



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 06:12 AM UTC

PDB ID : 7VMP / pdb_00007vmp
EMDB ID : EMD-33939
Title : Structure of recombinant RyR2 (Ca²⁺ dataset, class 2, 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

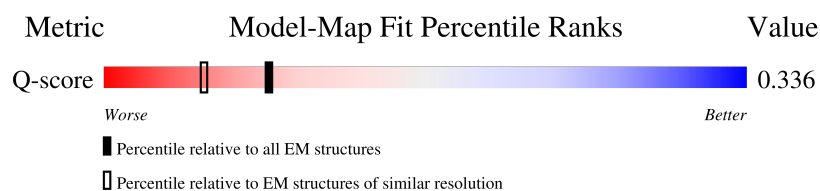
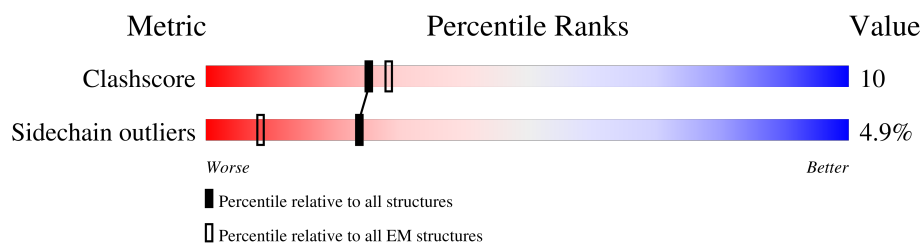
1 Overall quality at a glance

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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13085 (3.01 - 4.01)

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	
1	B	4966	
1	C	4966	
1	D	4966	
2	G	176	

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Mol	Chain	Length	Quality of chain
2	H	176	10% 40% 19% 39%
2	I	176	11% 41% 20% 39%
2	J	176	10% 40% 19% 39%

2 Entry composition

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
1	A	3991	Total	C	N	O	S	0	0
			29688	18782	5180	5553	173		
1	B	3991	Total	C	N	O	S	0	0
			29688	18782	5180	5553	173		
1	C	3991	Total	C	N	O	S	0	0
			29688	18782	5180	5553	173		
1	D	3991	Total	C	N	O	S	0	0
			29688	18782	5180	5553	173		

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

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

There are 276 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

- Molecule 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 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	C	1	Total 1	Ca 1	0
4	D	1	Total 1	Ca 1	0

