1:A:1988:PRO:HD2	1.86	0.57
1:A:2065:MET:HE3	1:A:2086:LEU:HD23	1.86	0.57
1:A:2887:LYS:O	1:A:2891:ILE:HG22	2.03	0.57
1:C:329:PHE:HB3	1:C:363:ILE:HD11	1.85	0.57
1:D:1006:VAL:HG23	1:D:1009:ARG:HH12	1.68	0.57
1:D:2728:HIS:HA	1:D:2767:LYS:HZ1	1.70	0.57
1:A:1272:ARG:NH2	1:A:1584:PRO:O	2.35	0.57
1:B:188:SER:HB3	1:B:190:ARG:HD2	1.86	0.57
1:B:4106:GLU:OE1	1:B:4134:ARG:NH1	2.37	0.57
1:A:188:SER:HB3	1:A:190:ARG:HD2	1.86	0.57
1:B:1272:ARG:NH2	1:B:1584:PRO:O	2.35	0.57
1:B:1609:VAL:HG23	1:B:1610:SER:H	1.68	0.57
1:C:921:PHE:HA	1:C:924:LEU:HD23	1.86	0.57
1:C:694:ARG:HG2	1:C:728:ASP:HB3	1.87	0.57
1:D:694:ARG:HG2	1:D:728:ASP:HB3	1.87	0.57
1:A:694:ARG:HG2	1:A:728:ASP:HB3	1.87	0.57
1:A:921:PHE:HA	1:A:924:LEU:HD23	1.86	0.57
1:A:1730:MET:SD	1:A:2106:THR:OG1	2.63	0.57
1:B:799:LYS:HG2	1:B:1621:GLN:HG3	1.86	0.57
1:B:1730:MET:SD	1:B:2106:THR:OG1	2.63	0.57
1:C:226:GLY:O	1:C:356:TYR:N	2.33	0.57
1:C:799:LYS:HG2	1:C:1621:GLN:HG3	1.86	0.57
1:C:1730:MET:SD	1:C:2106:THR:OG1	2.63	0.57
1:C:4106:GLU:OE1	1:C:4134:ARG:NH1	2.37	0.57
1:D:329:PHE:HB3	1:D:363:ILE:HD11	1.85	0.57
1:D:799:LYS:HG2	1:D:1621:GLN:HG3	1.86	0.57
1:A:2343:LEU:O	1:A:2347:GLU:HG3	2.05	0.57
1:B:694:ARG:HG2	1:B:728:ASP:HB3	1.87	0.57
1:B:1060:TYR:HB2	1:B:1062:TYR:CE1	2.40	0.57
1:C:2065:MET:HE3	1:C:2086:LEU:HD23	1.86	0.57
1:D:1060:TYR:HB2	1:D:1062:TYR:CE1	2.40	0.57
1:D:2065:MET:HE3	1:D:2086:LEU:HD23	1.86	0.57
1:D:4121:ALA:O	1:D:4125:LEU:HG	2.04	0.57
1:B:2343:LEU:O	1:B:2347:GLU:HG3	2.05	0.57
1:C:1986:PRO:HB2	1:C:1988:PRO:HD2	1.86	0.57
1:C:2343:LEU:O	1:C:2347:GLU:HG3	2.05	0.57
1:D:271:ALA:O	1:D:301:THR:OG1	2.23	0.57
1:D:921:PHE:HA	1:D:924:LEU:HD23	1.86	0.57
1:D:2343:LEU:O	1:D:2347:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1609:VAL:HG23	1:A:1610:SER:H	1.68	0.56
1:B:1986:PRO:HB2	1:B:1988:PRO:HD2	1.86	0.56
1:C:1060:TYR:HB2	1:C:1062:TYR:CE1	2.40	0.56
1:D:4195:THR:HB	1:D:4918:LEU:HD11	1.87	0.56
1:A:1060:TYR:HB2	1:A:1062:TYR:CE1	2.40	0.56
1:A:4195:THR:HB	1:A:4918:LEU:HD11	1.88	0.56
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.87	0.56
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.87	0.56
1:D:3831:ASP:HB2	1:D:3834:PHE:HB3	1.88	0.56
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.87	0.56
1:A:271:ALA:O	1:A:301:THR:OG1	2.23	0.56
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.38	0.56
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.39	0.56
1:A:226:GLY:O	1:A:356:TYR:N	2.33	0.56
1:B:4195:THR:HB	1:B:4918:LEU:HD11	1.88	0.56
1:C:1588:HIS:HE1	1:C:1590:GLN:HE21	1.53	0.56
1:A:2723:TYR:HD1	1:A:2894:PHE:HD2	1.53	0.56
1:C:1989:GLU:HA	1:C:1992:ARG:HD3	1.85	0.56
1:D:1986:PRO:HB2	1:D:1988:PRO:HD2	1.86	0.56
1:C:3831:ASP:HB2	1:C:3834:PHE:HB3	1.88	0.56
1:D:1989:GLU:HA	1:D:1992:ARG:HD3	1.85	0.56
1:B:836:HIS:NE2	1:B:842:GLN:OE1	2.35	0.56
1:D:2723:TYR:HD1	1:D:2894:PHE:HD2	1.53	0.56
1:A:655:MET:SD	1:A:836:HIS:ND1	2.79	0.56
1:C:271:ALA:O	1:C:301:THR:OG1	2.23	0.56
1:C:933:LEU:HD23	1:C:937:LEU:HD23	1.87	0.56
1:C:4195:THR:HB	1:C:4918:LEU:HD11	1.88	0.56
1:D:2159:ASN:HD22	1:D:2162:ARG:HH22	1.54	0.56
1:D:3840:ARG:HH21	1:D:3844:LEU:HD21	1.71	0.56
1:A:1272:ARG:NH2	1:A:1583:CYS:SG	2.79	0.56
1:B:271:ALA:O	1:B:301:THR:OG1	2.23	0.56
1:B:933:LEU:HD23	1:B:937:LEU:HD23	1.87	0.56
1:B:1272:ARG:NH2	1:B:1583:CYS:SG	2.79	0.56
1:C:2728:HIS:HA	1:C:2767:LYS:HZ1	1.70	0.56
1:A:3831:ASP:HB2	1:A:3834:PHE:HB3	1.88	0.56
1:B:655:MET:SD	1:B:836:HIS:ND1	2.79	0.56
1:B:1294:ASN:O	1:B:1348:LYS:NZ	2.35	0.56
1:B:2723:TYR:HD1	1:B:2894:PHE:HD2	1.53	0.56
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.79	0.56
1:B:503:ASP:HA	1:B:561:ARG:HH12	1.71	0.55
1:B:1588:HIS:HE1	1:B:1590:GLN:HE21	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3840:ARG:HH21	1:B:3844:LEU:HD21	1.71	0.55
1:C:655:MET:SD	1:C:836:HIS:ND1	2.79	0.55
1:D:387:ILE:O	1:D:388:GLN:NE2	2.39	0.55
1:D:1730:MET:SD	1:D:2106:THR:OG1	2.63	0.55
1:A:340:VAL:HG23	1:A:341:GLY:H	1.71	0.55
1:A:799:LYS:HG2	1:A:1621:GLN:HG3	1.86	0.55
1:A:2003:MET:HB3	1:A:2008:ILE:HD11	1.88	0.55
1:A:3840:ARG:HH21	1:A:3844:LEU:HD21	1.71	0.55
1:B:2003:MET:HB3	1:B:2008:ILE:HD11	1.88	0.55
1:C:2839:MET:HE1	1:C:2904:ARG:HE	1.71	0.55
1:D:655:MET:SD	1:D:836:HIS:ND1	2.79	0.55
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.79	0.55
1:D:1294:ASN:O	1:D:1348:LYS:NZ	2.34	0.55
1:A:891:GLU:HA	1:A:894:VAL:HG22	1.88	0.55
1:A:2839:MET:HE1	1:A:2904:ARG:HE	1.71	0.55
1:C:340:VAL:HG23	1:C:341:GLY:H	1.71	0.55
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.39	0.55
1:A:503:ASP:HA	1:A:561:ARG:HH12	1.72	0.55
1:A:933:LEU:HD23	1:A:937:LEU:HD23	1.87	0.55
1:A:938:GLU:O	1:A:942:THR:HG23	2.07	0.55
1:A:999:LEU:HD21	1:A:1050:LEU:HD12	1.89	0.55
1:B:3831:ASP:HB2	1:B:3834:PHE:HB3	1.88	0.55
1:C:2159:ASN:HD22	1:C:2162:ARG:HH22	1.54	0.55
1:D:938:GLU:O	1:D:942:THR:HG23	2.07	0.55
1:B:938:GLU:O	1:B:942:THR:HG23	2.07	0.55
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.87	0.55
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.39	0.55
1:D:1588:HIS:HE1	1:D:1590:GLN:HE21	1.53	0.55
1:B:2087:LEU:HD21	1:B:3643:LEU:HD11	1.88	0.55
1:B:2159:ASN:HD22	1:B:2162:ARG:HH22	1.54	0.55
1:C:498:VAL:HG13	1:C:533:LEU:HD22	1.89	0.55
1:D:226:GLY:O	1:D:356:TYR:N	2.33	0.55
1:D:933:LEU:HD23	1:D:937:LEU:HD23	1.87	0.55
1:B:387:ILE:O	1:B:388:GLN:NE2	2.40	0.55
1:B:498:VAL:HG13	1:B:533:LEU:HD22	1.89	0.55
1:B:1680:HIS:CE1	2:H:91:VAL:HG22	2.41	0.55
1:C:1294:ASN:ND2	1:C:1296:ASN:O	2.40	0.55
1:C:1684:PRO:HD3	2:I:42:ASP:HB3	1.87	0.55
1:A:498:VAL:HG13	1:A:533:LEU:HD22	1.89	0.55
1:C:503:ASP:HA	1:C:561:ARG:HH12	1.71	0.55
1:C:1985:CYS:SG	1:C:1992:ARG:NH1	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3840:ARG:HH21	1:C:3844:LEU:HD21	1.71	0.55
1:A:1166:VAL:HG22	1:A:1173:MET:HG2	1.89	0.55
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.89	0.55
1:B:891:GLU:HA	1:B:894:VAL:HG22	1.88	0.55
1:B:999:LEU:HD21	1:B:1050:LEU:HD12	1.89	0.55
1:B:1166:VAL:HG22	1:B:1173:MET:HG2	1.89	0.55
1:B:1985:CYS:SG	1:B:1992:ARG:NH1	2.80	0.55
1:C:938:GLU:O	1:C:942:THR:HG23	2.07	0.55
1:C:2442:PRO:HG2	1:C:2506:LEU:HD21	1.89	0.55
1:A:387:ILE:O	1:A:388:GLN:NE2	2.40	0.55
1:A:1985:CYS:SG	1:A:1992:ARG:NH1	2.80	0.55
1:B:4608:LYS:HD3	1:B:4614:LEU:HD22	1.89	0.55
1:D:503:ASP:HA	1:D:561:ARG:HH12	1.72	0.55
1:D:1985:CYS:SG	1:D:1992:ARG:NH1	2.80	0.55
1:D:2839:MET:HE1	1:D:2904:ARG:HE	1.71	0.55
1:A:2087:LEU:HD21	1:A:3643:LEU:HD11	1.89	0.54
1:A:2159:ASN:HD22	1:A:2162:ARG:HH22	1.54	0.54
1:B:2839:MET:HE1	1:B:2904:ARG:HE	1.71	0.54
1:C:1166:VAL:HG22	1:C:1173:MET:HG2	1.89	0.54
1:C:2723:TYR:HD1	1:C:2894:PHE:HD2	1.53	0.54
1:C:4608:LYS:HD3	1:C:4614:LEU:HD22	1.89	0.54
1:D:2087:LEU:HD21	1:D:3643:LEU:HD11	1.89	0.54
1:D:2442:PRO:HG2	1:D:2506:LEU:HD21	1.89	0.54
1:A:1588:HIS:HE1	1:A:1590:GLN:HE21	1.54	0.54
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.89	0.54
1:C:2087:LEU:HD21	1:C:3643:LEU:HD11	1.89	0.54
1:D:836:HIS:NE2	1:D:842:GLN:OE1	2.35	0.54
1:B:2442:PRO:HG2	1:B:2506:LEU:HD21	1.89	0.54
1:A:3975:LYS:HB2	1:A:4093:ILE:HG13	1.89	0.54
1:B:2099:ARG:O	1:B:2103:LYS:NZ	2.39	0.54
1:B:3975:LYS:HB2	1:B:4093:ILE:HG13	1.89	0.54
1:C:387:ILE:O	1:C:388:GLN:NE2	2.39	0.54
1:D:1166:VAL:HG22	1:D:1173:MET:HG2	1.89	0.54
1:B:1609:VAL:HG12	1:B:1620:VAL:HG23	1.89	0.54
1:C:1769:PHE:O	2:I:83:TYR:OH	2.26	0.54
1:D:340:VAL:HG23	1:D:341:GLY:H	1.71	0.54
1:A:1953:SER:HB3	1:A:1956:LEU:HD23	1.90	0.54
1:B:915:HIS:HD2	1:B:916:PRO:HD2	1.73	0.54
1:C:1810:PRO:HB3	1:C:1818:LEU:HD22	1.89	0.54
1:D:2003:MET:HB3	1:D:2008:ILE:HD11	1.88	0.54
1:A:1294:ASN:ND2	1:A:1296:ASN:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:HG23	1:B:341:GLY:H	1.71	0.54
1:C:3975:LYS:HB2	1:C:4093:ILE:HG13	1.89	0.54
1:D:891:GLU:HA	1:D:894:VAL:HG22	1.88	0.54
1:C:678:MET:HG3	1:C:801:ARG:HB3	1.90	0.54
1:C:2003:MET:HB3	1:C:2008:ILE:HD11	1.88	0.54
1:D:1294:ASN:ND2	1:D:1296:ASN:O	2.40	0.54
1:D:3975:LYS:HB2	1:D:4093:ILE:HG13	1.89	0.54
1:A:2442:PRO:HG2	1:A:2506:LEU:HD21	1.89	0.54
1:B:1810:PRO:HB3	1:B:1818:LEU:HD22	1.89	0.54
1:B:3796:MET:HE1	1:B:3869:ILE:HG23	1.90	0.54
1:C:836:HIS:NE2	1:C:842:GLN:OE1	2.35	0.54
1:C:999:LEU:HD21	1:C:1050:LEU:HD12	1.89	0.54
1:D:498:VAL:HG13	1:D:533:LEU:HD22	1.89	0.54
1:A:915:HIS:HD2	1:A:916:PRO:HD2	1.73	0.54
1:B:1294:ASN:ND2	1:B:1296:ASN:O	2.40	0.54
1:B:1929:ASP:OD1	1:B:3612:ARG:NH2	2.41	0.54
1:D:678:MET:HG3	1:D:801:ARG:HB3	1.90	0.54
1:D:999:LEU:HD21	1:D:1050:LEU:HD12	1.89	0.54
1:A:1609:VAL:HG12	1:A:1620:VAL:HG23	1.89	0.53
1:B:2728:HIS:HA	1:B:2767:LYS:HZ1	1.72	0.53
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.89	0.53
1:D:1953:SER:HB3	1:D:1956:LEU:HD23	1.90	0.53
1:A:678:MET:HG3	1:A:801:ARG:HB3	1.90	0.53
1:A:3796:MET:HE1	1:A:3869:ILE:HG23	1.89	0.53
1:B:503:ASP:O	1:B:507:VAL:HG13	2.09	0.53
1:B:678:MET:HG3	1:B:801:ARG:HB3	1.90	0.53
1:C:891:GLU:HA	1:C:894:VAL:HG22	1.88	0.53
1:C:1929:ASP:OD1	1:C:3612:ARG:NH2	2.41	0.53
1:C:4018:MET:HE2	1:C:4061:GLU:HG2	1.90	0.53
1:A:1294:ASN:O	1:A:1348:LYS:NZ	2.35	0.53
1:A:1968:PRO:HB2	1:A:3618:LEU:HD13	1.91	0.53
1:A:4608:LYS:HD3	1:A:4614:LEU:HD22	1.89	0.53
1:B:1174:MET:HG2	1:B:1190:LEU:HA	1.90	0.53
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.89	0.53
1:B:4018:MET:HE2	1:B:4061:GLU:HG2	1.90	0.53
1:C:1609:VAL:HG12	1:C:1620:VAL:HG23	1.89	0.53
1:D:1609:VAL:HG12	1:D:1620:VAL:HG23	1.89	0.53
1:D:1968:PRO:HB2	1:D:3618:LEU:HD13	1.90	0.53
1:D:3796:MET:HE1	1:D:3869:ILE:HG23	1.89	0.53
1:D:4608:LYS:HD3	1:D:4614:LEU:HD22	1.89	0.53
1:A:1810:PRO:HB3	1:A:1818:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4942:MET:HE1	1:B:4949:GLU:HB2	1.91	0.53
1:C:915:HIS:HD2	1:C:916:PRO:HD2	1.73	0.53
1:C:1968:PRO:HB2	1:C:3618:LEU:HD13	1.91	0.53
1:A:4558:TYR:OH	1:D:4789:ARG:NH1	2.42	0.53
1:B:2731:TRP:O	1:B:2735:LYS:HG2	2.09	0.53
1:C:1294:ASN:O	1:C:1348:LYS:NZ	2.35	0.53
1:A:503:ASP:O	1:A:507:VAL:HG13	2.09	0.53
1:A:1119:ARG:NH2	1:A:1196:ASP:OD1	2.42	0.53
1:A:4942:MET:HE1	1:A:4949:GLU:HB2	1.91	0.53
1:B:1968:PRO:HB2	1:B:3618:LEU:HD13	1.91	0.53
1:C:2731:TRP:O	1:C:2735:LYS:HG2	2.09	0.53
1:D:915:HIS:HD2	1:D:916:PRO:HD2	1.73	0.53
1:D:1810:PRO:HB3	1:D:1818:LEU:HD22	1.89	0.53
1:C:997:ASP:HA	1:C:1047:LYS:HD2	1.91	0.53
1:C:4633:VAL:HG12	1:C:4703:LYS:HG2	1.91	0.53
1:D:62:LEU:O	1:D:66:THR:HG23	2.09	0.53
1:D:503:ASP:O	1:D:507:VAL:HG13	2.09	0.53
1:D:4018:MET:HE2	1:D:4061:GLU:HG2	1.90	0.53
1:A:2325:ARG:NH1	1:D:191:TYR:OH	2.39	0.53
1:C:1119:ARG:NH2	1:C:1196:ASP:OD1	2.42	0.53
1:C:1174:MET:HG2	1:C:1190:LEU:HA	1.90	0.53
1:D:4942:MET:HE1	1:D:4949:GLU:HB2	1.91	0.53
1:B:1119:ARG:NH2	1:B:1196:ASP:OD1	2.42	0.53
1:C:503:ASP:O	1:C:507:VAL:HG13	2.09	0.53
1:D:997:ASP:HA	1:D:1047:LYS:HD2	1.91	0.53
1:D:4633:VAL:HG12	1:D:4703:LYS:HG2	1.91	0.53
1:A:78:LEU:O	1:A:82:LEU:HG	2.09	0.53
1:A:1174:MET:HG2	1:A:1190:LEU:HA	1.90	0.53
1:B:62:LEU:O	1:B:66:THR:HG23	2.09	0.53
1:B:4494:ALA:HB2	1:B:4591:CYS:SG	2.49	0.53
1:C:4494:ALA:HB2	1:C:4591:CYS:SG	2.49	0.53
1:D:1119:ARG:NH2	1:D:1196:ASP:OD1	2.42	0.53
1:A:62:LEU:O	1:A:66:THR:HG23	2.09	0.52
1:A:4494:ALA:HB2	1:A:4591:CYS:SG	2.49	0.52
1:D:1929:ASP:OD1	1:D:3612:ARG:NH2	2.41	0.52
1:A:4018:MET:HE2	1:A:4061:GLU:HG2	1.90	0.52
1:B:78:LEU:O	1:B:82:LEU:HG	2.09	0.52
1:B:1953:SER:HB3	1:B:1956:LEU:HD23	1.90	0.52
1:C:1680:HIS:CE1	2:I:91:VAL:HG22	2.45	0.52
1:C:3796:MET:HE1	1:C:3869:ILE:HG23	1.90	0.52
1:A:1012:ILE:HG13	1:A:1013:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:O	1:C:82:LEU:HG	2.09	0.52
1:C:1953:SER:HB3	1:C:1956:LEU:HD23	1.90	0.52
1:A:2853:LYS:O	1:A:2857:LEU:HG	2.10	0.52
1:B:997:ASP:HA	1:B:1047:LYS:HD2	1.91	0.52
1:B:2853:LYS:O	1:B:2857:LEU:HG	2.10	0.52
1:D:4494:ALA:HB2	1:D:4591:CYS:SG	2.49	0.52
1:A:4671:MET:HG3	1:A:4674:ALA:HB3	1.91	0.52
1:C:1245:ARG:NH1	1:C:1809:ASP:O	2.43	0.52
1:D:2731:TRP:O	1:D:2735:LYS:HG2	2.09	0.52
1:A:2731:TRP:O	1:A:2735:LYS:HG2	2.09	0.52
1:C:2853:LYS:O	1:C:2857:LEU:HG	2.10	0.52
1:C:4942:MET:HE1	1:C:4949:GLU:HB2	1.91	0.52
1:A:997:ASP:HA	1:A:1047:LYS:HD2	1.91	0.52
1:A:1929:ASP:OD1	1:A:3612:ARG:NH2	2.41	0.52
1:B:1245:ARG:NH1	1:B:1809:ASP:O	2.43	0.52
1:C:989:THR:HG23	1:C:992:GLN:H	1.75	0.52
1:D:1174:MET:HG2	1:D:1190:LEU:HA	1.90	0.52
1:A:3919:LEU:O	1:A:3923:ILE:HG12	2.10	0.52
1:B:4671:MET:HG3	1:B:4674:ALA:HB3	1.91	0.52
1:C:4013:LEU:HD22	1:C:4124:VAL:HG21	1.91	0.52
1:D:1257:GLN:HA	1:D:1384:LEU:HD23	1.92	0.52
1:D:1578:ASN:HD22	1:D:1582:GLN:HE22	1.58	0.52
1:B:4633:VAL:HG12	1:B:4703:LYS:HG2	1.91	0.52
1:C:62:LEU:O	1:C:66:THR:HG23	2.09	0.51
1:C:1012:ILE:HG13	1:C:1013:ARG:HD2	1.92	0.51
1:C:1257:GLN:HA	1:C:1384:LEU:HD23	1.92	0.51
1:D:49:LEU:HD12	1:D:201:TRP:HB3	1.92	0.51
1:A:671:LYS:HB3	1:A:761:LEU:HB2	1.92	0.51
1:A:1245:ARG:NH1	1:A:1809:ASP:O	2.43	0.51
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.76	0.51
1:C:3728:ALA:HA	1:C:3731:HIS:ND1	2.25	0.51
1:D:2853:LYS:O	1:D:2857:LEU:HG	2.10	0.51
1:D:3728:ALA:HA	1:D:3731:HIS:ND1	2.25	0.51
1:D:4671:MET:HG3	1:D:4674:ALA:HB3	1.91	0.51
1:A:1578:ASN:HD22	1:A:1582:GLN:HE22	1.58	0.51
1:A:4013:LEU:HD22	1:A:4124:VAL:HG21	1.91	0.51
1:C:1578:ASN:HD22	1:C:1582:GLN:HE22	1.58	0.51
1:C:4833:PRO:HD3	1:C:4842:ARG:HE	1.76	0.51
1:D:3919:LEU:O	1:D:3923:ILE:HG12	2.10	0.51
1:D:4044:LYS:NZ	1:D:4071:THR:H	2.09	0.51
1:A:989:THR:HG23	1:A:992:GLN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2315:ASN:O	1:A:2319:VAL:HG23	2.11	0.51
1:A:3878:LEU:HD22	1:A:3938:ARG:HE	1.76	0.51
1:D:78:LEU:O	1:D:82:LEU:HG	2.09	0.51
1:D:3878:LEU:HD22	1:D:3938:ARG:HE	1.76	0.51
1:A:926:GLU:HA	1:A:929:ARG:HB3	1.92	0.51
1:A:1257:GLN:HA	1:A:1384:LEU:HD23	1.92	0.51
1:A:4633:VAL:HG12	1:A:4703:LYS:HG2	1.91	0.51
1:B:1257:GLN:HA	1:B:1384:LEU:HD23	1.92	0.51
1:B:3878:LEU:HD22	1:B:3938:ARG:HE	1.76	0.51
1:B:4044:LYS:NZ	1:B:4071:THR:H	2.09	0.51
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.76	0.51
1:C:671:LYS:HB3	1:C:761:LEU:HB2	1.92	0.51
1:D:671:LYS:HB3	1:D:761:LEU:HB2	1.92	0.51
1:D:989:THR:HG23	1:D:992:GLN:H	1.75	0.51
1:D:1245:ARG:NH1	1:D:1809:ASP:O	2.43	0.51
1:D:4046:ASP:OD1	1:D:4046:ASP:N	2.43	0.51
1:D:4640:PRO:HG2	1:D:4646:LYS:HA	1.92	0.51
1:B:1012:ILE:HG13	1:B:1013:ARG:HD2	1.91	0.51
1:B:2315:ASN:O	1:B:2319:VAL:HG23	2.11	0.51
1:B:4013:LEU:HD22	1:B:4124:VAL:HG21	1.91	0.51
1:C:4671:MET:HG3	1:C:4674:ALA:HB3	1.91	0.51
1:D:2315:ASN:O	1:D:2319:VAL:HG23	2.11	0.51
1:D:4013:LEU:HD22	1:D:4124:VAL:HG21	1.91	0.51
1:D:4833:PRO:HD3	1:D:4842:ARG:HE	1.76	0.51
1:A:1586:ARG:NH2	1:A:1635:GLU:OE1	2.44	0.51
1:A:3989:VAL:HG12	1:A:3990:VAL:H	1.75	0.51
1:B:1578:ASN:HD22	1:B:1582:GLN:HE22	1.58	0.51
1:B:4640:PRO:HG2	1:B:4646:LYS:HA	1.92	0.51
1:C:3989:VAL:HG12	1:C:3990:VAL:H	1.76	0.51
1:A:49:LEU:HD12	1:A:201:TRP:HB3	1.92	0.51
1:C:926:GLU:HA	1:C:929:ARG:HB3	1.92	0.51
1:C:3919:LEU:O	1:C:3923:ILE:HG12	2.10	0.51
1:D:1012:ILE:HG13	1:D:1013:ARG:HD2	1.91	0.51
1:D:3989:VAL:HG12	1:D:3990:VAL:H	1.75	0.51
1:A:2099:ARG:O	1:A:2103:LYS:NZ	2.39	0.51
1:A:3728:ALA:HA	1:A:3731:HIS:ND1	2.25	0.51
1:B:1631:LEU:HD22	1:B:1645:LEU:HD11	1.93	0.51
1:B:3728:ALA:HA	1:B:3731:HIS:ND1	2.25	0.51
1:B:3919:LEU:O	1:B:3923:ILE:HG12	2.10	0.51
1:C:1586:ARG:NH2	1:C:1635:GLU:OE1	2.44	0.51
1:C:3878:LEU:HD22	1:C:3938:ARG:HE	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ILE:N	1:D:160:TRP:O	2.44	0.51
1:D:1586:ARG:NH2	1:D:1635:GLU:OE1	2.44	0.51
1:D:1953:SER:OG	1:D:1954:ALA:N	2.44	0.51
1:A:1631:LEU:HD22	1:A:1645:LEU:HD11	1.93	0.50
1:B:4833:PRO:HD3	1:B:4842:ARG:HE	1.76	0.50
1:C:1090:ALA:HB3	1:C:1202:ILE:HG23	1.93	0.50
1:C:1631:LEU:HD22	1:C:1645:LEU:HD11	1.93	0.50
1:C:4044:LYS:NZ	1:C:4071:THR:H	2.09	0.50
1:B:309:MET:HB2	1:B:312:LYS:HZ2	1.76	0.50
1:B:989:THR:HG23	1:B:992:GLN:H	1.75	0.50
1:C:49:LEU:HD12	1:C:201:TRP:HB3	1.92	0.50
1:C:4046:ASP:OD1	1:C:4046:ASP:N	2.43	0.50
1:D:757:CYS:HG	1:D:768:PHE:HD1	1.58	0.50
1:D:1631:LEU:HD22	1:D:1645:LEU:HD11	1.93	0.50
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.76	0.50
1:A:370:LEU:HB2	1:A:393:MET:HE3	1.94	0.50
1:A:661:LEU:HD13	1:A:673:TRP:CD1	2.47	0.50
1:B:671:LYS:HB3	1:B:761:LEU:HB2	1.92	0.50
1:B:1090:ALA:HB3	1:B:1202:ILE:HG23	1.93	0.50
1:B:1586:ARG:NH2	1:B:1635:GLU:OE1	2.44	0.50
1:C:1086:ARG:HH21	1:C:1251:LEU:HD13	1.77	0.50
1:C:4029:ASP:OD2	1:C:4054:HIS:NE2	2.45	0.50
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.76	0.50
1:A:119:ILE:N	1:A:160:TRP:O	2.45	0.50
1:B:1086:ARG:HH21	1:B:1251:LEU:HD13	1.77	0.50
1:C:119:ILE:N	1:C:160:TRP:O	2.44	0.50
1:C:1838:GLU:OE1	1:C:1838:GLU:N	2.43	0.50
1:D:370:LEU:HB2	1:D:393:MET:HE3	1.94	0.50
1:D:4029:ASP:OD2	1:D:4054:HIS:NE2	2.45	0.50
1:A:1829:LEU:HB3	1:A:1834:ILE:HD11	1.94	0.50
1:A:2728:HIS:HA	1:A:2767:LYS:HZ1	1.75	0.50
1:A:4046:ASP:OD1	1:A:4046:ASP:N	2.43	0.50
1:A:4649:LYS:NZ	1:A:4669:LEU:O	2.45	0.50
1:B:2753:GLN:HG2	1:B:2755:LEU:H	1.77	0.50
1:B:3989:VAL:HG12	1:B:3990:VAL:H	1.76	0.50
1:B:4046:ASP:N	1:B:4046:ASP:OD1	2.43	0.50
1:C:1829:LEU:HB3	1:C:1834:ILE:HD11	1.94	0.50
1:C:2315:ASN:O	1:C:2319:VAL:HG23	2.11	0.50
1:C:4640:PRO:HG2	1:C:4646:LYS:HA	1.92	0.50
1:C:4830:ILE:HG13	1:C:4842:ARG:HH22	1.77	0.50
1:D:926:GLU:HA	1:D:929:ARG:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1829:LEU:HB3	1:D:1834:ILE:HD11	1.94	0.50
1:A:4830:ILE:HG13	1:A:4842:ARG:HH22	1.77	0.50
1:B:661:LEU:HD13	1:B:673:TRP:CD1	2.47	0.50
1:B:926:GLU:HA	1:B:929:ARG:HB3	1.92	0.50
1:C:934:GLN:O	1:C:937:LEU:HG	2.12	0.50
1:D:1362:ASP:OD1	1:D:1362:ASP:N	2.45	0.50
1:A:934:GLN:O	1:A:937:LEU:HG	2.12	0.50
1:A:4640:PRO:HG2	1:A:4646:LYS:HA	1.92	0.50
1:B:1609:VAL:HA	1:B:1620:VAL:HA	1.94	0.50
1:C:2753:GLN:HG2	1:C:2755:LEU:H	1.77	0.50
1:C:4649:LYS:NZ	1:C:4669:LEU:O	2.45	0.50
1:D:4830:ILE:HG13	1:D:4842:ARG:HH22	1.77	0.50
1:A:1090:ALA:HB3	1:A:1202:ILE:HG23	1.93	0.50
1:A:4044:LYS:NZ	1:A:4071:THR:H	2.09	0.50
1:B:1953:SER:OG	1:B:1954:ALA:N	2.44	0.50
1:B:4029:ASP:OD2	1:B:4054:HIS:NE2	2.45	0.50
1:B:4051:MET:HG3	1:B:4062:THR:HG22	1.94	0.50
1:D:309:MET:HB2	1:D:312:LYS:HZ1	1.77	0.50
1:D:1838:GLU:OE1	1:D:1838:GLU:N	2.43	0.50
1:D:2753:GLN:HG2	1:D:2755:LEU:H	1.77	0.50
1:B:49:LEU:HD12	1:B:201:TRP:HB3	1.92	0.50
1:B:370:LEU:HB2	1:B:393:MET:HE3	1.94	0.50
1:B:1829:LEU:HB3	1:B:1834:ILE:HD11	1.94	0.50
1:B:4830:ILE:HG13	1:B:4842:ARG:HH22	1.77	0.50
1:A:2206:SER:OG	1:A:2207:ARG:N	2.45	0.49
1:A:3831:ASP:N	1:A:3831:ASP:OD1	2.45	0.49
1:B:2478:GLU:HG2	1:B:2479:VAL:HG13	1.95	0.49
1:C:1397:UNK:HA	1:C:1412:UNK:HA	1.94	0.49
1:C:1786:ASP:OD1	1:C:1786:ASP:N	2.45	0.49
1:D:661:LEU:HD13	1:D:673:TRP:CD1	2.47	0.49
1:D:1090:ALA:HB3	1:D:1202:ILE:HG23	1.93	0.49
1:D:2839:MET:HB2	1:D:2892:PHE:HE2	1.77	0.49
1:A:4833:PRO:HD3	1:A:4842:ARG:HE	1.76	0.49
1:B:1397:UNK:HA	1:B:1412:UNK:HA	1.94	0.49
1:A:4029:ASP:OD2	1:A:4054:HIS:NE2	2.45	0.49
1:A:4051:MET:HG3	1:A:4062:THR:HG22	1.94	0.49
1:B:119:ILE:N	1:B:160:TRP:O	2.44	0.49
1:B:2839:MET:HB2	1:B:2892:PHE:HE2	1.77	0.49
1:B:4507:VAL:HG23	1:B:4574:LEU:HD22	1.94	0.49
1:B:4832:ASP:OD1	1:B:4832:ASP:N	2.45	0.49
1:C:2478:GLU:HG2	1:C:2479:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4660:TYR:HB3	1:C:4664:ARG:HH21	1.78	0.49
1:D:934:GLN:O	1:D:937:LEU:HG	2.12	0.49
1:D:1629:MET:HE3	1:D:1642:ILE:HG21	1.94	0.49
1:D:1786:ASP:OD1	1:D:1786:ASP:N	2.45	0.49
1:D:1972:ILE:HD13	1:D:1975:LEU:HD21	1.94	0.49
1:D:2206:SER:OG	1:D:2207:ARG:N	2.45	0.49
1:D:4660:TYR:HB3	1:D:4664:ARG:HH21	1.77	0.49
1:A:1972:ILE:HD13	1:A:1975:LEU:HD21	1.95	0.49
1:B:408:SER:O	1:B:408:SER:OG	2.31	0.49
1:C:1953:SER:OG	1:C:1954:ALA:N	2.44	0.49
1:C:2781:MET:HE3	1:C:2843:MET:HE3	1.95	0.49
1:C:4051:MET:HG3	1:C:4062:THR:HG22	1.94	0.49
1:D:1086:ARG:HH21	1:D:1251:LEU:HD13	1.77	0.49
1:D:2478:GLU:HG2	1:D:2479:VAL:HG13	1.94	0.49
1:D:4051:MET:HG3	1:D:4062:THR:HG22	1.94	0.49
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.45	0.49
1:A:1629:MET:HE3	1:A:1642:ILE:HG21	1.94	0.49
1:A:1953:SER:OG	1:A:1954:ALA:N	2.44	0.49
1:A:2352:ILE:HD12	1:A:2358:ARG:HG3	1.95	0.49
1:B:1362:ASP:N	1:B:1362:ASP:OD1	2.45	0.49
1:B:1629:MET:HE3	1:B:1642:ILE:HG21	1.95	0.49
1:B:1720:LEU:HD21	1:B:1831:ILE:HD13	1.95	0.49
1:C:191:TYR:OH	1:D:2325:ARG:NH1	2.45	0.49
1:C:370:LEU:HB2	1:C:393:MET:HE3	1.94	0.49
1:C:661:LEU:HD13	1:C:673:TRP:CD1	2.47	0.49
1:C:4120:LEU:O	1:C:4124:VAL:HG23	2.13	0.49
1:C:4775:VAL:HG21	1:D:4745:ILE:HD11	1.94	0.49
1:D:1609:VAL:HA	1:D:1620:VAL:HA	1.94	0.49
1:A:52:THR:OG1	1:A:282:VAL:HG11	2.13	0.49
1:A:1086:ARG:HH21	1:A:1251:LEU:HD13	1.77	0.49
1:A:1397:UNK:HA	1:A:1412:UNK:HA	1.94	0.49
1:A:1677:LEU:O	1:A:1681:VAL:HG22	2.13	0.49
1:A:2781:MET:HE3	1:A:2843:MET:HE3	1.95	0.49
1:B:3898:ASP:OD1	1:B:3898:ASP:N	2.45	0.49
1:C:1629:MET:HE3	1:C:1642:ILE:HG21	1.94	0.49
1:C:1715:TYR:CZ	1:C:1762:MET:HB3	2.48	0.49
1:C:3712:SER:OG	1:C:3716:LYS:NZ	2.38	0.49
1:D:3898:ASP:OD1	1:D:3898:ASP:N	2.45	0.49
1:A:1609:VAL:HA	1:A:1620:VAL:HA	1.94	0.49
1:A:1715:TYR:CZ	1:A:1762:MET:HB3	2.48	0.49
1:A:1720:LEU:HD21	1:A:1831:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2478:GLU:HG2	1:A:2479:VAL:HG13	1.95	0.49
1:A:2753:GLN:HG2	1:A:2755:LEU:H	1.77	0.49
1:A:2839:MET:HB2	1:A:2892:PHE:HE2	1.77	0.49
1:B:2428:LEU:HD21	1:B:2482:PHE:CE1	2.48	0.49
1:B:4120:LEU:O	1:B:4124:VAL:HG23	2.13	0.49
1:B:4660:TYR:HB3	1:B:4664:ARG:HH21	1.77	0.49
1:C:200:SER:HG	1:C:202:HIS:CE1	2.30	0.49
1:C:408:SER:O	1:C:408:SER:OG	2.31	0.49
1:C:1720:LEU:HD21	1:C:1831:ILE:HD13	1.95	0.49
1:C:2839:MET:HB2	1:C:2892:PHE:HE2	1.77	0.49
1:D:1677:LEU:O	1:D:1681:VAL:HG22	2.13	0.49
1:D:1720:LEU:HD21	1:D:1831:ILE:HD13	1.95	0.49
1:D:2352:ILE:HD12	1:D:2358:ARG:HG3	1.95	0.49
1:A:4660:TYR:HB3	1:A:4664:ARG:HH21	1.78	0.49
1:B:934:GLN:O	1:B:937:LEU:HG	2.12	0.49
1:C:2428:LEU:HD21	1:C:2482:PHE:CE1	2.48	0.49
1:D:946:LEU:HD21	1:D:998:LYS:HB3	1.95	0.49
1:D:3831:ASP:OD1	1:D:3831:ASP:N	2.45	0.49
1:D:4649:LYS:NZ	1:D:4669:LEU:O	2.45	0.49
1:B:200:SER:HG	1:B:202:HIS:CE1	2.30	0.49
1:B:1727:ILE:HG22	1:B:1758:LEU:HD23	1.95	0.49
1:B:2895:LEU:HD11	1:B:2900:TYR:CD1	2.48	0.49
1:B:4775:VAL:HG21	1:C:4745:ILE:HD11	1.94	0.49
1:C:2206:SER:OG	1:C:2207:ARG:N	2.45	0.49
1:C:2352:ILE:HD12	1:C:2358:ARG:HG3	1.95	0.49
1:A:677:LEU:HD11	1:A:800:VAL:HG13	1.95	0.49
1:A:2895:LEU:HD11	1:A:2900:TYR:CD1	2.48	0.49
1:B:763:ALA:HB3	1:B:764:PRO:HD3	1.94	0.49
1:B:1677:LEU:O	1:B:1681:VAL:HG22	2.13	0.49
1:C:946:LEU:HD21	1:C:998:LYS:HB3	1.95	0.49
1:D:1989:GLU:HG2	1:D:1992:ARG:HD3	1.95	0.49
1:A:408:SER:O	1:A:408:SER:OG	2.31	0.48
1:A:2428:LEU:HD21	1:A:2482:PHE:CE1	2.48	0.48
1:B:1572:PHE:HZ	1:B:1587:LEU:HD11	1.77	0.48
1:B:2442:PRO:HG3	1:B:2454:ASP:HB2	1.95	0.48
1:C:763:ALA:HB3	1:C:764:PRO:HD3	1.94	0.48
1:C:1572:PHE:HZ	1:C:1587:LEU:HD11	1.78	0.48
1:C:1727:ILE:HG22	1:C:1758:LEU:HD23	1.95	0.48
1:C:2317:ASN:O	1:C:2321:ARG:HG2	2.13	0.48
1:D:763:ALA:HB3	1:D:764:PRO:HD3	1.94	0.48
1:D:1572:PHE:HZ	1:D:1587:LEU:HD11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1727:ILE:HG22	1:D:1758:LEU:HD23	1.95	0.48
1:D:2428:LEU:HD21	1:D:2482:PHE:CE1	2.48	0.48
1:D:4507:VAL:HG23	1:D:4574:LEU:HD22	1.94	0.48
1:D:4832:ASP:N	1:D:4832:ASP:OD1	2.45	0.48
1:B:677:LEU:HD11	1:B:800:VAL:HG13	1.96	0.48
1:B:4649:LYS:NZ	1:B:4669:LEU:O	2.45	0.48
1:C:1609:VAL:HA	1:C:1620:VAL:HA	1.94	0.48
1:C:4111:ASP:HB2	1:C:4114:LEU:HB3	1.95	0.48
1:D:2317:ASN:O	1:D:2321:ARG:HG2	2.13	0.48
1:D:4120:LEU:O	1:D:4124:VAL:HG23	2.13	0.48
1:A:76:ARG:O	1:A:80:GLU:HG2	2.14	0.48
1:A:1989:GLU:HG2	1:A:1992:ARG:HD3	1.95	0.48
1:A:4112:THR:HA	1:A:4115:GLN:HB2	1.95	0.48
1:A:4775:VAL:HG21	1:B:4745:ILE:HD11	1.95	0.48
1:B:2206:SER:OG	1:B:2207:ARG:N	2.45	0.48
1:B:2352:ILE:HD12	1:B:2358:ARG:HG3	1.95	0.48
1:C:76:ARG:O	1:C:80:GLU:HG2	2.14	0.48
1:C:2442:PRO:HG3	1:C:2454:ASP:HB2	1.95	0.48
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.94	0.48
1:A:1572:PHE:HZ	1:A:1587:LEU:HD11	1.77	0.48
1:A:1727:ILE:HG22	1:A:1758:LEU:HD23	1.95	0.48
1:A:2442:PRO:HG3	1:A:2454:ASP:HB2	1.95	0.48
1:B:76:ARG:O	1:B:80:GLU:HG2	2.14	0.48
1:B:4112:THR:HA	1:B:4115:GLN:HB2	1.95	0.48
1:C:1362:ASP:N	1:C:1362:ASP:OD1	2.45	0.48
1:D:76:ARG:O	1:D:80:GLU:HG2	2.14	0.48
1:D:1715:TYR:CZ	1:D:1762:MET:HB3	2.48	0.48
1:D:4111:ASP:HB2	1:D:4114:LEU:HB3	1.95	0.48
1:A:1827:TYR:CZ	1:A:1831:ILE:HD11	2.49	0.48
1:A:2718:TYR:CD1	1:A:2718:TYR:C	2.92	0.48
1:A:4116:THR:O	1:A:4119:GLU:HG2	2.14	0.48
2:G:79:PRO:HB3	2:G:95:ASN:HA	1.95	0.48
1:B:1972:ILE:HD13	1:B:1975:LEU:HD21	1.95	0.48
1:B:4116:THR:O	1:B:4119:GLU:HG2	2.14	0.48
1:C:1273:ILE:HD11	1:C:1287:GLN:HB2	1.96	0.48
1:C:1677:LEU:HA	1:C:1680:HIS:HB2	1.95	0.48
1:C:2718:TYR:CD1	1:C:2718:TYR:C	2.92	0.48
1:C:3898:ASP:OD1	1:C:3898:ASP:N	2.45	0.48
1:C:3961:SER:OG	1:C:3962:SER:N	2.47	0.48
1:D:2718:TYR:CD1	1:D:2718:TYR:C	2.92	0.48
1:D:2781:MET:HE3	1:D:2843:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:SER:HG	1:A:202:HIS:CE1	2.31	0.48
1:A:4507:VAL:HG23	1:A:4574:LEU:HD22	1.94	0.48
1:B:52:THR:OG1	1:B:282:VAL:HG11	2.13	0.48
1:B:3420:UNK:HA	1:B:3421:UNK:HA	1.65	0.48
1:C:1972:ILE:HD13	1:C:1975:LEU:HD21	1.95	0.48
1:C:2895:LEU:HD11	1:C:2900:TYR:CD1	2.48	0.48
1:D:1397:UNK:HA	1:D:1412:UNK:HA	1.94	0.48
1:B:234:LEU:HD12	1:B:405:LEU:HB3	1.96	0.48
1:B:1578:ASN:OD1	1:B:1578:ASN:N	2.46	0.48
1:B:1715:TYR:CZ	1:B:1762:MET:HB3	2.48	0.48
1:B:1989:GLU:HG2	1:B:1992:ARG:HD3	1.95	0.48
2:H:79:PRO:HB3	2:H:95:ASN:HA	1.95	0.48
1:C:3831:ASP:OD1	1:C:3831:ASP:N	2.45	0.48
1:C:4026:THR:HG21	1:C:4083:VAL:HG11	1.96	0.48
1:A:1750:PRO:HG3	1:A:2057:LEU:HD22	1.96	0.48
1:A:3961:SER:OG	1:A:3962:SER:N	2.47	0.48
1:A:4832:ASP:N	1:A:4832:ASP:OD1	2.45	0.48
1:B:1683:GLU:HB3	2:H:42:ASP:HB3	1.96	0.48
2:H:83:TYR:HB3	2:H:87:GLY:HA2	1.96	0.48
1:C:1207:LEU:HB3	1:C:1211:GLN:HB2	1.96	0.48
1:C:2851:TRP:HA	1:C:2854:LYS:HE2	1.96	0.48
1:C:4044:LYS:HZ3	1:C:4069:ALA:HB1	1.79	0.48
1:D:52:THR:OG1	1:D:282:VAL:HG11	2.13	0.48
1:D:3961:SER:OG	1:D:3962:SER:N	2.47	0.48
1:D:4515:LEU:O	1:D:4518:TYR:HB2	2.14	0.48
1:A:4120:LEU:O	1:A:4124:VAL:HG23	2.13	0.48
2:G:57:ILE:HG13	2:G:60:PHE:HB2	1.96	0.48
1:B:3934:LEU:HD23	1:B:3939:LEU:HD22	1.96	0.48
1:B:4883:MET:HE1	1:B:4888:PHE:HD1	1.79	0.48
1:C:950:VAL:HG11	1:C:1057:LEU:HD21	1.96	0.48
1:C:1677:LEU:O	1:C:1681:VAL:HG22	2.13	0.48
1:C:4883:MET:HE1	1:C:4888:PHE:HD1	1.79	0.48
1:D:1273:ILE:HD11	1:D:1287:GLN:HB2	1.96	0.48
1:D:1677:LEU:HA	1:D:1680:HIS:HB2	1.95	0.48
1:D:2895:LEU:HD11	1:D:2900:TYR:CD1	2.48	0.48
2:J:79:PRO:HB3	2:J:95:ASN:HA	1.95	0.48
1:A:2432:VAL:HG12	1:A:2486:LEU:HD13	1.96	0.48
2:G:83:TYR:HB3	2:G:87:GLY:HA2	1.96	0.48
1:B:721:ASP:OD1	1:B:721:ASP:N	2.46	0.48
1:B:1709:ASP:HA	1:B:1713:SER:HB2	1.96	0.48
1:B:4111:ASP:HB2	1:B:4114:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1685:GLN:NE2	1:C:1703:TYR:OH	2.47	0.48
1:C:1727:ILE:HD12	1:C:2119:LEU:HD11	1.95	0.48
1:C:3934:LEU:HD23	1:C:3939:LEU:HD22	1.96	0.48
1:C:4832:ASP:N	1:C:4832:ASP:OD1	2.45	0.48
1:D:4044:LYS:HZ3	1:D:4069:ALA:HB1	1.79	0.48
2:J:57:ILE:HG13	2:J:60:PHE:HB2	1.96	0.48
1:A:2317:ASN:O	1:A:2321:ARG:HG2	2.13	0.47
1:A:3950:PHE:HZ	1:A:3973:LEU:HG	1.79	0.47
1:A:4111:ASP:HB2	1:A:4114:LEU:HB3	1.95	0.47
1:B:1677:LEU:HA	1:B:1680:HIS:HB2	1.95	0.47
1:B:1827:TYR:CZ	1:B:1831:ILE:HD11	2.49	0.47
1:B:2781:MET:HE3	1:B:2843:MET:HE3	1.95	0.47
1:B:3905:PHE:O	1:B:3909:ILE:HG12	2.14	0.47
1:C:309:MET:HB2	1:C:312:LYS:HZ2	1.79	0.47
1:C:2346:MET:HE3	1:C:2388:MET:HG2	1.95	0.47
2:I:79:PRO:HB3	2:I:95:ASN:HA	1.95	0.47
1:D:677:LEU:HD11	1:D:800:VAL:HG13	1.95	0.47
1:D:2184:LYS:HE2	1:D:2184:LYS:HB3	1.75	0.47
1:D:2442:PRO:HG3	1:D:2454:ASP:HB2	1.95	0.47
1:A:721:ASP:N	1:A:721:ASP:OD1	2.46	0.47
1:A:946:LEU:HD21	1:A:998:LYS:HB3	1.95	0.47
1:A:1727:ILE:HD12	1:A:2119:LEU:HD11	1.95	0.47
1:A:2346:MET:HE3	1:A:2388:MET:HG2	1.95	0.47
1:A:2765:LYS:O	1:A:2765:LYS:HD3	2.14	0.47
1:A:3898:ASP:OD1	1:A:3898:ASP:N	2.45	0.47
1:B:946:LEU:HD21	1:B:998:LYS:HB3	1.95	0.47
1:B:950:VAL:HG11	1:B:1057:LEU:HD21	1.96	0.47
1:B:2346:MET:HE3	1:B:2388:MET:HG2	1.95	0.47
1:B:2432:VAL:HG12	1:B:2486:LEU:HD13	1.96	0.47
1:B:2718:TYR:C	1:B:2718:TYR:CD1	2.92	0.47
1:B:3961:SER:OG	1:B:3962:SER:N	2.47	0.47
2:H:57:ILE:HG13	2:H:60:PHE:HB2	1.96	0.47
1:C:52:THR:OG1	1:C:282:VAL:HG11	2.13	0.47
1:C:677:LEU:HD11	1:C:800:VAL:HG13	1.95	0.47
2:I:83:TYR:HB3	2:I:87:GLY:HA2	1.96	0.47
1:D:950:VAL:HG11	1:D:1057:LEU:HD21	1.96	0.47
1:D:1685:GLN:NE2	1:D:1703:TYR:OH	2.47	0.47
1:D:2355:ASP:OD2	1:D:2357:SER:OG	2.30	0.47
1:D:4112:THR:HA	1:D:4115:GLN:HB2	1.95	0.47
1:D:4116:THR:O	1:D:4119:GLU:HG2	2.14	0.47
2:J:83:TYR:HB3	2:J:87:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:LEU:HD13	1:A:995:MET:HB3	1.97	0.47
1:B:1207:LEU:HB3	1:B:1211:GLN:HB2	1.96	0.47
1:B:1655:HIS:HB3	1:B:1699:LEU:HD11	1.97	0.47
1:B:2851:TRP:HA	1:B:2854:LYS:HE2	1.96	0.47
1:B:3950:PHE:HZ	1:B:3973:LEU:HG	1.79	0.47
1:C:304:LYS:HB2	1:C:316:LEU:HD23	1.96	0.47
1:C:1655:HIS:HB3	1:C:1699:LEU:HD11	1.96	0.47
1:C:1827:TYR:CZ	1:C:1831:ILE:HD11	2.49	0.47
1:C:4507:VAL:HG23	1:C:4574:LEU:HD22	1.94	0.47
1:D:4883:MET:HE1	1:D:4888:PHE:HD1	1.79	0.47
1:A:1655:HIS:HB3	1:A:1699:LEU:HD11	1.97	0.47
1:A:1677:LEU:HA	1:A:1680:HIS:HB2	1.95	0.47
1:A:1786:ASP:OD1	1:A:1786:ASP:N	2.45	0.47
1:A:3905:PHE:O	1:A:3909:ILE:HG12	2.14	0.47
1:A:4044:LYS:HZ3	1:A:4069:ALA:HB1	1.78	0.47
1:C:4112:THR:HA	1:C:4115:GLN:HB2	1.95	0.47
1:C:4116:THR:O	1:C:4119:GLU:HG2	2.14	0.47
1:C:4515:LEU:O	1:C:4518:TYR:HB2	2.14	0.47
1:D:1827:TYR:CZ	1:D:1831:ILE:HD11	2.49	0.47
1:A:2159:ASN:HD22	1:A:2162:ARG:NH2	2.13	0.47
1:B:1217:PHE:HD2	1:B:1247:ILE:HG13	1.80	0.47
1:C:1704:TYR:O	1:C:1708:ILE:HG12	2.15	0.47
1:D:946:LEU:HD13	1:D:995:MET:HB3	1.97	0.47
1:D:1655:HIS:HB3	1:D:1699:LEU:HD11	1.96	0.47
1:A:1207:LEU:HB3	1:A:1211:GLN:HB2	1.96	0.47
1:A:4026:THR:HG21	1:A:4083:VAL:HG11	1.96	0.47
1:A:4630:ASP:O	1:A:4634:ILE:HG23	2.15	0.47
1:B:2159:ASN:HD22	1:B:2162:ARG:NH2	2.13	0.47
1:B:4630:ASP:O	1:B:4634:ILE:HG23	2.15	0.47
1:C:1709:ASP:HA	1:C:1713:SER:HB2	1.96	0.47
1:C:1750:PRO:HG3	1:C:2057:LEU:HD22	1.96	0.47
1:C:2404:GLU:HG3	1:C:2405:MET:H	1.79	0.47
1:D:1578:ASN:OD1	1:D:1578:ASN:N	2.46	0.47
1:D:2346:MET:HE3	1:D:2388:MET:HG2	1.95	0.47
1:A:59:PRO:HB3	1:A:296:ARG:NH1	2.29	0.47
1:A:1685:GLN:NE2	1:A:1703:TYR:OH	2.47	0.47
1:A:4883:MET:HE1	1:A:4888:PHE:HD1	1.79	0.47
1:B:1273:ILE:HD11	1:B:1287:GLN:HB2	1.96	0.47
1:B:1750:PRO:HG3	1:B:2057:LEU:HD22	1.96	0.47
1:B:1965:ARG:O	1:B:1966:SER:OG	2.33	0.47
1:B:3909:ILE:HG21	1:B:3969:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4135:ILE:HB	1:B:4147:VAL:HG22	1.96	0.47
1:C:946:LEU:HD13	1:C:995:MET:HB3	1.97	0.47
1:C:2355:ASP:OD2	1:C:2357:SER:OG	2.30	0.47
1:C:4859:ALA:HB1	1:D:4866:ILE:HD11	1.97	0.47
1:D:234:LEU:HD12	1:D:405:LEU:HB3	1.96	0.47
1:D:304:LYS:HB2	1:D:316:LEU:HD23	1.96	0.47
1:D:2404:GLU:HG3	1:D:2405:MET:H	1.79	0.47
1:D:2851:TRP:HA	1:D:2854:LYS:HE2	1.96	0.47
1:D:3934:LEU:HD23	1:D:3939:LEU:HD22	1.96	0.47
1:D:3950:PHE:HZ	1:D:3973:LEU:HG	1.78	0.47
1:A:950:VAL:HG11	1:A:1057:LEU:HD21	1.96	0.47
1:A:1965:ARG:O	1:A:1966:SER:OG	2.33	0.47
1:A:4515:LEU:O	1:A:4518:TYR:HB2	2.14	0.47
1:B:946:LEU:HD13	1:B:995:MET:HB3	1.97	0.47
1:B:4026:THR:HG21	1:B:4083:VAL:HG11	1.96	0.47
1:C:1578:ASN:OD1	1:C:1578:ASN:N	2.46	0.47
1:C:4135:ILE:HB	1:C:4147:VAL:HG22	1.96	0.47
1:C:4601:ARG:HD2	1:C:4711:VAL:HG21	1.97	0.47
2:I:57:ILE:HG13	2:I:60:PHE:HB2	1.96	0.47
1:D:1727:ILE:HD12	1:D:2119:LEU:HD11	1.95	0.47
1:A:304:LYS:HB2	1:A:316:LEU:HD23	1.96	0.47
1:A:1704:TYR:O	1:A:1708:ILE:HG12	2.15	0.47
1:A:3934:LEU:HD23	1:A:3939:LEU:HD22	1.96	0.47
1:B:1727:ILE:HD12	1:B:2119:LEU:HD11	1.95	0.47
1:C:234:LEU:HD12	1:C:405:LEU:HB3	1.96	0.47
1:C:2330:PHE:HD1	1:C:2394:LEU:HD21	1.80	0.47
1:C:3905:PHE:O	1:C:3909:ILE:HG12	2.14	0.47
1:D:1207:LEU:HB3	1:D:1211:GLN:HB2	1.96	0.47
1:D:2765:LYS:O	1:D:2765:LYS:HD3	2.14	0.47
1:A:234:LEU:HA	1:A:408:SER:HB3	1.97	0.47
1:A:4135:ILE:HB	1:A:4147:VAL:HG22	1.96	0.47
1:B:2404:GLU:HG3	1:B:2405:MET:H	1.79	0.47
1:C:2265:VAL:HG12	1:C:2326:ARG:HD2	1.97	0.47
1:C:4601:ARG:HD3	1:C:4707:TRP:CZ2	2.50	0.47
1:D:59:PRO:HB3	1:D:296:ARG:NH1	2.29	0.47
1:D:1676:ALA:HB1	2:J:91:VAL:CG2	2.45	0.47
1:D:1704:TYR:O	1:D:1708:ILE:HG12	2.15	0.47
1:D:1709:ASP:HA	1:D:1713:SER:HB2	1.97	0.47
1:D:3661:ASP:OD2	1:D:3733:ARG:NH2	2.48	0.47
1:D:4135:ILE:HB	1:D:4147:VAL:HG22	1.96	0.47
1:D:4630:ASP:O	1:D:4634:ILE:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:PHE:HD2	1:A:1247:ILE:HG13	1.80	0.46
1:A:1273:ILE:HD11	1:A:1287:GLN:HB2	1.96	0.46
1:A:1972:ILE:HA	1:A:1975:LEU:HG	1.97	0.46
1:A:2404:GLU:HG3	1:A:2405:MET:H	1.79	0.46
1:A:2735:LYS:HD3	1:A:2740:TRP:CE3	2.51	0.46
1:B:304:LYS:HB2	1:B:316:LEU:HD23	1.96	0.46
1:B:1311:ALA:HA	1:B:1312:UNK:HA	1.50	0.46
1:B:1685:GLN:NE2	1:B:1703:TYR:OH	2.47	0.46
1:B:4515:LEU:O	1:B:4518:TYR:HB2	2.14	0.46
1:C:1361:LYS:HA	1:C:1566:PRO:HA	1.98	0.46
1:C:1989:GLU:HG2	1:C:1992:ARG:HD3	1.95	0.46
1:C:2184:LYS:HE2	1:C:2184:LYS:HB3	1.75	0.46
1:C:3950:PHE:HZ	1:C:3973:LEU:HG	1.79	0.46
1:C:4630:ASP:O	1:C:4634:ILE:HG23	2.15	0.46
1:D:1750:PRO:HG3	1:D:2057:LEU:HD22	1.96	0.46
1:D:2154:PHE:HD2	1:D:2205:ILE:HD11	1.81	0.46
1:D:2330:PHE:HD1	1:D:2394:LEU:HD21	1.80	0.46
1:D:2432:VAL:HG12	1:D:2486:LEU:HD13	1.96	0.46
1:D:4026:THR:HG21	1:D:4083:VAL:HG11	1.96	0.46
1:A:336:GLU:HG3	1:A:338:LEU:HD22	1.98	0.46
1:A:2851:TRP:HA	1:A:2854:LYS:HE2	1.96	0.46
1:B:59:PRO:HB3	1:B:296:ARG:NH1	2.29	0.46
1:B:1361:LYS:HA	1:B:1566:PRO:HA	1.98	0.46
1:B:2735:LYS:HD3	1:B:2740:TRP:CE3	2.51	0.46
1:C:1217:PHE:HD2	1:C:1247:ILE:HG13	1.80	0.46
1:C:2159:ASN:HD22	1:C:2162:ARG:NH2	2.13	0.46
1:C:2432:VAL:HG12	1:C:2486:LEU:HD13	1.96	0.46
1:C:3909:ILE:HG21	1:C:3969:GLU:HB3	1.96	0.46
1:D:1972:ILE:HA	1:D:1975:LEU:HG	1.97	0.46
1:D:2159:ASN:HD22	1:D:2162:ARG:NH2	2.13	0.46
1:D:3909:ILE:HG21	1:D:3969:GLU:HB3	1.96	0.46
1:D:4079:TYR:O	1:D:4083:VAL:HG22	2.16	0.46
1:A:2522:UNK:C	1:A:2524:UNK:H	2.29	0.46
1:B:336:GLU:HG3	1:B:338:LEU:HD22	1.98	0.46
1:B:2184:LYS:HE2	1:B:2184:LYS:HB3	1.75	0.46
1:B:3661:ASP:OD2	1:B:3733:ARG:NH2	2.48	0.46
1:B:4044:LYS:HZ1	1:B:4071:THR:H	1.63	0.46
1:B:4601:ARG:HD3	1:B:4707:TRP:CZ2	2.50	0.46
1:C:1965:ARG:O	1:C:1966:SER:OG	2.33	0.46
1:C:3661:ASP:OD2	1:C:3733:ARG:NH2	2.48	0.46
1:D:2522:UNK:C	1:D:2524:UNK:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:OD1	1:A:233:VAL:N	2.49	0.46
1:A:718:VAL:HG13	1:A:793:SER:HB3	1.98	0.46
1:B:234:LEU:HA	1:B:408:SER:HB3	1.98	0.46
1:B:2317:ASN:O	1:B:2321:ARG:HG2	2.13	0.46
1:B:2330:PHE:HD1	1:B:2394:LEU:HD21	1.80	0.46
1:B:3831:ASP:OD1	1:B:3831:ASP:N	2.45	0.46
1:B:4601:ARG:HD2	1:B:4711:VAL:HG21	1.97	0.46
1:C:200:SER:HG	1:C:202:HIS:HD1	1.56	0.46
1:C:2839:MET:HB2	1:C:2892:PHE:CE2	2.51	0.46
1:C:4079:TYR:O	1:C:4083:VAL:HG22	2.16	0.46
1:D:1361:LYS:HA	1:D:1566:PRO:HA	1.97	0.46
1:D:2321:ARG:O	1:D:2325:ARG:HG2	2.15	0.46
1:A:234:LEU:HD12	1:A:405:LEU:HB3	1.96	0.46
1:A:2154:PHE:HD1	1:A:2205:ILE:HD11	1.81	0.46
1:A:3909:ILE:HG21	1:A:3969:GLU:HB3	1.96	0.46
1:B:1786:ASP:OD1	1:B:1786:ASP:N	2.45	0.46
1:B:2265:VAL:HG12	1:B:2326:ARG:HD2	1.97	0.46
1:B:2765:LYS:O	1:B:2765:LYS:HD3	2.14	0.46
1:C:59:PRO:HB3	1:C:296:ARG:NH1	2.29	0.46
1:C:232:ASP:OD1	1:C:233:VAL:N	2.49	0.46
1:C:336:GLU:HG3	1:C:338:LEU:HD22	1.98	0.46
1:D:234:LEU:HA	1:D:408:SER:HB3	1.98	0.46
1:D:336:GLU:HG3	1:D:338:LEU:HD22	1.98	0.46
1:D:718:VAL:HG13	1:D:793:SER:HB3	1.98	0.46
1:D:2265:VAL:HG12	1:D:2326:ARG:HD2	1.97	0.46
1:D:3905:PHE:O	1:D:3909:ILE:HG12	2.14	0.46
1:D:4029:ASP:OD1	1:D:4029:ASP:N	2.49	0.46
1:A:1709:ASP:HA	1:A:1713:SER:HB2	1.96	0.46
1:A:4050:ALA:O	1:A:4054:HIS:ND1	2.49	0.46
1:A:4601:ARG:HD2	1:A:4711:VAL:HG21	1.97	0.46
1:B:1738:THR:HG22	1:B:1926:ALA:HB1	1.98	0.46
1:B:2718:TYR:C	1:B:2718:TYR:HD1	2.24	0.46
2:H:28:THR:HA	2:H:39:SER:HA	1.98	0.46
1:C:1683:GLU:HB3	2:I:42:ASP:HB3	1.97	0.46
1:C:2321:ARG:O	1:C:2325:ARG:HG2	2.15	0.46
1:C:2425:LEU:HD13	1:C:2425:LEU:HA	1.85	0.46
1:C:2735:LYS:HD3	1:C:2740:TRP:CE3	2.51	0.46
1:D:2718:TYR:C	1:D:2718:TYR:HD1	2.24	0.46
1:D:2735:LYS:HD3	1:D:2740:TRP:CE3	2.51	0.46
1:A:2430:ASP:O	1:A:2434:VAL:HG23	2.15	0.46
1:C:721:ASP:OD1	1:C:721:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2099:ARG:O	1:C:2103:LYS:NZ	2.39	0.46
1:D:408:SER:O	1:D:408:SER:OG	2.31	0.46
1:D:4601:ARG:HD2	1:D:4711:VAL:HG21	1.97	0.46
1:A:1361:LYS:HA	1:A:1566:PRO:HA	1.97	0.46
1:A:2355:ASP:OD2	1:A:2357:SER:OG	2.30	0.46
1:A:2425:LEU:HD13	1:A:2425:LEU:HA	1.85	0.46
1:A:3639:LEU:HD23	1:A:3693:ILE:HG21	1.98	0.46
1:A:3661:ASP:OD2	1:A:3733:ARG:NH2	2.48	0.46
1:B:2430:ASP:O	1:B:2434:VAL:HG23	2.15	0.46
1:B:4050:ALA:O	1:B:4054:HIS:ND1	2.49	0.46
1:C:3420:UNK:HA	1:C:3421:UNK:HA	1.65	0.46
1:C:4653:MET:HE2	1:C:4666:SER:HA	1.98	0.46
1:D:274:LEU:HD22	1:D:408:SER:HB2	1.98	0.46
1:D:1359:ILE:HG13	1:D:1360:ASP:H	1.81	0.46
1:D:4108:MET:HE2	1:D:4108:MET:HB3	1.89	0.46
1:D:4601:ARG:HD3	1:D:4707:TRP:CZ2	2.50	0.46
1:A:672:LYS:NZ	1:A:760:ASP:OD2	2.36	0.46
1:A:4014:LYS:HB3	1:A:4018:MET:HE3	1.98	0.46
1:B:232:ASP:OD1	1:B:233:VAL:N	2.49	0.46
1:B:555:LEU:HD11	1:B:585:ALA:HB1	1.98	0.46
1:B:2321:ARG:O	1:B:2325:ARG:HG2	2.15	0.46
1:C:2430:ASP:O	1:C:2434:VAL:HG23	2.15	0.46
1:D:2430:ASP:O	1:D:2434:VAL:HG23	2.15	0.46
1:A:1359:ILE:HG13	1:A:1360:ASP:H	1.81	0.46
1:A:1981:ASP:OD1	1:A:1981:ASP:N	2.49	0.46
1:A:4745:ILE:HD11	1:D:4775:VAL:HG21	1.97	0.46
1:B:1704:TYR:O	1:B:1708:ILE:HG12	2.15	0.46
1:B:2522:UNK:C	1:B:2524:UNK:H	2.29	0.46
1:B:2715:LYS:O	1:B:2718:TYR:HB3	2.16	0.46
1:B:4014:LYS:HB3	1:B:4018:MET:HE3	1.98	0.46
1:B:4653:MET:HE2	1:B:4666:SER:HA	1.98	0.46
1:B:4731:GLY:HA2	1:B:4737:PHE:HB2	1.98	0.46
1:C:1738:THR:HG22	1:C:1926:ALA:HB1	1.98	0.46
2:I:28:THR:HA	2:I:39:SER:HA	1.98	0.46
1:D:4023:LYS:HG2	1:D:4087:HIS:CE1	2.51	0.46
2:J:28:THR:HA	2:J:39:SER:HA	1.98	0.46
1:A:2265:VAL:HG12	1:A:2326:ARG:HD2	1.97	0.45
1:A:4731:GLY:HA2	1:A:4737:PHE:HB2	1.97	0.45
1:C:1100:ARG:HB3	1:C:1236:TYR:CD2	2.51	0.45
1:C:1359:ILE:HG13	1:C:1360:ASP:H	1.81	0.45
1:C:2765:LYS:O	1:C:2765:LYS:HD3	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4653:MET:HE2	1:D:4666:SER:HA	1.98	0.45
1:A:1738:THR:HG22	1:A:1926:ALA:HB1	1.98	0.45
1:A:2091:TYR:CD2	1:A:3639:LEU:HD13	2.52	0.45
1:A:2839:MET:HB2	1:A:2892:PHE:CE2	2.51	0.45
1:B:541:ILE:HG22	1:B:547:ASN:HB3	1.98	0.45
1:B:3639:LEU:HD23	1:B:3693:ILE:HG21	1.98	0.45
1:C:234:LEU:HA	1:C:408:SER:HB3	1.98	0.45
1:C:2325:ARG:HA	1:C:2325:ARG:HD3	1.77	0.45
1:C:4050:ALA:O	1:C:4054:HIS:ND1	2.49	0.45
1:D:232:ASP:OD1	1:D:233:VAL:N	2.49	0.45
1:D:1100:ARG:HB3	1:D:1236:TYR:CD2	2.52	0.45
1:A:2321:ARG:O	1:A:2325:ARG:HG2	2.15	0.45
1:A:2330:PHE:HD1	1:A:2394:LEU:HD21	1.80	0.45
1:A:4108:MET:HE2	1:A:4108:MET:HB3	1.89	0.45
1:A:4653:MET:HE2	1:A:4666:SER:HA	1.98	0.45
2:G:28:THR:HA	2:G:39:SER:HA	1.98	0.45
1:C:541:ILE:HG22	1:C:547:ASN:HB3	1.98	0.45
1:D:1217:PHE:HD2	1:D:1247:ILE:HG13	1.80	0.45
1:D:2715:LYS:O	1:D:2718:TYR:HB3	2.16	0.45
1:D:2839:MET:HB2	1:D:2892:PHE:CE2	2.51	0.45
1:D:2855:LYS:O	1:D:2859:LEU:HG	2.17	0.45
1:D:3712:SER:OG	1:D:3716:LYS:NZ	2.38	0.45
1:D:4596:LEU:HG	1:D:4600:LYS:HE3	1.98	0.45
1:A:1936:GLN:O	1:A:1939:GLN:HG3	2.17	0.45
1:B:606:ARG:NH1	1:B:1635:GLU:OE2	2.50	0.45
1:B:1936:GLN:O	1:B:1939:GLN:HG3	2.17	0.45
1:B:1981:ASP:OD1	1:B:1981:ASP:N	2.49	0.45
1:B:2091:TYR:CD2	1:B:3639:LEU:HD13	2.52	0.45
1:B:3712:SER:OG	1:B:3716:LYS:NZ	2.38	0.45
1:C:244:CYS:SG	1:C:273:SER:HB2	2.56	0.45
1:C:718:VAL:HG13	1:C:793:SER:HB3	1.98	0.45
1:C:4014:LYS:HB3	1:C:4018:MET:HE3	1.98	0.45
1:D:245:LEU:HD11	1:D:260:VAL:HG12	1.99	0.45
1:A:2238:PRO:O	1:A:2241:VAL:HG12	2.17	0.45
1:A:2715:LYS:O	1:A:2718:TYR:HB3	2.16	0.45
1:A:2718:TYR:O	1:A:2718:TYR:HD1	2.00	0.45
1:A:4079:TYR:O	1:A:4083:VAL:HG22	2.16	0.45
1:B:244:CYS:SG	1:B:273:SER:HB2	2.56	0.45
1:B:274:LEU:HD22	1:B:408:SER:HB2	1.98	0.45
1:B:718:VAL:HG13	1:B:793:SER:HB3	1.98	0.45
1:B:1095:ALA:HB1	1:B:1200:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:GLN:NE2	1:C:390:LYS:O	2.49	0.45
1:C:555:LEU:HD11	1:C:585:ALA:HB1	1.98	0.45
1:D:1190:LEU:HD11	1:D:1193:LYS:HE3	1.98	0.45
1:D:1738:THR:HG22	1:D:1926:ALA:HB1	1.98	0.45