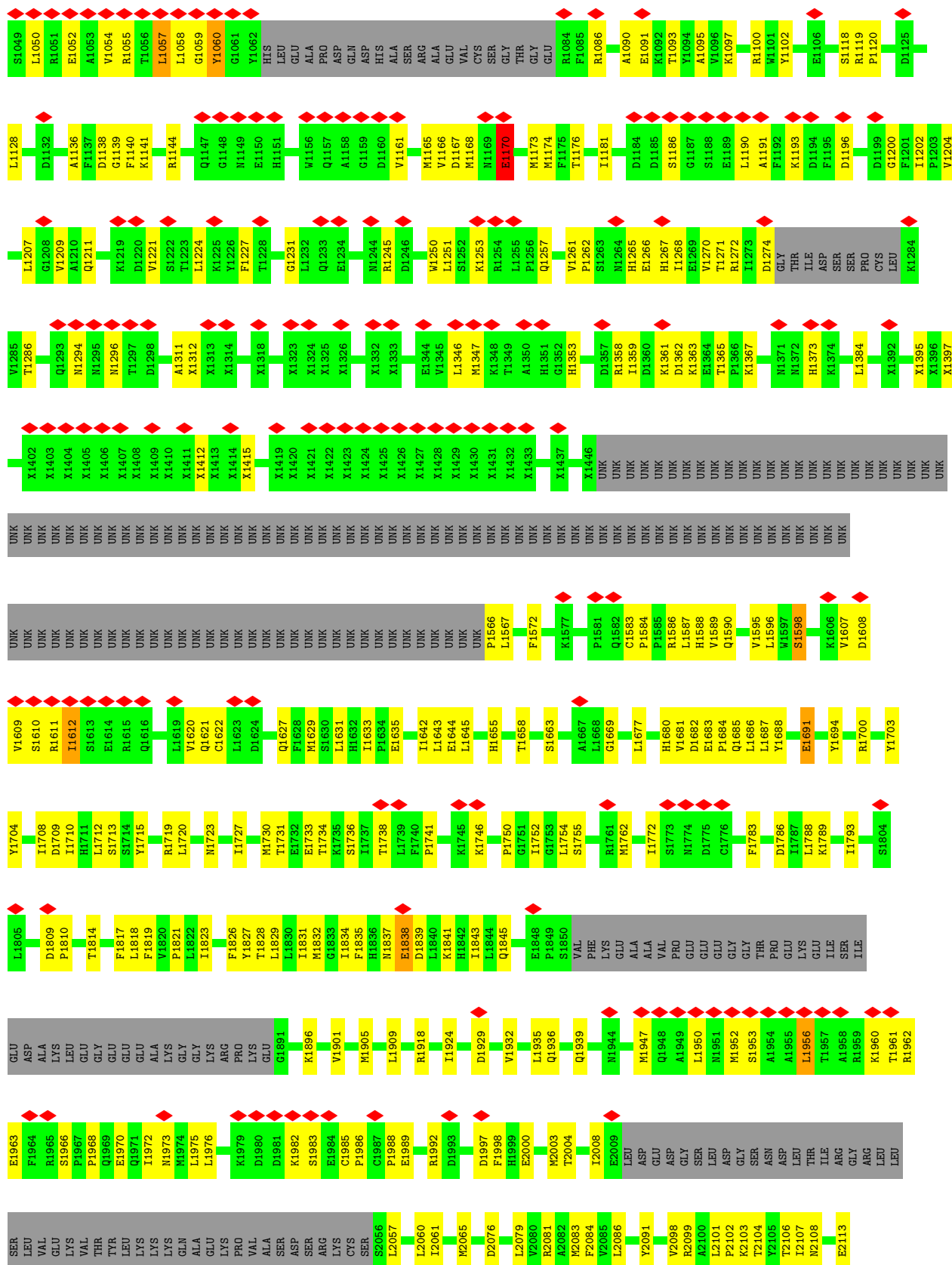






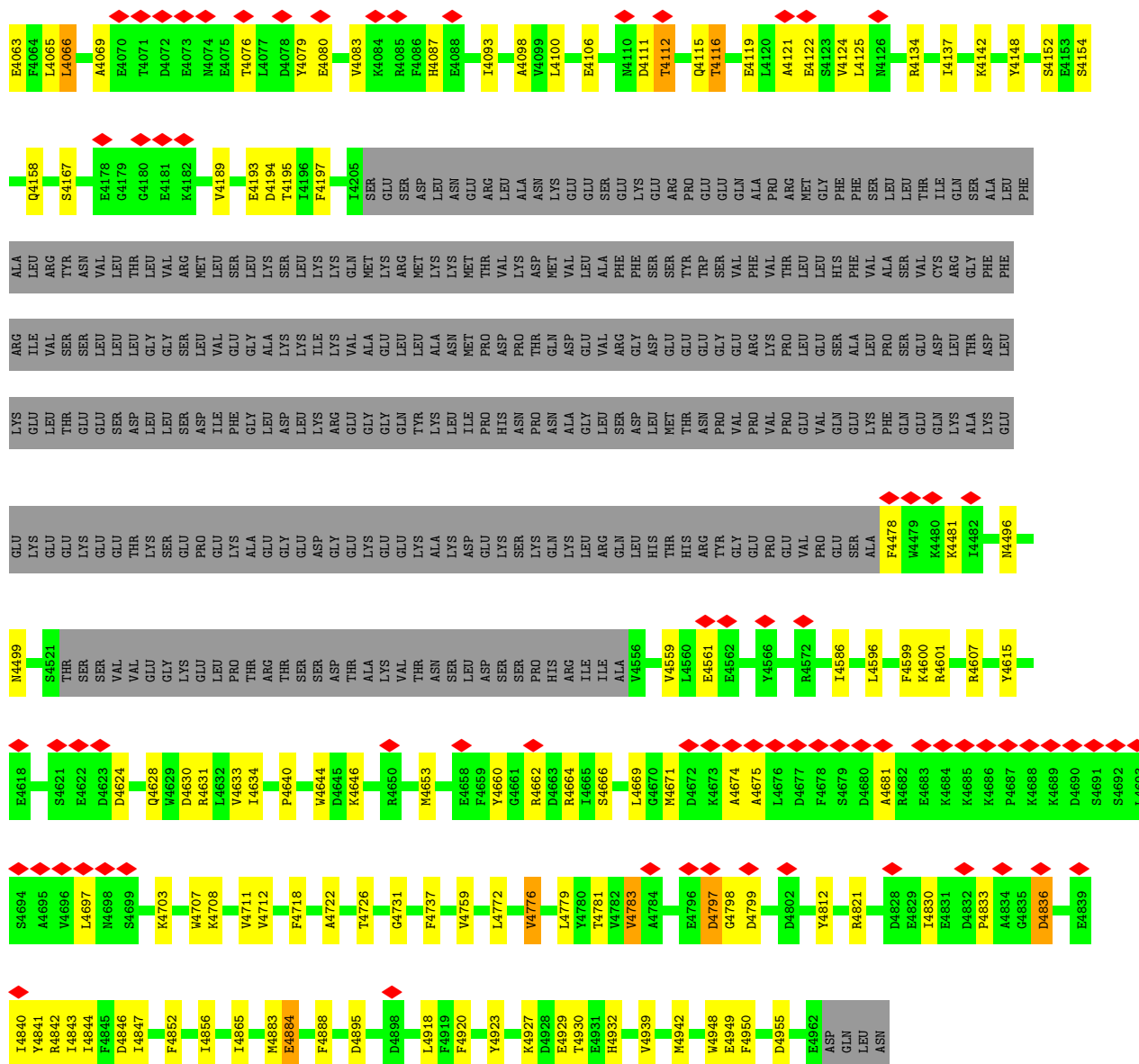




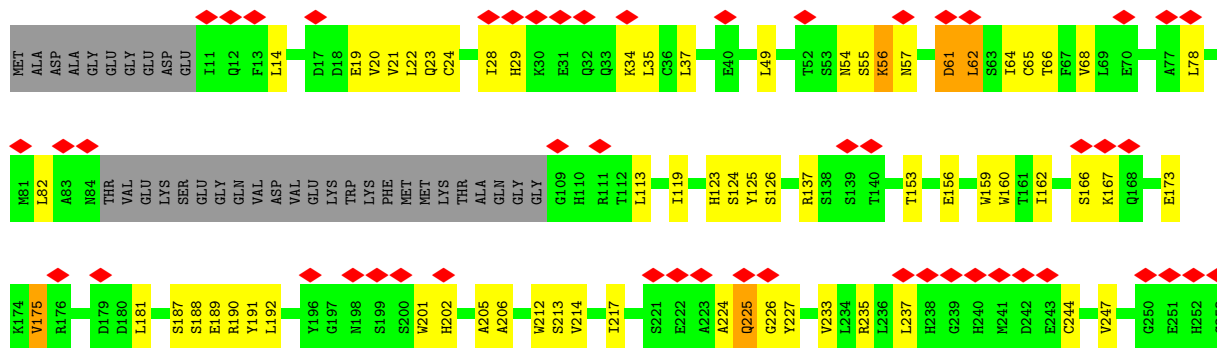


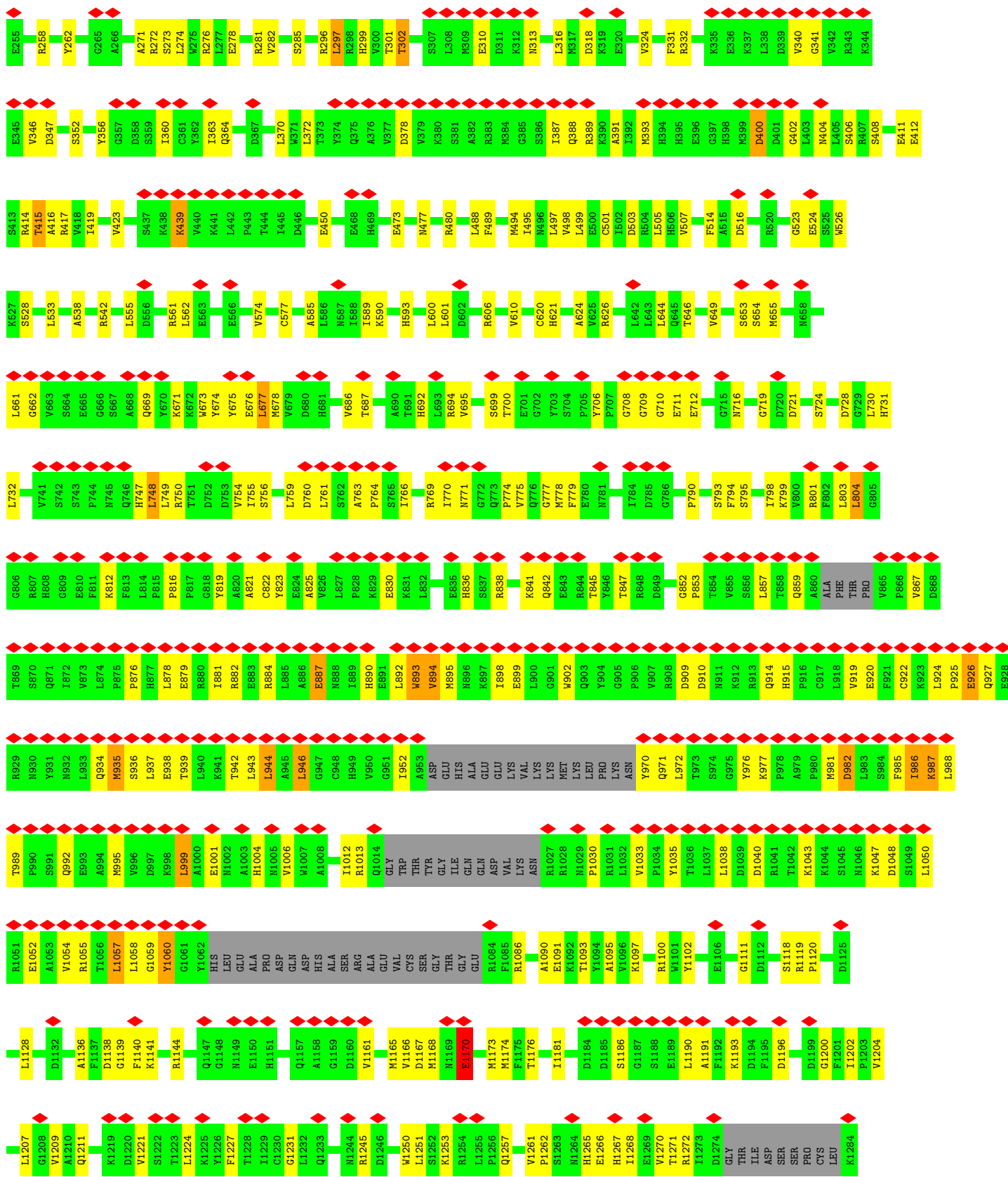






• Molecule 1: Ryanodine receptor 2

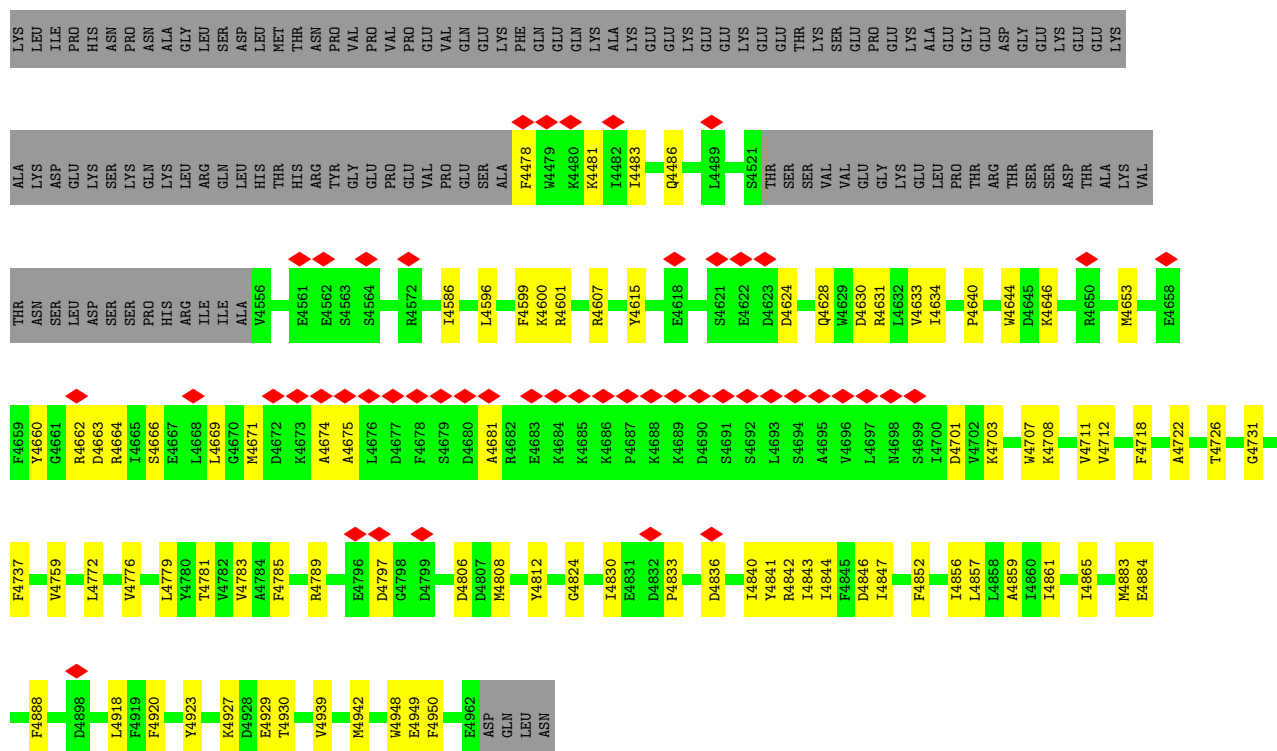




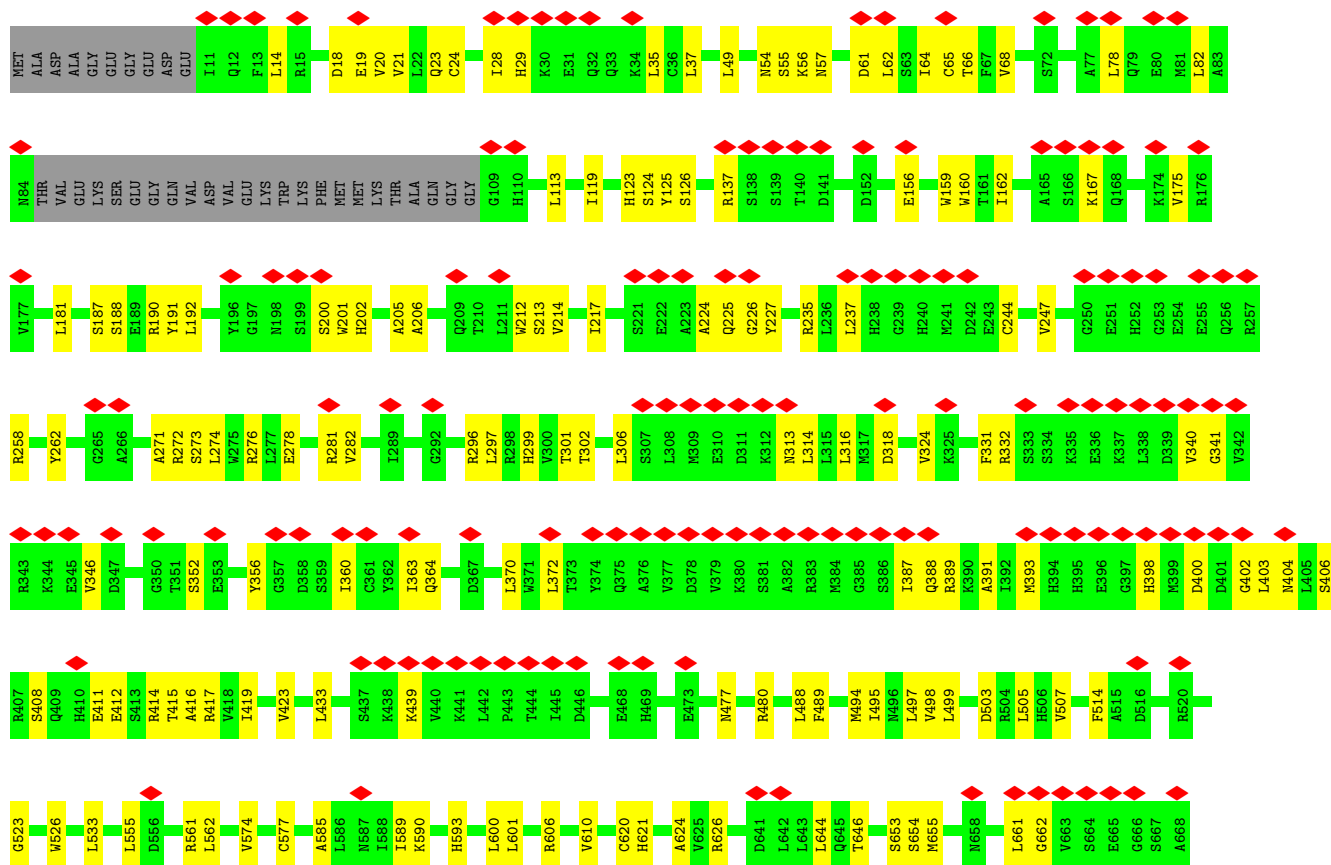








• Molecule 1: Ryanodine receptor 2



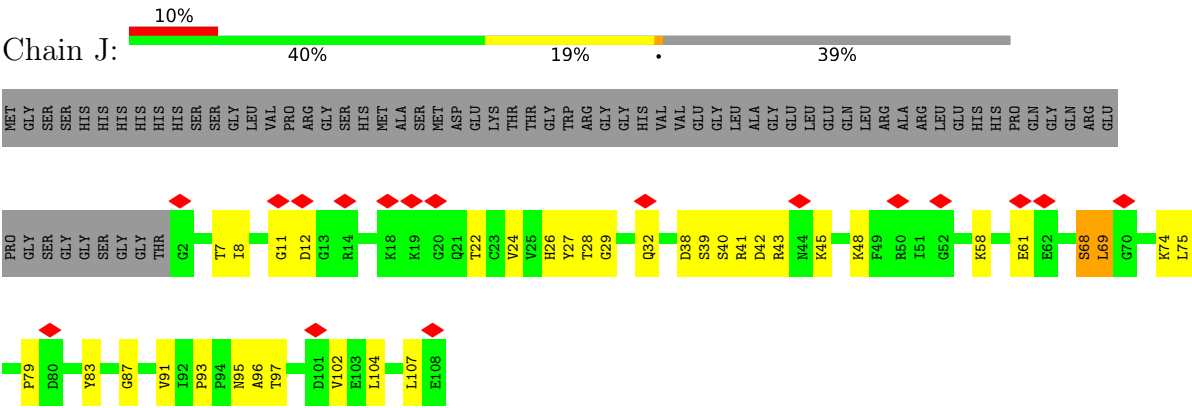








● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42375	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	0.165	Depositor
Minimum map value	-0.096	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/26573	0.38	7/35881 (0.0%)
1	B	0.14	0/26573	0.38	7/35881 (0.0%)
1	C	0.14	0/26573	0.38	7/35881 (0.0%)
1	D	0.14	0/26573	0.38	7/35881 (0.0%)
2	G	0.13	0/835	0.38	0/1123
2	H	0.13	0/835	0.38	0/1123
2	I	0.13	0/835	0.38	0/1123
2	J	0.13	0/835	0.38	0/1123
All	All	0.14	0/109632	0.38	28/148016 (0.0%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1170	GLU	CA-CB-CG	6.12	126.33	114.10
1	D	1170	GLU	CA-CB-CG	6.11	126.33	114.10
1	A	1170	GLU	CA-CB-CG	6.09	126.29	114.10
1	B	1170	GLU	CA-CB-CG	6.09	126.28	114.10
1	A	1838	GLU	CA-CB-CG	5.87	125.85	114.10
1	C	1838	GLU	CA-CB-CG	5.87	125.85	114.10
1	B	1838	GLU	CA-CB-CG	5.87	125.83	114.10
1	D	1838	GLU	CA-CB-CG	5.87	125.83	114.10
1	B	2257	ARG	CA-C-N	-5.73	115.95	123.34
1	B	2257	ARG	C-N-CA	-5.73	115.95	123.34
1	D	2257	ARG	CA-C-N	-5.71	115.97	123.34
1	D	2257	ARG	C-N-CA	-5.71	115.97	123.34
1	C	2257	ARG	CA-C-N	-5.69	116.00	123.34
1	C	2257	ARG	C-N-CA	-5.69	116.00	123.34
1	A	2257	ARG	CA-C-N	-5.69	116.00	123.34
1	A	2257	ARG	C-N-CA	-5.69	116.00	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2725	GLU	CA-CB-CG	5.31	124.71	114.10
1	D	2725	GLU	CA-CB-CG	5.30	124.70	114.10
1	B	2725	GLU	CA-CB-CG	5.28	124.66	114.10
1	C	2725	GLU	CA-CB-CG	5.28	124.66	114.10
1	B	1612	ILE	N-CA-C	-5.11	108.85	113.71
1	D	1612	ILE	N-CA-C	-5.08	108.88	113.71
1	C	1612	ILE	N-CA-C	-5.06	108.90	113.71
1	A	1612	ILE	N-CA-C	-5.04	108.92	113.71
1	B	1838	GLU	CB-CG-CD	5.04	121.16	112.60
1	C	1838	GLU	CB-CG-CD	5.01	121.12	112.60
1	A	1838	GLU	CB-CG-CD	5.01	121.11	112.60
1	D	1838	GLU	CB-CG-CD	5.00	121.11	112.60

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	585	0
1	B	29688	0	26383	586	0
1	C	29688	0	26383	583	0
1	D	29688	0	26383	594	0
2	G	819	0	821	23	0
2	H	819	0	821	23	0
2	I	819	0	821	25	0
2	J	819	0	821	23	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	2398	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 10.

All (2398) 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:1687:LEU:O	1:A:1691:GLU:HB3	1.78	0.84
1:B:1687:LEU:O	1:B:1691:GLU:HB3	1.78	0.84
1:A:1170:GLU:OE1	1:A:1170:GLU:N	2.11	0.84
1:C:1687:LEU:O	1:C:1691:GLU:HB3	1.78	0.84
1:D:1687:LEU:O	1:D:1691:GLU:HB3	1.78	0.84
1:B:1170:GLU:OE1	1:B:1170:GLU:N	2.11	0.83
1:D:760:ASP:HB3	1:D:764:PRO:HG2	1.61	0.83
1:C:1170:GLU:N	1:C:1170:GLU:OE1	2.11	0.83
1:C:748:LEU:HD23	2:I:8:ILE:HG23	1.59	0.83
1:A:760:ASP:HB3	1:A:764:PRO:HG2	1.61	0.83
1:D:1170:GLU:OE1	1:D:1170:GLU:N	2.11	0.82
1:C:760:ASP:HB3	1:C:764:PRO:HG2	1.61	0.82
1:B:760:ASP:HB3	1:B:764:PRO:HG2	1.61	0.81
1:D:1165:MET:HE1	1:D:1231:GLY:HA3	1.63	0.81
1:C:1165:MET:HE1	1:C:1231:GLY:HA3	1.63	0.81
1:B:1165:MET:HE1	1:B:1231:GLY:HA3	1.63	0.80
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.65	0.79
1:C:4833:PRO:HD3	1:C:4842:ARG:HE	1.48	0.79
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.65	0.78
1:A:1165:MET:HE1	1:A:1231:GLY:HA3	1.63	0.78
1:A:4833:PRO:HD3	1:A:4842:ARG:HE	1.48	0.78
1:B:4833:PRO:HD3	1:B:4842:ARG:HE	1.48	0.78
1:D:4833:PRO:HD3	1:D:4842:ARG:HE	1.48	0.78
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.65	0.77
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.65	0.76
1:C:156:GLU:HG2	1:C:187:SER:HB3	1.68	0.75
1:B:156:GLU:HG2	1:B:187:SER:HB3	1.68	0.74
1:D:4844:ILE:HD12	1:D:4847:ILE:HD11	1.70	0.74
1:D:156:GLU:HG2	1:D:187:SER:HB3	1.68	0.74
1:B:189:GLU:OE2	1:C:2321:ARG:NH1	2.21	0.73
1:A:156:GLU:HG2	1:A:187:SER:HB3	1.68	0.73
1:A:4844:ILE:HD12	1:A:4847:ILE:HD11	1.70	0.73
1:C:4844:ILE:HD12	1:C:4847:ILE:HD11	1.70	0.72
1:B:719:GLY:H	1:B:724:SER:HB3	1.54	0.72
1:C:2740:TRP:HD1	1:C:2751:LYS:HE3	1.55	0.72
1:A:3773:GLN:OE1	1:A:3850:ASN:ND2	2.23	0.72
1:C:719:GLY:H	1:C:724:SER:HB3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:GLY:H	1:A:724:SER:HB3	1.54	0.72
1:B:1060:TYR:HD1	1:B:1060:TYR:H	1.38	0.72
1:A:2765:LYS:O	1:A:2769:ILE:HG23	1.90	0.71
1:B:4844:ILE:HD12	1:B:4847:ILE:HD11	1.70	0.71
1:D:981:MET:HE1	1:D:1059:GLY:HA3	1.73	0.71
1:C:981:MET:HE1	1:C:1059:GLY:HA3	1.73	0.71
1:C:1060:TYR:H	1:C:1060:TYR:HD1	1.38	0.71
1:B:2765:LYS:O	1:B:2769:ILE:HG23	1.90	0.71
1:C:3773:GLN:OE1	1:C:3850:ASN:ND2	2.23	0.71
1:D:1060:TYR:HD1	1:D:1060:TYR:H	1.38	0.71
1:D:2765:LYS:O	1:D:2769:ILE:HG23	1.90	0.71
1:A:1681:VAL:HG23	1:A:1682:ASP:H	1.55	0.71
1:C:1700:ARG:NH1	1:C:1817:PHE:O	2.24	0.71
1:B:981:MET:HE1	1:B:1059:GLY:HA3	1.73	0.71
1:A:1060:TYR:H	1:A:1060:TYR:HD1	1.38	0.71
1:B:924:LEU:HG	1:B:925:PRO:HD2	1.73	0.71
1:A:924:LEU:HG	1:A:925:PRO:HD2	1.73	0.71
1:B:3773:GLN:OE1	1:B:3850:ASN:ND2	2.23	0.71
1:D:1700:ARG:NH1	1:D:1817:PHE:O	2.24	0.71
1:C:1681:VAL:HG23	1:C:1682:ASP:H	1.56	0.70
1:D:3773:GLN:OE1	1:D:3850:ASN:ND2	2.23	0.70
1:A:981:MET:HE1	1:A:1059:GLY:HA3	1.73	0.70
1:B:2740:TRP:HD1	1:B:2751:LYS:HE3	1.54	0.70
1:A:4866:ILE:HD11	1:D:4859:ALA:HB1	1.74	0.70
1:B:1700:ARG:NH1	1:B:1817:PHE:O	2.24	0.70
1:D:719:GLY:H	1:D:724:SER:HB3	1.54	0.70
2:G:75:LEU:HD22	2:G:102:VAL:HG21	1.74	0.70
1:B:1681:VAL:HG23	1:B:1682:ASP:H	1.56	0.70
1:D:924:LEU:HG	1:D:925:PRO:HD2	1.73	0.70
1:A:2740:TRP:HD1	1:A:2751:LYS:HE3	1.54	0.69
1:D:2740:TRP:HD1	1:D:2751:LYS:HE3	1.54	0.69
2:H:75:LEU:HD22	2:H:102:VAL:HG21	1.74	0.69
1:C:924:LEU:HG	1:C:925:PRO:HD2	1.73	0.69
1:C:1684:PRO:HD3	2:I:42:ASP:HB3	1.73	0.69
1:C:2765:LYS:O	1:C:2769:ILE:HG23	1.90	0.69
1:A:1700:ARG:NH1	1:A:1817:PHE:O	2.24	0.69
2:J:75:LEU:HD22	2:J:102:VAL:HG21	1.74	0.69
1:D:1681:VAL:HG23	1:D:1682:ASP:H	1.56	0.69
2:I:75:LEU:HD22	2:I:102:VAL:HG21	1.74	0.69
1:D:1262:PRO:HG2	1:D:1265:HIS:HB2	1.75	0.69
1:B:1970:GLU:HA	1:B:1973:ASN:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2171:MET:HE2	1:D:2216:HIS:HB3	1.76	0.68
1:A:2171:MET:HE2	1:A:2216:HIS:HB3	1.76	0.68
1:C:3802:LEU:HD11	1:C:3908:ALA:HB2	1.76	0.68
1:A:2406:HIS:HA	1:A:2409:HIS:HB3	1.76	0.68
1:B:2406:HIS:HA	1:B:2409:HIS:HB3	1.76	0.68
1:C:1262:PRO:HG2	1:C:1265:HIS:HB2	1.75	0.68
1:B:191:TYR:OH	1:C:2325:ARG:NH1	2.26	0.68
1:A:1262:PRO:HG2	1:A:1265:HIS:HB2	1.75	0.68
1:C:1970:GLU:HA	1:C:1973:ASN:HB2	1.75	0.68
1:C:4830:ILE:HG13	1:C:4842:ARG:HH22	1.59	0.67
1:A:3802:LEU:HD11	1:A:3908:ALA:HB2	1.76	0.67
1:A:759:LEU:HD13	1:A:766:ILE:HG22	1.77	0.67
1:A:970:TYR:HE2	1:A:977:LYS:HG2	1.60	0.67
1:A:1682:ASP:HB2	1:A:1685:GLN:HB3	1.76	0.67
1:B:1682:ASP:HB2	1:B:1685:GLN:HB3	1.76	0.67
1:B:4830:ILE:HG13	1:B:4842:ARG:HH22	1.59	0.67
1:C:970:TYR:HE2	1:C:977:LYS:HG2	1.60	0.67
1:C:1682:ASP:HB2	1:C:1685:GLN:HB3	1.75	0.67
1:C:2171:MET:HE2	1:C:2216:HIS:HB3	1.76	0.67
1:D:3802:LEU:HD11	1:D:3908:ALA:HB2	1.76	0.67
1:B:2171:MET:HE2	1:B:2216:HIS:HB3	1.76	0.67
1:B:759:LEU:HD13	1:B:766:ILE:HG22	1.77	0.67
1:D:1970:GLU:HA	1:D:1973:ASN:HB2	1.75	0.67
1:A:49:LEU:HD12	1:A:201:TRP:HB3	1.77	0.67
1:A:4830:ILE:HG13	1:A:4842:ARG:HH22	1.60	0.67
1:C:759:LEU:HD13	1:C:766:ILE:HG22	1.77	0.67
1:D:759:LEU:HD13	1:D:766:ILE:HG22	1.77	0.67
1:B:3802:LEU:HD11	1:B:3908:ALA:HB2	1.76	0.67
1:D:1682:ASP:HB2	1:D:1685:GLN:HB3	1.76	0.67
1:D:2406:HIS:HA	1:D:2409:HIS:HB3	1.76	0.67
1:A:1970:GLU:HA	1:A:1973:ASN:HB2	1.75	0.66
1:B:1262:PRO:HG2	1:B:1265:HIS:HB2	1.75	0.66
1:C:748:LEU:CD2	2:I:8:ILE:HG23	2.25	0.66
1:D:970:TYR:HE2	1:D:977:LYS:HG2	1.60	0.66
1:C:2081:ARG:HG3	1:C:3686:LEU:HD22	1.76	0.66
1:D:654:SER:H	1:D:841:LYS:NZ	1.93	0.66
1:C:2406:HIS:HA	1:C:2409:HIS:HB3	1.76	0.66
1:C:2893:LYS:O	1:C:2897:ILE:HG13	1.96	0.66
1:A:804:LEU:HD22	1:A:822:CYS:HB2	1.78	0.66
1:A:2081:ARG:HG3	1:A:3686:LEU:HD22	1.76	0.66
1:B:970:TYR:HE2	1:B:977:LYS:HG2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:SER:H	1:C:841:LYS:NZ	1.93	0.66
1:C:1720:LEU:HD21	1:C:1831:ILE:HD13	1.78	0.66
2:I:104:LEU:HD21	2:I:107:LEU:HD21	1.78	0.66
1:B:49:LEU:HD12	1:B:201:TRP:HB3	1.77	0.66
1:C:804:LEU:HD22	1:C:822:CYS:HB2	1.78	0.66
1:D:4830:ILE:HG13	1:D:4842:ARG:HH22	1.59	0.66
1:A:2893:LYS:O	1:A:2897:ILE:HG13	1.96	0.66
1:D:49:LEU:HD12	1:D:201:TRP:HB3	1.77	0.66
1:D:804:LEU:HD22	1:D:822:CYS:HB2	1.78	0.66
2:G:104:LEU:HD21	2:G:107:LEU:HD21	1.78	0.66
1:B:1720:LEU:HD21	1:B:1831:ILE:HD13	1.78	0.66
1:D:2081:ARG:HG3	1:D:3686:LEU:HD22	1.76	0.66
1:D:2893:LYS:O	1:D:2897:ILE:HG13	1.96	0.66
1:B:2893:LYS:O	1:B:2897:ILE:HG13	1.95	0.66
1:D:590:LYS:H	1:D:593:HIS:HD2	1.44	0.66
1:A:654:SER:H	1:A:841:LYS:NZ	1.93	0.65
1:B:412:GLU:HG3	1:B:488:LEU:HD11	1.78	0.65
1:D:412:GLU:HG3	1:D:488:LEU:HD11	1.79	0.65
1:A:1266:GLU:O	1:A:1267:HIS:ND1	2.29	0.65
1:B:1266:GLU:O	1:B:1267:HIS:ND1	2.29	0.65
1:D:1266:GLU:O	1:D:1267:HIS:ND1	2.29	0.65
1:D:3786:VAL:O	1:D:3790:GLN:HG3	1.97	0.65
1:B:2081:ARG:HG3	1:B:3686:LEU:HD22	1.76	0.65
1:B:3826:GLU:HG2	1:B:3827:LYS:H	1.62	0.65
1:B:804:LEU:HD22	1:B:822:CYS:HB2	1.78	0.65
1:B:3786:VAL:O	1:B:3790:GLN:HG3	1.97	0.65
1:C:49:LEU:HD12	1:C:201:TRP:HB3	1.77	0.65
1:C:1719:ARG:O	1:C:1723:ASN:HB2	1.97	0.65
1:C:1985:CYS:SG	1:C:1992:ARG:NH1	2.70	0.65
1:C:3786:VAL:O	1:C:3790:GLN:HG3	1.96	0.65
1:C:3826:GLU:HG2	1:C:3827:LYS:H	1.62	0.65
1:D:4840:ILE:HD12	1:D:4843:ILE:HD11	1.78	0.65
2:J:104:LEU:HD21	2:J:107:LEU:HD21	1.78	0.65
1:A:1985:CYS:SG	1:A:1992:ARG:NH1	2.70	0.65
1:B:654:SER:H	1:B:841:LYS:NZ	1.93	0.65
1:C:590:LYS:H	1:C:593:HIS:HD2	1.44	0.65
1:C:1266:GLU:O	1:C:1267:HIS:ND1	2.29	0.65
1:A:412:GLU:HG3	1:A:488:LEU:HD11	1.78	0.65
1:B:1985:CYS:SG	1:B:1992:ARG:NH1	2.70	0.65
2:I:28:THR:HA	2:I:39:SER:HA	1.79	0.65
1:A:3826:GLU:HG2	1:A:3827:LYS:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1793:ILE:HG12	1:B:1843:ILE:HD11	1.79	0.65
1:C:412:GLU:HG3	1:C:488:LEU:HD11	1.78	0.65
1:C:1793:ILE:HG12	1:C:1843:ILE:HD11	1.79	0.65
1:D:1720:LEU:HD21	1:D:1831:ILE:HD13	1.78	0.65
1:A:4840:ILE:HD12	1:A:4843:ILE:HD11	1.78	0.64
1:D:1688:TYR:HA	1:D:1691:GLU:HG2	1.79	0.64
1:C:2844:ALA:HB1	1:C:2884:ASP:HB3	1.78	0.64
1:D:1719:ARG:O	1:D:1723:ASN:HB2	1.97	0.64
1:D:3826:GLU:HG2	1:D:3827:LYS:H	1.62	0.64
1:C:3611:PRO:HD2	1:C:3614:ARG:HD3	1.79	0.64
1:A:1720:LEU:HD21	1:A:1831:ILE:HD13	1.78	0.64
1:B:1719:ARG:O	1:B:1723:ASN:HB2	1.97	0.64
1:B:4840:ILE:HD12	1:B:4843:ILE:HD11	1.78	0.64
2:H:28:THR:HA	2:H:39:SER:HA	1.79	0.64
2:H:104:LEU:HD21	2:H:107:LEU:HD21	1.78	0.64
1:A:3786:VAL:O	1:A:3790:GLN:HG3	1.97	0.64
1:B:2844:ALA:HB1	1:B:2884:ASP:HB3	1.78	0.64
1:D:1985:CYS:SG	1:D:1992:ARG:NH1	2.70	0.64
2:G:28:THR:HA	2:G:39:SER:HA	1.79	0.64
1:A:590:LYS:H	1:A:593:HIS:HD2	1.44	0.64
1:A:2844:ALA:HB1	1:A:2884:ASP:HB3	1.78	0.64
1:A:3611:PRO:HD2	1:A:3614:ARG:HD3	1.79	0.64
1:D:943:LEU:HG	1:D:999:LEU:HD13	1.80	0.64
1:A:943:LEU:HG	1:A:999:LEU:HD13	1.80	0.64
1:D:2844:ALA:HB1	1:D:2884:ASP:HB3	1.78	0.64
1:A:1719:ARG:O	1:A:1723:ASN:HB2	1.97	0.63
1:B:3611:PRO:HD2	1:B:3614:ARG:HD3	1.79	0.63
1:C:1257:GLN:HA	1:C:1384:LEU:HD23	1.81	0.63
1:D:1793:ILE:HG12	1:D:1843:ILE:HD11	1.79	0.63
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.31	0.63
1:C:1688:TYR:HA	1:C:1691:GLU:HG2	1.79	0.63
1:C:4840:ILE:HD12	1:C:4843:ILE:HD11	1.78	0.63
1:D:3611:PRO:HD2	1:D:3614:ARG:HD3	1.79	0.63
1:A:644:LEU:HD13	1:A:1631:LEU:HD21	1.81	0.63
1:A:1793:ILE:HG12	1:A:1843:ILE:HD11	1.79	0.63
1:C:943:LEU:HG	1:C:999:LEU:HD13	1.80	0.63
1:D:644:LEU:HD13	1:D:1631:LEU:HD21	1.81	0.63
1:A:1688:TYR:HA	1:A:1691:GLU:HG2	1.79	0.63
1:D:3613:HIS:O	1:D:3617:ASN:ND2	2.32	0.63
1:B:2485:HIS:O	1:B:2489:VAL:HG22	1.99	0.63
1:C:3613:HIS:O	1:C:3617:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:LYS:H	1:B:593:HIS:HD2	1.44	0.63
1:C:4624:ASP:O	1:C:4628:GLN:NE2	2.32	0.63
1:D:1257:GLN:HA	1:D:1384:LEU:HD23	1.81	0.63
1:D:2485:HIS:O	1:D:2489:VAL:HG22	1.99	0.63
2:J:28:THR:HA	2:J:39:SER:HA	1.79	0.63
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.31	0.63
1:A:2414:GLU:OE1	1:A:2414:GLU:N	2.32	0.63
1:B:2414:GLU:OE1	1:B:2414:GLU:N	2.32	0.63
1:B:4624:ASP:O	1:B:4628:GLN:NE2	2.32	0.63
1:D:1166:VAL:HG22	1:D:1173:MET:HG2	1.80	0.63
1:B:207:PHE:CE1	1:C:2324:ILE:HD12	2.34	0.62
1:B:2442:PRO:HG2	1:B:2506:LEU:HD21	1.81	0.62
1:B:1257:GLN:HA	1:B:1384:LEU:HD23	1.81	0.62
1:C:4042:ILE:HG22	1:C:4044:LYS:H	1.64	0.62
1:D:4624:ASP:O	1:D:4628:GLN:NE2	2.32	0.62
1:A:2485:HIS:O	1:A:2489:VAL:HG22	1.99	0.62
1:B:1166:VAL:HG22	1:B:1173:MET:HG2	1.81	0.62
1:C:2414:GLU:N	1:C:2414:GLU:OE1	2.32	0.62
1:B:943:LEU:HG	1:B:999:LEU:HD13	1.80	0.62
1:C:2485:HIS:O	1:C:2489:VAL:HG22	1.99	0.62
2:J:11:GLY:O	2:J:68:SER:OG	2.18	0.62
1:B:1663:SER:OG	1:B:1709:ASP:OD2	2.17	0.62
1:C:1789:LYS:HG3	1:C:1835:PHE:HE1	1.65	0.62
1:D:2442:PRO:HG2	1:D:2506:LEU:HD21	1.81	0.62
1:B:4042:ILE:HG22	1:B:4044:LYS:H	1.64	0.62
1:A:2442:PRO:HG2	1:A:2506:LEU:HD21	1.82	0.62
1:A:4624:ASP:O	1:A:4628:GLN:NE2	2.32	0.62
1:A:1257:GLN:HA	1:A:1384:LEU:HD23	1.81	0.62
1:B:644:LEU:HD13	1:B:1631:LEU:HD21	1.81	0.62
1:B:1688:TYR:HA	1:B:1691:GLU:HG2	1.79	0.62
1:D:2414:GLU:OE1	1:D:2414:GLU:N	2.32	0.62
1:A:276:ARG:NE	1:A:278:GLU:OE2	2.31	0.62
1:A:1663:SER:OG	1:A:1709:ASP:OD2	2.17	0.62
1:A:4660:TYR:HB3	1:A:4664:ARG:HH21	1.65	0.62
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.81	0.62
1:C:2442:PRO:HG2	1:C:2506:LEU:HD21	1.81	0.62
1:B:4660:TYR:HB3	1:B:4664:ARG:HH21	1.65	0.61
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.82	0.61
1:B:676:GLU:HB2	1:B:803:LEU:HB2	1.81	0.61
1:C:644:LEU:HD13	1:C:1631:LEU:HD21	1.81	0.61
1:C:1294:ASN:ND2	1:C:1296:ASN:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ARG:NH1	1:D:316:LEU:O	2.33	0.61
1:D:1789:LYS:HG3	1:D:1835:PHE:HE1	1.65	0.61
2:G:11:GLY:O	2:G:68:SER:OG	2.18	0.61
1:B:732:LEU:HD23	1:B:779:PHE:CZ	2.35	0.61
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.82	0.61
1:A:4042:ILE:HG22	1:A:4044:LYS:H	1.64	0.61
1:B:1839:ASP:O	1:B:1843:ILE:HG12	2.01	0.61
1:C:1166:VAL:HG22	1:C:1173:MET:HG2	1.81	0.61
1:D:1839:ASP:O	1:D:1843:ILE:HG12	2.01	0.61
1:D:4042:ILE:HG22	1:D:4044:LYS:H	1.65	0.61
1:D:4842:ARG:NH1	1:D:4846:ASP:OD2	2.34	0.61
1:A:671:LYS:HA	1:A:761:LEU:HD12	1.82	0.61
1:A:1166:VAL:HG22	1:A:1173:MET:HG2	1.81	0.61
1:A:732:LEU:HD23	1:A:779:PHE:CZ	2.35	0.61
1:C:4779:LEU:O	1:C:4783:VAL:HG23	2.01	0.61
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.81	0.61
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.83	0.61
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.82	0.61
1:B:258:ARG:NH1	1:B:316:LEU:O	2.33	0.61
1:B:1095:ALA:HB1	1:B:1200:GLY:HA3	1.82	0.61
1:C:732:LEU:HD23	1:C:779:PHE:CZ	2.35	0.61
1:C:1741:PRO:HB3	1:C:1746:LYS:HE3	1.83	0.61
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.31	0.61