1:D:1981:ASP:N	1:D:1981:ASP:OD1	2.49	0.45
1:D:3420:UNK:HA	1:D:3421:UNK:HA	1.65	0.45
1:D:3639:LEU:HD23	1:D:3693:ILE:HG21	1.98	0.45
1:A:1100:ARG:HB3	1:A:1236:TYR:CD2	2.51	0.45
1:A:1190:LEU:HD11	1:A:1193:LYS:HE3	1.98	0.45
1:A:2718:TYR:C	1:A:2718:TYR:HD1	2.24	0.45
1:A:4023:LYS:HG2	1:A:4087:HIS:CE1	2.51	0.45
1:A:4029:ASP:OD1	1:A:4029:ASP:N	2.49	0.45
1:A:4601:ARG:HD3	1:A:4707:TRP:CZ2	2.50	0.45
1:B:2217:LEU:HA	1:B:2220:LEU:HG	1.98	0.45
1:B:2753:GLN:HE22	1:B:2762:LEU:HD12	1.82	0.45
1:B:3974:GLN:HE22	1:B:4012:ILE:HG21	1.81	0.45
1:B:4023:LYS:HG2	1:B:4087:HIS:CE1	2.51	0.45
1:C:122:ARG:HD3	1:C:129:TYR:CZ	2.52	0.45
1:C:606:ARG:NH1	1:C:1635:GLU:OE2	2.50	0.45
1:C:1972:ILE:HA	1:C:1975:LEU:HG	1.97	0.45
1:C:2154:PHE:HD1	1:C:2205:ILE:HD11	1.81	0.45
1:C:2522:UNK:C	1:C:2524:UNK:H	2.29	0.45
1:C:2855:LYS:HZ3	1:C:2867:HIS:HB2	1.81	0.45
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.25	0.45
1:D:2718:TYR:HD1	1:D:2718:TYR:O	2.00	0.45
1:D:4048:HIS:CE1	1:D:4059:GLN:HE22	2.35	0.45
1:A:881:ILE:O	1:A:884:ARG:HG3	2.17	0.45
1:A:4118:LEU:HD23	1:A:4118:LEU:HA	1.81	0.45
1:B:2238:PRO:O	1:B:2241:VAL:HG12	2.17	0.45
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.25	0.45
1:B:4619:GLN:OE1	1:B:4631:ARG:NH2	2.50	0.45
1:C:692:HIS:HB3	1:C:795:SER:HB3	1.99	0.45
1:D:244:CYS:SG	1:D:273:SER:HB2	2.57	0.45
1:D:1769:PHE:O	2:J:83:TYR:OH	2.35	0.45
1:D:2217:LEU:HA	1:D:2220:LEU:HG	1.98	0.45
1:D:4050:ALA:O	1:D:4054:HIS:ND1	2.49	0.45
1:A:21:VAL:HG12	1:A:23:GLN:HG3	1.99	0.45
1:A:375:GLN:NE2	1:A:390:LYS:O	2.49	0.45
1:A:555:LEU:HD11	1:A:585:ALA:HB1	1.98	0.45
1:A:1311:ALA:HA	1:A:1312:UNK:HA	1.50	0.45
1:A:2753:GLN:HE22	1:A:2762:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1972:ILE:HA	1:B:1975:LEU:HG	1.97	0.45
1:B:4079:TYR:O	1:B:4083:VAL:HG22	2.16	0.45
1:D:1965:ARG:O	1:D:1966:SER:OG	2.33	0.45
1:D:3974:GLN:HE22	1:D:4012:ILE:HG21	1.81	0.45
1:A:274:LEU:HD22	1:A:408:SER:HB2	1.98	0.45
1:A:4044:LYS:NZ	1:A:4069:ALA:HB1	2.32	0.45
1:B:122:ARG:HD3	1:B:129:TYR:CZ	2.52	0.45
1:B:1100:ARG:HB3	1:B:1236:TYR:CD2	2.51	0.45
1:B:1769:PHE:O	2:H:83:TYR:OH	2.34	0.45
1:B:2718:TYR:HD1	1:B:2718:TYR:O	2.00	0.45
1:C:1190:LEU:HD11	1:C:1193:LYS:HE3	1.98	0.45
1:C:1936:GLN:O	1:C:1939:GLN:HG3	2.17	0.45
1:C:1981:ASP:OD1	1:C:1981:ASP:N	2.49	0.45
1:C:2091:TYR:CD2	1:C:3639:LEU:HD13	2.52	0.45
1:C:2718:TYR:HD1	1:C:2718:TYR:O	2.00	0.45
1:C:2753:GLN:HE22	1:C:2762:LEU:HD12	1.82	0.45
1:C:4596:LEU:HG	1:C:4600:LYS:HE3	1.98	0.45
1:D:1668:LEU:HD23	1:D:2131:VAL:HG12	1.99	0.45
1:D:4014:LYS:HB3	1:D:4018:MET:HE3	1.98	0.45
1:A:122:ARG:HD3	1:A:129:TYR:CZ	2.52	0.45
1:A:244:CYS:SG	1:A:273:SER:HB2	2.57	0.45
1:A:245:LEU:HD11	1:A:260:VAL:HG12	1.99	0.45
1:A:1095:ALA:HB1	1:A:1200:GLY:HA3	1.99	0.45
1:A:2217:LEU:HA	1:A:2220:LEU:HG	1.98	0.45
1:A:3974:GLN:HE22	1:A:4012:ILE:HG21	1.81	0.45
1:B:692:HIS:HB3	1:B:795:SER:HB3	1.99	0.45
1:B:907:VAL:HB	1:B:914:GLN:HE22	1.82	0.45
1:B:1359:ILE:HG13	1:B:1360:ASP:H	1.81	0.45
1:B:2839:MET:HB2	1:B:2892:PHE:CE2	2.51	0.45
1:B:3964:ILE:HG21	1:B:4085:ARG:HD2	1.99	0.45
1:B:4118:LEU:HD23	1:B:4118:LEU:HA	1.80	0.45
1:C:35:LEU:HD23	1:C:51:SER:HA	1.99	0.45
1:D:1165:MET:HB3	1:D:1236:TYR:CE2	2.52	0.45
1:D:3951:ALA:O	1:D:3954:GLN:HG2	2.17	0.45
1:B:35:LEU:HD23	1:B:51:SER:HA	1.99	0.44
1:B:1190:LEU:HD11	1:B:1193:LYS:HE3	1.99	0.44
1:B:2855:LYS:O	1:B:2859:LEU:HG	2.17	0.44
1:C:274:LEU:HD22	1:C:408:SER:HB2	1.98	0.44
1:C:686:VAL:HG13	1:C:687:THR:H	1.82	0.44
1:C:2855:LYS:O	1:C:2859:LEU:HG	2.17	0.44
1:C:4048:HIS:CE1	1:C:4059:GLN:HE22	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:881:ILE:O	1:D:884:ARG:HG3	2.17	0.44
1:D:4619:GLN:OE1	1:D:4631:ARG:NH2	2.50	0.44
1:A:299:HIS:HD2	1:A:302:THR:HG22	1.82	0.44
1:A:2735:LYS:HA	1:A:2740:TRP:CE3	2.47	0.44
1:A:3694:MET:HE1	1:A:3738:MET:HE1	1.98	0.44
1:A:3951:ALA:O	1:A:3954:GLN:HG2	2.18	0.44
1:B:1666:CYS:SG	1:B:1710:ILE:HG22	2.57	0.44
1:B:2735:LYS:HA	1:B:2740:TRP:CE3	2.47	0.44
1:B:3698:CYS:SG	1:B:3730:LEU:HD21	2.58	0.44
1:B:3871:ILE:HA	1:B:3874:VAL:HG12	1.99	0.44
1:B:4662:ARG:NH2	1:B:4675:ALA:O	2.51	0.44
1:C:1165:MET:HB3	1:C:1236:TYR:CE2	2.52	0.44
1:C:2238:PRO:O	1:C:2241:VAL:HG12	2.17	0.44
1:C:2715:LYS:O	1:C:2718:TYR:HB3	2.16	0.44
1:C:2718:TYR:C	1:C:2718:TYR:HD1	2.24	0.44
1:C:3639:LEU:HD23	1:C:3693:ILE:HG21	1.98	0.44
1:C:3694:MET:HE1	1:C:3738:MET:HE1	1.98	0.44
1:C:3974:GLN:HE22	1:C:4012:ILE:HG21	1.81	0.44
1:D:122:ARG:HD3	1:D:129:TYR:CZ	2.52	0.44
1:D:541:ILE:HG22	1:D:547:ASN:HB3	1.98	0.44
1:D:555:LEU:HD11	1:D:585:ALA:HB1	1.98	0.44
1:D:686:VAL:HG13	1:D:687:THR:H	1.82	0.44
1:D:2091:TYR:CD2	1:D:3639:LEU:HD13	2.52	0.44
1:D:3694:MET:HE1	1:D:3738:MET:HE1	1.98	0.44
1:A:1666:CYS:SG	1:A:1710:ILE:HG22	2.57	0.44
1:A:4048:HIS:CE1	1:A:4059:GLN:HE22	2.35	0.44
1:A:4662:ARG:NH2	1:A:4675:ALA:O	2.50	0.44
1:B:686:VAL:HG13	1:B:687:THR:H	1.82	0.44
1:B:4044:LYS:NZ	1:B:4069:ALA:HB1	2.32	0.44
1:C:712:GLU:CD	1:C:839:GLU:HG2	2.43	0.44
1:C:2774:ILE:H	1:C:2774:ILE:HG12	1.57	0.44
1:C:4044:LYS:NZ	1:C:4069:ALA:HB1	2.32	0.44
1:C:4619:GLN:OE1	1:C:4631:ARG:NH2	2.50	0.44
2:I:19:LYS:HD3	2:I:51:ILE:HG22	1.99	0.44
1:D:907:VAL:HB	1:D:914:GLN:HE22	1.83	0.44
1:D:1936:GLN:O	1:D:1939:GLN:HG3	2.17	0.44
1:D:2238:PRO:O	1:D:2241:VAL:HG12	2.17	0.44
1:D:2753:GLN:HE22	1:D:2762:LEU:HD12	1.82	0.44
1:D:3964:ILE:HG21	1:D:4085:ARG:HD2	1.99	0.44
1:D:4044:LYS:NZ	1:D:4069:ALA:HB1	2.32	0.44
1:D:4731:GLY:HA2	1:D:4737:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:19:LYS:HD3	2:J:51:ILE:HG22	1.99	0.44
1:A:606:ARG:NH1	1:A:1635:GLU:OE2	2.50	0.44
1:A:1217:PHE:O	1:A:1240:ALA:N	2.50	0.44
1:A:2855:LYS:O	1:A:2859:LEU:HG	2.17	0.44
1:A:4619:GLN:OE1	1:A:4631:ARG:NH2	2.50	0.44
1:B:881:ILE:O	1:B:884:ARG:HG3	2.17	0.44
1:C:299:HIS:HD2	1:C:302:THR:HG22	1.82	0.44
1:C:881:ILE:O	1:C:884:ARG:HG3	2.17	0.44
1:C:3698:CYS:SG	1:C:3730:LEU:HD21	2.58	0.44
1:D:297:LEU:HD12	1:D:329:PHE:HD2	1.82	0.44
1:D:299:HIS:HD2	1:D:302:THR:HG22	1.82	0.44
1:D:3698:CYS:SG	1:D:3730:LEU:HD21	2.58	0.44
1:A:35:LEU:HD23	1:A:51:SER:HA	1.99	0.44
1:A:123:HIS:CD2	1:A:126:SER:H	2.32	0.44
1:A:695:VAL:HG12	1:A:792:VAL:HG23	2.00	0.44
1:B:562:LEU:HD21	1:B:600:LEU:HD22	2.00	0.44
1:B:816:PRO:HB2	1:B:819:TYR:CD1	2.53	0.44
2:H:19:LYS:HD3	2:H:51:ILE:HG22	1.99	0.44
1:C:245:LEU:HD11	1:C:260:VAL:HG12	1.99	0.44
1:C:893:TRP:O	1:C:897:LYS:HD3	2.18	0.44
1:C:2217:LEU:HA	1:C:2220:LEU:HG	1.98	0.44
1:C:4662:ARG:NH2	1:C:4675:ALA:O	2.51	0.44
1:C:4731:GLY:HA2	1:C:4737:PHE:HB2	1.98	0.44
1:D:712:GLU:CD	1:D:839:GLU:HG2	2.43	0.44
1:D:721:ASP:N	1:D:721:ASP:OD1	2.46	0.44
1:D:892:LEU:HA	1:D:895:MET:HG3	2.00	0.44
1:D:1652:LEU:HD12	1:D:1699:LEU:HD13	2.00	0.44
1:D:2231:PRO:HG3	1:D:2381:ILE:HG12	2.00	0.44
1:D:4112:THR:O	1:D:4116:THR:HG23	2.18	0.44
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.25	0.44
1:D:4701:ASP:OD1	1:D:4701:ASP:N	2.31	0.44
1:D:4781:THR:HG21	1:D:4812:TYR:HB2	2.00	0.44
1:A:233:VAL:HA	1:A:276:ARG:HA	2.00	0.44
1:A:686:VAL:HG13	1:A:687:THR:H	1.82	0.44
1:A:1793:ILE:HG12	1:A:1843:ILE:HD11	1.99	0.44
1:B:514:PHE:HD2	1:B:523:GLY:HA2	1.82	0.44
1:B:1977:ASN:N	1:B:1977:ASN:OD1	2.51	0.44
1:B:2154:PHE:HD1	1:B:2205:ILE:HD11	1.81	0.44
1:C:514:PHE:HD2	1:C:523:GLY:HA2	1.82	0.44
1:C:555:LEU:HD21	1:C:578:VAL:HG11	2.00	0.44
1:C:606:ARG:HH22	1:C:1633:ILE:HG23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:907:VAL:HB	1:C:914:GLN:HE22	1.83	0.44
1:C:1039:ASP:OD1	1:C:1039:ASP:N	2.51	0.44
1:C:2231:PRO:HG3	1:C:2381:ILE:HG12	2.00	0.44
1:C:3951:ALA:O	1:C:3954:GLN:HG2	2.18	0.44
1:C:4023:LYS:HG2	1:C:4087:HIS:CE1	2.51	0.44
1:D:606:ARG:HH22	1:D:1633:ILE:HG23	1.83	0.44
1:D:1666:CYS:SG	1:D:1710:ILE:HG22	2.57	0.44
1:D:1977:ASN:OD1	1:D:1977:ASN:N	2.51	0.44
1:D:2855:LYS:HZ3	1:D:2867:HIS:HB2	1.82	0.44
1:A:2431:LEU:HD13	1:A:2471:LEU:HG	2.00	0.44
1:B:233:VAL:HA	1:B:276:ARG:HA	2.00	0.44
1:B:477:ASN:OD1	1:B:480:ARG:NH2	2.51	0.44
1:B:1165:MET:HB3	1:B:1236:TYR:CE2	2.52	0.44
1:C:562:LEU:HD21	1:C:600:LEU:HD22	2.00	0.44
1:C:1095:ALA:HB1	1:C:1200:GLY:HA3	1.99	0.44
1:C:3871:ILE:HA	1:C:3874:VAL:HG12	1.99	0.44
1:D:695:VAL:HG12	1:D:792:VAL:HG23	2.00	0.44
1:D:1095:ALA:HB1	1:D:1200:GLY:HA3	1.99	0.44
1:D:1395:UNK:HA	1:D:1415:UNK:HA	2.00	0.44
1:A:541:ILE:HG22	1:A:547:ASN:HB3	1.98	0.44
1:A:892:LEU:HA	1:A:895:MET:HG3	2.00	0.44
1:A:1165:MET:HB3	1:A:1236:TYR:CE2	2.52	0.44
1:A:3920:THR:HG22	1:A:3980:MET:HA	2.00	0.44
1:A:3964:ILE:HG21	1:A:4085:ARG:HD2	1.99	0.44
1:A:4154:SER:O	1:A:4158:GLN:HG2	2.18	0.44
2:G:19:LYS:HD3	2:G:51:ILE:HG22	1.99	0.44
1:B:892:LEU:HA	1:B:895:MET:HG3	2.00	0.44
1:B:2231:PRO:HG3	1:B:2381:ILE:HG12	2.00	0.44
1:B:3694:MET:HE1	1:B:3738:MET:HE1	1.98	0.44
1:C:235:ARG:HB2	1:C:406:SER:OG	2.18	0.44
1:C:816:PRO:HB2	1:C:819:TYR:CD1	2.53	0.44
1:C:1652:LEU:HD12	1:C:1699:LEU:HD13	2.00	0.44
1:C:2431:LEU:HD13	1:C:2471:LEU:HG	2.00	0.44
1:C:4781:THR:HG21	1:C:4812:TYR:HB2	2.00	0.44
1:D:606:ARG:NH1	1:D:1635:GLU:OE2	2.50	0.44
1:D:893:TRP:O	1:D:897:LYS:HD3	2.18	0.44
1:D:4662:ARG:NH2	1:D:4675:ALA:O	2.50	0.44
1:A:606:ARG:HH22	1:A:1633:ILE:HG23	1.83	0.44
1:A:2062:SER:O	1:A:2066:VAL:HG22	2.18	0.44
1:A:3871:ILE:HA	1:A:3874:VAL:HG12	1.99	0.44
1:A:4596:LEU:HG	1:A:4600:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:VAL:HG12	1:B:792:VAL:HG23	2.00	0.44
1:B:1395:UNK:HA	1:B:1415:UNK:HA	2.00	0.44
1:B:1668:LEU:HD23	1:B:2131:VAL:HG12	1.99	0.44
1:B:1793:ILE:HG12	1:B:1843:ILE:HD11	2.00	0.44
1:B:1838:GLU:OE1	1:B:1838:GLU:N	2.43	0.44
1:B:2107:ILE:HG13	1:B:2108:ASN:N	2.33	0.44
1:B:2118:LEU:HD12	1:B:2148:ILE:HG22	2.00	0.44
1:B:4048:HIS:CE1	1:B:4059:GLN:HE22	2.35	0.44
1:C:892:LEU:HA	1:C:895:MET:HG3	2.00	0.44
1:C:1666:CYS:SG	1:C:1710:ILE:HG22	2.57	0.44
1:C:1668:LEU:HD23	1:C:2131:VAL:HG12	1.99	0.44
1:A:323:ASP:O	1:A:327:THR:OG1	2.28	0.43
1:A:555:LEU:HD21	1:A:578:VAL:HG11	2.00	0.43
1:A:1395:UNK:HA	1:A:1415:UNK:HA	2.00	0.43
1:A:1928:SER:O	1:A:1932:VAL:HG12	2.18	0.43
1:A:3698:CYS:SG	1:A:3730:LEU:HD21	2.58	0.43
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.25	0.43
1:A:4859:ALA:HB1	1:B:4866:ILE:HD11	2.00	0.43
1:B:21:VAL:HG12	1:B:23:GLN:HG3	1.99	0.43
1:B:712:GLU:CD	1:B:839:GLU:HG2	2.43	0.43
1:B:1004:HIS:HB3	1:B:1035:TYR:HB2	2.00	0.43
1:B:3802:LEU:HD23	1:B:3802:LEU:HA	1.89	0.43
1:B:4107:HIS:O	1:B:4109:PRO:HD3	2.18	0.43
1:C:1928:SER:O	1:C:1932:VAL:HG12	2.18	0.43
1:C:3955:MET:HE2	1:C:3955:MET:HB3	1.94	0.43
1:C:4154:SER:O	1:C:4158:GLN:HG2	2.18	0.43
1:D:1004:HIS:HB3	1:D:1035:TYR:HB2	2.00	0.43
1:A:1652:LEU:HD12	1:A:1699:LEU:HD13	2.00	0.43
1:A:2231:PRO:HG3	1:A:2381:ILE:HG12	2.00	0.43
1:A:2463:HIS:O	1:A:2467:MET:HG2	2.19	0.43
1:B:245:LEU:HD11	1:B:260:VAL:HG12	1.99	0.43
1:B:555:LEU:HD21	1:B:578:VAL:HG11	2.00	0.43
1:B:2128:LEU:HA	1:B:2131:VAL:HG22	2.00	0.43
1:B:2431:LEU:HD13	1:B:2471:LEU:HG	2.00	0.43
1:C:2844:ALA:HB1	1:C:2884:ASP:OD1	2.18	0.43
1:C:3964:ILE:HG21	1:C:4085:ARG:HD2	1.99	0.43
1:D:555:LEU:HD21	1:D:578:VAL:HG11	2.00	0.43
1:D:1034:PRO:HD2	1:D:1037:LEU:HD13	2.01	0.43
1:D:2062:SER:O	1:D:2066:VAL:HG22	2.18	0.43
1:D:2844:ALA:HB1	1:D:2884:ASP:OD1	2.19	0.43
1:D:3920:THR:HG22	1:D:3980:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:43:ARG:HG3	2:J:45:LYS:HG2	2.00	0.43
1:A:626:ARG:HH21	1:A:2131:VAL:HG11	1.83	0.43
1:A:712:GLU:CD	1:A:839:GLU:HG2	2.43	0.43
1:A:907:VAL:HB	1:A:914:GLN:HE22	1.83	0.43
1:A:1838:GLU:OE1	1:A:1838:GLU:N	2.43	0.43
1:A:2118:LEU:HD12	1:A:2148:ILE:HG22	2.00	0.43
1:A:4112:THR:O	1:A:4116:THR:HG23	2.18	0.43
2:G:69:LEU:HD12	2:G:107:LEU:HB2	2.00	0.43
1:B:299:HIS:HD2	1:B:302:THR:HG22	1.82	0.43
1:B:2197:ARG:HB2	1:B:2236:SER:HB3	2.00	0.43
1:B:2844:ALA:HB1	1:B:2884:ASP:OD1	2.18	0.43
1:B:4596:LEU:HG	1:B:4600:LYS:HE3	1.98	0.43
1:C:21:VAL:HG12	1:C:23:GLN:HG3	1.99	0.43
1:C:1395:UNK:HA	1:C:1415:UNK:HA	2.00	0.43
1:C:2092:ASP:OD1	1:C:2095:GLY:N	2.49	0.43
1:C:2197:ARG:HB2	1:C:2236:SER:HB3	2.00	0.43
1:C:4029:ASP:OD1	1:C:4029:ASP:N	2.49	0.43
1:D:35:LEU:HD23	1:D:51:SER:HA	1.99	0.43
1:D:514:PHE:HD2	1:D:523:GLY:HA2	1.82	0.43
1:D:692:HIS:HB3	1:D:795:SER:HB3	1.99	0.43
1:D:1311:ALA:HA	1:D:1312:UNK:HA	1.50	0.43
1:D:4154:SER:O	1:D:4158:GLN:HG2	2.18	0.43
1:A:816:PRO:HB2	1:A:819:TYR:CD1	2.53	0.43
1:A:1668:LEU:HD23	1:A:2131:VAL:HG12	1.99	0.43
1:A:2279:LEU:HB3	1:A:2284:TYR:HB2	2.00	0.43
1:A:2844:ALA:HB1	1:A:2884:ASP:OD1	2.18	0.43
1:A:2855:LYS:HZ3	1:A:2867:HIS:HB2	1.83	0.43
1:B:2335:ARG:HE	1:B:2335:ARG:HB3	1.67	0.43
1:B:2346:MET:HE2	1:B:2346:MET:HB3	1.87	0.43
1:B:4154:SER:O	1:B:4158:GLN:HG2	2.18	0.43
1:C:1004:HIS:HB3	1:C:1035:TYR:HB2	2.00	0.43
1:C:1157:GLN:N	1:C:1160:ASP:OD2	2.41	0.43
1:C:2735:LYS:HA	1:C:2740:TRP:CE3	2.47	0.43
1:C:4112:THR:O	1:C:4116:THR:HG23	2.18	0.43
2:I:69:LEU:HD12	2:I:107:LEU:HB2	2.00	0.43
1:D:816:PRO:HB2	1:D:819:TYR:CD1	2.53	0.43
1:D:1793:ILE:HG12	1:D:1843:ILE:HD11	1.99	0.43
1:D:2431:LEU:HD13	1:D:2471:LEU:HG	2.00	0.43
1:D:4107:HIS:O	1:D:4109:PRO:HD3	2.18	0.43
1:A:1977:ASN:OD1	1:A:1977:ASN:N	2.51	0.43
1:A:2500:SER:O	1:A:2500:SER:OG	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2852:ALA:O	1:A:2855:LYS:HG3	2.19	0.43
1:A:3916:PHE:O	1:A:3920:THR:HG23	2.19	0.43
1:B:200:SER:HG	1:B:202:HIS:HD1	1.60	0.43
1:B:606:ARG:HH22	1:B:1633:ILE:HG23	1.83	0.43
1:B:1928:SER:O	1:B:1932:VAL:HG12	2.18	0.43
1:B:2171:MET:O	1:B:2175:VAL:HG13	2.19	0.43
1:B:4029:ASP:OD1	1:B:4029:ASP:N	2.49	0.43
1:B:4051:MET:O	1:B:4057:TYR:HB2	2.19	0.43
1:B:4859:ALA:HB1	1:C:4866:ILE:HD11	2.01	0.43
1:C:695:VAL:HG12	1:C:792:VAL:HG23	2.00	0.43
1:D:477:ASN:OD1	1:D:480:ARG:NH2	2.51	0.43
1:D:769:ARG:HA	1:D:774:PRO:HA	2.01	0.43
1:D:1928:SER:O	1:D:1932:VAL:HG12	2.18	0.43
1:D:2197:ARG:HB2	1:D:2236:SER:HB3	2.00	0.43
1:A:235:ARG:HB2	1:A:406:SER:OG	2.18	0.43
1:A:297:LEU:HD12	1:A:329:PHE:HD2	1.82	0.43
1:A:4107:HIS:O	1:A:4109:PRO:HD3	2.18	0.43
1:B:297:LEU:HD12	1:B:329:PHE:HD2	1.82	0.43
1:B:1006:VAL:HG23	1:B:1009:ARG:NH1	2.34	0.43
1:B:1034:PRO:HD2	1:B:1037:LEU:HD13	2.00	0.43
1:B:2076:ASP:HB3	1:B:2079:LEU:HB3	2.01	0.43
1:B:3920:THR:HG22	1:B:3980:MET:HA	2.00	0.43
1:C:1977:ASN:OD1	1:C:1977:ASN:N	2.51	0.43
1:C:3916:PHE:O	1:C:3920:THR:HG23	2.19	0.43
1:C:4107:HIS:O	1:C:4109:PRO:HD3	2.18	0.43
1:D:1683:GLU:HB3	2:J:42:ASP:HB3	2.00	0.43
1:D:2118:LEU:HD12	1:D:2148:ILE:HG22	2.00	0.43
1:A:49:LEU:HD11	1:A:194:LEU:HD11	2.01	0.43
1:A:562:LEU:HD21	1:A:600:LEU:HD22	2.00	0.43
1:A:692:HIS:HB3	1:A:795:SER:HB3	1.99	0.43
1:A:1004:HIS:HB3	1:A:1035:TYR:HB2	2.00	0.43
1:A:1039:ASP:OD1	1:A:1039:ASP:N	2.51	0.43
1:A:2128:LEU:HA	1:A:2131:VAL:HG22	2.00	0.43
1:A:2171:MET:O	1:A:2175:VAL:HG13	2.19	0.43
1:A:2197:ARG:HB2	1:A:2236:SER:HB3	2.00	0.43
1:A:4781:THR:HG21	1:A:4812:TYR:HB2	2.00	0.43
1:B:49:LEU:HD11	1:B:194:LEU:HD11	2.01	0.43
1:B:1173:MET:O	1:B:1191:ALA:N	2.37	0.43
1:B:1652:LEU:HD12	1:B:1699:LEU:HD13	2.00	0.43
1:B:3951:ALA:O	1:B:3954:GLN:HG2	2.18	0.43
1:B:4112:THR:O	1:B:4116:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2062:SER:O	1:C:2066:VAL:HG22	2.18	0.43
1:D:1039:ASP:OD1	1:D:1039:ASP:N	2.51	0.43
1:D:2463:HIS:O	1:D:2467:MET:HG2	2.19	0.43
1:D:3832:ASP:OD1	1:D:3832:ASP:N	2.52	0.43
1:D:3871:ILE:HA	1:D:3874:VAL:HG12	2.00	0.43
2:J:69:LEU:HD12	2:J:107:LEU:HB2	2.00	0.43
1:A:769:ARG:HA	1:A:774:PRO:HA	2.00	0.43
1:A:4615:TYR:CE1	1:A:4631:ARG:HB2	2.54	0.43
1:B:235:ARG:HB2	1:B:406:SER:OG	2.18	0.43
1:B:893:TRP:O	1:B:897:LYS:HD3	2.18	0.43
2:H:43:ARG:HG3	2:H:45:LYS:HG2	2.00	0.43
2:H:69:LEU:HD12	2:H:107:LEU:HB2	2.00	0.43
1:C:556:ASP:OD1	1:C:556:ASP:N	2.50	0.43
1:C:3832:ASP:OD1	1:C:3832:ASP:N	2.51	0.43
1:C:3920:THR:HG22	1:C:3980:MET:HA	2.00	0.43
1:D:2128:LEU:HA	1:D:2131:VAL:HG22	2.00	0.43
1:D:4615:TYR:CE1	1:D:4631:ARG:HB2	2.54	0.43
1:A:514:PHE:HD2	1:A:523:GLY:HA2	1.82	0.43
1:A:1173:MET:O	1:A:1191:ALA:N	2.37	0.43
1:B:123:HIS:CD2	1:B:126:SER:H	2.32	0.43
1:B:2092:ASP:OD1	1:B:2095:GLY:N	2.49	0.43
1:B:4615:TYR:CE1	1:B:4631:ARG:HB2	2.54	0.43
1:B:4781:THR:HG21	1:B:4812:TYR:HB2	2.00	0.43
1:C:1676:ALA:HB1	2:I:91:VAL:CG2	2.48	0.43
1:D:21:VAL:HG12	1:D:23:GLN:HG3	1.99	0.43
1:D:562:LEU:HD21	1:D:600:LEU:HD22	2.00	0.43
1:D:2774:ILE:H	1:D:2774:ILE:HG12	1.57	0.43
1:A:893:TRP:O	1:A:897:LYS:HD3	2.18	0.43
1:A:1034:PRO:HD2	1:A:1037:LEU:HD13	2.00	0.43
1:A:1758:LEU:HD13	1:A:1758:LEU:HA	1.89	0.43
1:A:1764:PHE:HD1	1:A:1780:SER:HB2	1.84	0.43
1:A:3812:LYS:HB3	1:A:3812:LYS:HE2	1.81	0.43
1:A:4929:GLU:O	1:A:4930:THR:OG1	2.35	0.43
1:B:626:ARG:HH21	1:B:2131:VAL:HG11	1.83	0.43
1:B:1039:ASP:OD1	1:B:1039:ASP:N	2.51	0.43
1:C:297:LEU:HD12	1:C:329:PHE:HD2	1.82	0.43
1:C:318:ASP:N	1:C:318:ASP:OD1	2.52	0.43
1:C:1793:ILE:HG12	1:C:1843:ILE:HD11	1.99	0.43
1:A:318:ASP:N	1:A:318:ASP:OD1	2.52	0.42
1:A:876:PRO:HA	1:A:879:GLU:HG2	2.01	0.42
1:B:2062:SER:O	1:B:2066:VAL:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2859:LEU:HD11	1:B:2867:HIS:CD2	2.54	0.42
1:C:123:HIS:CD2	1:C:126:SER:H	2.32	0.42
1:C:1034:PRO:HD2	1:C:1037:LEU:HD13	2.01	0.42
1:C:2118:LEU:HD12	1:C:2148:ILE:HG22	2.00	0.42
1:C:3839:PHE:HE1	1:C:3873:THR:HG23	1.84	0.42
1:C:4106:GLU:OE2	1:C:4148:TYR:OH	2.33	0.42
1:C:4615:TYR:CE1	1:C:4631:ARG:HB2	2.54	0.42
2:I:43:ARG:HG3	2:I:45:LYS:HG2	2.00	0.42
1:D:224:ALA:HB3	1:D:227:TYR:HD2	1.84	0.42
1:D:2425:LEU:HD13	1:D:2425:LEU:HA	1.85	0.42
1:D:2859:LEU:HD11	1:D:2867:HIS:CD2	2.54	0.42
1:A:477:ASN:OD1	1:A:480:ARG:NH2	2.51	0.42
1:A:2107:ILE:HG13	1:A:2108:ASN:N	2.33	0.42
1:B:224:ALA:HB3	1:B:227:TYR:HD2	1.84	0.42
1:B:876:PRO:HA	1:B:879:GLU:HG2	2.01	0.42
1:B:2463:HIS:O	1:B:2467:MET:HG2	2.19	0.42
1:C:233:VAL:HA	1:C:276:ARG:HA	2.00	0.42
1:C:2107:ILE:HG13	1:C:2108:ASN:N	2.33	0.42
1:C:2279:LEU:HB3	1:C:2284:TYR:HB2	2.00	0.42
1:D:235:ARG:HB2	1:D:406:SER:OG	2.18	0.42
1:D:626:ARG:HH21	1:D:2131:VAL:HG11	1.83	0.42
1:A:1006:VAL:HG23	1:A:1009:ARG:NH1	2.34	0.42
1:A:2859:LEU:HD11	1:A:2867:HIS:CD2	2.54	0.42
1:A:4065:LEU:HD13	1:A:4065:LEU:HA	1.90	0.42
1:B:318:ASP:OD1	1:B:318:ASP:N	2.52	0.42
1:B:556:ASP:OD1	1:B:556:ASP:N	2.50	0.42
1:B:643:LEU:HD12	1:B:1658:THR:OG1	2.20	0.42
1:B:2501:LEU:HD11	1:B:2505:ALA:HB2	2.02	0.42
1:B:2852:ALA:O	1:B:2855:LYS:HG3	2.19	0.42
1:B:3916:PHE:O	1:B:3920:THR:HG23	2.19	0.42
1:C:224:ALA:HB3	1:C:227:TYR:HD2	1.84	0.42
1:C:410:HIS:HE1	1:C:414:ARG:HH21	1.68	0.42
1:C:1028:ARG:NH2	1:C:1033:VAL:HG23	2.35	0.42
1:C:2171:MET:O	1:C:2175:VAL:HG13	2.19	0.42
1:C:2463:HIS:O	1:C:2467:MET:HG2	2.19	0.42
1:C:2852:ALA:O	1:C:2855:LYS:HG3	2.19	0.42
1:C:4051:MET:O	1:C:4057:TYR:HB2	2.19	0.42
1:D:233:VAL:HA	1:D:276:ARG:HA	2.00	0.42
1:D:1028:ARG:NH2	1:D:1033:VAL:HG23	2.34	0.42
1:A:224:ALA:HB3	1:A:227:TYR:HD2	1.85	0.42
1:A:1932:VAL:HG11	1:A:3616:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2076:ASP:HB3	1:A:2079:LEU:HB3	2.01	0.42
1:A:2215:ASP:N	1:A:2215:ASP:OD1	2.52	0.42
1:A:2895:LEU:HD11	1:A:2900:TYR:HD1	1.84	0.42
1:B:1642:ILE:HG23	1:B:1643:LEU:HD23	2.01	0.42
1:C:626:ARG:HH21	1:C:2131:VAL:HG11	1.83	0.42
1:C:1764:PHE:HD1	1:C:1780:SER:HB2	1.84	0.42
1:C:2501:LEU:HD11	1:C:2505:ALA:HB2	2.02	0.42
1:D:556:ASP:OD1	1:D:556:ASP:N	2.50	0.42
1:D:2171:MET:O	1:D:2175:VAL:HG13	2.19	0.42
1:D:2852:ALA:O	1:D:2855:LYS:HG3	2.19	0.42
1:D:4051:MET:O	1:D:4057:TYR:HB2	2.19	0.42
1:A:1028:ARG:NH2	1:A:1033:VAL:HG23	2.35	0.42
1:A:1955:ALA:O	1:A:1959:ARG:HG2	2.19	0.42
1:B:769:ARG:HA	1:B:774:PRO:HA	2.01	0.42
1:B:1676:ALA:HB1	2:H:91:VAL:CG2	2.50	0.42
1:B:2065:MET:SD	1:B:2083:MET:HG3	2.60	0.42
1:B:2436:SER:OG	1:B:2489:VAL:HG12	2.20	0.42
1:C:162:ILE:HG22	1:C:181:LEU:HD13	2.02	0.42
1:C:562:LEU:HA	1:C:571:ILE:HD13	2.01	0.42
1:C:2076:ASP:HB3	1:C:2079:LEU:HB3	2.01	0.42
1:C:2128:LEU:HA	1:C:2131:VAL:HG22	2.00	0.42
1:C:4132:LEU:HD11	1:C:4134:ARG:HH21	1.85	0.42
1:D:550:GLN:HE21	1:D:550:GLN:HB2	1.73	0.42
1:D:1764:PHE:HD1	1:D:1780:SER:HB2	1.84	0.42
1:D:1955:ALA:O	1:D:1959:ARG:HG2	2.19	0.42
1:D:2099:ARG:O	1:D:2103:LYS:NZ	2.39	0.42
1:D:2215:ASP:OD1	1:D:2215:ASP:N	2.52	0.42
1:D:3916:PHE:O	1:D:3920:THR:HG23	2.19	0.42
1:D:4132:LEU:HD11	1:D:4134:ARG:HH21	1.85	0.42