1:D:1095:ALA:HB1	1:D:1200:GLY:HA3	1.82	0.61
1:D:2880:GLU:HA	1:D:2883:LYS:HB2	1.83	0.61
1:A:4842:ARG:NH1	1:A:4846:ASP:OD2	2.34	0.61
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.83	0.61
1:B:1789:LYS:HG3	1:B:1835:PHE:HE1	1.65	0.61
2:I:11:GLY:O	2:I:68:SER:OG	2.18	0.61
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.83	0.61
1:D:732:LEU:HD23	1:D:779:PHE:CZ	2.35	0.61
1:D:1294:ASN:ND2	1:D:1296:ASN:O	2.33	0.61
1:D:4779:LEU:O	1:D:4783:VAL:HG23	2.01	0.61
1:A:1839:ASP:O	1:A:1843:ILE:HG12	2.01	0.61
1:B:247:VAL:O	1:B:272:ARG:NH1	2.34	0.61
1:B:4772:LEU:O	1:B:4776:VAL:HG22	2.01	0.61
2:H:11:GLY:O	2:H:68:SER:OG	2.18	0.61
1:A:62:LEU:HA	1:A:65:CYS:HB2	1.82	0.61
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.81	0.61
1:A:4779:LEU:O	1:A:4783:VAL:HG23	2.01	0.61
1:B:2880:GLU:HA	1:B:2883:LYS:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4018:MET:HB3	1:B:4065:LEU:HD21	1.83	0.61
1:C:1663:SER:OG	1:C:1709:ASP:OD2	2.17	0.61
1:C:4660:TYR:HB3	1:C:4664:ARG:HH21	1.65	0.61
1:D:1663:SER:OG	1:D:1709:ASP:OD2	2.17	0.61
1:D:1741:PRO:HB3	1:D:1746:LYS:HE3	1.83	0.61
1:A:1741:PRO:HB3	1:A:1746:LYS:HE3	1.83	0.60
1:A:4772:LEU:O	1:A:4776:VAL:HG22	2.01	0.60
1:D:4660:TYR:HB3	1:D:4664:ARG:HH21	1.65	0.60
1:D:4772:LEU:O	1:D:4776:VAL:HG22	2.01	0.60
1:B:2003:MET:HB3	1:B:2008:ILE:HD11	1.83	0.60
1:B:3613:HIS:O	1:B:3617:ASN:ND2	2.32	0.60
1:C:247:VAL:O	1:C:272:ARG:NH1	2.34	0.60
1:C:258:ARG:NH1	1:C:316:LEU:O	2.33	0.60
1:C:276:ARG:NE	1:C:278:GLU:OE2	2.31	0.60
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.83	0.60
1:C:2385:ASN:O	1:C:2389:THR:HG22	2.01	0.60
1:A:258:ARG:NH1	1:A:316:LEU:O	2.33	0.60
1:A:2003:MET:HB3	1:A:2008:ILE:HD11	1.83	0.60
1:A:4018:MET:HB3	1:A:4065:LEU:HD21	1.83	0.60
1:B:4779:LEU:O	1:B:4783:VAL:HG23	2.01	0.60
1:C:1629:MET:HE3	1:C:1642:ILE:HG21	1.83	0.60
1:D:247:VAL:O	1:D:272:ARG:NH1	2.34	0.60
1:D:276:ARG:NE	1:D:278:GLU:OE2	2.31	0.60
1:A:1294:ASN:ND2	1:A:1296:ASN:O	2.33	0.60
1:A:2385:ASN:O	1:A:2389:THR:HG22	2.01	0.60
1:B:4046:ASP:HA	1:B:4049:LYS:HG2	1.84	0.60
1:C:671:LYS:HA	1:C:761:LEU:HD12	1.82	0.60
1:C:3891:TYR:OH	1:C:3898:ASP:OD2	2.19	0.60
1:C:4046:ASP:HA	1:C:4049:LYS:HG2	1.84	0.60
1:B:62:LEU:HA	1:B:65:CYS:HB2	1.82	0.60
1:D:3891:TYR:OH	1:D:3898:ASP:OD2	2.19	0.60
1:A:1095:ALA:HB1	1:A:1200:GLY:HA3	1.82	0.60
1:B:671:LYS:HA	1:B:761:LEU:HD12	1.83	0.60
1:C:1839:ASP:O	1:C:1843:ILE:HG12	2.01	0.60
1:C:1962:ARG:O	1:C:1966:SER:OG	2.20	0.60
1:A:1629:MET:HE3	1:A:1642:ILE:HG21	1.84	0.60
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.31	0.60
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.82	0.60
1:C:62:LEU:HA	1:C:65:CYS:HB2	1.82	0.60
1:C:1095:ALA:HB1	1:C:1200:GLY:HA3	1.82	0.60
1:C:4842:ARG:NH1	1:C:4846:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1629:MET:HE3	1:D:1642:ILE:HG21	1.84	0.60
1:D:4046:ASP:HA	1:D:4049:LYS:HG2	1.84	0.60
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.84	0.60
1:A:708:GLY:O	1:A:838:ARG:NH1	2.35	0.60
1:A:1789:LYS:HG3	1:A:1835:PHE:HE1	1.65	0.60
1:A:2880:GLU:HA	1:A:2883:LYS:HB2	1.83	0.60
1:B:1294:ASN:ND2	1:B:1296:ASN:O	2.33	0.60
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.84	0.60
1:C:2880:GLU:HA	1:C:2883:LYS:HB2	1.83	0.60
1:D:671:LYS:HA	1:D:761:LEU:HD12	1.82	0.60
1:D:1962:ARG:O	1:D:1966:SER:OG	2.20	0.60
1:A:1962:ARG:O	1:A:1966:SER:OG	2.20	0.60
1:B:1629:MET:HE3	1:B:1642:ILE:HG21	1.84	0.60
1:C:4111:ASP:O	1:C:4115:GLN:N	2.35	0.60
1:A:247:VAL:O	1:A:272:ARG:NH1	2.34	0.60
1:B:708:GLY:O	1:B:838:ARG:NH1	2.35	0.60
1:B:1741:PRO:HB3	1:B:1746:LYS:HE3	1.83	0.60
1:B:4842:ARG:NH1	1:B:4846:ASP:OD2	2.34	0.59
1:C:2003:MET:HB3	1:C:2008:ILE:HD11	1.83	0.59
1:D:2385:ASN:O	1:D:2389:THR:HG22	2.01	0.59
1:D:4111:ASP:O	1:D:4115:GLN:N	2.35	0.59
1:A:4046:ASP:HA	1:A:4049:LYS:HG2	1.84	0.59
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.84	0.59
1:B:1609:VAL:HA	1:B:1620:VAL:HA	1.84	0.59
1:B:2065:MET:HE3	1:B:2086:LEU:HD23	1.84	0.59
1:B:2385:ASN:O	1:B:2389:THR:HG22	2.01	0.59
1:D:62:LEU:HA	1:D:65:CYS:HB2	1.82	0.59
1:C:892:LEU:HD23	1:C:895:MET:HE2	1.85	0.59
1:D:360:ILE:HG23	1:D:402:GLY:HA2	1.84	0.59
2:H:32:GLN:NE2	2:H:97:THR:OG1	2.35	0.59
1:C:360:ILE:HG23	1:C:402:GLY:HA2	1.84	0.59
1:C:4018:MET:HB3	1:C:4065:LEU:HD21	1.83	0.59
1:C:4772:LEU:O	1:C:4776:VAL:HG22	2.01	0.59
1:D:708:GLY:O	1:D:838:ARG:NH1	2.35	0.59
1:A:890:HIS:O	1:A:894:VAL:HG22	2.03	0.59
1:A:2065:MET:HE3	1:A:2086:LEU:HD23	1.84	0.59
1:C:708:GLY:O	1:C:838:ARG:NH1	2.35	0.59
1:D:28:ILE:HG12	1:D:29:HIS:ND1	2.17	0.59
1:D:2003:MET:HB3	1:D:2008:ILE:HD11	1.83	0.59
1:D:2732:SER:HA	1:D:2735:LYS:HD2	1.84	0.59
2:J:32:GLN:NE2	2:J:97:THR:OG1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3613:HIS:O	1:A:3617:ASN:ND2	2.32	0.59
1:A:4813:MET:HG3	1:D:4843:ILE:HD13	1.84	0.59
1:B:28:ILE:HG12	1:B:29:HIS:ND1	2.17	0.59
1:B:4111:ASP:O	1:B:4115:GLN:N	2.35	0.59
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.36	0.59
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.36	0.59
1:A:1684:PRO:HD3	2:G:42:ASP:HB3	1.84	0.59
1:B:1962:ARG:O	1:B:1966:SER:OG	2.20	0.59
2:I:32:GLN:NE2	2:I:97:THR:OG1	2.35	0.59
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.84	0.59
1:D:2261:LEU:O	1:D:2265:VAL:HG22	2.03	0.59
1:D:4018:MET:HB3	1:D:4065:LEU:HD21	1.83	0.59
1:B:123:HIS:HD2	1:B:126:SER:H	1.51	0.59
1:B:3718:MET:HE3	1:B:4681:ALA:HB1	1.84	0.59
1:B:3891:TYR:OH	1:B:3898:ASP:OD2	2.19	0.59
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.36	0.59
1:A:946:LEU:HD13	1:A:995:MET:HG2	1.85	0.59
1:A:2732:SER:HA	1:A:2735:LYS:HD2	1.84	0.59
1:B:946:LEU:HD13	1:B:995:MET:HG2	1.85	0.59
1:B:1607:VAL:HG23	1:B:1622:CYS:HB2	1.85	0.59
1:B:2413:GLY:HA2	1:B:2416:ILE:HD12	1.85	0.59
1:B:2732:SER:HA	1:B:2735:LYS:HD2	1.84	0.59
1:C:890:HIS:O	1:C:894:VAL:HG22	2.03	0.59
1:C:3718:MET:HE3	1:C:4681:ALA:HB1	1.84	0.59
1:D:881:ILE:O	1:D:884:ARG:HG3	2.03	0.59
1:D:4633:VAL:HG12	1:D:4703:LYS:HG2	1.85	0.59
2:G:32:GLN:NE2	2:G:97:THR:OG1	2.35	0.58
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.36	0.58
1:C:28:ILE:HG12	1:C:29:HIS:ND1	2.17	0.58
1:C:4633:VAL:HG12	1:C:4703:LYS:HG2	1.85	0.58
1:D:892:LEU:HD23	1:D:895:MET:HE2	1.85	0.58
1:D:1607:VAL:HG23	1:D:1622:CYS:HB2	1.85	0.58
1:A:881:ILE:O	1:A:884:ARG:HG3	2.03	0.58
1:A:4111:ASP:O	1:A:4115:GLN:N	2.35	0.58
1:C:946:LEU:HD13	1:C:995:MET:HG2	1.85	0.58
1:C:2065:MET:HE3	1:C:2086:LEU:HD23	1.84	0.58
1:C:2413:GLY:HA2	1:C:2416:ILE:HD12	1.85	0.58
1:D:946:LEU:HD13	1:D:995:MET:HG2	1.85	0.58
1:D:2314:GLU:O	1:D:2318:VAL:HG22	2.03	0.58
1:D:3718:MET:HE3	1:D:4681:ALA:HB1	1.84	0.58
1:A:4478:PHE:HA	1:A:4481:LYS:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ILE:HG23	1:B:402:GLY:HA2	1.84	0.58
1:C:4797:ASP:OD1	1:C:4797:ASP:N	2.36	0.58
1:D:1989:GLU:HG2	1:D:1992:ARG:HD3	1.85	0.58
1:D:4478:PHE:HA	1:D:4481:LYS:HE2	1.84	0.58
1:A:123:HIS:HD2	1:A:126:SER:H	1.51	0.58
1:A:360:ILE:HG23	1:A:402:GLY:HA2	1.84	0.58
1:A:2261:LEU:O	1:A:2265:VAL:HG22	2.03	0.58
1:A:2314:GLU:O	1:A:2318:VAL:HG22	2.03	0.58
1:A:2413:GLY:HA2	1:A:2416:ILE:HD12	1.85	0.58
1:B:890:HIS:O	1:B:894:VAL:HG22	2.03	0.58
1:B:2314:GLU:O	1:B:2318:VAL:HG22	2.03	0.58
1:C:2732:SER:HA	1:C:2735:LYS:HD2	1.84	0.58
1:D:2065:MET:HE3	1:D:2086:LEU:HD23	1.84	0.58
1:A:1607:VAL:HG23	1:A:1622:CYS:HB2	1.85	0.58
1:A:3718:MET:HE3	1:A:4681:ALA:HB1	1.84	0.58
1:B:2261:LEU:O	1:B:2265:VAL:HG22	2.03	0.58
1:B:2348:GLU:O	1:B:2352:ILE:HG13	2.04	0.58
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.37	0.58
1:C:881:ILE:O	1:C:884:ARG:HG3	2.03	0.58
1:C:2261:LEU:O	1:C:2265:VAL:HG22	2.03	0.58
1:D:890:HIS:O	1:D:894:VAL:HG22	2.03	0.58
1:A:28:ILE:HG12	1:A:29:HIS:ND1	2.17	0.58
1:A:892:LEU:HD23	1:A:895:MET:HE2	1.85	0.58
1:B:4633:VAL:HG12	1:B:4703:LYS:HG2	1.85	0.58
1:B:881:ILE:O	1:B:884:ARG:HG3	2.03	0.58
1:C:2314:GLU:O	1:C:2318:VAL:HG22	2.04	0.58
1:D:1723:ASN:O	1:D:1918:ARG:NH2	2.36	0.58
1:D:3909:ILE:HG21	1:D:3969:GLU:HB3	1.86	0.58
1:A:671:LYS:HB3	1:A:761:LEU:HB2	1.86	0.58
1:A:1609:VAL:HA	1:A:1620:VAL:HA	1.84	0.58
1:A:1723:ASN:O	1:A:1918:ARG:NH2	2.36	0.58
1:A:4923:TYR:O	1:A:4927:LYS:HB2	2.03	0.58
1:C:1272:ARG:NH2	1:C:1584:PRO:O	2.37	0.58
1:C:1607:VAL:HG23	1:C:1622:CYS:HB2	1.85	0.58
1:C:1723:ASN:O	1:C:1918:ARG:NH2	2.36	0.58
1:C:2348:GLU:O	1:C:2352:ILE:HG13	2.04	0.58
1:D:2127:SER:O	1:D:2131:VAL:HG23	2.04	0.58
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.37	0.58
1:B:4478:PHE:HA	1:B:4481:LYS:HE2	1.84	0.58
1:C:1989:GLU:HG2	1:C:1992:ARG:HD3	1.85	0.58
1:A:400:ASP:OD1	1:A:400:ASP:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1253:LYS:HB3	1:B:1598:SER:HB2	1.86	0.58
1:B:1723:ASN:O	1:B:1918:ARG:NH2	2.36	0.58
1:B:1989:GLU:HA	1:B:1992:ARG:HD3	1.86	0.58
1:B:1989:GLU:HG2	1:B:1992:ARG:HD3	1.85	0.58
1:B:4923:TYR:O	1:B:4927:LYS:HB2	2.03	0.58
1:C:400:ASP:OD1	1:C:400:ASP:N	2.37	0.58
1:D:1609:VAL:HA	1:D:1620:VAL:HA	1.85	0.58
1:B:2127:SER:O	1:B:2131:VAL:HG23	2.04	0.57
1:C:1609:VAL:HA	1:C:1620:VAL:HA	1.84	0.57
1:C:2127:SER:O	1:C:2131:VAL:HG23	2.04	0.57
1:C:4923:TYR:O	1:C:4927:LYS:HB2	2.03	0.57
1:A:4797:ASP:OD1	1:A:4797:ASP:N	2.36	0.57
1:D:655:MET:SD	1:D:836:HIS:ND1	2.77	0.57
1:D:2413:GLY:HA2	1:D:2416:ILE:HD12	1.85	0.57
1:D:4923:TYR:O	1:D:4927:LYS:HB2	2.03	0.57
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.37	0.57
1:A:1989:GLU:HA	1:A:1992:ARG:HD3	1.86	0.57
1:A:4633:VAL:HG12	1:A:4703:LYS:HG2	1.86	0.57
1:B:276:ARG:NE	1:B:278:GLU:OE2	2.31	0.57
1:B:1272:ARG:NH2	1:B:1584:PRO:O	2.37	0.57
1:B:1684:PRO:HD3	2:H:42:ASP:HB3	1.85	0.57
1:C:1609:VAL:HG23	1:C:1610:SER:H	1.70	0.57
1:C:4478:PHE:HA	1:C:4481:LYS:HE2	1.84	0.57
1:D:1253:LYS:HB3	1:D:1598:SER:HB2	1.86	0.57
1:A:987:LYS:HD2	1:A:988:LEU:N	2.20	0.57
1:A:3891:TYR:OH	1:A:3898:ASP:OD2	2.19	0.57
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.37	0.57
1:D:671:LYS:HB3	1:D:761:LEU:HB2	1.86	0.57
1:D:1989:GLU:HA	1:D:1992:ARG:HD3	1.86	0.57
1:A:1989:GLU:HG2	1:A:1992:ARG:HD3	1.85	0.57
1:A:2145:LEU:HD23	1:A:2148:ILE:HD11	1.87	0.57
1:B:892:LEU:HD23	1:B:895:MET:HE2	1.85	0.57
1:B:2145:LEU:HD23	1:B:2148:ILE:HD11	1.87	0.57
1:C:1929:ASP:OD1	1:C:3612:ARG:NH2	2.38	0.57
1:C:1989:GLU:HA	1:C:1992:ARG:HD3	1.86	0.57
1:C:3909:ILE:HG21	1:C:3969:GLU:HB3	1.86	0.57
1:A:1929:ASP:OD1	1:A:3612:ARG:NH2	2.38	0.57
1:B:1929:ASP:OD1	1:B:3612:ARG:NH2	2.38	0.57
1:C:671:LYS:HB3	1:C:761:LEU:HB2	1.86	0.57
1:C:1054:VAL:HA	1:C:1057:LEU:HB2	1.87	0.57
1:D:400:ASP:N	1:D:400:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:853:PRO:HG2	1:D:1209:VAL:HA	1.87	0.57
1:A:655:MET:SD	1:A:836:HIS:ND1	2.77	0.57
1:A:853:PRO:HG2	1:A:1209:VAL:HA	1.87	0.57
1:A:2197:ARG:HB2	1:A:2236:SER:HB3	1.86	0.57
1:A:2348:GLU:O	1:A:2352:ILE:HG13	2.04	0.57
1:B:400:ASP:N	1:B:400:ASP:OD1	2.37	0.57
1:B:1353:HIS:CE1	1:B:1367:LYS:HB3	2.40	0.57
1:B:2099:ARG:O	1:B:2103:LYS:NZ	2.36	0.57
1:C:1353:HIS:CE1	1:C:1367:LYS:HB3	2.40	0.57
1:B:3909:ILE:HG21	1:B:3969:GLU:HB3	1.86	0.57
1:B:4797:ASP:OD1	1:B:4797:ASP:N	2.36	0.57
1:C:123:HIS:HD2	1:C:126:SER:H	1.51	0.57
1:C:498:VAL:HG13	1:C:533:LEU:HD22	1.87	0.57
1:C:1253:LYS:HB3	1:C:1598:SER:HB2	1.86	0.57
1:D:123:HIS:HD2	1:D:126:SER:H	1.51	0.57
1:A:1353:HIS:CE1	1:A:1367:LYS:HB3	2.40	0.57
1:B:989:THR:HG23	1:B:992:GLN:H	1.70	0.57
1:B:1054:VAL:HA	1:B:1057:LEU:HB2	1.87	0.57
1:D:987:LYS:HD2	1:D:988:LEU:N	2.20	0.57
1:A:498:VAL:HG13	1:A:533:LEU:HD22	1.87	0.56
1:A:989:THR:HG23	1:A:992:GLN:H	1.70	0.56
1:A:1272:ARG:NH2	1:A:1584:PRO:O	2.37	0.56
1:A:3712:SER:OG	1:A:3716:LYS:NZ	2.35	0.56
1:B:655:MET:SD	1:B:836:HIS:ND1	2.77	0.56
1:C:655:MET:SD	1:C:836:HIS:ND1	2.77	0.56
1:C:987:LYS:HD2	1:C:988:LEU:N	2.20	0.56
1:D:1353:HIS:CE1	1:D:1367:LYS:HB3	2.40	0.56
1:A:56:LYS:HD2	1:A:56:LYS:C	2.31	0.56
1:A:1253:LYS:HB3	1:A:1598:SER:HB2	1.86	0.56
1:A:2127:SER:O	1:A:2131:VAL:HG23	2.04	0.56
1:B:498:VAL:HG13	1:B:533:LEU:HD22	1.87	0.56
1:B:4662:ARG:NH2	1:B:4675:ALA:O	2.38	0.56
1:D:56:LYS:HD2	1:D:56:LYS:C	2.30	0.56
1:D:989:THR:HG23	1:D:992:GLN:H	1.70	0.56
1:D:2348:GLU:O	1:D:2352:ILE:HG13	2.04	0.56
1:A:1609:VAL:HG23	1:A:1610:SER:H	1.70	0.56
1:A:2881:LYS:O	1:A:2885:ARG:HD3	2.06	0.56
1:B:56:LYS:HD2	1:B:56:LYS:C	2.31	0.56
1:B:671:LYS:HB3	1:B:761:LEU:HB2	1.86	0.56
1:B:987:LYS:HD2	1:B:988:LEU:N	2.20	0.56
1:B:1609:VAL:HG23	1:B:1610:SER:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2197:ARG:HB2	1:B:2236:SER:HB3	1.86	0.56