1:A:434:ASP:OD2	1:A:504:ARG:NH1	2.53	0.42
1:A:2065:MET:SD	1:A:2083:MET:HG3	2.60	0.42
1:A:2425:LEU:HD22	1:D:143:LEU:HD11	2.02	0.42
1:B:4108:MET:HE2	1:B:4108:MET:HB3	1.89	0.42
1:C:3804:LEU:HD21	1:C:3890:TYR:HB2	2.02	0.42
1:D:3624:GLU:HA	1:D:3628:ILE:HD11	2.02	0.42
1:A:550:GLN:HE21	1:A:550:GLN:HB2	1.73	0.42
1:A:907:VAL:O	1:A:914:GLN:NE2	2.53	0.42
1:A:2234:ARG:HD2	1:A:2234:ARG:HA	1.91	0.42
1:A:4051:MET:O	1:A:4057:TYR:HB2	2.19	0.42
1:B:410:HIS:HE1	1:B:414:ARG:HH21	1.68	0.42
1:B:3832:ASP:OD1	1:B:3832:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:VAL:HG23	1:C:726:GLY:HA3	2.02	0.42
1:C:2215:ASP:OD1	1:C:2215:ASP:N	2.52	0.42
1:D:123:HIS:CD2	1:D:126:SER:H	2.32	0.42
1:D:562:LEU:HA	1:D:571:ILE:HD13	2.01	0.42
1:D:703:TYR:O	1:D:856:SER:OG	2.32	0.42
1:D:718:VAL:HG23	1:D:726:GLY:HA3	2.02	0.42
1:D:2162:ARG:HH21	1:D:2208:GLN:HE21	1.68	0.42
1:D:2279:LEU:HB3	1:D:2284:TYR:HB2	2.00	0.42
2:J:23:CYS:HB2	2:J:51:ILE:HD11	2.02	0.42
1:A:562:LEU:HA	1:A:571:ILE:HD13	2.01	0.42
1:A:2772:TRP:N	1:A:2773:PRO:HD2	2.35	0.42
1:A:4132:LEU:HD11	1:A:4134:ARG:HH21	1.85	0.42
1:B:1955:ALA:O	1:B:1959:ARG:HG2	2.19	0.42
1:B:2279:LEU:HB3	1:B:2284:TYR:HB2	2.00	0.42
1:B:4132:LEU:HD11	1:B:4134:ARG:HH21	1.85	0.42
1:C:49:LEU:HD11	1:C:194:LEU:HD11	2.01	0.42
1:C:1642:ILE:HG23	1:C:1643:LEU:HD23	2.01	0.42
1:C:1955:ALA:O	1:C:1959:ARG:HG2	2.19	0.42
1:D:3839:PHE:HE1	1:D:3873:THR:HG23	1.84	0.42
1:D:4792:TYR:HB2	1:D:4805:CYS:HB2	2.02	0.42
1:A:643:LEU:HD12	1:A:1658:THR:OG1	2.20	0.42
1:A:1196:ASP:OD1	1:A:1196:ASP:N	2.53	0.42
1:B:1157:GLN:N	1:B:1160:ASP:OD2	2.41	0.42
1:B:1296:ASN:OD1	1:B:1296:ASN:N	2.53	0.42
1:B:2325:ARG:HA	1:B:2325:ARG:HD3	1.77	0.42
1:B:2895:LEU:HD11	1:B:2900:TYR:HD1	1.84	0.42
1:C:434:ASP:OD2	1:C:504:ARG:NH1	2.53	0.42
1:C:643:LEU:HD12	1:C:1658:THR:OG1	2.20	0.42
1:C:769:ARG:HA	1:C:774:PRO:HA	2.01	0.42
1:C:1196:ASP:OD1	1:C:1196:ASP:N	2.53	0.42
1:C:2772:TRP:N	1:C:2773:PRO:HD2	2.35	0.42
1:D:410:HIS:HE1	1:D:414:ARG:HH21	1.68	0.42
1:D:643:LEU:HD12	1:D:1658:THR:OG1	2.20	0.42
1:D:1006:VAL:HG23	1:D:1009:ARG:NH1	2.33	0.42
1:D:1932:VAL:HG11	1:D:3616:VAL:HB	2.01	0.42
1:D:2065:MET:SD	1:D:2083:MET:HG3	2.60	0.42
1:A:410:HIS:HE1	1:A:414:ARG:HH21	1.68	0.42
1:A:556:ASP:N	1:A:556:ASP:OD1	2.50	0.42
1:A:1053:ALA:O	1:A:1056:THR:OG1	2.35	0.42
1:A:1353:HIS:CE1	1:A:1367:LYS:HE3	2.55	0.42
1:A:4792:TYR:HB2	1:A:4805:CYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4866:ILE:HD11	1:D:4859:ALA:HB1	2.02	0.42
2:G:43:ARG:HG3	2:G:45:LYS:HG2	2.00	0.42
1:B:434:ASP:OD2	1:B:504:ARG:NH1	2.53	0.42
1:B:2774:ILE:H	1:B:2774:ILE:HG12	1.57	0.42
1:B:3804:LEU:HD21	1:B:3890:TYR:HB2	2.02	0.42
1:B:3839:PHE:HE1	1:B:3873:THR:HG23	1.84	0.42
1:B:4601:ARG:NH2	1:B:4626:LYS:HG3	2.35	0.42
1:B:4701:ASP:OD1	1:B:4701:ASP:N	2.31	0.42
1:C:1109:THR:OG1	1:C:1110:ALA:N	2.53	0.42
1:C:2102:PRO:HD3	1:C:3624:GLU:HG3	2.01	0.42
1:C:2335:ARG:HE	1:C:2335:ARG:HB3	1.67	0.42
1:D:434:ASP:OD2	1:D:504:ARG:NH1	2.53	0.42
1:D:1047:LYS:HG3	1:D:1051:ARG:NH1	2.35	0.42
1:D:1289:SER:HA	1:D:1353:HIS:HB3	2.02	0.42
1:D:1642:ILE:HG23	1:D:1643:LEU:HD23	2.01	0.42
1:D:2735:LYS:HA	1:D:2735:LYS:HD3	1.96	0.42
1:A:703:TYR:O	1:A:856:SER:OG	2.32	0.41
1:A:1051:ARG:HD2	1:A:1055:ARG:HH21	1.84	0.41
1:A:1289:SER:HA	1:A:1353:HIS:HB3	2.02	0.41
1:A:2162:ARG:HH21	1:A:2208:GLN:HE21	1.68	0.41
1:A:3839:PHE:HE1	1:A:3873:THR:HG23	1.84	0.41
1:B:527:LYS:HE2	1:B:566:GLU:HG2	2.02	0.41
1:B:562:LEU:HA	1:B:571:ILE:HD13	2.01	0.41
1:B:1028:ARG:NH2	1:B:1033:VAL:HG23	2.35	0.41
1:B:1047:LYS:HG3	1:B:1051:ARG:NH1	2.35	0.41
1:B:1758:LEU:HD13	1:B:1758:LEU:HA	1.89	0.41
1:B:1841:LYS:O	1:B:1845:GLN:HG2	2.20	0.41
1:B:2102:PRO:HD3	1:B:3624:GLU:HG3	2.01	0.41
1:B:4042:ILE:O	1:B:4076:THR:HA	2.20	0.41
1:D:49:LEU:HD11	1:D:194:LEU:HD11	2.01	0.41
1:D:375:GLN:NE2	1:D:390:LYS:O	2.49	0.41
1:D:2335:ARG:HE	1:D:2335:ARG:HB3	1.67	0.41
1:D:2895:LEU:HD11	1:D:2900:TYR:HD1	1.84	0.41
1:A:826:VAL:HG21	1:A:832:LEU:HB2	2.02	0.41
1:A:1047:LYS:HG3	1:A:1051:ARG:NH1	2.35	0.41
1:A:1091:GLU:HG3	1:A:1250:TRP:NE1	2.35	0.41
1:A:1109:THR:OG1	1:A:1110:ALA:N	2.53	0.41
1:A:2102:PRO:HD3	1:A:3624:GLU:HG3	2.01	0.41
1:A:2228:LEU:HD22	1:A:2296:ARG:HG3	2.01	0.41
1:A:3712:SER:OG	1:A:3716:LYS:NZ	2.38	0.41
1:B:732:LEU:HB3	1:B:779:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1353:HIS:CE1	1:B:1367:LYS:HE3	2.55	0.41
1:B:1764:PHE:HD1	1:B:1780:SER:HB2	1.84	0.41
1:C:907:VAL:O	1:C:914:GLN:NE2	2.53	0.41
1:C:1841:LYS:O	1:C:1845:GLN:HG2	2.20	0.41
1:C:2065:MET:SD	1:C:2083:MET:HG3	2.60	0.41
1:C:2735:LYS:HA	1:C:2735:LYS:HD3	1.96	0.41
1:C:2859:LEU:HD11	1:C:2867:HIS:CD2	2.55	0.41
2:I:50:ARG:N	2:I:55:GLU:OE2	2.35	0.41
1:D:448:PRO:HB2	1:D:451:SER:HB3	2.02	0.41
1:D:826:VAL:HG21	1:D:832:LEU:HB2	2.03	0.41
1:A:1727:ILE:HD11	1:A:2164:LEU:HD21	2.03	0.41
1:A:2501:LEU:HD11	1:A:2505:ALA:HB2	2.02	0.41
1:A:3624:GLU:HA	1:A:3628:ILE:HD11	2.02	0.41
1:A:3802:LEU:HD23	1:A:3802:LEU:HA	1.89	0.41
1:A:4601:ARG:NH2	1:A:4626:LYS:HG3	2.35	0.41
1:B:907:VAL:O	1:B:914:GLN:NE2	2.53	0.41
1:B:3940:TRP:O	1:B:3944:VAL:HG23	2.20	0.41
1:B:4792:TYR:HB2	1:B:4805:CYS:HB2	2.02	0.41
1:C:459:LEU:HD12	1:C:459:LEU:HA	1.90	0.41
1:C:527:LYS:HE2	1:C:566:GLU:HG2	2.02	0.41
1:C:747:HIS:CD2	1:C:750:ARG:HG2	2.55	0.41
1:C:876:PRO:HA	1:C:879:GLU:HG2	2.01	0.41
1:C:902:TRP:HE3	1:C:915:HIS:HB2	1.85	0.41
1:C:1051:ARG:HD2	1:C:1055:ARG:HH21	1.85	0.41
1:C:1102:TYR:CD1	1:C:1165:MET:HG2	2.50	0.41
1:C:1976:LEU:HD11	1:C:3619:PHE:CE2	2.55	0.41
1:C:3624:GLU:HA	1:C:3628:ILE:HD11	2.02	0.41
1:D:2772:TRP:N	1:D:2773:PRO:HD2	2.35	0.41
1:A:309:MET:HB2	1:A:312:LYS:HZ2	1.84	0.41
1:A:869:THR:O	1:A:941:LYS:NZ	2.50	0.41
1:A:2092:ASP:OD1	1:A:2095:GLY:N	2.49	0.41
1:A:2713:PRO:HG2	1:A:2716:LEU:HD12	2.02	0.41
1:A:3832:ASP:N	1:A:3832:ASP:OD1	2.51	0.41
1:B:162:ILE:HG22	1:B:181:LEU:HD13	2.02	0.41
1:B:433:LEU:HD12	1:B:433:LEU:HA	1.93	0.41
1:B:718:VAL:HG23	1:B:726:GLY:HA3	2.02	0.41
1:B:1091:GLU:HG3	1:B:1250:TRP:NE1	2.35	0.41
1:B:1265:HIS:CD2	1:B:1268:ILE:HD12	2.56	0.41
1:B:1727:ILE:HD11	1:B:2164:LEU:HD21	2.03	0.41
1:B:1976:LEU:HD11	1:B:3619:PHE:CE2	2.55	0.41
1:B:4044:LYS:HZ3	1:B:4069:ALA:HB1	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1893:LEU:HD13	1:C:2064:THR:HG21	2.03	0.41
1:C:2162:ARG:HH21	1:C:2208:GLN:HE21	1.68	0.41
1:C:3940:TRP:O	1:C:3944:VAL:HG23	2.20	0.41
1:C:4792:TYR:HB2	1:C:4805:CYS:HB2	2.02	0.41
1:D:895:MET:O	1:D:899:GLU:HG3	2.21	0.41
1:D:907:VAL:O	1:D:914:GLN:NE2	2.53	0.41
1:D:2076:ASP:HB3	1:D:2079:LEU:HB3	2.01	0.41
1:D:2735:LYS:HA	1:D:2740:TRP:CE3	2.47	0.41
1:A:1265:HIS:CD2	1:A:1268:ILE:HD12	2.56	0.41
1:A:1663:SER:OG	1:A:1709:ASP:OD2	2.29	0.41
1:A:1841:LYS:O	1:A:1845:GLN:HG2	2.20	0.41
1:A:2335:ARG:HE	1:A:2335:ARG:HB3	1.67	0.41
1:A:3641:GLU:OE1	1:A:3729:ARG:NH1	2.54	0.41
1:A:4042:ILE:O	1:A:4076:THR:HA	2.20	0.41
1:B:375:GLN:NE2	1:B:390:LYS:O	2.49	0.41
1:B:1289:SER:HA	1:B:1353:HIS:HB3	2.02	0.41
1:B:1775:ASP:OD1	1:B:1776:CYS:N	2.51	0.41
1:B:1843:ILE:HD13	1:B:1843:ILE:HA	1.93	0.41
1:B:2101:LEU:O	1:B:2104:THR:HG22	2.21	0.41
1:B:2713:PRO:HG2	1:B:2716:LEU:HD12	2.02	0.41
1:C:732:LEU:HB3	1:C:779:PHE:CE1	2.56	0.41
1:C:1353:HIS:CE1	1:C:1367:LYS:HE3	2.55	0.41
1:C:1680:HIS:CE1	2:I:91:VAL:HA	2.55	0.41
1:C:2436:SER:OG	1:C:2489:VAL:HG12	2.20	0.41
1:C:2713:PRO:HG2	1:C:2716:LEU:HD12	2.03	0.41
1:D:606:ARG:HH22	1:D:1635:GLU:HG2	1.86	0.41
1:D:876:PRO:HA	1:D:879:GLU:HG2	2.01	0.41
1:D:1102:TYR:CD1	1:D:1165:MET:HG2	2.50	0.41
1:D:1841:LYS:O	1:D:1845:GLN:HG2	2.20	0.41
1:D:2436:SER:OG	1:D:2489:VAL:HG12	2.20	0.41
1:D:2735:LYS:HD3	1:D:2740:TRP:HE3	1.85	0.41
1:A:394:HIS:HD2	1:A:396:GLU:HG3	1.86	0.41
1:A:747:HIS:CD2	1:A:750:ARG:HG2	2.55	0.41
1:A:898:ILE:HG13	1:A:898:ILE:H	1.73	0.41
1:A:2101:LEU:O	1:A:2104:THR:HG22	2.21	0.41
2:G:23:CYS:HB2	2:G:51:ILE:HD11	2.02	0.41
1:B:394:HIS:HD2	1:B:396:GLU:HG3	1.86	0.41
1:B:1342:ASP:OD1	1:B:1342:ASP:N	2.53	0.41
1:B:2207:ARG:HD2	1:B:2207:ARG:HA	1.92	0.41
1:B:2215:ASP:OD1	1:B:2215:ASP:N	2.52	0.41
1:B:3795:LEU:HD22	1:B:3834:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2895:LEU:HD11	1:C:2900:TYR:HD1	1.84	0.41
1:C:3795:LEU:HD22	1:C:3834:PHE:HZ	1.85	0.41
1:C:4517:PHE:HD1	1:C:4517:PHE:HA	1.72	0.41
1:D:1353:HIS:CE1	1:D:1367:LYS:HE3	2.55	0.41
1:D:2102:PRO:HD3	1:D:3624:GLU:HG3	2.01	0.41
1:D:2228:LEU:HD22	1:D:2296:ARG:HG3	2.01	0.41
1:D:2501:LEU:HD11	1:D:2505:ALA:HB2	2.02	0.41
1:D:4000:ASP:O	1:D:4004:GLU:HG2	2.21	0.41
1:D:4042:ILE:O	1:D:4076:THR:HA	2.20	0.41
1:A:162:ILE:HG22	1:A:181:LEU:HD13	2.02	0.41
1:A:732:LEU:HB3	1:A:779:PHE:CE1	2.56	0.41
1:A:748:LEU:HD13	2:G:8:ILE:HG23	2.03	0.41
1:A:1893:LEU:HD13	1:A:2064:THR:HG21	2.03	0.41
1:A:3754:VAL:HA	1:A:3757:THR:HG22	2.03	0.41
1:A:4851:PHE:HA	1:A:4855:VAL:HG22	2.03	0.41
1:B:1196:ASP:OD1	1:B:1196:ASP:N	2.53	0.41
1:C:1311:ALA:HA	1:C:1312:UNK:HA	1.50	0.41
1:C:2228:LEU:HD22	1:C:2296:ARG:HG3	2.01	0.41
1:C:2479:VAL:HG23	1:C:2482:PHE:H	1.86	0.41
1:C:2879:LYS:O	1:C:2883:LYS:HG3	2.21	0.41
1:C:4042:ILE:O	1:C:4076:THR:HA	2.20	0.41
1:C:4044:LYS:HZ1	1:C:4071:THR:H	1.67	0.41
1:C:4601:ARG:NH2	1:C:4626:LYS:HG3	2.35	0.41
2:I:23:CYS:HB2	2:I:51:ILE:HD11	2.02	0.41
1:D:37:LEU:HD13	1:D:203:VAL:HG21	2.03	0.41
1:D:902:TRP:HE3	1:D:915:HIS:HB2	1.85	0.41
1:D:1091:GLU:HG3	1:D:1250:TRP:NE1	2.35	0.41
1:D:1265:HIS:CD2	1:D:1268:ILE:HD12	2.56	0.41
1:D:1296:ASN:OD1	1:D:1296:ASN:N	2.53	0.41
1:D:3754:VAL:HA	1:D:3757:THR:HG22	2.03	0.41
1:D:3804:LEU:HD21	1:D:3890:TYR:HB2	2.02	0.41
1:A:37:LEU:HD13	1:A:203:VAL:HG21	2.03	0.41
1:A:718:VAL:HG23	1:A:726:GLY:HA3	2.02	0.41
1:A:2325:ARG:HD3	1:A:2325:ARG:HA	1.77	0.41
1:A:2735:LYS:HD3	1:A:2740:TRP:HE3	1.85	0.41
1:B:898:ILE:HG13	1:B:898:ILE:H	1.74	0.41
1:B:1932:VAL:HG11	1:B:3616:VAL:HB	2.02	0.41
1:B:2772:TRP:N	1:B:2773:PRO:HD2	2.35	0.41
1:B:3624:GLU:HA	1:B:3628:ILE:HD11	2.02	0.41
1:B:4631:ARG:O	1:B:4634:ILE:HG12	2.21	0.41
1:B:4851:PHE:HA	1:B:4855:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:826:VAL:HG21	1:C:832:LEU:HB2	2.02	0.41
1:C:1289:SER:HA	1:C:1353:HIS:HB3	2.02	0.41
1:C:2095:GLY:HA2	1:C:2098:VAL:HG22	2.02	0.41
1:C:4851:PHE:HA	1:C:4855:VAL:HG22	2.03	0.41
1:D:162:ILE:HG22	1:D:181:LEU:HD13	2.02	0.41
1:D:165:ALA:HB1	1:D:211:LEU:HD22	2.03	0.41
1:D:527:LYS:HE2	1:D:566:GLU:HG2	2.02	0.41
1:D:2107:ILE:HG13	1:D:2108:ASN:N	2.33	0.41
1:D:4601:ARG:NH2	1:D:4626:LYS:HG3	2.35	0.41
1:A:134:SER:O	1:A:134:SER:OG	2.34	0.41
1:A:448:PRO:HB2	1:A:451:SER:HB3	2.02	0.41
1:A:527:LYS:HE2	1:A:566:GLU:HG2	2.02	0.41
1:A:727:PHE:HD1	1:A:732:LEU:HD23	1.86	0.41
1:A:1342:ASP:OD1	1:A:1342:ASP:N	2.53	0.41
1:A:2184:LYS:HE2	1:A:2184:LYS:HB3	1.75	0.41
1:A:2436:SER:OG	1:A:2489:VAL:HG12	2.20	0.41
1:A:3795:LEU:HD22	1:A:3834:PHE:HZ	1.85	0.41
1:A:3804:LEU:HD21	1:A:3890:TYR:HB2	2.02	0.41
1:B:533:LEU:HD23	1:B:533:LEU:HA	1.95	0.41
1:B:606:ARG:HH22	1:B:1635:GLU:HG2	1.86	0.41
1:B:895:MET:O	1:B:899:GLU:HG3	2.21	0.41
1:B:902:TRP:HE3	1:B:915:HIS:HB2	1.85	0.41
1:B:1587:LEU:HD23	1:B:1587:LEU:HA	1.96	0.41
1:B:2162:ARG:HH21	1:B:2208:GLN:HE21	1.68	0.41
1:B:3812:LYS:HB3	1:B:3812:LYS:HE2	1.81	0.41
1:B:3962:SER:O	1:B:3962:SER:OG	2.38	0.41
1:B:4000:ASP:O	1:B:4003:VAL:HG12	2.21	0.41
2:H:5:ILE:HG13	2:H:73:ALA:HB1	2.03	0.41
1:C:394:HIS:HD2	1:C:396:GLU:HG3	1.86	0.41
1:C:495:ILE:O	1:C:499:LEU:HG	2.21	0.41
1:C:606:ARG:HH22	1:C:1635:GLU:HG2	1.86	0.41
1:C:686:VAL:HG22	1:C:687:THR:HG23	2.03	0.41
1:C:976:TYR:HD1	1:C:977:LYS:N	2.19	0.41
1:C:1031:ARG:HA	1:C:1031:ARG:HD3	1.93	0.41
1:C:1047:LYS:HD3	1:C:1047:LYS:HA	1.91	0.41
1:C:3754:VAL:HA	1:C:3757:THR:HG22	2.03	0.41
1:C:4000:ASP:O	1:C:4003:VAL:HG12	2.21	0.41
1:D:495:ILE:O	1:D:499:LEU:HG	2.21	0.41
1:D:669:GLN:HB3	1:D:673:TRP:HZ2	1.86	0.41
1:D:727:PHE:HD1	1:D:732:LEU:HD23	1.86	0.41
1:D:747:HIS:CD2	1:D:750:ARG:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1051:ARG:HD2	1:D:1055:ARG:HH21	1.85	0.41
1:D:1113:MET:HG2	1:D:1207:LEU:HD22	2.03	0.41
1:D:1727:ILE:HD11	1:D:2164:LEU:HD21	2.03	0.41
1:D:1758:LEU:HD13	1:D:1758:LEU:HA	1.89	0.41
1:D:1789:LYS:HD3	1:D:1839:ASP:OD2	2.21	0.41
1:D:2101:LEU:O	1:D:2104:THR:HG22	2.21	0.41
1:D:3641:GLU:OE1	1:D:3729:ARG:NH1	2.54	0.41
1:D:3795:LEU:HD22	1:D:3834:PHE:HZ	1.85	0.41
1:D:3940:TRP:O	1:D:3944:VAL:HG23	2.20	0.41
2:J:104:LEU:HD12	2:J:104:LEU:HA	1.88	0.41
1:A:190:ARG:HD3	1:A:205:ALA:O	2.21	0.41
1:A:1712:LEU:HD22	1:A:1832:MET:SD	2.61	0.41
1:A:2095:GLY:HA2	1:A:2098:VAL:HG22	2.02	0.41
1:A:4000:ASP:O	1:A:4004:GLU:HG2	2.21	0.41
1:A:4598:ILE:HD13	1:A:4708:LYS:HE3	2.03	0.41
2:G:12:ASP:C	2:G:12:ASP:OD1	2.64	0.41
1:B:37:LEU:HD13	1:B:203:VAL:HG21	2.03	0.41
1:B:747:HIS:CD2	1:B:750:ARG:HG2	2.55	0.41
1:B:826:VAL:HG21	1:B:832:LEU:HB2	2.03	0.41
1:B:1051:ARG:HD2	1:B:1055:ARG:HH21	1.85	0.41
1:B:1113:MET:HG2	1:B:1207:LEU:HD22	2.03	0.41
1:B:2228:LEU:HD22	1:B:2296:ARG:HG3	2.01	0.41
1:C:448:PRO:HB2	1:C:451:SER:HB3	2.02	0.41
1:C:997:ASP:HA	1:C:1047:LYS:HZ2	1.86	0.41
1:C:1091:GLU:HG3	1:C:1250:TRP:NE1	2.35	0.41
1:C:1265:HIS:CD2	1:C:1268:ILE:HD12	2.56	0.41
1:C:1596:LEU:HD23	1:C:1596:LEU:HA	1.96	0.41
1:C:4108:MET:HE2	1:C:4108:MET:HB3	1.89	0.41
1:C:4631:ARG:O	1:C:4634:ILE:HG12	2.21	0.41
1:D:394:HIS:HD2	1:D:396:GLU:HG3	1.86	0.41
1:D:1109:THR:OG1	1:D:1110:ALA:N	2.53	0.41
1:D:1173:MET:O	1:D:1191:ALA:N	2.37	0.41
1:D:1893:LEU:HD13	1:D:2064:THR:HG21	2.03	0.41
1:D:2713:PRO:HG2	1:D:2716:LEU:HD12	2.03	0.41
1:D:4631:ARG:O	1:D:4634:ILE:HG12	2.21	0.41
1:D:4851:PHE:HA	1:D:4855:VAL:HG22	2.03	0.41
1:A:902:TRP:HE3	1:A:915:HIS:HB2	1.85	0.40
1:A:1035:TYR:HE2	1:A:1047:LYS:HZ3	1.69	0.40
1:A:1364:GLU:HG3	1:A:1364:GLU:O	2.21	0.40
1:A:1642:ILE:HG23	1:A:1643:LEU:HD23	2.01	0.40
1:B:1109:THR:OG1	1:B:1110:ALA:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2781:MET:HE2	1:B:2781:MET:HA	2.03	0.40
1:B:3641:GLU:OE1	1:B:3729:ARG:NH1	2.54	0.40
1:C:669:GLN:HB3	1:C:673:TRP:HZ2	1.86	0.40
1:C:1047:LYS:HG3	1:C:1051:ARG:NH1	2.35	0.40
1:C:1117:TRP:HB3	1:C:1201:PHE:HB3	2.03	0.40
1:C:1789:LYS:HD3	1:C:1839:ASP:OD2	2.21	0.40
1:C:1932:VAL:HG11	1:C:3616:VAL:HB	2.01	0.40
1:C:2327:PRO:HB2	1:C:2335:ARG:HD3	2.02	0.40
1:C:2859:LEU:HD21	1:C:2867:HIS:NE2	2.36	0.40
1:C:4798:GLY:HA3	1:C:4799:ASP:HA	1.77	0.40
1:D:281:ARG:NH1	1:D:346:VAL:O	2.37	0.40
1:D:318:ASP:OD1	1:D:318:ASP:N	2.52	0.40
1:D:686:VAL:HG22	1:D:687:THR:HG23	2.03	0.40
1:D:2346:MET:HB3	1:D:2346:MET:HE2	1.88	0.40
1:D:3613:HIS:HA	1:D:3616:VAL:HG12	2.03	0.40
1:D:3812:LYS:HB3	1:D:3812:LYS:HE2	1.81	0.40
1:A:669:GLN:HB3	1:A:673:TRP:HZ2	1.86	0.40
1:A:3940:TRP:O	1:A:3944:VAL:HG23	2.20	0.40
1:A:4731:GLY:HA2	1:A:4734:ASN:O	2.22	0.40
1:B:152:ASP:OD1	1:B:152:ASP:N	2.52	0.40
1:B:686:VAL:HG22	1:B:687:THR:HG23	2.03	0.40
1:B:727:PHE:HD1	1:B:732:LEU:HD23	1.86	0.40
1:B:1364:GLU:HG3	1:B:1364:GLU:O	2.21	0.40
1:B:4598:ILE:HD13	1:B:4708:LYS:HE3	2.03	0.40
1:C:37:LEU:HD13	1:C:203:VAL:HG21	2.03	0.40
1:C:190:ARG:HD3	1:C:205:ALA:O	2.21	0.40
1:C:640:ARG:HB3	1:C:645:GLN:CD	2.46	0.40
1:C:703:TYR:O	1:C:856:SER:OG	2.32	0.40
1:C:2735:LYS:HD3	1:C:2740:TRP:HE3	1.85	0.40
1:C:2781:MET:HE2	1:C:2781:MET:HA	2.03	0.40
1:C:3613:HIS:HA	1:C:3616:VAL:HG12	2.03	0.40
1:D:190:ARG:HD3	1:D:205:ALA:O	2.21	0.40
1:D:1944:ASN:O	1:D:1948:GLN:HG2	2.22	0.40
1:D:2095:GLY:HA2	1:D:2098:VAL:HG22	2.02	0.40
1:D:2428:LEU:HD12	1:D:2475:TYR:CD1	2.56	0.40
1:D:2879:LYS:O	1:D:2883:LYS:HG3	2.21	0.40
1:D:4044:LYS:HZ1	1:D:4071:THR:H	1.67	0.40
1:A:410:HIS:CE1	1:A:414:ARG:HH21	2.40	0.40
1:A:1587:LEU:HD23	1:A:1587:LEU:HA	1.96	0.40
1:A:2859:LEU:HD21	1:A:2867:HIS:NE2	2.36	0.40
1:A:4033:GLU:OE1	1:A:4033:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:PRO:HB2	1:B:451:SER:HB3	2.02	0.40
1:B:976:TYR:HD1	1:B:977:LYS:N	2.19	0.40
1:B:981:MET:HE2	1:B:1056:THR:HA	2.03	0.40
1:B:2095:GLY:HA2	1:B:2098:VAL:HG22	2.02	0.40
1:B:4000:ASP:O	1:B:4004:GLU:HG2	2.21	0.40
1:C:433:LEU:HD12	1:C:433:LEU:HA	1.93	0.40
1:C:1342:ASP:OD1	1:C:1342:ASP:N	2.53	0.40
1:C:1663:SER:OG	1:C:1709:ASP:OD2	2.29	0.40
1:C:1727:ILE:HD11	1:C:2164:LEU:HD21	2.03	0.40
1:C:1758:LEU:HD13	1:C:1758:LEU:HA	1.89	0.40
1:C:1944:ASN:O	1:C:1948:GLN:HG2	2.22	0.40
1:C:2428:LEU:HD12	1:C:2475:TYR:CD1	2.56	0.40
1:C:2480:GLN:HG3	1:C:2484:LEU:HD23	2.04	0.40
1:C:3641:GLU:OE1	1:C:3729:ARG:NH1	2.54	0.40
1:C:4000:ASP:O	1:C:4004:GLU:HG2	2.21	0.40
1:C:4033:GLU:OE1	1:C:4033:GLU:N	2.54	0.40
2:I:12:ASP:OD1	2:I:12:ASP:C	2.64	0.40
1:D:732:LEU:HB3	1:D:779:PHE:CE1	2.56	0.40
1:D:2327:PRO:HB2	1:D:2335:ARG:HD3	2.03	0.40
1:D:3860:GLN:N	1:D:3860:GLN:OE1	2.54	0.40
1:D:4507:VAL:HG13	1:D:4578:HIS:HD2	1.86	0.40
1:D:4731:GLY:HA2	1:D:4734:ASN:O	2.22	0.40
2:J:12:ASP:OD1	2:J:12:ASP:C	2.64	0.40
1:A:200:SER:OG	1:A:202:HIS:ND1	2.47	0.40
1:A:396:GLU:HG3	1:A:396:GLU:H	1.66	0.40
1:A:1157:GLN:N	1:A:1160:ASP:OD2	2.41	0.40
1:A:1789:LYS:HG3	1:A:1835:PHE:HE1	1.86	0.40
1:A:1789:LYS:HD3	1:A:1839:ASP:OD2	2.21	0.40
1:A:1976:LEU:HD11	1:A:3619:PHE:CE2	2.55	0.40
1:A:2428:LEU:HD12	1:A:2475:TYR:CD1	2.56	0.40
1:A:2836:LEU:H	1:A:2836:LEU:HD12	1.87	0.40
1:A:2879:LYS:O	1:A:2883:LYS:HG3	2.21	0.40
1:B:190:ARG:HD3	1:B:205:ALA:O	2.21	0.40
1:B:495:ILE:O	1:B:499:LEU:HG	2.21	0.40
1:B:669:GLN:HB3	1:B:673:TRP:HZ2	1.86	0.40
1:B:722:LEU:HD13	1:B:722:LEU:HA	1.96	0.40
1:B:3754:VAL:HA	1:B:3757:THR:HG22	2.03	0.40
1:B:4896:TYR:CZ	1:B:4959:LYS:HG2	2.56	0.40
2:H:12:ASP:OD1	2:H:12:ASP:C	2.64	0.40
1:C:895:MET:O	1:C:899:GLU:HG3	2.21	0.40
1:C:981:MET:HE2	1:C:1056:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2207:ARG:HD2	1:C:2207:ARG:HA	1.92	0.40
1:C:2835:ASP:O	1:C:2839:MET:HG2	2.22	0.40
2:I:104:LEU:HD12	2:I:104:LEU:HA	1.88	0.40
1:D:1342:ASP:OD1	1:D:1342:ASP:N	2.53	0.40
1:D:1956:LEU:HD13	1:D:1956:LEU:HA	1.98	0.40
1:D:2264:VAL:HG21	1:D:2300:PHE:HE2	1.87	0.40
1:D:2836:LEU:H	1:D:2836:LEU:HD12	1.87	0.40
1:A:143:LEU:HD11	1:B:2425:LEU:HD22	2.04	0.40
1:A:606:ARG:HH2	1:A:1635:GLU:HG2	1.86	0.40
1:A:640:ARG:HB3	1:A:645:GLN:CD	2.46	0.40
1:A:1117:TRP:HB3	1:A:1201:PHE:HB3	2.03	0.40
1:A:2074:ILE:HG22	1:A:2075:GLU:O	2.22	0.40
1:A:2479:VAL:HG23	1:A:2482:PHE:H	1.86	0.40
1:B:640:ARG:HB3	1:B:645:GLN:CD	2.46	0.40
1:B:997:ASP:HA	1:B:1047:LYS:HZ2	1.85	0.40
1:B:1970:GLU:O	1:B:1974:MET:HG3	2.22	0.40
1:B:3613:HIS:HA	1:B:3616:VAL:HG12	2.03	0.40
1:B:3779:TYR:HA	1:B:3782:GLU:HG2	2.04	0.40
1:B:3998:MET:HE3	1:B:3998:MET:HB2	1.98	0.40
1:B:4731:GLY:HA2	1:B:4734:ASN:O	2.22	0.40
1:B:4762:ASN:O	1:B:4766:LEU:HB2	2.22	0.40
1:C:410:HIS:CE1	1:C:414:ARG:HH21	2.40	0.40
1:C:727:PHE:HD1	1:C:732:LEU:HD23	1.86	0.40
1:C:1138:ASP:OD1	1:C:1139:GLY:N	2.54	0.40
1:C:1217:PHE:O	1:C:1240:ALA:N	2.50	0.40
1:C:1364:GLU:O	1:C:1364:GLU:HG3	2.21	0.40
1:C:1792:THR:HG21	1:C:1829:LEU:HD12	2.03	0.40
1:C:4507:VAL:HG13	1:C:4578:HIS:HD2	1.86	0.40
2:I:5:ILE:HG13	2:I:73:ALA:HB1	2.03	0.40
1:D:410:HIS:CE1	1:D:414:ARG:HH21	2.39	0.40
1:D:997:ASP:HA	1:D:1047:LYS:HZ2	1.87	0.40
1:D:1138:ASP:OD1	1:D:1139:GLY:N	2.54	0.40
1:D:1976:LEU:HD11	1:D:3619:PHE:CE2	2.55	0.40
1:D:4033:GLU:OE1	1:D:4033:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3218/4966 (65%)	3005 (93%)	213 (7%)	0	100	100
1	B	3218/4966 (65%)	3005 (93%)	213 (7%)	0	100	100
1	C	3218/4966 (65%)	3005 (93%)	213 (7%)	0	100	100
1	D	3218/4966 (65%)	3006 (93%)	212 (7%)	0	100	100
2	G	105/176 (60%)	98 (93%)	7 (7%)	0	100	100
2	H	105/176 (60%)	97 (92%)	8 (8%)	0	100	100
2	I	105/176 (60%)	98 (93%)	7 (7%)	0	100	100
2	J	105/176 (60%)	98 (93%)	7 (7%)	0	100	100
All	All	13292/20568 (65%)	12412 (93%)	880 (7%)	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	2827/3387 (84%)	2746 (97%)	81 (3%)	37	60
1	B	2827/3387 (84%)	2746 (97%)	81 (3%)	37	60
1	C	2827/3387 (84%)	2746 (97%)	81 (3%)	37	60
1	D	2827/3387 (84%)	2746 (97%)	81 (3%)	37	60
2	G	88/140 (63%)	85 (97%)	3 (3%)	32	57
2	H	88/140 (63%)	85 (97%)	3 (3%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	88/140 (63%)	85 (97%)	3 (3%)	32	57
2	J	88/140 (63%)	85 (97%)	3 (3%)	32	57
All	All	11660/14108 (83%)	11324 (97%)	336 (3%)	38	60

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	233	VAL
1	A	255	GLU
1	A	430	ILE
1	A	446	ASP
1	A	548	CYS
1	A	551	PHE
1	A	611	LEU
1	A	637	LEU
1	A	643	LEU
1	A	665	GLU
1	A	686	VAL
1	A	800	VAL
1	A	883	GLU
1	A	884	ARG
1	A	892	LEU
1	A	898	ILE
1	A	918	LEU
1	A	920	GLU
1	A	922	CYS
1	A	923	LYS
1	A	924	LEU
1	A	926	GLU
1	A	950	VAL
1	A	952	ILE
1	A	970	TYR
1	A	971	GLN
1	A	972	LEU
1	A	976	TYR
1	A	1001	GLU
1	A	1033	VAL
1	A	1045	SER
1	A	1062	TYR
1	A	1109	THR

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Mol	Chain	Res	Type
1	A	1162	VAL
1	A	1202	ILE
1	A	1209	VAL
1	A	1271	THR
1	A	1340	ASP
1	A	1359	ILE
1	A	1376	TYR
1	A	1685	GLN
1	A	1758	LEU
1	A	1771	SER
1	A	1847	ILE
1	A	1977	ASN
1	A	1987	CYS
1	A	2106	THR
1	A	2217	LEU
1	A	2271	CYS
1	A	2425	LEU
1	A	2714	GLU
1	A	2715	LYS
1	A	2718	TYR
1	A	2745	ILE
1	A	2748	ASP
1	A	2750	SER
1	A	2762	LEU
1	A	2763	SER
1	A	2768	GLU
1	A	2774	ILE
1	A	2778	LEU
1	A	2891	ILE
1	A	3628	ILE
1	A	3643	LEU
1	A	3663	LEU
1	A	3731	HIS
1	A	3786	VAL
1	A	3870	ILE
1	A	3990	VAL
1	A	4003	VAL
1	A	4041	VAL
1	A	4065	LEU
1	A	4147	VAL
1	A	4175	VAL
1	A	4509	PHE