1:C:853:PRO:HG2	1:C:1209:VAL:HA	1.87	0.56
1:C:4662:ARG:NH2	1:C:4675:ALA:O	2.38	0.56
1:D:1929:ASP:OD1	1:D:3612:ARG:NH2	2.38	0.56
1:D:4195:THR:HB	1:D:4918:LEU:HD11	1.88	0.56
1:A:1054:VAL:HA	1:A:1057:LEU:HB2	1.87	0.56
1:A:1715:TYR:CZ	1:A:1762:MET:HB3	2.41	0.56
1:A:4026:THR:HG21	1:A:4083:VAL:HG11	1.88	0.56
1:B:4137:ILE:HG23	1:B:4950:PHE:HB2	1.88	0.56
1:C:2145:LEU:HD23	1:C:2148:ILE:HD11	1.87	0.56
1:D:4026:THR:HG21	1:D:4083:VAL:HG11	1.88	0.56
1:A:1952:MET:HA	1:A:1956:LEU:HD12	1.87	0.56
1:A:4662:ARG:NH2	1:A:4675:ALA:O	2.38	0.56
1:C:2197:ARG:HB2	1:C:2236:SER:HB3	1.86	0.56
1:C:4137:ILE:HG23	1:C:4950:PHE:HB2	1.88	0.56
1:D:1609:VAL:HG23	1:D:1610:SER:H	1.70	0.56
1:D:4662:ARG:NH2	1:D:4675:ALA:O	2.38	0.56
1:A:1789:LYS:HG3	1:A:1835:PHE:CE1	2.40	0.56
1:A:3909:ILE:HG21	1:A:3969:GLU:HB3	1.86	0.56
1:A:4195:THR:HB	1:A:4918:LEU:HD11	1.88	0.56
1:D:1715:TYR:CZ	1:D:1762:MET:HB3	2.41	0.56
1:B:2723:TYR:O	1:B:2727:SER:OG	2.23	0.56
1:C:1060:TYR:N	1:C:1060:TYR:CD1	2.74	0.56
1:D:1054:VAL:HA	1:D:1057:LEU:HB2	1.87	0.56
1:D:2145:LEU:HD23	1:D:2148:ILE:HD11	1.87	0.56
1:B:853:PRO:HG2	1:B:1209:VAL:HA	1.87	0.56
1:B:2881:LYS:O	1:B:2885:ARG:HD3	2.06	0.56
1:B:4195:THR:HB	1:B:4918:LEU:HD11	1.88	0.56
1:D:1952:MET:HA	1:D:1956:LEU:HD12	1.86	0.56
1:D:3712:SER:OG	1:D:3716:LYS:NZ	2.35	0.56
1:B:748:LEU:HD23	2:H:8:ILE:HG23	1.88	0.56
1:B:1060:TYR:N	1:B:1060:TYR:CD1	2.74	0.56
1:C:3974:GLN:HE22	1:C:4012:ILE:HG21	1.71	0.56
1:C:4195:THR:HB	1:C:4918:LEU:HD11	1.88	0.56
1:D:503:ASP:HA	1:D:561:ARG:HH12	1.71	0.56
1:B:226:GLY:O	1:B:356:TYR:N	2.35	0.56
1:B:3864:ASN:OD1	1:B:3865:THR:N	2.39	0.56
1:B:3974:GLN:HE22	1:B:4012:ILE:HG21	1.71	0.56
1:C:503:ASP:HA	1:C:561:ARG:HH12	1.71	0.56
1:A:857:LEU:HB3	1:A:859:GLN:HG3	1.88	0.55
1:A:1810:PRO:HB3	1:A:1818:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:LEU:HB3	1:B:859:GLN:HG3	1.88	0.55
1:B:1715:TYR:CZ	1:B:1762:MET:HB3	2.41	0.55
1:B:1789:LYS:HG3	1:B:1835:PHE:CE1	2.40	0.55
1:D:694:ARG:HG2	1:D:728:ASP:HB3	1.88	0.55
1:D:1272:ARG:NH2	1:D:1584:PRO:O	2.37	0.55
1:B:3712:SER:OG	1:B:3716:LYS:NZ	2.35	0.55
1:C:989:THR:HG23	1:C:992:GLN:H	1.70	0.55
1:C:2723:TYR:O	1:C:2727:SER:OG	2.23	0.55
1:D:411:GLU:O	1:D:415:THR:OG1	2.25	0.55
1:D:878:LEU:HG	1:D:881:ILE:HB	1.88	0.55
1:D:1060:TYR:N	1:D:1060:TYR:CD1	2.74	0.55
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.89	0.55
1:B:207:PHE:CZ	1:C:2324:ILE:HD12	2.41	0.55
1:B:1631:LEU:HD22	1:B:1645:LEU:HD11	1.89	0.55
1:C:857:LEU:HB3	1:C:859:GLN:HG3	1.88	0.55
1:C:878:LEU:HG	1:C:881:ILE:HB	1.88	0.55
1:C:1715:TYR:CZ	1:C:1762:MET:HB3	2.41	0.55
1:D:498:VAL:HG13	1:D:533:LEU:HD22	1.87	0.55
1:D:2881:LYS:O	1:D:2885:ARG:HD3	2.06	0.55
1:A:1091:GLU:OE1	1:A:1093:THR:OG1	2.25	0.55
1:B:411:GLU:O	1:B:415:THR:OG1	2.25	0.55
1:B:1810:PRO:HB3	1:B:1818:LEU:HD22	1.88	0.55
1:D:857:LEU:HB3	1:D:859:GLN:HG3	1.88	0.55
1:D:2197:ARG:HB2	1:D:2236:SER:HB3	1.86	0.55
1:A:4862:GLN:HG3	1:D:4855:VAL:O	2.06	0.55
1:B:878:LEU:HG	1:B:881:ILE:HB	1.88	0.55
1:D:119:ILE:N	1:D:160:TRP:O	2.39	0.55
1:D:1972:ILE:HA	1:D:1975:LEU:HG	1.89	0.55
1:D:2723:TYR:O	1:D:2727:SER:OG	2.23	0.55
1:D:3840:ARG:HH21	1:D:3844:LEU:HD21	1.72	0.55
1:D:3864:ASN:OD1	1:D:3865:THR:N	2.39	0.55
1:A:411:GLU:O	1:A:415:THR:OG1	2.25	0.55
1:A:1631:LEU:HD22	1:A:1645:LEU:HD11	1.89	0.55
1:A:1956:LEU:O	1:A:1960:LYS:HG2	2.07	0.55
1:B:503:ASP:HA	1:B:561:ARG:HH12	1.71	0.55
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.89	0.55
1:B:1952:MET:HA	1:B:1956:LEU:HD12	1.87	0.55
1:C:2881:LYS:O	1:C:2885:ARG:HD3	2.06	0.55
1:D:1789:LYS:HG3	1:D:1835:PHE:CE1	2.40	0.55
1:A:119:ILE:N	1:A:160:TRP:O	2.39	0.55
1:A:902:TRP:HE3	1:A:915:HIS:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:TYR:N	1:A:1060:TYR:CD1	2.74	0.55
1:A:2723:TYR:O	1:A:2727:SER:OG	2.23	0.55
1:A:4137:ILE:HG23	1:A:4950:PHE:HB2	1.88	0.55
1:B:1968:PRO:HB2	1:B:3618:LEU:HD13	1.89	0.55
1:C:119:ILE:N	1:C:160:TRP:O	2.39	0.55
1:D:1631:LEU:HD22	1:D:1645:LEU:HD11	1.89	0.55
1:D:3974:GLN:HE22	1:D:4012:ILE:HG21	1.71	0.55
1:C:226:GLY:O	1:C:356:TYR:N	2.35	0.55
1:C:694:ARG:HG2	1:C:728:ASP:HB3	1.88	0.55
1:C:902:TRP:HE3	1:C:915:HIS:HB2	1.72	0.55
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.89	0.55
1:C:1952:MET:HA	1:C:1956:LEU:HD12	1.87	0.55
1:A:503:ASP:HA	1:A:561:ARG:HH12	1.71	0.55
1:B:4026:THR:HG21	1:B:4083:VAL:HG11	1.88	0.55
1:C:56:LYS:HD2	1:C:56:LYS:C	2.30	0.55
1:C:1956:LEU:O	1:C:1960:LYS:HG2	2.07	0.55
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.89	0.55
1:D:1176:THR:HG22	1:D:1181:ILE:HG12	1.89	0.55
1:D:1265:HIS:HD2	1:D:1268:ILE:HB	1.72	0.55
1:D:2099:ARG:O	1:D:2103:LYS:NZ	2.36	0.55
1:A:1176:THR:HG22	1:A:1181:ILE:HG12	1.89	0.55
1:D:4797:ASP:OD1	1:D:4797:ASP:N	2.36	0.55
1:A:878:LEU:HG	1:A:881:ILE:HB	1.89	0.54
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.89	0.54
1:A:3860:GLN:HE22	1:A:3867:VAL:H	1.55	0.54
1:B:3840:ARG:HH21	1:B:3844:LEU:HD21	1.72	0.54
1:C:1030:PRO:O	1:C:1033:VAL:HG12	2.07	0.54
1:C:1176:THR:HG22	1:C:1181:ILE:HG12	1.89	0.54
1:C:1789:LYS:HG3	1:C:1835:PHE:CE1	2.40	0.54
1:C:1986:PRO:HB2	1:C:1988:PRO:HD2	1.89	0.54
1:D:1221:VAL:HA	1:D:1224:LEU:HB2	1.89	0.54
1:D:1683:GLU:HB3	2:J:42:ASP:HB3	1.88	0.54
1:D:1956:LEU:O	1:D:1960:LYS:HG2	2.07	0.54
1:D:2851:TRP:CZ3	1:D:2855:LYS:HG2	2.42	0.54
1:D:3860:GLN:HE22	1:D:3867:VAL:H	1.55	0.54
1:B:188:SER:HB3	1:B:190:ARG:HD2	1.89	0.54
1:B:694:ARG:HG2	1:B:728:ASP:HB3	1.88	0.54
1:B:1091:GLU:OE1	1:B:1093:THR:OG1	2.25	0.54
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.89	0.54
1:C:1631:LEU:HD22	1:C:1645:LEU:HD11	1.89	0.54
1:C:1968:PRO:HB2	1:C:3618:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2858:GLU:O	1:C:2862:LYS:HG2	2.08	0.54
1:C:4026:THR:HG21	1:C:4083:VAL:HG11	1.88	0.54
1:A:992:GLN:HE22	1:A:1058:LEU:HD13	1.73	0.54
1:A:1030:PRO:O	1:A:1033:VAL:HG12	2.07	0.54
1:A:1682:ASP:HB3	1:A:1684:PRO:HD2	1.89	0.54
1:B:756:SER:OG	1:B:769:ARG:HB2	2.08	0.54
1:C:4859:ALA:HB1	1:D:4866:ILE:HD11	1.88	0.54
1:D:756:SER:OG	1:D:769:ARG:HB2	2.07	0.54
1:D:3975:LYS:HB2	1:D:4093:ILE:HG13	1.90	0.54
1:D:4137:ILE:HG23	1:D:4950:PHE:HB2	1.88	0.54
1:A:1968:PRO:HB2	1:A:3618:LEU:HD13	1.89	0.54
1:C:1810:PRO:HB3	1:C:1818:LEU:HD22	1.88	0.54
1:C:3864:ASN:OD1	1:C:3865:THR:N	2.39	0.54
1:D:992:GLN:HE22	1:D:1058:LEU:HD13	1.73	0.54
1:A:756:SER:OG	1:A:769:ARG:HB2	2.07	0.54
1:A:2851:TRP:CZ3	1:A:2855:LYS:HG2	2.43	0.54
1:A:2858:GLU:O	1:A:2862:LYS:HG2	2.08	0.54
1:A:3840:ARG:HH21	1:A:3844:LEU:HD21	1.72	0.54
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.89	0.54
1:D:1091:GLU:OE1	1:D:1093:THR:OG1	2.25	0.54
1:D:1810:PRO:HB3	1:D:1818:LEU:HD22	1.88	0.54
1:D:1968:PRO:HB2	1:D:3618:LEU:HD13	1.89	0.54
1:D:2738:ASN:N	1:D:2738:ASN:OD1	2.41	0.54
1:A:1265:HIS:HD2	1:A:1268:ILE:HB	1.72	0.54
1:A:1972:ILE:HA	1:A:1975:LEU:HG	1.89	0.54
1:A:1986:PRO:HB2	1:A:1988:PRO:HD2	1.89	0.54
1:B:988:LEU:HD22	1:B:1055:ARG:HG2	1.90	0.54
1:B:1176:THR:HG22	1:B:1181:ILE:HG12	1.89	0.54
1:D:678:MET:HG3	1:D:801:ARG:HB3	1.90	0.54
1:D:988:LEU:HD22	1:D:1055:ARG:HG2	1.90	0.54
1:D:1030:PRO:O	1:D:1033:VAL:HG12	2.07	0.54
1:A:694:ARG:HG2	1:A:728:ASP:HB3	1.88	0.54
1:A:3974:GLN:HE22	1:A:4012:ILE:HG21	1.71	0.54
1:B:1956:LEU:O	1:B:1960:LYS:HG2	2.07	0.54
1:C:1982:LYS:NZ	1:C:1983:SER:O	2.29	0.54
1:D:1682:ASP:HB3	1:D:1684:PRO:HD2	1.89	0.54
1:A:226:GLY:O	1:A:356:TYR:N	2.35	0.54
1:A:1221:VAL:HA	1:A:1224:LEU:HB2	1.90	0.54
1:A:1829:LEU:HB3	1:A:1834:ILE:HD11	1.90	0.54
1:A:3975:LYS:HB2	1:A:4093:ILE:HG13	1.89	0.54
1:A:4044:LYS:HZ2	1:A:4069:ALA:HB1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:TRP:HE3	1:B:915:HIS:HB2	1.72	0.54
1:B:992:GLN:HE22	1:B:1058:LEU:HD13	1.73	0.54
1:B:1030:PRO:O	1:B:1033:VAL:HG12	2.07	0.54
1:B:1972:ILE:HA	1:B:1975:LEU:HG	1.89	0.54
1:B:2851:TRP:CZ3	1:B:2855:LYS:HG2	2.42	0.54
1:C:2851:TRP:CZ3	1:C:2855:LYS:HG2	2.42	0.54
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.89	0.54
1:B:55:SER:O	1:B:296:ARG:NH2	2.34	0.54
1:B:1682:ASP:HB3	1:B:1684:PRO:HD2	1.89	0.54
1:B:1986:PRO:HB2	1:B:1988:PRO:HD2	1.89	0.54
1:C:125:TYR:HE1	1:C:414:ARG:HA	1.73	0.54
1:D:1608:ASP:HB2	1:D:1611:ARG:HD3	1.90	0.54
1:A:988:LEU:HD22	1:A:1055:ARG:HG2	1.90	0.54
1:A:1608:ASP:HB2	1:A:1611:ARG:HD3	1.90	0.54
1:A:4106:GLU:OE2	1:A:4148:TYR:OH	2.19	0.54
1:B:1265:HIS:HD2	1:B:1268:ILE:HB	1.72	0.54
1:C:678:MET:HG3	1:C:801:ARG:HB3	1.90	0.54
1:C:1265:HIS:HD2	1:C:1268:ILE:HB	1.72	0.54
1:C:2257:ARG:NH1	1:C:3806:ALA:HB2	2.24	0.54
1:D:188:SER:HB3	1:D:190:ARG:HD2	1.89	0.54
1:D:970:TYR:CE2	1:D:977:LYS:HG2	2.43	0.54
1:D:2858:GLU:O	1:D:2862:LYS:HG2	2.08	0.54
1:A:188:SER:HB3	1:A:190:ARG:HD2	1.89	0.53
1:B:2858:GLU:O	1:B:2862:LYS:HG2	2.08	0.53
1:C:1221:VAL:HA	1:C:1224:LEU:HB2	1.90	0.53
1:C:2738:ASN:N	1:C:2738:ASN:OD1	2.41	0.53
1:C:3860:GLN:HE22	1:C:3867:VAL:H	1.55	0.53
1:C:4883:MET:HE1	1:C:4888:PHE:HD1	1.73	0.53
1:D:4883:MET:HE1	1:D:4888:PHE:HD1	1.73	0.53
1:A:363:ILE:HD11	1:A:372:LEU:HB3	1.90	0.53
1:A:2099:ARG:O	1:A:2103:LYS:NZ	2.36	0.53
1:A:2257:ARG:NH1	1:A:3806:ALA:HB2	2.23	0.53
1:A:3864:ASN:OD1	1:A:3865:THR:N	2.39	0.53
1:B:2738:ASN:OD1	1:B:2738:ASN:N	2.41	0.53
1:B:3860:GLN:HE22	1:B:3867:VAL:H	1.55	0.53
1:C:188:SER:HB3	1:C:190:ARG:HD2	1.89	0.53
1:C:1012:ILE:HG13	1:C:1013:ARG:HD2	1.90	0.53
1:D:902:TRP:HE3	1:D:915:HIS:HB2	1.72	0.53
1:B:370:LEU:HB2	1:B:393:MET:HE3	1.90	0.53
1:B:1829:LEU:HB3	1:B:1834:ILE:HD11	1.90	0.53
1:B:4731:GLY:HA2	1:B:4737:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4883:MET:HE1	1:B:4888:PHE:HD1	1.73	0.53
1:C:411:GLU:O	1:C:415:THR:OG1	2.25	0.53
1:C:756:SER:OG	1:C:769:ARG:HB2	2.07	0.53
1:C:1682:ASP:HB3	1:C:1684:PRO:HD2	1.89	0.53
1:C:3840:ARG:HH21	1:C:3844:LEU:HD21	1.72	0.53
1:D:125:TYR:HE1	1:D:414:ARG:HA	1.73	0.53
1:A:748:LEU:HD23	2:G:8:ILE:HG23	1.89	0.53
1:A:2107:ILE:HG13	1:A:2108:ASN:H	1.74	0.53
1:B:125:TYR:HE1	1:B:414:ARG:HA	1.73	0.53
1:A:1012:ILE:HG13	1:A:1013:ARG:HD2	1.90	0.53
1:C:370:LEU:HB2	1:C:393:MET:HE3	1.90	0.53
1:D:78:LEU:HD11	1:D:159:TRP:CG	2.44	0.53
1:D:370:LEU:HB2	1:D:393:MET:HE3	1.90	0.53
1:D:878:LEU:HD23	1:D:882:ARG:HG3	1.91	0.53
1:A:125:TYR:HE1	1:A:414:ARG:HA	1.73	0.53
1:A:2738:ASN:N	1:A:2738:ASN:OD1	2.41	0.53
1:A:4731:GLY:HA2	1:A:4737:PHE:HB2	1.91	0.53
1:C:653:SER:O	1:C:793:SER:HA	2.09	0.53
1:C:1972:ILE:HA	1:C:1975:LEU:HG	1.89	0.53
1:D:653:SER:O	1:D:793:SER:HA	2.09	0.53
1:A:370:LEU:HB2	1:A:393:MET:HE3	1.90	0.53
1:A:4883:MET:HE1	1:A:4888:PHE:HD1	1.73	0.53
1:B:119:ILE:N	1:B:160:TRP:O	2.39	0.53
1:C:363:ILE:HD11	1:C:372:LEU:HB3	1.90	0.53
1:C:988:LEU:HD22	1:C:1055:ARG:HG2	1.90	0.53
1:C:3975:LYS:HB2	1:C:4093:ILE:HG13	1.89	0.53
1:D:1709:ASP:HA	1:D:1713:SER:HB3	1.91	0.53
1:D:2107:ILE:HG13	1:D:2108:ASN:H	1.74	0.53
2:J:43:ARG:HG3	2:J:45:LYS:HG2	1.91	0.53
1:A:653:SER:O	1:A:793:SER:HA	2.09	0.53
1:B:363:ILE:HD11	1:B:372:LEU:HB3	1.90	0.53
1:B:2257:ARG:NH1	1:B:3806:ALA:HB2	2.24	0.53
1:B:4042:ILE:H	1:B:4076:THR:HG23	1.74	0.53
1:C:992:GLN:HE22	1:C:1058:LEU:HD13	1.73	0.53
1:C:2859:LEU:HD12	1:C:2867:HIS:CE1	2.44	0.53
1:A:678:MET:HG3	1:A:801:ARG:HB3	1.90	0.53
1:B:1221:VAL:HA	1:B:1224:LEU:HB2	1.89	0.53
1:B:3975:LYS:HB2	1:B:4093:ILE:HG13	1.90	0.53
1:D:799:LYS:HG2	1:D:1621:GLN:HG3	1.91	0.53
1:D:1986:PRO:HB2	1:D:1988:PRO:HD2	1.89	0.53
1:D:2722:LYS:NZ	1:D:2726:HIS:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD11	1:A:159:TRP:CG	2.44	0.53
1:B:1608:ASP:HB2	1:B:1611:ARG:HD3	1.90	0.53
1:C:799:LYS:HG2	1:C:1621:GLN:HG3	1.91	0.53
1:C:878:LEU:HD23	1:C:882:ARG:HG3	1.91	0.53
1:C:4042:ILE:H	1:C:4076:THR:HG23	1.74	0.53
1:D:363:ILE:HD11	1:D:372:LEU:HB3	1.90	0.53
1:D:2257:ARG:NH1	1:D:3806:ALA:HB2	2.24	0.53
1:A:4042:ILE:H	1:A:4076:THR:HG23	1.74	0.52
1:B:878:LEU:HD23	1:B:882:ARG:HG3	1.91	0.52
1:B:2859:LEU:HD12	1:B:2867:HIS:CE1	2.44	0.52
1:C:763:ALA:HB3	1:C:764:PRO:HD3	1.91	0.52
1:C:1091:GLU:OE1	1:C:1093:THR:OG1	2.25	0.52
1:C:1608:ASP:HB2	1:C:1611:ARG:HD3	1.90	0.52
2:I:8:ILE:HD11	2:I:74:LYS:HB2	1.91	0.52
1:D:226:GLY:O	1:D:356:TYR:N	2.35	0.52
1:D:763:ALA:HB3	1:D:764:PRO:HD3	1.91	0.52
1:D:4042:ILE:H	1:D:4076:THR:HG23	1.74	0.52
1:B:1012:ILE:HG13	1:B:1013:ARG:HD2	1.90	0.52
1:B:2084:PHE:O	1:B:3690:TYR:OH	2.25	0.52
2:H:43:ARG:HG3	2:H:45:LYS:HG2	1.91	0.52
1:C:4059:GLN:O	1:C:4063:GLU:HG3	2.10	0.52
1:D:4059:GLN:O	1:D:4063:GLU:HG3	2.10	0.52
1:A:799:LYS:HG2	1:A:1621:GLN:HG3	1.91	0.52
1:B:678:MET:HG3	1:B:801:ARG:HB3	1.90	0.52