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Mol	Chain	Res	Type
1	A	4594	VAL
1	A	4668	LEU
1	A	4700	ILE
1	A	4701	ASP
1	A	4742	LEU
2	G	5	ILE
2	G	25	VAL
2	G	81	VAL
1	B	58	VAL
1	B	233	VAL
1	B	255	GLU
1	B	430	ILE
1	B	446	ASP
1	B	548	CYS
1	B	551	PHE
1	B	611	LEU
1	B	637	LEU
1	B	643	LEU
1	B	665	GLU
1	B	686	VAL
1	B	800	VAL
1	B	883	GLU
1	B	884	ARG
1	B	892	LEU
1	B	898	ILE
1	B	918	LEU
1	B	920	GLU
1	B	922	CYS
1	B	923	LYS
1	B	924	LEU
1	B	926	GLU
1	B	950	VAL
1	B	952	ILE
1	B	970	TYR
1	B	971	GLN
1	B	972	LEU
1	B	976	TYR
1	B	1001	GLU
1	B	1033	VAL
1	B	1045	SER
1	B	1062	TYR
1	B	1109	THR

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Mol	Chain	Res	Type
1	B	1162	VAL
1	B	1202	ILE
1	B	1209	VAL
1	B	1271	THR
1	B	1340	ASP
1	B	1359	ILE
1	B	1376	TYR
1	B	1685	GLN
1	B	1758	LEU
1	B	1771	SER
1	B	1847	ILE
1	B	1977	ASN
1	B	1987	CYS
1	B	2106	THR
1	B	2217	LEU
1	B	2271	CYS
1	B	2425	LEU
1	B	2714	GLU
1	B	2715	LYS
1	B	2718	TYR
1	B	2745	ILE
1	B	2748	ASP
1	B	2750	SER
1	B	2762	LEU
1	B	2763	SER
1	B	2768	GLU
1	B	2774	ILE
1	B	2778	LEU
1	B	2891	ILE
1	B	3628	ILE
1	B	3643	LEU
1	B	3663	LEU
1	B	3731	HIS
1	B	3786	VAL
1	B	3870	ILE
1	B	3990	VAL
1	B	4003	VAL
1	B	4041	VAL
1	B	4065	LEU
1	B	4147	VAL
1	B	4175	VAL
1	B	4509	PHE

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Mol	Chain	Res	Type
1	B	4594	VAL
1	B	4668	LEU
1	B	4700	ILE
1	B	4701	ASP
1	B	4742	LEU
2	H	5	ILE
2	H	25	VAL
2	H	81	VAL
1	C	58	VAL
1	C	233	VAL
1	C	255	GLU
1	C	430	ILE
1	C	446	ASP
1	C	548	CYS
1	C	551	PHE
1	C	611	LEU
1	C	637	LEU
1	C	643	LEU
1	C	665	GLU
1	C	686	VAL
1	C	800	VAL
1	C	883	GLU
1	C	884	ARG
1	C	892	LEU
1	C	898	ILE
1	C	918	LEU
1	C	920	GLU
1	C	922	CYS
1	C	923	LYS
1	C	924	LEU
1	C	926	GLU
1	C	950	VAL
1	C	952	ILE
1	C	970	TYR
1	C	971	GLN
1	C	972	LEU
1	C	976	TYR
1	C	1001	GLU
1	C	1033	VAL
1	C	1045	SER
1	C	1062	TYR
1	C	1109	THR

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Mol	Chain	Res	Type
1	C	1162	VAL
1	C	1202	ILE
1	C	1209	VAL
1	C	1271	THR
1	C	1340	ASP
1	C	1359	ILE
1	C	1376	TYR
1	C	1685	GLN
1	C	1758	LEU
1	C	1771	SER
1	C	1847	ILE
1	C	1977	ASN
1	C	1987	CYS
1	C	2106	THR
1	C	2217	LEU
1	C	2271	CYS
1	C	2425	LEU
1	C	2714	GLU
1	C	2715	LYS
1	C	2718	TYR
1	C	2745	ILE
1	C	2748	ASP
1	C	2750	SER
1	C	2762	LEU
1	C	2763	SER
1	C	2768	GLU
1	C	2774	ILE
1	C	2778	LEU
1	C	2891	ILE
1	C	3628	ILE
1	C	3643	LEU
1	C	3663	LEU
1	C	3731	HIS
1	C	3786	VAL
1	C	3870	ILE
1	C	3990	VAL
1	C	4003	VAL
1	C	4041	VAL
1	C	4065	LEU
1	C	4147	VAL
1	C	4175	VAL
1	C	4509	PHE

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Mol	Chain	Res	Type
1	C	4594	VAL
1	C	4668	LEU
1	C	4700	ILE
1	C	4701	ASP
1	C	4742	LEU
2	I	5	ILE
2	I	25	VAL
2	I	81	VAL
1	D	58	VAL
1	D	233	VAL
1	D	255	GLU
1	D	430	ILE
1	D	446	ASP
1	D	548	CYS
1	D	551	PHE
1	D	611	LEU
1	D	637	LEU
1	D	643	LEU
1	D	665	GLU
1	D	686	VAL
1	D	800	VAL
1	D	883	GLU
1	D	884	ARG
1	D	892	LEU
1	D	898	ILE
1	D	918	LEU
1	D	920	GLU
1	D	922	CYS
1	D	923	LYS
1	D	924	LEU
1	D	926	GLU
1	D	950	VAL
1	D	952	ILE
1	D	970	TYR
1	D	971	GLN
1	D	972	LEU
1	D	976	TYR
1	D	1001	GLU
1	D	1033	VAL
1	D	1045	SER
1	D	1062	TYR
1	D	1109	THR

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Mol	Chain	Res	Type
1	D	1162	VAL
1	D	1202	ILE
1	D	1209	VAL
1	D	1271	THR
1	D	1340	ASP
1	D	1359	ILE
1	D	1376	TYR
1	D	1685	GLN
1	D	1758	LEU
1	D	1771	SER
1	D	1847	ILE
1	D	1977	ASN
1	D	1987	CYS
1	D	2106	THR
1	D	2217	LEU
1	D	2271	CYS
1	D	2425	LEU
1	D	2714	GLU
1	D	2715	LYS
1	D	2718	TYR
1	D	2745	ILE
1	D	2748	ASP
1	D	2750	SER
1	D	2762	LEU
1	D	2763	SER
1	D	2768	GLU
1	D	2774	ILE
1	D	2778	LEU
1	D	2891	ILE
1	D	3628	ILE
1	D	3643	LEU
1	D	3663	LEU
1	D	3731	HIS
1	D	3786	VAL
1	D	3870	ILE
1	D	3990	VAL
1	D	4003	VAL
1	D	4041	VAL
1	D	4065	LEU
1	D	4147	VAL
1	D	4175	VAL
1	D	4509	PHE

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Mol	Chain	Res	Type
1	D	4594	VAL
1	D	4668	LEU
1	D	4700	ILE
1	D	4701	ASP
1	D	4742	LEU
2	J	5	ILE
2	J	25	VAL
2	J	81	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (255) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	GLN
1	A	79	GLN
1	A	123	HIS
1	A	150	GLN
1	A	168	GLN
1	A	299	HIS
1	A	388	GLN
1	A	394	HIS
1	A	395	HIS
1	A	410	HIS
1	A	469	HIS
1	A	472	HIS
1	A	476	GLN
1	A	487	ASN
1	A	496	ASN
1	A	550	GLN
1	A	593	HIS
1	A	629	GLN
1	A	650	ASN
1	A	745	ASN
1	A	746	GLN
1	A	903	GLN
1	A	914	GLN
1	A	915	HIS
1	A	1005	ASN
1	A	1257	GLN
1	A	1582	GLN
1	A	1590	GLN
1	A	1653	GLN

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Mol	Chain	Res	Type
1	A	1685	GLN
1	A	1711	HIS
1	A	1806	HIS
1	A	1938	ASN
1	A	1999	HIS
1	A	2150	ASN
1	A	2157	HIS
1	A	2159	ASN
1	A	2317	ASN
1	A	2382	HIS
1	A	2485	HIS
1	A	2753	GLN
1	A	2867	HIS
1	A	3613	HIS
1	A	3721	GLN
1	A	3805	ASN
1	A	3881	GLN
1	A	3932	GLN
1	A	3959	GLN
1	A	3974	GLN
1	A	4059	GLN
1	A	4087	HIS
1	A	4096	ASN
1	A	4170	GLN
1	A	4491	ASN
1	A	4496	ASN
1	A	4637	GLN
1	A	4642	ASN
1	A	4698	ASN
1	A	4765	GLN
1	A	4786	ASN
1	A	4793	ASN
1	A	4960	GLN
2	G	21	GLN
2	G	26	HIS
1	B	12	GLN
1	B	23	GLN
1	B	79	GLN
1	B	123	HIS
1	B	150	GLN
1	B	168	GLN
1	B	240	HIS

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Mol	Chain	Res	Type
1	B	299	HIS
1	B	388	GLN
1	B	394	HIS
1	B	395	HIS
1	B	410	HIS
1	B	469	HIS
1	B	472	HIS
1	B	476	GLN
1	B	487	ASN
1	B	496	ASN
1	B	550	GLN
1	B	576	HIS
1	B	593	HIS
1	B	629	GLN
1	B	650	ASN
1	B	651	HIS
1	B	776	GLN
1	B	903	GLN
1	B	914	GLN
1	B	915	HIS
1	B	1005	ASN
1	B	1257	GLN
1	B	1582	GLN
1	B	1590	GLN
1	B	1653	GLN
1	B	1685	GLN
1	B	1711	HIS
1	B	1806	HIS
1	B	1936	GLN
1	B	1938	ASN
1	B	1999	HIS
1	B	2157	HIS
1	B	2159	ASN
1	B	2317	ASN
1	B	2382	HIS
1	B	2485	HIS
1	B	2753	GLN
1	B	2867	HIS
1	B	3613	HIS
1	B	3721	GLN
1	B	3805	ASN
1	B	3881	GLN

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Mol	Chain	Res	Type
1	B	3932	GLN
1	B	3936	HIS
1	B	3959	GLN
1	B	3974	GLN
1	B	4059	GLN
1	B	4087	HIS
1	B	4096	ASN
1	B	4170	GLN
1	B	4491	ASN
1	B	4496	ASN
1	B	4642	ASN
1	B	4698	ASN
1	B	4765	GLN
1	B	4786	ASN
1	B	4793	ASN
1	B	4960	GLN
2	H	21	GLN
1	C	12	GLN
1	C	23	GLN
1	C	79	GLN
1	C	123	HIS
1	C	150	GLN
1	C	240	HIS
1	C	299	HIS
1	C	388	GLN
1	C	394	HIS
1	C	395	HIS
1	C	410	HIS
1	C	469	HIS
1	C	472	HIS
1	C	476	GLN
1	C	487	ASN
1	C	496	ASN
1	C	550	GLN
1	C	593	HIS
1	C	629	GLN
1	C	650	ASN
1	C	903	GLN
1	C	914	GLN
1	C	915	HIS
1	C	1005	ASN
1	C	1257	GLN

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Mol	Chain	Res	Type
1	C	1264	ASN
1	C	1582	GLN
1	C	1590	GLN
1	C	1653	GLN
1	C	1685	GLN
1	C	1711	HIS
1	C	1806	HIS
1	C	1999	HIS
1	C	2157	HIS
1	C	2159	ASN
1	C	2317	ASN
1	C	2382	HIS
1	C	2485	HIS
1	C	2753	GLN
1	C	2867	HIS
1	C	3613	HIS
1	C	3721	GLN
1	C	3805	ASN
1	C	3881	GLN
1	C	3932	GLN
1	C	3959	GLN
1	C	3974	GLN
1	C	4048	HIS
1	C	4087	HIS
1	C	4096	ASN
1	C	4170	GLN
1	C	4491	ASN
1	C	4496	ASN
1	C	4642	ASN
1	C	4698	ASN
1	C	4786	ASN
1	C	4793	ASN
1	C	4960	GLN
2	I	21	GLN
1	D	12	GLN
1	D	23	GLN
1	D	79	GLN
1	D	123	HIS
1	D	150	GLN
1	D	240	HIS
1	D	299	HIS
1	D	388	GLN

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Mol	Chain	Res	Type
1	D	394	HIS
1	D	395	HIS
1	D	410	HIS
1	D	469	HIS
1	D	472	HIS
1	D	476	GLN
1	D	487	ASN
1	D	496	ASN
1	D	550	GLN
1	D	576	HIS
1	D	593	HIS
1	D	629	GLN
1	D	650	ASN
1	D	746	GLN
1	D	903	GLN
1	D	914	GLN
1	D	915	HIS
1	D	1005	ASN
1	D	1257	GLN
1	D	1582	GLN
1	D	1590	GLN
1	D	1653	GLN
1	D	1685	GLN
1	D	1711	HIS
1	D	1806	HIS
1	D	1842	HIS
1	D	1936	GLN
1	D	1999	HIS
1	D	2150	ASN
1	D	2157	HIS
1	D	2159	ASN
1	D	2317	ASN
1	D	2382	HIS
1	D	2485	HIS
1	D	2753	GLN
1	D	2867	HIS
1	D	3613	HIS
1	D	3721	GLN
1	D	3805	ASN
1	D	3881	GLN
1	D	3932	GLN
1	D	3959	GLN

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Mol	Chain	Res	Type
1	D	3974	GLN
1	D	4059	GLN
1	D	4087	HIS
1	D	4096	ASN
1	D	4170	GLN
1	D	4491	ASN
1	D	4496	ASN
1	D	4642	ASN
1	D	4698	ASN
1	D	4765	GLN
1	D	4786	ASN
1	D	4793	ASN
1	D	4960	GLN
2	J	21	GLN
2	J	26	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

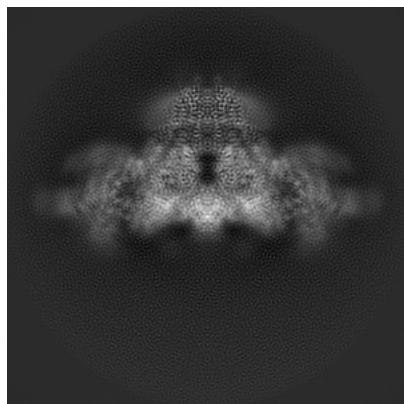
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33938. These allow visual inspection of the internal detail of the map and identification of artifacts.

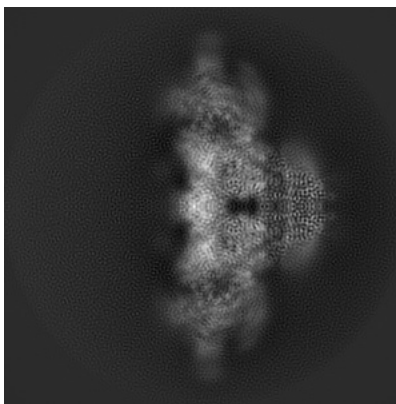
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

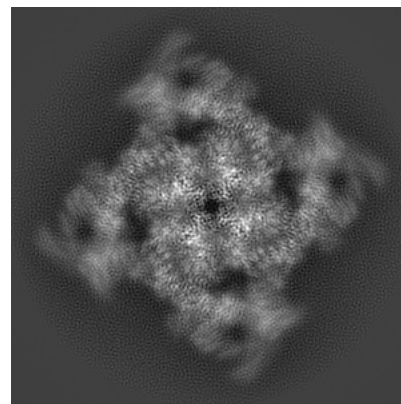
6.1.1 Primary map



X

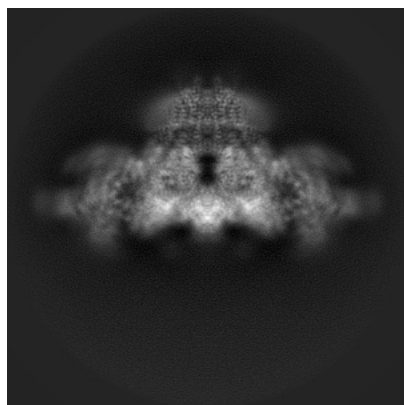


Y

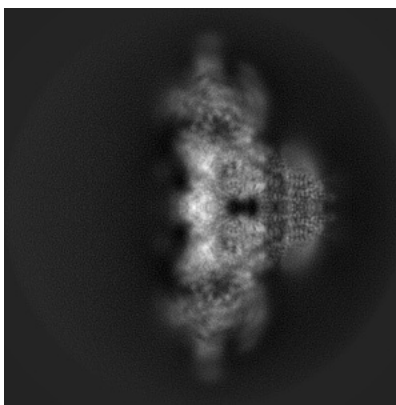


Z

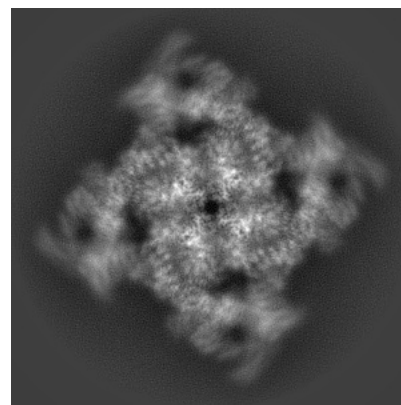
6.1.2 Raw map



X



Y

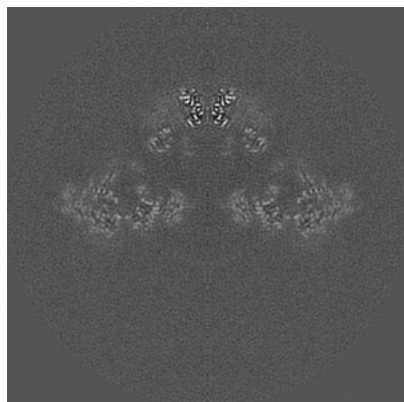


Z

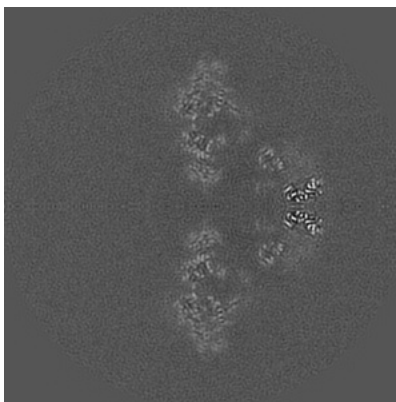
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

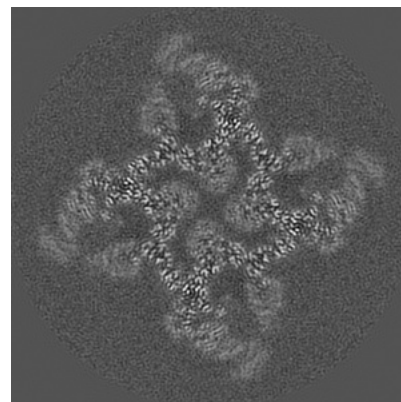
6.2.1 Primary map



X Index: 170

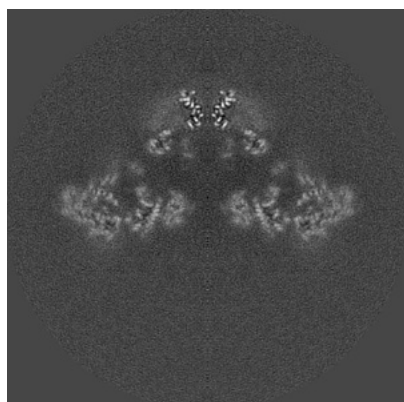


Y Index: 170

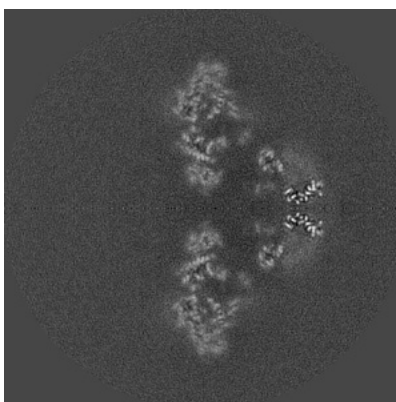


Z Index: 170

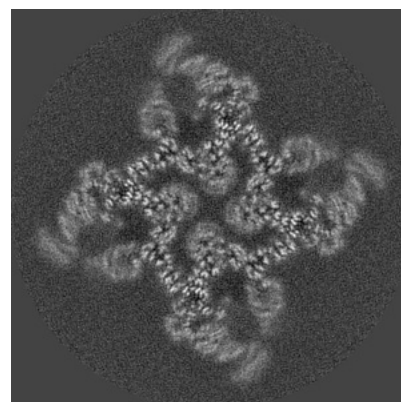
6.2.2 Raw map



X Index: 170



Y Index: 170

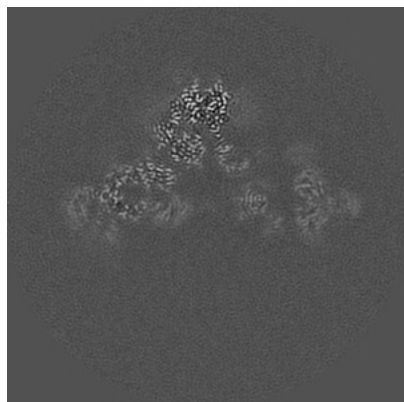


Z Index: 170

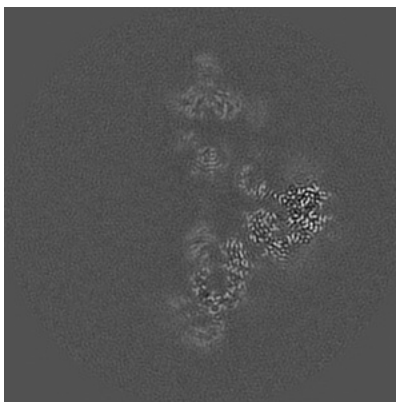
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