1:B:2107:ILE:HG13	1:B:2108:ASN:H	1.74	0.52
1:C:1207:LEU:HB3	1:C:1211:GLN:HB2	1.92	0.52
1:C:4106:GLU:OE1	1:C:4134:ARG:NH1	2.43	0.52
1:D:1012:ILE:HG13	1:D:1013:ARG:HD2	1.90	0.52
1:A:878:LEU:HD23	1:A:882:ARG:HG3	1.91	0.52
1:C:1829:LEU:HB3	1:C:1834:ILE:HD11	1.90	0.52
1:C:2722:LYS:NZ	1:C:2726:HIS:HB2	2.24	0.52
1:C:4884:GLU:HA	1:C:4884:GLU:OE2	2.10	0.52
1:D:1829:LEU:HB3	1:D:1834:ILE:HD11	1.90	0.52
1:A:271:ALA:O	1:A:301:THR:OG1	2.28	0.52
1:A:2722:LYS:NZ	1:A:2726:HIS:HB2	2.24	0.52
1:B:78:LEU:HD11	1:B:159:TRP:CG	2.44	0.52
1:D:4106:GLU:OE1	1:D:4134:ARG:NH1	2.43	0.52
1:B:1207:LEU:HB3	1:B:1211:GLN:HB2	1.92	0.52
1:C:78:LEU:HD11	1:C:159:TRP:CG	2.44	0.52
1:C:1680:HIS:CE1	2:I:91:VAL:HA	2.44	0.52
1:C:3639:LEU:HD23	1:C:3693:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4731:GLY:HA2	1:C:4737:PHE:HB2	1.91	0.52
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.91	0.52
1:B:1709:ASP:HA	1:B:1713:SER:HB3	1.91	0.52
1:B:1727:ILE:HD12	1:B:2119:LEU:HD11	1.91	0.52
1:C:2107:ILE:HG13	1:C:2108:ASN:H	1.74	0.52
1:D:4046:ASP:OD1	1:D:4046:ASP:N	2.43	0.52
1:B:653:SER:O	1:B:793:SER:HA	2.09	0.52
1:B:2722:LYS:NZ	1:B:2726:HIS:HB2	2.24	0.52
1:C:620:CYS:SG	1:C:621:HIS:N	2.83	0.52
1:C:1727:ILE:HD12	1:C:2119:LEU:HD11	1.91	0.52
1:D:706:TYR:OH	1:D:852:GLY:O	2.28	0.52
1:D:2859:LEU:HD12	1:D:2867:HIS:CE1	2.44	0.52
1:A:620:CYS:SG	1:A:621:HIS:N	2.83	0.52
1:A:1709:ASP:HA	1:A:1713:SER:HB3	1.91	0.52
1:C:271:ALA:O	1:C:301:THR:OG1	2.28	0.52
1:C:1683:GLU:HB3	2:I:42:ASP:HB3	1.92	0.52
1:C:2091:TYR:CD2	1:C:3639:LEU:HD13	2.45	0.52
1:D:2091:TYR:CD2	1:D:3639:LEU:HD13	2.45	0.52
1:D:4884:GLU:HA	1:D:4884:GLU:OE2	2.10	0.52
2:J:8:ILE:HD11	2:J:74:LYS:HB2	1.91	0.52
1:A:2859:LEU:HD12	1:A:2867:HIS:CE1	2.44	0.52
1:A:4050:ALA:O	1:A:4054:HIS:ND1	2.43	0.52
2:G:43:ARG:HG3	2:G:45:LYS:HG2	1.91	0.52
1:B:970:TYR:CE2	1:B:977:LYS:HG2	2.43	0.52
1:C:1709:ASP:HA	1:C:1713:SER:HB3	1.91	0.52
2:I:43:ARG:HG3	2:I:45:LYS:HG2	1.91	0.52
1:D:4731:GLY:HA2	1:D:4737:PHE:HB2	1.91	0.52
1:A:1609:VAL:H	1:A:1611:ARG:NH1	2.08	0.51
1:A:1677:LEU:O	1:A:1681:VAL:HG22	2.10	0.51
1:A:4106:GLU:OE1	1:A:4134:ARG:NH1	2.43	0.51
1:B:763:ALA:HB3	1:B:764:PRO:HD3	1.91	0.51
1:A:2118:LEU:HD12	1:A:2148:ILE:HG22	1.93	0.51
1:A:4884:GLU:HA	1:A:4884:GLU:OE2	2.10	0.51
2:G:8:ILE:HD11	2:G:74:LYS:HB2	1.91	0.51
1:B:620:CYS:SG	1:B:621:HIS:N	2.83	0.51
1:B:1090:ALA:HB3	1:B:1202:ILE:HG23	1.92	0.51
1:A:37:LEU:HD22	1:A:192:LEU:HD21	1.92	0.51
1:A:1090:ALA:HB3	1:A:1202:ILE:HG23	1.92	0.51
1:A:3639:LEU:HD23	1:A:3693:ILE:HG21	1.92	0.51
1:B:4050:ALA:O	1:B:4054:HIS:ND1	2.43	0.51
1:B:4059:GLN:O	1:B:4063:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ALA:O	1:D:301:THR:OG1	2.28	0.51
1:D:754:VAL:HG13	1:D:771:ASN:HA	1.93	0.51
1:D:1245:ARG:NH1	1:D:1809:ASP:O	2.44	0.51
1:D:1731:THR:O	1:D:1734:THR:OG1	2.27	0.51
1:A:2487:LEU:O	1:A:2492:LEU:HG	2.11	0.51
1:B:2118:LEU:HD12	1:B:2148:ILE:HG22	1.93	0.51
1:B:4836:ASP:OD1	1:B:4836:ASP:N	2.42	0.51
1:C:1609:VAL:H	1:C:1611:ARG:NH1	2.08	0.51
1:D:1207:LEU:HB3	1:D:1211:GLN:HB2	1.92	0.51
1:B:2487:LEU:O	1:B:2492:LEU:HG	2.11	0.51
1:B:4106:GLU:OE1	1:B:4134:ARG:NH1	2.43	0.51
1:C:1786:ASP:OD1	1:C:1786:ASP:N	2.44	0.51
1:C:4929:GLU:HG2	1:C:4930:THR:N	2.26	0.51
1:D:1609:VAL:H	1:D:1611:ARG:NH1	2.08	0.51
1:D:1677:LEU:O	1:D:1681:VAL:HG22	2.10	0.51
1:D:1769:PHE:O	2:J:83:TYR:OH	2.27	0.51
1:A:942:THR:HB	1:A:999:LEU:HD12	1.93	0.51
1:A:1727:ILE:HD12	1:A:2119:LEU:HD11	1.91	0.51
1:A:4929:GLU:HG2	1:A:4930:THR:N	2.26	0.51
1:B:1677:LEU:O	1:B:1681:VAL:HG22	2.10	0.51
1:B:3639:LEU:HD23	1:B:3693:ILE:HG21	1.92	0.51
1:B:4884:GLU:OE2	1:B:4884:GLU:HA	2.10	0.51
2:H:8:ILE:HD11	2:H:74:LYS:HB2	1.91	0.51
1:C:754:VAL:HG13	1:C:771:ASN:HA	1.93	0.51
1:C:4050:ALA:O	1:C:4054:HIS:ND1	2.43	0.51
1:D:942:THR:HB	1:D:999:LEU:HD12	1.93	0.51
1:A:754:VAL:HG13	1:A:771:ASN:HA	1.93	0.51
1:B:37:LEU:HD22	1:B:192:LEU:HD21	1.92	0.51
1:C:37:LEU:HD22	1:C:192:LEU:HD21	1.92	0.51
1:D:721:ASP:N	1:D:721:ASP:OD1	2.44	0.51
1:D:1786:ASP:OD1	1:D:1786:ASP:N	2.44	0.51
2:J:69:LEU:HD12	2:J:107:LEU:HD23	1.93	0.51
1:A:706:TYR:OH	1:A:852:GLY:O	2.28	0.51
1:C:1677:LEU:O	1:C:1681:VAL:HG22	2.11	0.51
1:C:1731:THR:O	1:C:1734:THR:OG1	2.27	0.51
1:C:2118:LEU:HD12	1:C:2148:ILE:HG22	1.93	0.51
1:D:620:CYS:SG	1:D:621:HIS:N	2.83	0.51
1:D:699:SER:OG	1:D:700:THR:N	2.44	0.51
1:D:1727:ILE:HD12	1:D:2119:LEU:HD11	1.91	0.51
1:A:970:TYR:CE2	1:A:977:LYS:HG2	2.43	0.51
1:B:2091:TYR:CD2	1:B:3639:LEU:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4063:GLU:HA	1:B:4066:LEU:HG	1.93	0.51
1:B:4929:GLU:HG2	1:B:4930:THR:N	2.26	0.51
1:D:37:LEU:HD22	1:D:192:LEU:HD21	1.92	0.51
1:D:1086:ARG:HH21	1:D:1251:LEU:HD13	1.76	0.51
1:D:4106:GLU:OE2	1:D:4148:TYR:OH	2.19	0.51
1:A:1245:ARG:NH1	1:A:1809:ASP:O	2.44	0.51
2:G:69:LEU:HD12	2:G:107:LEU:HD23	1.93	0.51
1:B:799:LYS:HG2	1:B:1621:GLN:HG3	1.91	0.51
1:B:2471:LEU:HD11	1:B:2482:PHE:HZ	1.76	0.51
1:D:1655:HIS:HA	1:D:1658:THR:HG22	1.93	0.51
1:D:2118:LEU:HD12	1:D:2148:ILE:HG22	1.93	0.51
1:A:1207:LEU:HB3	1:A:1211:GLN:HB2	1.92	0.50
1:A:4059:GLN:O	1:A:4063:GLU:HG3	2.10	0.50
1:C:706:TYR:OH	1:C:852:GLY:O	2.28	0.50
1:C:1090:ALA:HB3	1:C:1202:ILE:HG23	1.92	0.50
1:D:1090:ALA:HB3	1:D:1202:ILE:HG23	1.92	0.50
1:D:4050:ALA:O	1:D:4054:HIS:ND1	2.43	0.50
1:A:54:ASN:ND2	1:A:57:ASN:OD1	2.45	0.50
1:A:4063:GLU:HA	1:A:4066:LEU:HG	1.93	0.50
1:B:754:VAL:HG13	1:B:771:ASN:HA	1.93	0.50
1:B:1245:ARG:NH1	1:B:1809:ASP:O	2.44	0.50
1:B:1972:ILE:HD13	1:B:1975:LEU:HD21	1.93	0.50
1:B:4640:PRO:HG2	1:B:4646:LYS:HA	1.93	0.50
1:B:4781:THR:HG21	1:B:4812:TYR:HB2	1.94	0.50
1:D:677:LEU:HD23	1:D:755:ILE:HD13	1.94	0.50
1:A:1086:ARG:HH21	1:A:1251:LEU:HD13	1.76	0.50
1:A:2471:LEU:HD11	1:A:2482:PHE:HZ	1.76	0.50
1:A:4781:THR:HG21	1:A:4812:TYR:HB2	1.94	0.50
1:B:706:TYR:OH	1:B:852:GLY:O	2.28	0.50
1:B:1588:HIS:HE1	1:B:1590:GLN:HE21	1.59	0.50
1:B:1609:VAL:H	1:B:1611:ARG:NH1	2.08	0.50
1:C:674:TYR:CE1	1:C:756:SER:HB2	2.47	0.50
1:C:1972:ILE:HD13	1:C:1975:LEU:HD21	1.93	0.50
1:C:2471:LEU:HD11	1:C:2482:PHE:HZ	1.77	0.50
1:D:3639:LEU:HD23	1:D:3693:ILE:HG21	1.92	0.50
1:A:1731:THR:O	1:A:1734:THR:OG1	2.27	0.50
1:A:2330:PHE:HD1	1:A:2394:LEU:HD21	1.76	0.50
1:A:4653:MET:HE3	1:A:4669:LEU:HD23	1.94	0.50
1:B:699:SER:OG	1:B:700:THR:N	2.44	0.50
1:B:4023:LYS:HG3	1:B:4087:HIS:CD2	2.47	0.50
1:B:4653:MET:HE3	1:B:4669:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASN:ND2	1:C:57:ASN:OD1	2.45	0.50
1:C:970:TYR:CE2	1:C:977:LYS:HG2	2.43	0.50
1:C:4640:PRO:HG2	1:C:4646:LYS:HA	1.93	0.50
1:D:55:SER:O	1:D:296:ARG:NH2	2.34	0.50
1:A:1595:VAL:O	1:A:1595:VAL:HG23	2.12	0.50
1:A:1655:HIS:HA	1:A:1658:THR:HG22	1.93	0.50
1:A:4046:ASP:OD1	1:A:4046:ASP:N	2.43	0.50
1:A:4640:PRO:HG2	1:A:4646:LYS:HA	1.93	0.50
1:D:1947:MET:HE1	1:D:1960:LYS:HE3	1.94	0.50
1:D:2084:PHE:O	1:D:3690:TYR:OH	2.25	0.50
1:D:2442:PRO:HG3	1:D:2454:ASP:HB2	1.94	0.50
1:A:893:TRP:CE3	1:A:893:TRP:HA	2.47	0.50
1:A:4836:ASP:OD1	1:A:4836:ASP:N	2.42	0.50
1:A:4858:LEU:HD21	1:D:4855:VAL:HG11	1.93	0.50
1:B:271:ALA:O	1:B:301:THR:OG1	2.28	0.50
1:B:1048:ASP:O	1:B:1052:GLU:HG3	2.12	0.50
1:B:1595:VAL:HG23	1:B:1595:VAL:O	2.12	0.50
1:C:677:LEU:HD23	1:C:755:ILE:HD13	1.94	0.50
1:C:1086:ARG:HH21	1:C:1251:LEU:HD13	1.76	0.50
1:C:1588:HIS:HE1	1:C:1590:GLN:HE21	1.59	0.50
1:C:4046:ASP:OD1	1:C:4046:ASP:N	2.43	0.50
1:B:54:ASN:ND2	1:B:57:ASN:OD1	2.45	0.50
1:C:1655:HIS:HA	1:C:1658:THR:HG22	1.93	0.50
1:C:2099:ARG:O	1:C:2103:LYS:NZ	2.36	0.50
1:C:4023:LYS:HG3	1:C:4087:HIS:CD2	2.47	0.50
1:D:54:ASN:ND2	1:D:57:ASN:OD1	2.45	0.50
1:D:2220:LEU:HD11	1:D:2242:ALA:HB2	1.94	0.50
1:A:1102:TYR:HD1	1:A:1165:MET:HG2	1.76	0.50
1:B:674:TYR:CE1	1:B:756:SER:HB2	2.47	0.50
1:B:942:THR:HB	1:B:999:LEU:HD12	1.93	0.50
1:B:1086:ARG:HH21	1:B:1251:LEU:HD13	1.76	0.50
1:B:1102:TYR:HD1	1:B:1165:MET:HG2	1.76	0.50
1:C:2084:PHE:O	1:C:3690:TYR:OH	2.25	0.50
1:C:2487:LEU:O	1:C:2492:LEU:HG	2.11	0.50
1:D:893:TRP:CE3	1:D:893:TRP:HA	2.47	0.50
1:D:2487:LEU:O	1:D:2492:LEU:HG	2.11	0.50
1:D:4653:MET:HE3	1:D:4669:LEU:HD23	1.94	0.50
1:A:1750:PRO:HG3	1:A:2057:LEU:HD22	1.94	0.50
1:A:1947:MET:HE1	1:A:1960:LYS:HE3	1.94	0.50
1:A:4023:LYS:HG3	1:A:4087:HIS:CD2	2.47	0.50
1:B:1947:MET:HE1	1:B:1960:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4046:ASP:N	1:B:4046:ASP:OD1	2.43	0.50
1:C:1947:MET:HE1	1:C:1960:LYS:HE3	1.94	0.50
1:C:2777:SER:OG	1:C:2843:MET:SD	2.68	0.50
1:A:3989:VAL:HG12	1:A:3990:VAL:H	1.77	0.49
1:B:1950:LEU:O	1:B:1956:LEU:HD11	2.12	0.49
1:B:3971:MET:HB3	1:B:4093:ILE:HD13	1.94	0.49
1:C:699:SER:OG	1:C:700:THR:N	2.44	0.49
1:C:4009:VAL:HA	1:C:4012:ILE:HD12	1.94	0.49
1:D:674:TYR:CE1	1:D:756:SER:HB2	2.47	0.49
1:D:1595:VAL:O	1:D:1595:VAL:HG23	2.12	0.49
1:D:3989:VAL:HG12	1:D:3990:VAL:H	1.76	0.49
1:D:4063:GLU:HA	1:D:4066:LEU:HG	1.93	0.49
1:D:4781:THR:HG21	1:D:4812:TYR:HB2	1.94	0.49
1:A:982:ASP:OD1	1:A:985:PHE:HB3	2.12	0.49
1:A:2220:LEU:HD11	1:A:2242:ALA:HB2	1.93	0.49
1:A:3698:CYS:SG	1:A:3730:LEU:HD21	2.52	0.49
1:B:624:ALA:HB3	1:B:2131:VAL:HG13	1.94	0.49
1:B:759:LEU:HD11	1:B:761:LEU:HD23	1.94	0.49
1:B:2076:ASP:HB3	1:B:2079:LEU:HB3	1.94	0.49
1:B:2414:GLU:H	1:B:2414:GLU:CD	2.20	0.49
1:B:3989:VAL:HG12	1:B:3990:VAL:H	1.76	0.49
1:C:942:THR:HB	1:C:999:LEU:HD12	1.93	0.49
1:C:1102:TYR:HD1	1:C:1165:MET:HG2	1.76	0.49
1:C:3989:VAL:HG12	1:C:3990:VAL:H	1.77	0.49
1:C:4063:GLU:HA	1:C:4066:LEU:HG	1.93	0.49
1:C:4836:ASP:OD1	1:C:4836:ASP:N	2.42	0.49
1:D:1048:ASP:O	1:D:1052:GLU:HG3	2.12	0.49
1:D:1972:ILE:HD13	1:D:1975:LEU:HD21	1.93	0.49
1:D:4929:GLU:HG2	1:D:4930:THR:N	2.26	0.49
1:A:721:ASP:N	1:A:721:ASP:OD1	2.44	0.49
1:A:1827:TYR:CZ	1:A:1831:ILE:HD11	2.48	0.49
1:A:1924:ILE:HA	1:A:1998:PHE:HZ	1.78	0.49
1:A:1950:LEU:O	1:A:1956:LEU:HD11	2.12	0.49
1:A:2091:TYR:CD2	1:A:3639:LEU:HD13	2.45	0.49
1:B:721:ASP:OD1	1:B:721:ASP:N	2.44	0.49
1:B:1655:HIS:HA	1:B:1658:THR:HG22	1.93	0.49
1:B:1683:GLU:HB3	2:H:42:ASP:HB3	1.93	0.49
1:B:1715:TYR:CE2	1:B:1719:ARG:HD2	2.48	0.49
1:B:1719:ARG:NE	1:B:1831:ILE:O	2.46	0.49
1:B:4106:GLU:OE2	1:B:4148:TYR:OH	2.19	0.49
1:C:3728:ALA:HA	1:C:3731:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4808:MET:HB2	1:D:4518:TYR:HD2	1.78	0.49
1:A:1048:ASP:O	1:A:1052:GLU:HG3	2.12	0.49
1:B:893:TRP:HA	1:B:893:TRP:CE3	2.47	0.49
1:B:2442:PRO:HG3	1:B:2454:ASP:HB2	1.94	0.49
1:C:340:VAL:HG23	1:C:341:GLY:H	1.78	0.49
1:C:2220:LEU:HD11	1:C:2242:ALA:HB2	1.93	0.49
2:I:69:LEU:HD12	2:I:107:LEU:HD23	1.93	0.49
1:D:1924:ILE:HA	1:D:1998:PHE:HZ	1.78	0.49
1:D:3698:CYS:SG	1:D:3730:LEU:HD21	2.52	0.49
1:D:3971:MET:HB3	1:D:4093:ILE:HD13	1.94	0.49
1:D:4023:LYS:HG3	1:D:4087:HIS:CD2	2.47	0.49
1:C:624:ALA:HB3	1:C:2131:VAL:HG13	1.94	0.49
1:C:721:ASP:OD1	1:C:721:ASP:N	2.44	0.49
1:C:1595:VAL:HG23	1:C:1595:VAL:O	2.12	0.49
1:C:1950:LEU:O	1:C:1956:LEU:HD11	2.12	0.49
1:C:4781:THR:HG21	1:C:4812:TYR:HB2	1.94	0.49
1:D:1102:TYR:HD1	1:D:1165:MET:HG2	1.76	0.49
1:D:1750:PRO:HG3	1:D:2057:LEU:HD22	1.94	0.49
1:A:674:TYR:CE1	1:A:756:SER:HB2	2.47	0.49
1:A:1588:HIS:HE1	1:A:1590:GLN:HE21	1.59	0.49
1:A:4009:VAL:HA	1:A:4012:ILE:HD12	1.94	0.49
1:B:909:ASP:OD1	1:B:910:ASP:N	2.45	0.49
1:B:1750:PRO:HG3	1:B:2057:LEU:HD22	1.94	0.49
1:C:794:PHE:CD1	1:C:798:ILE:HG21	2.48	0.49
1:C:1048:ASP:O	1:C:1052:GLU:HG3	2.12	0.49
1:C:1257:GLN:HB2	1:C:1596:LEU:HD11	1.95	0.49
1:C:1924:ILE:HA	1:C:1998:PHE:HZ	1.78	0.49
1:C:2343:LEU:O	1:C:2347:GLU:HG2	2.13	0.49
1:C:4653:MET:HE3	1:C:4669:LEU:HD23	1.94	0.49
1:D:1588:HIS:HE1	1:D:1590:GLN:HE21	1.59	0.49
1:A:794:PHE:CD1	1:A:798:ILE:HG21	2.48	0.49
1:A:1715:TYR:CE2	1:A:1719:ARG:HD2	2.48	0.49
1:A:1733:GLU:O	1:A:1736:SER:OG	2.30	0.49
1:A:1786:ASP:OD1	1:A:1786:ASP:N	2.44	0.49
1:A:1972:ILE:HD13	1:A:1975:LEU:HD21	1.93	0.49
1:B:730:LEU:HD22	1:B:731:HIS:CE1	2.48	0.49
2:H:38:ASP:OD1	2:H:39:SER:N	2.46	0.49
1:C:606:ARG:NH1	1:C:1635:GLU:OE2	2.46	0.49
1:D:982:ASP:OD1	1:D:985:PHE:HB3	2.12	0.49
1:D:2076:ASP:HB3	1:D:2079:LEU:HB3	1.94	0.49
1:D:4044:LYS:HZ2	1:D:4069:ALA:HB1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2442:PRO:HG3	1:A:2454:ASP:HB2	1.94	0.49
1:A:3786:VAL:HG11	1:A:3865:THR:HG23	1.95	0.49
1:B:1827:TYR:CZ	1:B:1831:ILE:HD11	2.48	0.49
1:B:3698:CYS:SG	1:B:3730:LEU:HD21	2.53	0.49
1:B:3796:MET:HE1	1:B:3869:ILE:HG23	1.95	0.49
1:C:730:LEU:HD22	1:C:731:HIS:CE1	2.48	0.49
2:I:38:ASP:OD1	2:I:39:SER:N	2.46	0.49
1:D:624:ALA:HB3	1:D:2131:VAL:HG13	1.94	0.49
1:D:730:LEU:HD22	1:D:731:HIS:CE1	2.48	0.49
1:D:759:LEU:HD11	1:D:761:LEU:HD23	1.94	0.49
1:D:1257:GLN:HB2	1:D:1596:LEU:HD11	1.95	0.49
1:D:2471:LEU:HD11	1:D:2482:PHE:HZ	1.76	0.49
1:D:4836:ASP:OD1	1:D:4836:ASP:N	2.42	0.49
1:A:125:TYR:OH	1:A:417:ARG:HB3	2.13	0.49
1:A:699:SER:OG	1:A:700:THR:N	2.44	0.49
1:A:759:LEU:HD11	1:A:761:LEU:HD23	1.94	0.49
1:A:2076:ASP:HB3	1:A:2079:LEU:HB3	1.94	0.49
1:A:2343:LEU:O	1:A:2347:GLU:HG2	2.13	0.49
1:C:125:TYR:OH	1:C:417:ARG:HB3	2.13	0.49
1:C:2442:PRO:HG3	1:C:2454:ASP:HB2	1.94	0.49
1:C:4806:ASP:O	1:D:4520:VAL:HG12	2.13	0.49
1:D:225:GLN:OE1	1:D:225:GLN:HA	2.13	0.49
1:D:893:TRP:HA	1:D:893:TRP:HE3	1.78	0.49
1:D:1950:LEU:O	1:D:1956:LEU:HD11	2.12	0.49
1:D:2330:PHE:HD1	1:D:2394:LEU:HD21	1.76	0.49
1:A:235:ARG:HB2	1:A:406:SER:OG	2.13	0.49
1:A:340:VAL:HG23	1:A:341:GLY:H	1.78	0.49
1:A:677:LEU:HD23	1:A:755:ILE:HD13	1.94	0.49
1:B:982:ASP:OD1	1:B:985:PHE:HB3	2.12	0.49
1:B:1932:VAL:HG11	1:B:3616:VAL:HB	1.95	0.49
1:B:2220:LEU:HD11	1:B:2242:ALA:HB2	1.93	0.49
1:C:28:ILE:HG12	1:C:29:HIS:CE1	2.48	0.49
1:C:1715:TYR:CE2	1:C:1719:ARG:HD2	2.48	0.49
1:C:2265:VAL:HG21	1:C:2322:LEU:HB3	1.95	0.49
1:C:2317:ASN:O	1:C:2321:ARG:HG2	2.13	0.49
1:C:2330:PHE:HD1	1:C:2394:LEU:HD21	1.77	0.49
1:C:2414:GLU:CD	1:C:2414:GLU:H	2.20	0.49
1:C:3971:MET:HB3	1:C:4093:ILE:HD13	1.94	0.49
1:D:416:ALA:HA	1:D:419:ILE:HD12	1.95	0.49
1:D:1715:TYR:CE2	1:D:1719:ARG:HD2	2.48	0.49
1:D:4009:VAL:HA	1:D:4012:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4653:MET:HE2	1:D:4666:SER:HA	1.95	0.49
1:A:477:ASN:OD1	1:A:480:ARG:NH2	2.45	0.48
1:A:893:TRP:HA	1:A:893:TRP:HE3	1.78	0.48
1:A:3796:MET:HE1	1:A:3869:ILE:HG23	1.95	0.48
1:B:2265:VAL:HG21	1:B:2322:LEU:HB3	1.95	0.48
1:B:2343:LEU:O	1:B:2347:GLU:HG2	2.13	0.48
1:B:3905:PHE:O	1:B:3909:ILE:HG12	2.13	0.48
1:B:4009:VAL:HA	1:B:4012:ILE:HD12	1.94	0.48
1:B:4029:ASP:OD2	1:B:4054:HIS:NE2	2.46	0.48
1:B:4044:LYS:HZ2	1:B:4069:ALA:HB1	1.77	0.48
1:B:4671:MET:HG2	1:B:4674:ALA:HB3	1.95	0.48
1:C:759:LEU:HD11	1:C:761:LEU:HD23	1.94	0.48
1:C:1719:ARG:NE	1:C:1831:ILE:O	2.46	0.48
1:C:2076:ASP:HB3	1:C:2079:LEU:HB3	1.94	0.48
1:D:28:ILE:HG12	1:D:29:HIS:CE1	2.48	0.48
1:D:3957:LEU:HG	1:D:3966:LEU:HD22	1.95	0.48
1:D:4640:PRO:HG2	1:D:4646:LYS:HA	1.93	0.48
1:D:4671:MET:HG2	1:D:4674:ALA:HB3	1.95	0.48
1:A:28:ILE:HG12	1:A:29:HIS:CE1	2.48	0.48
1:A:624:ALA:HB3	1:A:2131:VAL:HG13	1.94	0.48
1:A:4671:MET:HG2	1:A:4674:ALA:HB3	1.95	0.48
2:G:38:ASP:OD1	2:G:39:SER:N	2.46	0.48
1:B:125:TYR:OH	1:B:417:ARG:HB3	2.13	0.48
1:B:677:LEU:HD23	1:B:755:ILE:HD13	1.94	0.48
1:B:1924:ILE:HA	1:B:1998:PHE:HZ	1.78	0.48
1:B:2888:ALA:O	1:B:2892:PHE:HD1	1.96	0.48
1:B:3728:ALA:HA	1:B:3731:HIS:CE1	2.48	0.48
2:H:69:LEU:HD12	2:H:107:LEU:HD23	1.93	0.48
1:C:1685:GLN:NE2	1:C:1703:TYR:OH	2.46	0.48
1:C:1750:PRO:HG3	1:C:2057:LEU:HD22	1.94	0.48
1:D:340:VAL:HG23	1:D:341:GLY:H	1.78	0.48
1:D:2478:GLU:HG2	1:D:2479:VAL:HG22	1.95	0.48
1:D:3728:ALA:HA	1:D:3731:HIS:CE1	2.48	0.48
2:J:38:ASP:OD1	2:J:39:SER:N	2.46	0.48
1:A:730:LEU:HD22	1:A:731:HIS:CE1	2.48	0.48
1:A:909:ASP:OD1	1:A:910:ASP:N	2.45	0.48
1:A:2253:ALA:O	1:A:2315:ASN:ND2	2.40	0.48
1:A:2777:SER:OG	1:A:2843:MET:SD	2.68	0.48
1:A:2888:ALA:O	1:A:2892:PHE:HD1	1.96	0.48
1:A:3905:PHE:O	1:A:3909:ILE:HG12	2.13	0.48
1:A:3971:MET:HB3	1:A:4093:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ALA:HA	1:B:419:ILE:HD12	1.95	0.48
1:B:794:PHE:CD1	1:B:798:ILE:HG21	2.48	0.48
1:B:1733:GLU:O	1:B:1736:SER:OG	2.30	0.48
1:C:982:ASP:OD1	1:C:985:PHE:HB3	2.13	0.48
1:C:1827:TYR:CZ	1:C:1831:ILE:HD11	2.48	0.48
1:D:1827:TYR:CZ	1:D:1831:ILE:HD11	2.47	0.48
1:D:2522:UNK:C	1:D:2524:UNK:H	2.27	0.48
1:D:4596:LEU:HG	1:D:4600:LYS:HE3	1.95	0.48
1:A:3728:ALA:HA	1:A:3731:HIS:CE1	2.48	0.48
1:A:3957:LEU:HG	1:A:3966:LEU:HD22	1.95	0.48
1:A:4722:ALA:O	1:A:4726:THR:HG23	2.13	0.48
1:B:606:ARG:NH1	1:B:1635:GLU:OE2	2.46	0.48
1:B:893:TRP:HA	1:B:893:TRP:HE3	1.78	0.48
1:B:3786:VAL:HG11	1:B:3865:THR:HG23	1.95	0.48
1:C:235:ARG:HB2	1:C:406:SER:OG	2.13	0.48
1:C:416:ALA:HA	1:C:419:ILE:HD12	1.95	0.48
1:C:893:TRP:HE3	1:C:893:TRP:HA	1.78	0.48
1:C:1245:ARG:NH1	1:C:1809:ASP:O	2.44	0.48
1:C:1704:TYR:O	1:C:1708:ILE:HG12	2.14	0.48
1:C:1932:VAL:HG11	1:C:3616:VAL:HB	1.95	0.48
1:C:3698:CYS:SG	1:C:3730:LEU:HD21	2.52	0.48
1:C:4194:ASP:HA	1:C:4599:PHE:HE2	1.79	0.48
1:C:4942:MET:HE1	1:C:4949:GLU:HB2	1.96	0.48
1:D:1982:LYS:NZ	1:D:1983:SER:O	2.29	0.48
1:A:606:ARG:NH1	1:A:1635:GLU:OE2	2.46	0.48
1:A:3420:UNK:HA	1:A:3421:UNK:HA	1.66	0.48
1:A:4112:THR:HA	1:A:4115:GLN:HB2	1.96	0.48
1:A:4653:MET:HE2	1:A:4666:SER:HA	1.95	0.48
1:B:340:VAL:HG23	1:B:341:GLY:H	1.78	0.48
1:B:2330:PHE:HD1	1:B:2394:LEU:HD21	1.76	0.48
1:B:2405:MET:H	1:B:2405:MET:HG3	1.48	0.48
1:B:4112:THR:HA	1:B:4115:GLN:HB2	1.96	0.48
1:C:125:TYR:CE1	1:C:414:ARG:HA	2.49	0.48
1:C:2742:TYR:HD1	1:C:2756:MET:H	1.60	0.48
1:C:4596:LEU:HG	1:C:4600:LYS:HE3	1.95	0.48
1:D:235:ARG:HB2	1:D:406:SER:OG	2.13	0.48
1:D:794:PHE:CD1	1:D:798:ILE:HG21	2.48	0.48
1:D:1685:GLN:NE2	1:D:1703:TYR:OH	2.46	0.48
1:D:2317:ASN:O	1:D:2321:ARG:HG2	2.13	0.48
1:D:4942:MET:HE1	1:D:4949:GLU:HB2	1.96	0.48
1:A:769:ARG:HA	1:A:774:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1935:LEU:HD11	1:A:1975:LEU:HD13	1.96	0.48
1:A:2735:LYS:HD3	1:A:2756:MET:SD	2.54	0.48
1:A:4029:ASP:OD2	1:A:4054:HIS:NE2	2.46	0.48
1:B:4194:ASP:HA	1:B:4599:PHE:HE2	1.79	0.48
1:D:313:ASN:ND2	1:D:391:ALA:O	2.45	0.48
1:D:1704:TYR:O	1:D:1708:ILE:HG12	2.14	0.48
1:D:1719:ARG:NE	1:D:1831:ILE:O	2.46	0.48
1:D:2414:GLU:H	1:D:2414:GLU:CD	2.20	0.48
1:D:2735:LYS:HD3	1:D:2756:MET:SD	2.54	0.48
1:D:2742:TYR:HD1	1:D:2756:MET:H	1.60	0.48
1:D:3611:PRO:HD2	1:D:3614:ARG:HH21	1.79	0.48
1:A:225:GLN:OE1	1:A:225:GLN:HA	2.13	0.48
1:A:1257:GLN:HB2	1:A:1596:LEU:HD11	1.95	0.48
1:A:1704:TYR:O	1:A:1708:ILE:HG12	2.14	0.48
1:B:1786:ASP:OD1	1:B:1786:ASP:N	2.44	0.48
1:B:2522:UNK:C	1:B:2524:UNK:H	2.27	0.48
1:B:4722:ALA:O	1:B:4726:THR:HG23	2.13	0.48
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.79	0.48
1:C:439:LYS:HE2	1:C:439:LYS:HB3	1.59	0.48
1:C:876:PRO:HA	1:C:879:GLU:HG2	1.95	0.48
1:C:893:TRP:HA	1:C:893:TRP:CE3	2.47	0.48
1:C:2888:ALA:O	1:C:2892:PHE:HD1	1.96	0.48
1:C:3796:MET:HE1	1:C:3869:ILE:HG23	1.95	0.48
1:D:318:ASP:OD1	1:D:318:ASP:N	2.47	0.48
1:D:876:PRO:HA	1:D:879:GLU:HG2	1.95	0.48
1:A:2414:GLU:CD	1:A:2414:GLU:H	2.20	0.48
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.79	0.48
1:B:225:GLN:OE1	1:B:225:GLN:HA	2.13	0.48
1:B:2478:GLU:HG2	1:B:2479:VAL:HG22	1.95	0.48
1:B:2735:LYS:HD3	1:B:2756:MET:SD	2.54	0.48
1:C:3905:PHE:O	1:C:3909:ILE:HG12	2.13	0.48
1:D:606:ARG:NH1	1:D:1635:GLU:OE2	2.46	0.48
1:D:1730:MET:SD	1:D:2106:THR:OG1	2.69	0.48
1:A:2742:TYR:HD1	1:A:2756:MET:H	1.60	0.48
1:B:235:ARG:HB2	1:B:406:SER:OG	2.13	0.48
1:B:1685:GLN:NE2	1:B:1703:TYR:OH	2.46	0.48
1:B:2742:TYR:HD1	1:B:2756:MET:H	1.60	0.48
1:B:3420:UNK:HA	1:B:3421:UNK:HA	1.66	0.48
1:C:4722:ALA:O	1:C:4726:THR:HG23	2.13	0.48
1:D:606:ARG:HH22	1:D:1633:ILE:HG23	1.79	0.48
1:D:986:ILE:HG13	1:D:987:LYS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ALA:HA	1:A:419:ILE:HD12	1.95	0.48
1:A:606:ARG:HH22	1:A:1633:ILE:HG23	1.79	0.48
1:A:2217:LEU:HA	1:A:2220:LEU:HG	1.96	0.48
1:A:4013:LEU:HD22	1:A:4124:VAL:HG21	1.96	0.48
1:B:1257:GLN:HB2	1:B:1596:LEU:HD11	1.95	0.48
1:C:1120:PRO:HG3	1:C:1202:ILE:HD11	1.96	0.48
1:C:2522:UNK:C	1:C:2524:UNK:H	2.27	0.48
1:C:3712:SER:OG	1:C:3716:LYS:NZ	2.35	0.48
1:C:3786:VAL:HG11	1:C:3865:THR:HG23	1.95	0.48
1:C:4653:MET:HE2	1:C:4666:SER:HA	1.95	0.48
1:D:125:TYR:OH	1:D:417:ARG:HB3	2.13	0.48
1:D:4029:ASP:OD2	1:D:4054:HIS:NE2	2.46	0.48
1:A:2434:VAL:HG11	1:A:2467:MET:HE3	1.96	0.47
1:B:28:ILE:HG12	1:B:29:HIS:CE1	2.48	0.47
1:B:125:TYR:CE1	1:B:414:ARG:HA	2.49	0.47
1:C:503:ASP:O	1:C:507:VAL:HG13	2.14	0.47
1:C:4029:ASP:OD2	1:C:4054:HIS:NE2	2.46	0.47
1:D:769:ARG:HA	1:D:774:PRO:HA	1.96	0.47
1:D:2217:LEU:HA	1:D:2220:LEU:HG	1.96	0.47
1:D:2343:LEU:O	1:D:2347:GLU:HG2	2.13	0.47
1:D:2888:ALA:O	1:D:2892:PHE:HD1	1.96	0.47
1:D:3786:VAL:HG11	1:D:3865:THR:HG23	1.95	0.47
1:D:4722:ALA:O	1:D:4726:THR:HG23	2.13	0.47
1:A:1719:ARG:NE	1:A:1831:ILE:O	2.46	0.47
1:A:2478:GLU:HG2	1:A:2479:VAL:HG22	1.95	0.47
1:A:3611:PRO:HD2	1:A:3614:ARG:HH21	1.79	0.47
1:B:162:ILE:HG23	1:B:181:LEU:HB2	1.97	0.47
1:B:1935:LEU:HD11	1:B:1975:LEU:HD13	1.96	0.47
1:B:3611:PRO:HD2	1:B:3614:ARG:HH21	1.79	0.47
1:C:4027:SER:HA	1:C:4032:LYS:HG2	1.96	0.47
1:D:1935:LEU:HD11	1:D:1975:LEU:HD13	1.96	0.47
1:D:3796:MET:HE1	1:D:3869:ILE:HG23	1.95	0.47
1:D:3905:PHE:O	1:D:3909:ILE:HG12	2.13	0.47
1:A:125:TYR:CE1	1:A:414:ARG:HA	2.49	0.47
1:A:313:ASN:ND2	1:A:391:ALA:O	2.45	0.47
1:A:2522:UNK:C	1:A:2524:UNK:H	2.27	0.47
1:A:4189:VAL:HG21	1:A:4948:TRP:CD1	2.49	0.47
1:C:1733:GLU:O	1:C:1736:SER:OG	2.30	0.47
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.79	0.47
1:D:125:TYR:CE1	1:D:414:ARG:HA	2.49	0.47
1:D:1932:VAL:HG11	1:D:3616:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4112:THR:HA	1:D:4115:GLN:HB2	1.96	0.47
1:A:2265:VAL:HG21	1:A:2322:LEU:HB3	1.95	0.47
1:A:2317:ASN:O	1:A:2321:ARG:HG2	2.13	0.47
1:B:2781:MET:HE2	1:B:2781:MET:HA	1.97	0.47
1:C:606:ARG:HH22	1:C:1633:ILE:HG23	1.79	0.47
1:C:2217:LEU:HA	1:C:2220:LEU:HG	1.96	0.47
1:C:3611:PRO:HD2	1:C:3614:ARG:HH21	1.79	0.47
1:D:2434:VAL:HG11	1:D:2467:MET:HE3	1.96	0.47
1:D:3839:PHE:HE1	1:D:3873:THR:HG23	1.80	0.47
1:D:4189:VAL:HG21	1:D:4948:TRP:CD1	2.49	0.47
1:A:1932:VAL:HG11	1:A:3616:VAL:HB	1.95	0.47
1:A:2850:ILE:O	1:A:2854:LYS:HG2	2.15	0.47
1:B:503:ASP:O	1:B:507:VAL:HG13	2.14	0.47
1:B:1120:PRO:HG3	1:B:1202:ILE:HD11	1.96	0.47
1:B:2217:LEU:HA	1:B:2220:LEU:HG	1.96	0.47
1:B:3839:PHE:HE1	1:B:3873:THR:HG23	1.80	0.47
1:B:4189:VAL:HG21	1:B:4948:TRP:CD1	2.50	0.47
1:B:4942:MET:HE1	1:B:4949:GLU:HB2	1.96	0.47
1:C:3712:SER:HG	1:C:3716:LYS:HZ3	1.57	0.47
1:C:4112:THR:HA	1:C:4115:GLN:HB2	1.96	0.47
1:C:4671:MET:HG2	1:C:4674:ALA:HB3	1.95	0.47
1:A:162:ILE:HG23	1:A:181:LEU:HB2	1.97	0.47
1:A:423:VAL:HG23	1:A:497:LEU:HD22	1.97	0.47
1:A:2779:LYS:HE3	1:A:2779:LYS:HB3	1.72	0.47
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.97	0.47
1:B:318:ASP:OD1	1:B:318:ASP:N	2.47	0.47
1:B:2779:LYS:HE3	1:B:2779:LYS:HB3	1.72	0.47
1:B:3957:LEU:HG	1:B:3966:LEU:HD22	1.95	0.47
1:B:4142:LYS:HD3	1:B:4142:LYS:HA	1.71	0.47
1:C:225:GLN:HA	1:C:225:GLN:OE1	2.13	0.47
1:C:2735:LYS:HD3	1:C:2756:MET:SD	2.54	0.47
1:D:162:ILE:HG23	1:D:181:LEU:HB2	1.97	0.47
1:D:1120:PRO:HG3	1:D:1202:ILE:HD11	1.96	0.47
1:D:2265:VAL:HG21	1:D:2322:LEU:HB3	1.95	0.47
1:D:4194:ASP:HA	1:D:4599:PHE:HE2	1.79	0.47
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.79	0.47
1:A:167:LYS:HB2	1:A:167:LYS:HE2	1.48	0.47
1:A:503:ASP:O	1:A:507:VAL:HG13	2.14	0.47
1:A:686:VAL:HG13	1:A:687:THR:H	1.80	0.47
1:A:1224:LEU:HB3	1:A:1227:PHE:HB3	1.97	0.47
1:A:1685:GLN:NE2	1:A:1703:TYR:OH	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4942:MET:HE1	1:A:4949:GLU:HB2	1.96	0.47
1:B:769:ARG:HA	1:B:774:PRO:HA	1.96	0.47
1:B:876:PRO:HA	1:B:879:GLU:HG2	1.95	0.47
1:B:1174:MET:HG2	1:B:1190:LEU:HA	1.96	0.47
1:B:1224:LEU:HB3	1:B:1227:PHE:HB3	1.97	0.47
1:B:2723:TYR:CE1	1:B:2770:TYR:HE2	2.33	0.47
1:B:4029:ASP:OD1	1:B:4029:ASP:N	2.48	0.47
1:C:909:ASP:OD1	1:C:910:ASP:N	2.45	0.47
1:C:986:ILE:HG13	1:C:987:LYS:N	2.29	0.47
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.23	0.47
1:C:4601:ARG:HD3	1:C:4707:TRP:CZ2	2.50	0.47
1:D:909:ASP:OD1	1:D:910:ASP:N	2.45	0.47
1:D:2764:GLU:O	1:D:2768:GLU:HG2	2.15	0.47
1:D:4027:SER:HA	1:D:4032:LYS:HG2	1.96	0.47
1:A:4033:GLU:OE1	1:A:4033:GLU:N	2.48	0.47
1:B:606:ARG:HH22	1:B:1633:ILE:HG23	1.79	0.47
1:B:2317:ASN:O	1:B:2321:ARG:HG2	2.13	0.47
1:B:2777:SER:OG	1:B:2843:MET:SD	2.68	0.47
1:B:4653:MET:HE2	1:B:4666:SER:HA	1.95	0.47
1:C:55:SER:O	1:C:296:ARG:NH2	2.34	0.47
1:C:162:ILE:HG23	1:C:181:LEU:HB2	1.97	0.47
1:C:3839:PHE:HE1	1:C:3873:THR:HG23	1.80	0.47
1:C:4044:LYS:HZ2	1:C:4069:ALA:HB1	1.78	0.47
1:D:423:VAL:HG23	1:D:497:LEU:HD22	1.97	0.47
1:D:748:LEU:HD13	1:D:748:LEU:HA	1.77	0.47
1:A:207:PHE:CZ	1:B:2324:ILE:HD12	2.50	0.47
1:A:1174:MET:HG2	1:A:1190:LEU:HA	1.96	0.47
1:A:1311:ALA:HA	1:A:1312:UNK:HA	1.50	0.47
1:A:3839:PHE:HE1	1:A:3873:THR:HG23	1.80	0.47
1:B:423:VAL:HG23	1:B:497:LEU:HD22	1.97	0.47
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.23	0.47
1:B:4596:LEU:HG	1:B:4600:LYS:HE3	1.95	0.47
1:C:2723:TYR:CE1	1:C:2770:TYR:HE2	2.33	0.47