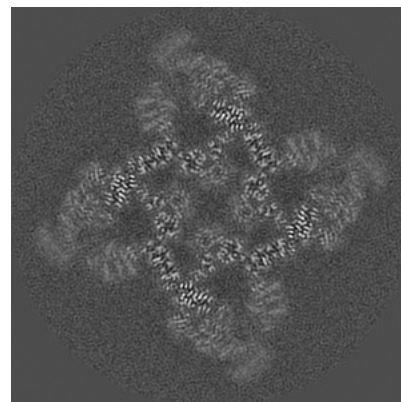
6.3.1 Primary map



X Index: 159

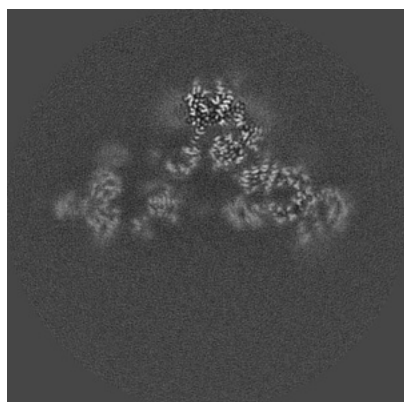


Y Index: 181

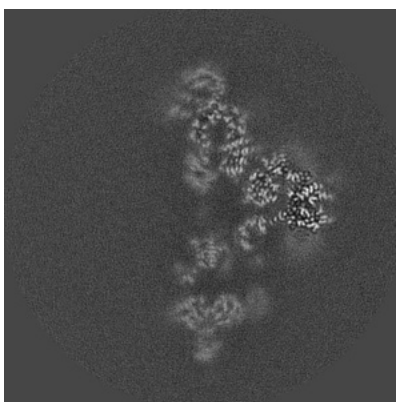


Z Index: 174

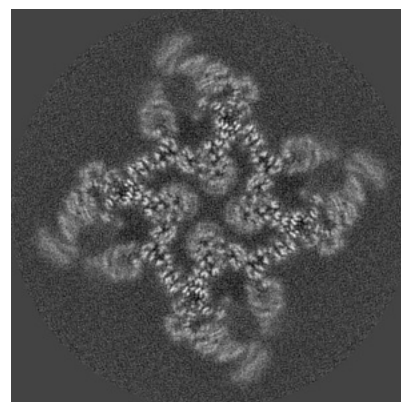
6.3.2 Raw map



X Index: 181



Y Index: 159

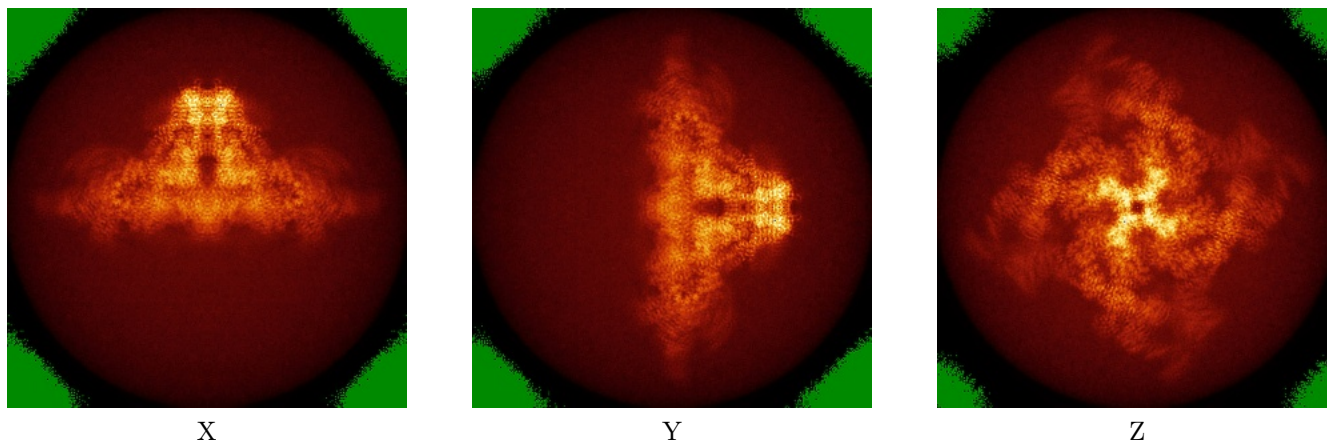


Z Index: 170

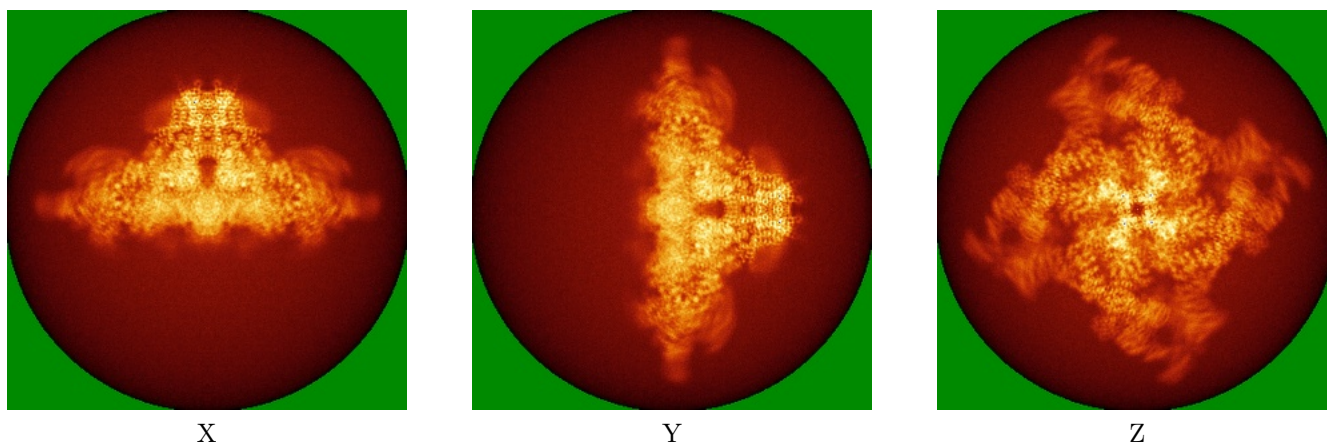
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

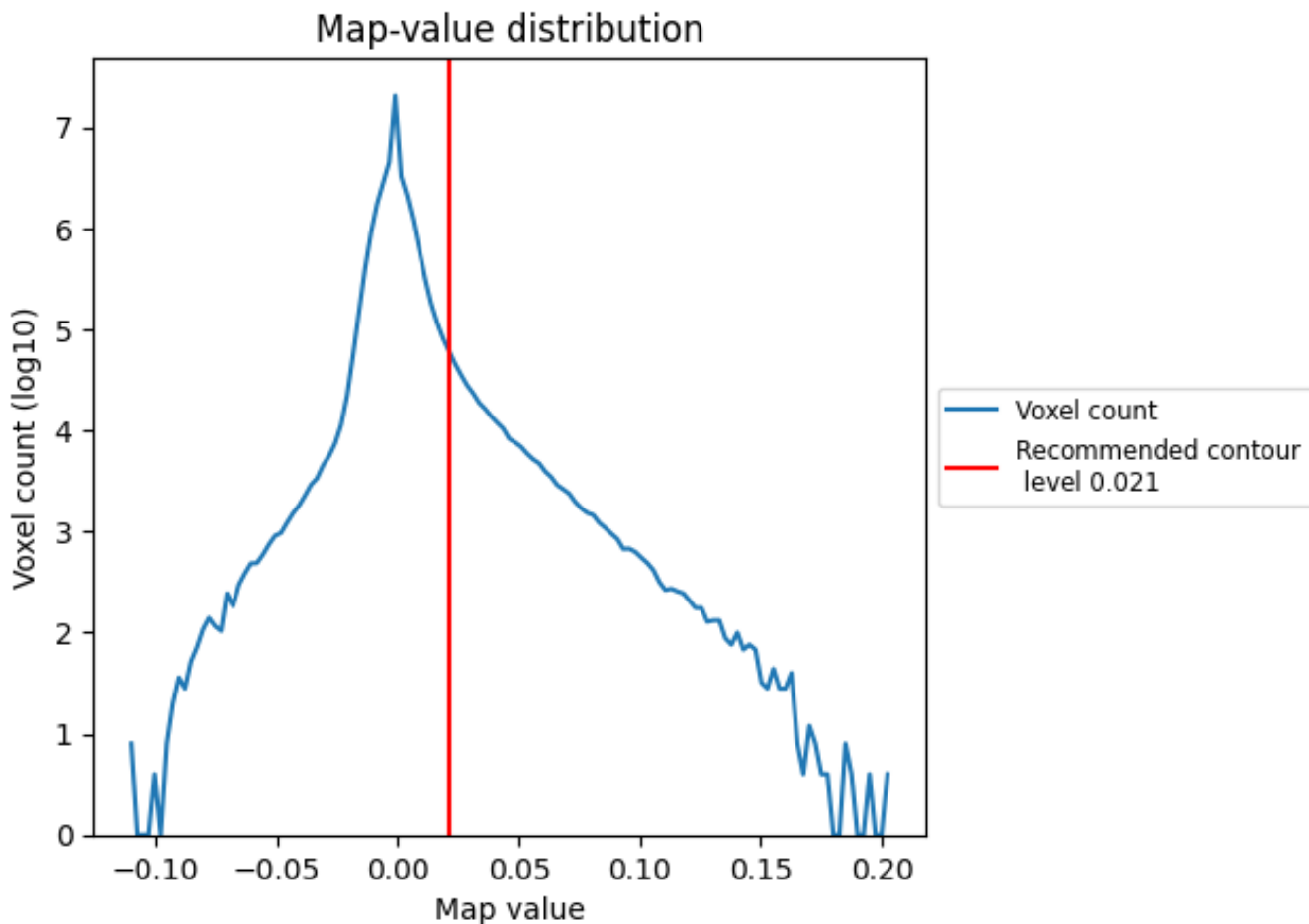
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

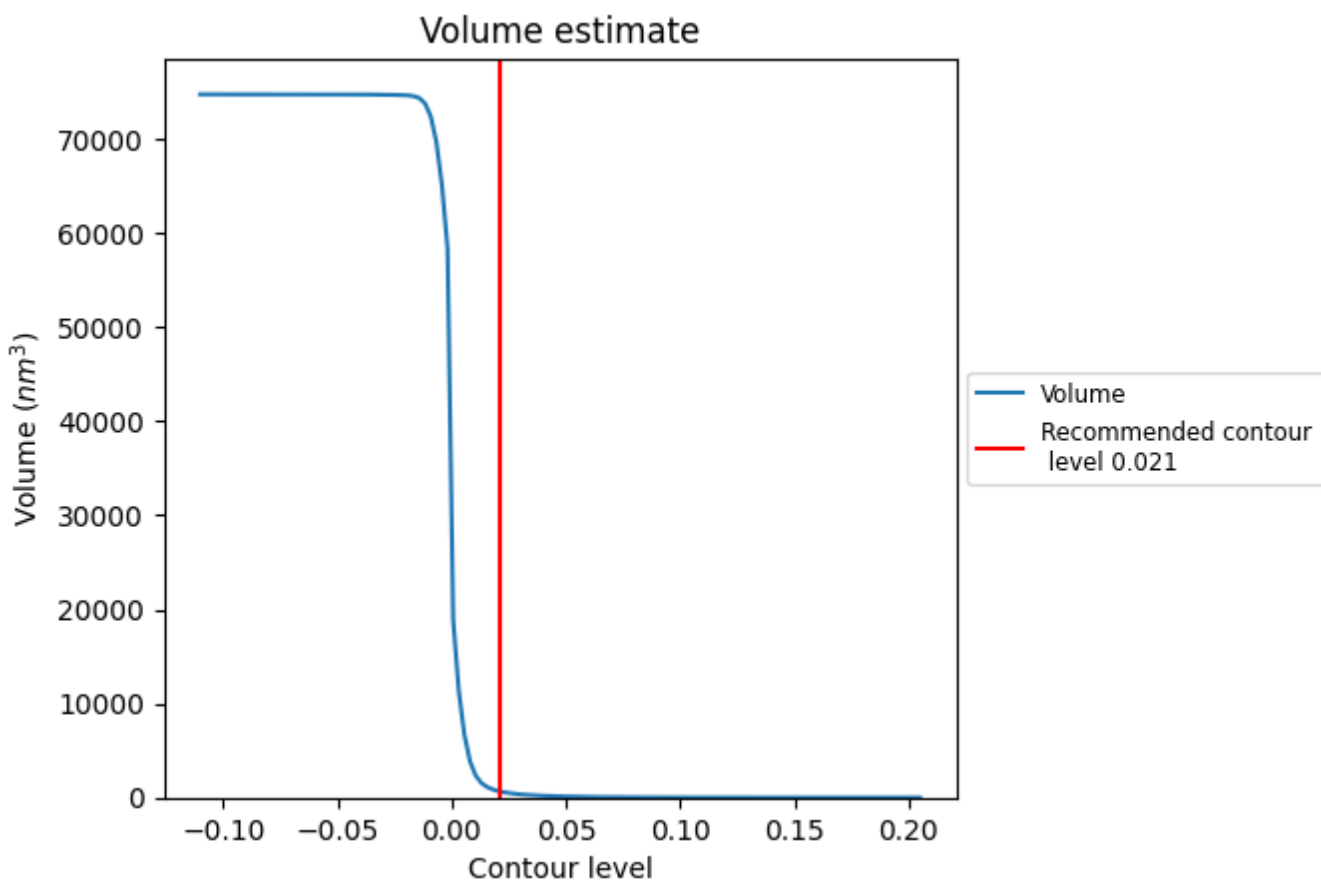
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

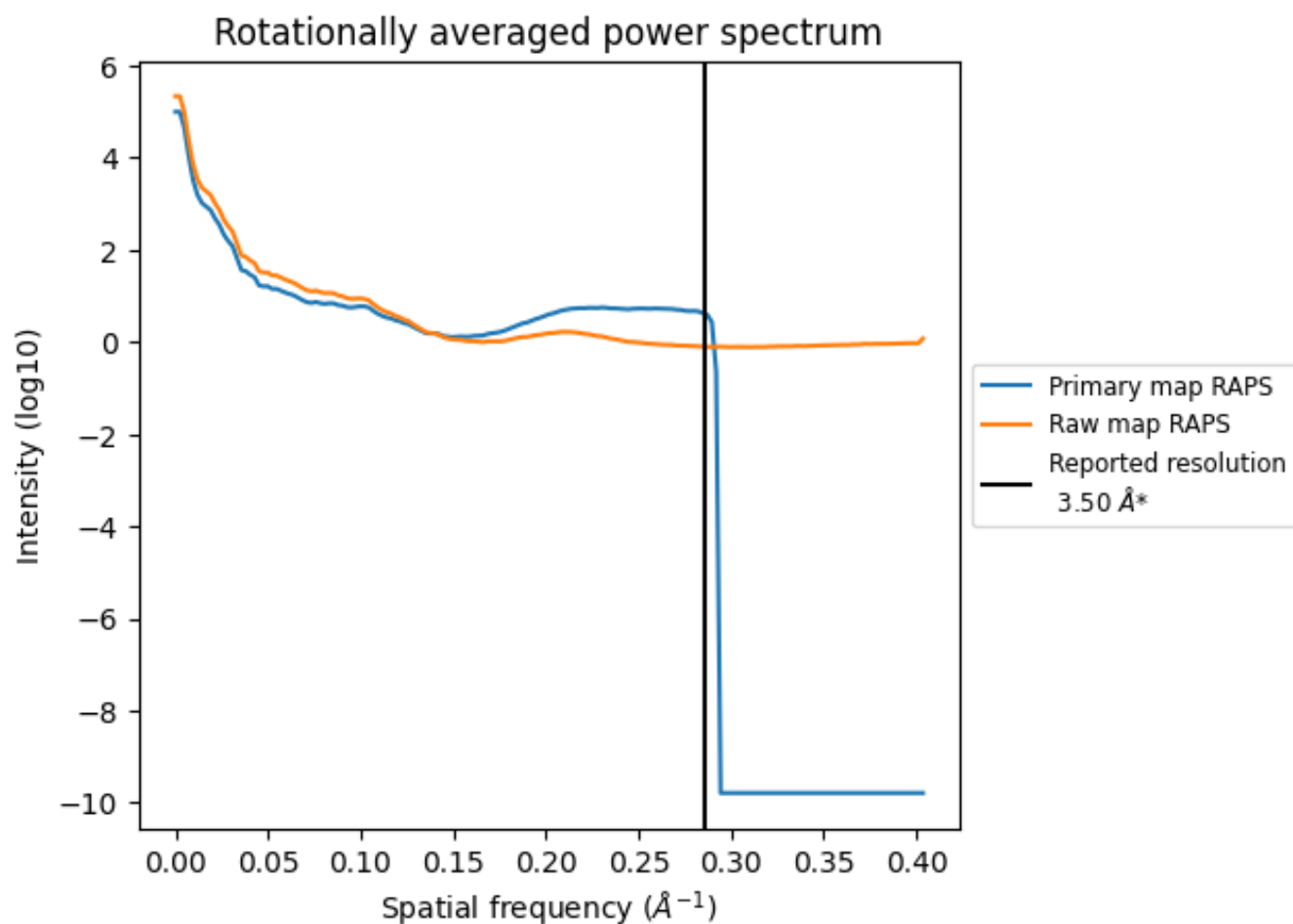
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 659 nm³; this corresponds to an approximate mass of 596 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](#)

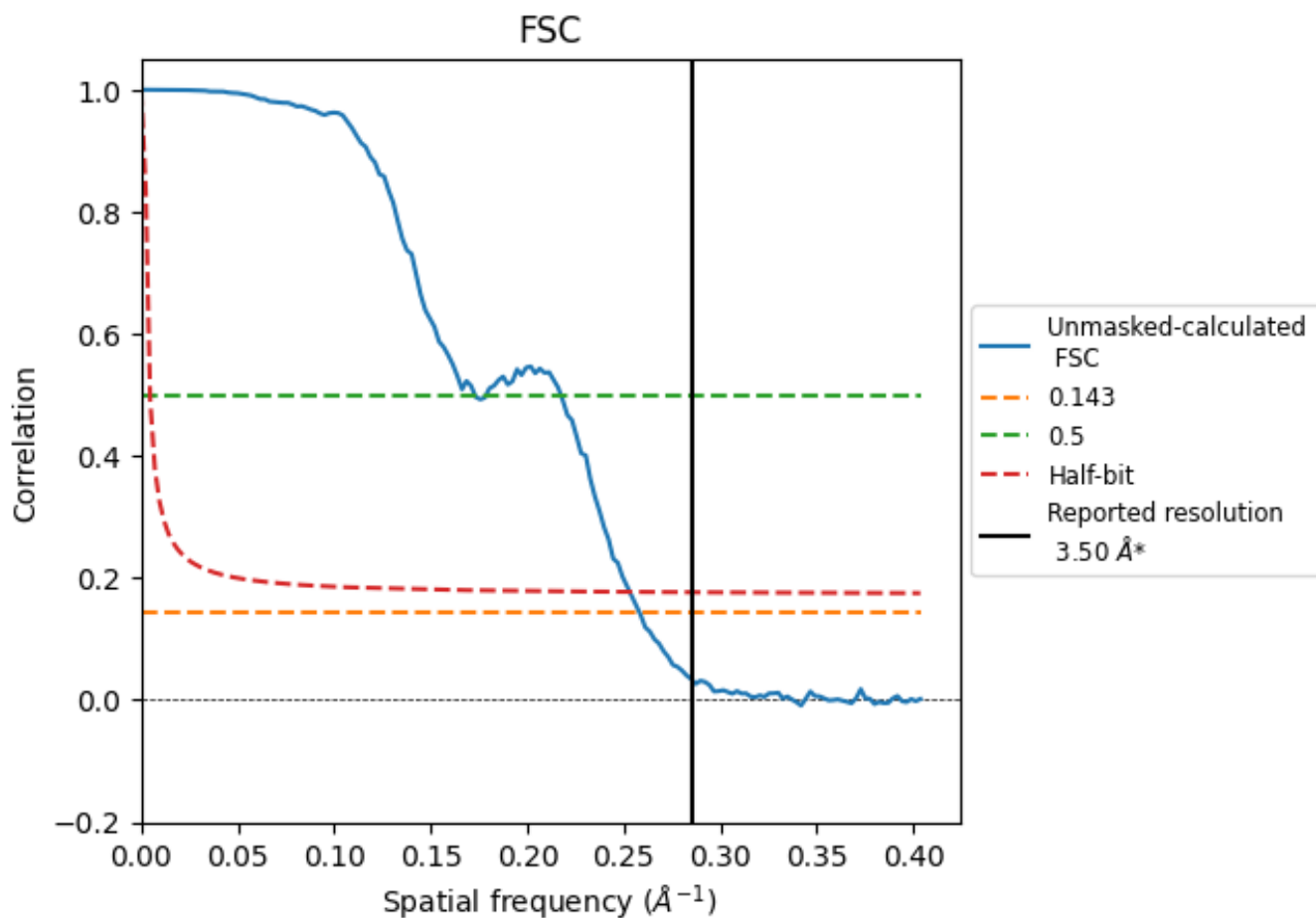


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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*	3.87	5.79	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.5 by more than 10 %

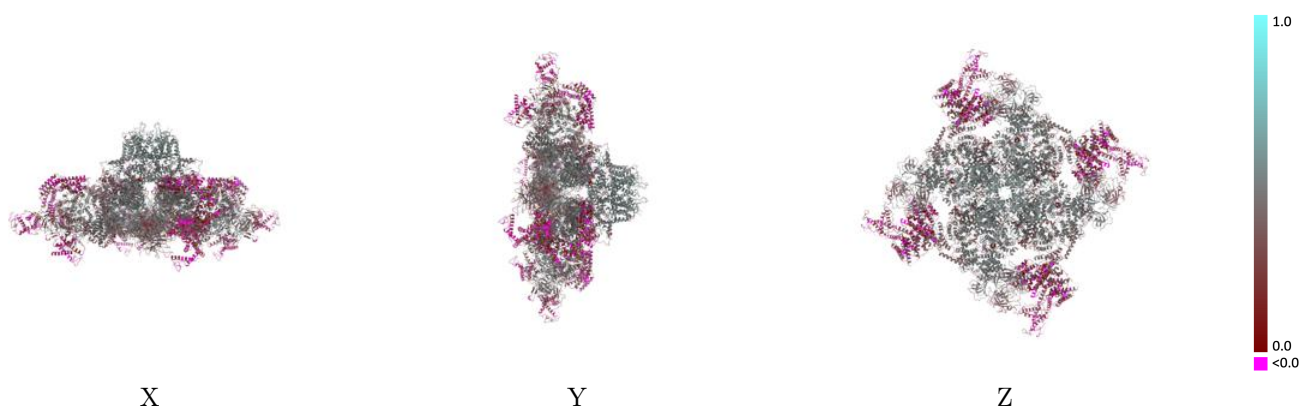
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33938 and PDB model 7VMO. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

This section was not generated.

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

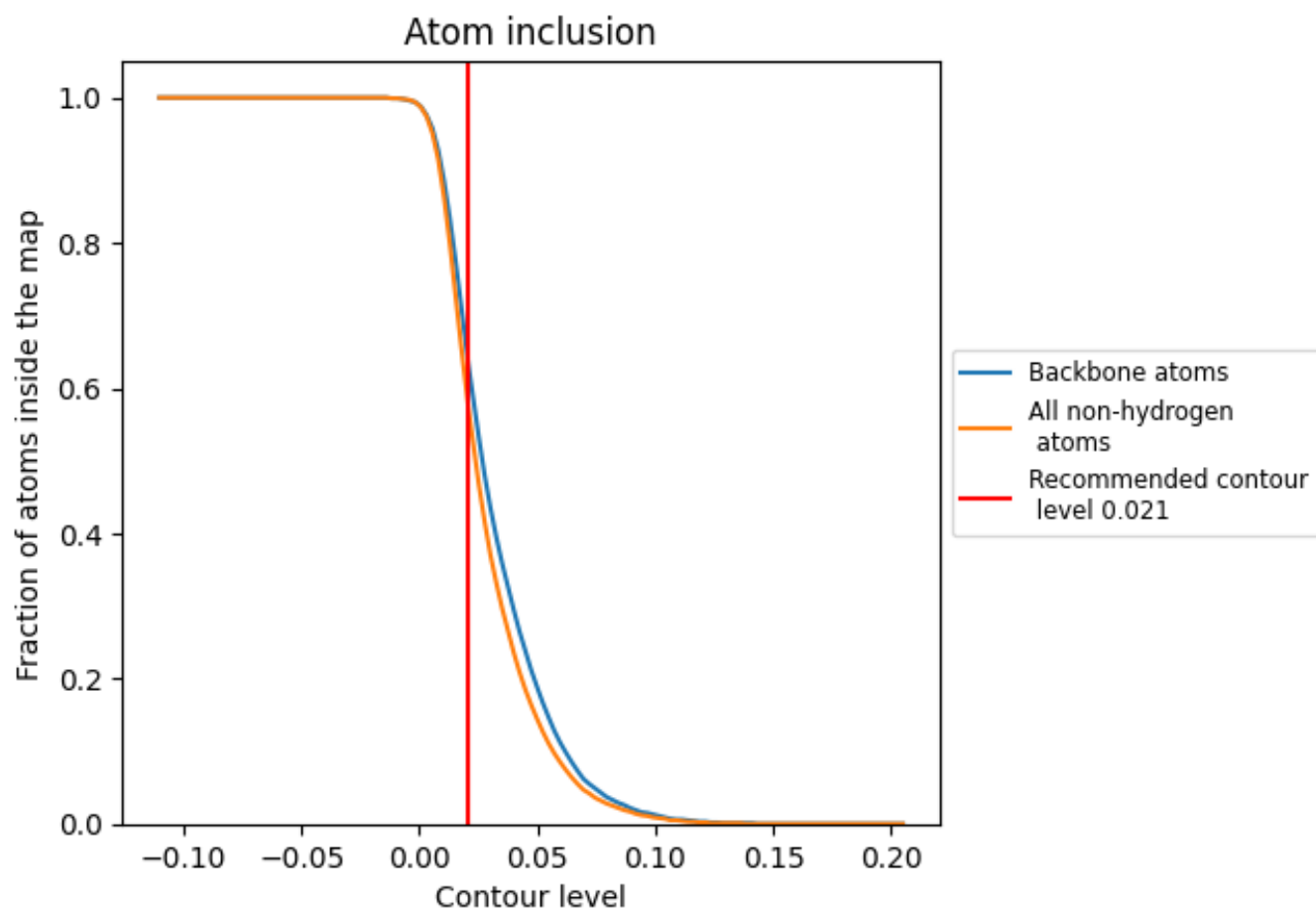


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.



















9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5680	 0.3790
A	 0.5660	 0.3770
B	 0.5660	 0.3770
C	 0.5660	 0.3770
D	 0.5650	 0.3770
G	 0.6570	 0.4500
H	 0.6550	 0.4520
I	 0.6530	 0.4540
J	 0.6580	 0.4500