1:D:946:LEU:HD11	1:D:995:MET:HE3	1.97	0.47
1:D:4601:ARG:HD3	1:D:4707:TRP:CZ2	2.50	0.47
1:A:2781:MET:HE2	1:A:2781:MET:HA	1.96	0.47
1:A:4596:LEU:HG	1:A:4600:LYS:HE3	1.96	0.47
1:B:816:PRO:HB2	1:B:819:TYR:CD1	2.50	0.47
1:B:1704:TYR:O	1:B:1708:ILE:HG12	2.14	0.47
1:C:2478:GLU:HG2	1:C:2479:VAL:HG22	1.95	0.47
1:C:3957:LEU:HG	1:C:3966:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4013:LEU:HD22	1:C:4124:VAL:HG21	1.96	0.47
1:C:4033:GLU:N	1:C:4033:GLU:OE1	2.48	0.47
1:C:4785:PHE:CZ	1:D:4518:TYR:HE2	2.33	0.47
1:C:4789:ARG:NH1	1:D:4558:TYR:OH	2.48	0.47
1:D:662:GLY:O	1:D:669:GLN:NE2	2.48	0.47
1:D:686:VAL:HG13	1:D:687:THR:H	1.80	0.47
1:D:1174:MET:HG2	1:D:1190:LEU:HA	1.97	0.47
1:D:2101:LEU:HA	1:D:2104:THR:HG22	1.97	0.47
1:D:2850:ILE:O	1:D:2854:LYS:HG2	2.15	0.47
1:A:986:ILE:HG13	1:A:987:LYS:N	2.29	0.46
1:A:2723:TYR:CE1	1:A:2770:TYR:HE2	2.33	0.46
1:B:2850:ILE:O	1:B:2854:LYS:HG2	2.15	0.46
1:C:686:VAL:HG13	1:C:687:THR:H	1.80	0.46
1:C:1358:ARG:HB2	1:C:1567:LEU:HD21	1.97	0.46
1:C:1361:LYS:HA	1:C:1566:PRO:HA	1.98	0.46
1:C:1935:LEU:HD11	1:C:1975:LEU:HD13	1.96	0.46
1:C:2101:LEU:HA	1:C:2104:THR:HG22	1.97	0.46
1:C:2781:MET:HE2	1:C:2781:MET:HA	1.97	0.46
1:D:503:ASP:O	1:D:507:VAL:HG13	2.14	0.46
1:D:4029:ASP:OD1	1:D:4029:ASP:N	2.48	0.46
1:A:876:PRO:HA	1:A:879:GLU:HG2	1.95	0.46
1:A:4601:ARG:HD3	1:A:4707:TRP:CZ2	2.50	0.46
1:B:1358:ARG:HB2	1:B:1567:LEU:HD21	1.98	0.46
1:B:1362:ASP:N	1:B:1362:ASP:OD1	2.49	0.46
1:B:3729:ARG:O	1:B:3733:ARG:NH1	2.48	0.46
1:C:313:ASN:ND2	1:C:391:ALA:O	2.45	0.46
1:C:423:VAL:HG23	1:C:497:LEU:HD22	1.97	0.46
1:C:654:SER:H	1:C:841:LYS:HZ1	1.59	0.46
1:C:692:HIS:HB3	1:C:795:SER:HB3	1.97	0.46
1:C:769:ARG:HA	1:C:774:PRO:HA	1.96	0.46
1:C:4106:GLU:OE2	1:C:4148:TYR:OH	2.19	0.46
1:C:4189:VAL:HG21	1:C:4948:TRP:CD1	2.50	0.46
1:D:1362:ASP:OD1	1:D:1362:ASP:N	2.49	0.46
1:D:1982:LYS:HD2	1:D:1983:SER:H	1.81	0.46
1:D:4033:GLU:OE1	1:D:4033:GLU:N	2.48	0.46
1:A:1120:PRO:HG3	1:A:1202:ILE:HD11	1.96	0.46
1:A:1936:GLN:O	1:A:1939:GLN:HG3	2.16	0.46
1:A:3899:GLU:OE2	1:A:3900:GLN:HG2	2.15	0.46
1:B:686:VAL:HG13	1:B:687:THR:H	1.80	0.46
1:B:2771:ARG:O	1:B:2775:LYS:HD3	2.15	0.46
1:C:816:PRO:HB2	1:C:819:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2405:MET:H	1:C:2405:MET:HG3	1.48	0.46
1:C:2764:GLU:O	1:C:2768:GLU:HG2	2.15	0.46
1:D:1733:GLU:O	1:D:1736:SER:OG	2.30	0.46
1:D:3727:GLN:C	1:D:3731:HIS:HD1	2.23	0.46
1:D:4013:LEU:HD22	1:D:4124:VAL:HG21	1.96	0.46
1:B:662:GLY:O	1:B:669:GLN:NE2	2.48	0.46
1:B:946:LEU:HD11	1:B:995:MET:HE3	1.97	0.46
1:B:4013:LEU:HD22	1:B:4124:VAL:HG21	1.96	0.46
1:B:4033:GLU:OE1	1:B:4033:GLU:N	2.48	0.46
1:C:23:GLN:HG3	1:C:213:SER:HB2	1.98	0.46
1:C:1677:LEU:HA	1:C:1680:HIS:HB2	1.97	0.46
1:C:2434:VAL:HG11	1:C:2467:MET:HE3	1.96	0.46
1:C:3420:UNK:HA	1:C:3421:UNK:HA	1.65	0.46
2:J:24:VAL:HG22	2:J:48:LYS:HG2	1.97	0.46
1:A:816:PRO:HB2	1:A:819:TYR:CD1	2.50	0.46
1:A:1677:LEU:HA	1:A:1680:HIS:HB2	1.97	0.46
1:A:2231:PRO:HG3	1:A:2381:ILE:HG12	1.98	0.46
1:A:4154:SER:O	1:A:4158:GLN:HG2	2.16	0.46
1:A:4194:ASP:HA	1:A:4599:PHE:HE2	1.79	0.46
1:B:646:THR:HG21	1:B:1685:GLN:NE2	2.31	0.46
1:B:1361:LYS:HA	1:B:1566:PRO:HA	1.98	0.46
1:B:4154:SER:O	1:B:4158:GLN:HG2	2.16	0.46
1:C:646:THR:HG21	1:C:1685:GLN:NE2	2.31	0.46
1:C:1224:LEU:HB3	1:C:1227:PHE:HB3	1.97	0.46
1:C:4154:SER:O	1:C:4158:GLN:HG2	2.16	0.46
1:D:1358:ARG:HB2	1:D:1567:LEU:HD21	1.97	0.46
1:A:750:ARG:NH2	2:G:9:SER:OG	2.47	0.46
1:A:946:LEU:HD11	1:A:995:MET:HE3	1.97	0.46
1:B:1936:GLN:O	1:B:1939:GLN:HG3	2.16	0.46
1:B:4601:ARG:HD3	1:B:4707:TRP:CZ2	2.50	0.46
1:C:2228:LEU:HD22	1:C:2296:ARG:HG3	1.98	0.46
1:C:2850:ILE:O	1:C:2854:LYS:HG2	2.15	0.46
1:D:23:GLN:HG3	1:D:213:SER:HB2	1.98	0.46
1:D:281:ARG:NH1	1:D:346:VAL:O	2.38	0.46
1:A:662:GLY:O	1:A:669:GLN:NE2	2.48	0.46
1:A:2477:ILE:O	1:A:2477:ILE:HG13	2.16	0.46
1:A:2740:TRP:CD1	1:A:2751:LYS:HE3	2.43	0.46
1:A:2764:GLU:O	1:A:2768:GLU:HG2	2.15	0.46
1:B:943:LEU:HG	1:B:999:LEU:CD1	2.46	0.46
1:B:986:ILE:HG13	1:B:987:LYS:N	2.29	0.46
1:B:1004:HIS:HB3	1:B:1035:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3899:GLU:OE2	1:B:3900:GLN:HG2	2.15	0.46
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.97	0.46
1:C:1174:MET:HG2	1:C:1190:LEU:HA	1.96	0.46
1:C:1311:ALA:HA	1:C:1312:UNK:HA	1.50	0.46
1:C:2325:ARG:HA	1:C:2325:ARG:HD3	1.82	0.46
1:C:3727:GLN:C	1:C:3731:HIS:HD1	2.23	0.46
1:C:4601:ARG:HD2	1:C:4711:VAL:HG21	1.98	0.46
1:D:646:THR:HG21	1:D:1685:GLN:NE2	2.31	0.46
1:A:934:GLN:O	1:A:938:GLU:HG2	2.16	0.46
1:A:999:LEU:HD23	1:A:1050:LEU:HG	1.98	0.46
1:A:4027:SER:HA	1:A:4032:LYS:HG2	1.96	0.46
1:B:1677:LEU:HA	1:B:1680:HIS:HB2	1.97	0.46
1:B:4027:SER:HA	1:B:4032:LYS:HG2	1.96	0.46
1:C:1004:HIS:HB3	1:C:1035:TYR:HB2	1.98	0.46
1:C:1100:ARG:HG3	1:C:1167:ASP:CG	2.41	0.46
1:C:2771:ARG:O	1:C:2775:LYS:HD3	2.15	0.46
1:D:1677:LEU:HA	1:D:1680:HIS:HB2	1.97	0.46
1:D:2228:LEU:HD22	1:D:2296:ARG:HG3	1.98	0.46
1:D:2771:ARG:O	1:D:2775:LYS:HD3	2.15	0.46
1:D:4142:LYS:HA	1:D:4142:LYS:HD3	1.71	0.46
1:A:23:GLN:HG3	1:A:213:SER:HB2	1.98	0.46
1:A:1982:LYS:HD2	1:A:1983:SER:H	1.80	0.46
1:A:4601:ARG:HD2	1:A:4711:VAL:HG21	1.98	0.46
1:B:692:HIS:HB3	1:B:795:SER:HB3	1.98	0.46
1:B:895:MET:O	1:B:899:GLU:HG3	2.16	0.46
1:B:2477:ILE:HG13	1:B:2477:ILE:O	2.16	0.46
1:C:662:GLY:O	1:C:669:GLN:NE2	2.48	0.46
1:C:946:LEU:HD11	1:C:995:MET:HE3	1.97	0.46
1:C:3729:ARG:O	1:C:3733:ARG:NH1	2.48	0.46
1:D:1224:LEU:HB3	1:D:1227:PHE:HB3	1.97	0.46
1:D:3729:ARG:O	1:D:3733:ARG:NH1	2.48	0.46
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.23	0.46
1:A:1358:ARG:HB2	1:A:1567:LEU:HD21	1.98	0.46
1:A:2228:LEU:HD22	1:A:2296:ARG:HG3	1.98	0.46
1:A:4029:ASP:N	1:A:4029:ASP:OD1	2.48	0.46
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.23	0.46
1:B:555:LEU:HD11	1:B:585:ALA:HB1	1.98	0.46
1:C:934:GLN:O	1:C:938:GLU:HG2	2.16	0.46
1:C:943:LEU:HG	1:C:999:LEU:CD1	2.46	0.46
1:C:3899:GLU:OE2	1:C:3900:GLN:HG2	2.15	0.46
1:C:4121:ALA:O	1:C:4125:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:24:VAL:HG22	2:I:48:LYS:HG2	1.97	0.46
1:D:3899:GLU:OE2	1:D:3900:GLN:HG2	2.15	0.46
1:D:4121:ALA:O	1:D:4125:LEU:HG	2.16	0.46
1:A:895:MET:O	1:A:899:GLU:HG3	2.16	0.45
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.49	0.45
1:A:2771:ARG:O	1:A:2775:LYS:HD3	2.15	0.45
1:B:1038:LEU:O	1:B:1043:LYS:HE3	2.16	0.45
1:B:1982:LYS:HD2	1:B:1983:SER:H	1.81	0.45
1:B:2764:GLU:O	1:B:2768:GLU:HG2	2.15	0.45
1:B:4586:ILE:HD11	1:B:4718:PHE:CE2	2.51	0.45
1:B:4852:PHE:HA	1:B:4856:ILE:HD12	1.99	0.45
1:C:318:ASP:N	1:C:318:ASP:OD1	2.47	0.45
1:C:2231:PRO:HG3	1:C:2381:ILE:HG12	1.98	0.45
1:C:4586:ILE:HD11	1:C:4718:PHE:CE2	2.51	0.45
1:D:934:GLN:O	1:D:938:GLU:HG2	2.16	0.45
1:D:2723:TYR:CE1	1:D:2770:TYR:HE2	2.33	0.45
1:D:4586:ILE:HD11	1:D:4718:PHE:CE2	2.51	0.45
1:A:3729:ARG:O	1:A:3733:ARG:NH1	2.48	0.45
1:B:1311:ALA:HA	1:B:1312:UNK:HA	1.50	0.45
1:B:4615:TYR:CE1	1:B:4631:ARG:HB2	2.51	0.45
1:D:1100:ARG:HG3	1:D:1167:ASP:CG	2.41	0.45
1:D:1361:LYS:HA	1:D:1566:PRO:HA	1.98	0.45
1:D:2740:TRP:CD1	1:D:2751:LYS:HE3	2.43	0.45
1:B:2101:LEU:HA	1:B:2104:THR:HG22	1.97	0.45
1:B:2228:LEU:HD22	1:B:2296:ARG:HG3	1.98	0.45
1:C:1936:GLN:O	1:C:1939:GLN:HG3	2.16	0.45
1:C:4824:GLY:O	1:D:4821:ARG:NH2	2.49	0.45
2:I:68:SER:C	2:I:104:LEU:HD23	2.42	0.45
1:D:2781:MET:HA	1:D:2781:MET:HE2	1.97	0.45
1:D:4615:TYR:CE1	1:D:4631:ARG:HB2	2.51	0.45
1:A:55:SER:O	1:A:296:ARG:NH2	2.34	0.45
1:A:189:GLU:OE2	1:B:2321:ARG:NH1	2.49	0.45
1:A:1730:MET:SD	1:A:2106:THR:OG1	2.69	0.45
1:A:4929:GLU:HG2	1:A:4930:THR:H	1.82	0.45
1:B:2434:VAL:HG11	1:B:2467:MET:HE3	1.96	0.45
1:C:555:LEU:HD11	1:C:585:ALA:HB1	1.99	0.45
1:C:1982:LYS:HD2	1:C:1983:SER:H	1.80	0.45
1:D:477:ASN:OD1	1:D:480:ARG:NH2	2.45	0.45
1:D:710:GLY:H	1:D:716:ASN:HD22	1.64	0.45
1:D:816:PRO:HB2	1:D:819:TYR:CD1	2.50	0.45
1:D:1936:GLN:O	1:D:1939:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2405:MET:H	1:D:2405:MET:HG3	1.48	0.45
1:A:836:HIS:NE2	1:A:842:GLN:OE1	2.46	0.45
1:A:1004:HIS:HB3	1:A:1035:TYR:HB2	1.97	0.45
1:A:4615:TYR:CE1	1:A:4631:ARG:HB2	2.51	0.45
1:B:23:GLN:HG3	1:B:213:SER:HB2	1.98	0.45
1:B:477:ASN:OD1	1:B:480:ARG:NH2	2.45	0.45
1:B:934:GLN:O	1:B:938:GLU:HG2	2.16	0.45
1:B:999:LEU:HD23	1:B:1050:LEU:HG	1.98	0.45
1:B:2231:PRO:HG3	1:B:2381:ILE:HG12	1.97	0.45
2:H:68:SER:C	2:H:104:LEU:HD23	2.42	0.45
1:C:895:MET:O	1:C:899:GLU:HG3	2.16	0.45
1:C:2154:PHE:CD2	1:C:2205:ILE:HD11	2.52	0.45
1:D:167:LYS:HB2	1:D:167:LYS:HE2	1.48	0.45
1:D:1586:ARG:NH2	1:D:1635:GLU:OE1	2.50	0.45
2:J:68:SER:C	2:J:104:LEU:HD23	2.42	0.45
1:A:555:LEU:HD11	1:A:585:ALA:HB1	1.98	0.45
1:A:2101:LEU:HA	1:A:2104:THR:HG22	1.97	0.45
1:A:2154:PHE:CD2	1:A:2205:ILE:HD11	2.52	0.45
1:D:439:LYS:HE2	1:D:439:LYS:HB3	1.59	0.45
1:D:1982:LYS:HD2	1:D:1983:SER:N	2.31	0.45
1:D:3420:UNK:HA	1:D:3421:UNK:HA	1.65	0.45
1:D:4601:ARG:HD2	1:D:4711:VAL:HG21	1.98	0.45
1:D:4929:GLU:HG2	1:D:4930:THR:H	1.82	0.45
1:A:318:ASP:N	1:A:318:ASP:OD1	2.47	0.45
1:A:439:LYS:HB3	1:A:439:LYS:HE2	1.59	0.45
1:A:1982:LYS:HD2	1:A:1983:SER:N	2.31	0.45
1:A:4586:ILE:HD11	1:A:4718:PHE:CE2	2.51	0.45
1:A:4850:PHE:CD2	1:B:4821:ARG:HG2	2.52	0.45
1:B:1730:MET:SD	1:B:2106:THR:OG1	2.69	0.45
1:B:2134:GLY:H	1:B:2137:GLU:HB2	1.82	0.45
1:B:4121:ALA:O	1:B:4125:LEU:HG	2.17	0.45
1:B:4122:GLU:HA	1:B:4125:LEU:HD12	1.99	0.45
1:D:895:MET:O	1:D:899:GLU:HG3	2.16	0.45
1:D:4154:SER:O	1:D:4158:GLN:HG2	2.16	0.45
1:A:710:GLY:H	1:A:716:ASN:HD22	1.64	0.45
1:A:1038:LEU:O	1:A:1043:LYS:HE3	2.16	0.45
1:A:1272:ARG:NH2	1:A:1583:CYS:SG	2.90	0.45
1:A:1361:LYS:HA	1:A:1566:PRO:HA	1.98	0.45
1:A:2091:TYR:CE2	1:A:3639:LEU:HD13	2.52	0.45
2:G:68:SER:C	2:G:104:LEU:HD23	2.42	0.45
1:B:2154:PHE:CD2	1:B:2205:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3860:GLN:NE2	1:B:3867:VAL:H	2.15	0.45
1:C:477:ASN:OD1	1:C:480:ARG:NH2	2.45	0.45
1:C:661:LEU:HD22	1:C:673:TRP:NE1	2.32	0.45
1:C:1572:PHE:HZ	1:C:1587:LEU:HD11	1.82	0.45
1:C:1982:LYS:HD2	1:C:1983:SER:N	2.31	0.45
1:C:4142:LYS:HD3	1:C:4142:LYS:HA	1.71	0.45
1:D:2134:GLY:H	1:D:2137:GLU:HB2	1.82	0.45
1:A:646:THR:HG21	1:A:1685:GLN:NE2	2.31	0.45
1:A:2134:GLY:H	1:A:2137:GLU:HB2	1.82	0.45
1:A:2206:SER:HB2	1:A:2209:ASN:HD22	1.82	0.45
1:B:299:HIS:HD2	1:B:302:THR:HG22	1.82	0.45
1:B:1100:ARG:HG3	1:B:1167:ASP:CG	2.41	0.45
1:C:299:HIS:HD2	1:C:302:THR:HG22	1.82	0.45
2:I:58:LYS:HA	2:I:61:GLU:HG3	1.99	0.45
1:D:24:CYS:HB3	1:D:212:TRP:CE3	2.52	0.45
1:D:692:HIS:HB3	1:D:795:SER:HB3	1.98	0.45
1:D:999:LEU:HD23	1:D:1050:LEU:HG	1.98	0.45
1:D:2206:SER:HB2	1:D:2209:ASN:HD22	1.82	0.45
1:D:2477:ILE:HG13	1:D:2477:ILE:O	2.16	0.45
1:A:1100:ARG:HG3	1:A:1167:ASP:CG	2.41	0.45
1:A:4813:MET:HG3	1:D:4843:ILE:CD1	2.45	0.45
1:B:710:GLY:H	1:B:716:ASN:ND2	2.15	0.45
1:B:1982:LYS:HD2	1:B:1983:SER:N	2.31	0.45
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.90	0.45
1:C:1586:ARG:NH2	1:C:1635:GLU:OE1	2.50	0.45
1:C:2206:SER:HB2	1:C:2209:ASN:HD22	1.82	0.45
1:C:4852:PHE:HA	1:C:4856:ILE:HD12	1.99	0.45
1:D:836:HIS:CG	1:D:841:LYS:HB3	2.52	0.45
1:D:1004:HIS:HB3	1:D:1035:TYR:HB2	1.98	0.45
1:D:1572:PHE:HZ	1:D:1587:LEU:HD11	1.82	0.45
1:D:2231:PRO:HG3	1:D:2381:ILE:HG12	1.98	0.45
1:D:4852:PHE:HA	1:D:4856:ILE:HD12	1.99	0.45
1:A:61:ASP:HB3	1:A:64:ILE:HG12	1.99	0.44
1:A:297:LEU:HD13	1:A:297:LEU:HA	1.81	0.44
1:A:606:ARG:HH22	1:A:1635:GLU:HG2	1.82	0.44
1:A:943:LEU:HG	1:A:999:LEU:CD1	2.46	0.44
1:A:1001:GLU:OE2	1:A:1035:TYR:HB3	2.17	0.44
1:A:2084:PHE:O	1:A:3690:TYR:OH	2.25	0.44
1:A:3920:THR:HG22	1:A:3980:MET:HA	1.99	0.44
1:B:313:ASN:ND2	1:B:391:ALA:O	2.45	0.44
1:B:1272:ARG:NH2	1:B:1583:CYS:SG	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:999:LEU:HD23	1:C:1050:LEU:HG	1.98	0.44
1:C:1362:ASP:N	1:C:1362:ASP:OD1	2.49	0.44
1:C:4929:GLU:HG2	1:C:4930:THR:H	1.82	0.44
1:D:675:TYR:CE1	1:D:790:PRO:HB3	2.52	0.44
1:D:775:VAL:HG23	1:D:777:GLY:H	1.82	0.44
1:D:1965:ARG:O	1:D:1966:SER:OG	2.35	0.44
1:A:14:LEU:HD11	1:A:214:VAL:HG21	1.99	0.44
1:A:836:HIS:CG	1:A:841:LYS:HB3	2.52	0.44
1:A:4121:ALA:O	1:A:4125:LEU:HG	2.16	0.44
1:A:4852:PHE:HA	1:A:4856:ILE:HD12	1.99	0.44
1:B:24:CYS:HB3	1:B:212:TRP:CE3	2.52	0.44
1:B:61:ASP:HB3	1:B:64:ILE:HG12	1.99	0.44
1:B:2741:ILE:HD12	1:B:2741:ILE:HA	1.72	0.44
1:B:3876:TYR:HD1	1:B:3879:ARG:HH21	1.66	0.44
1:C:710:GLY:H	1:C:716:ASN:ND2	2.15	0.44
1:C:775:VAL:HG23	1:C:777:GLY:H	1.82	0.44
1:C:1001:GLU:OE2	1:C:1035:TYR:HB3	2.17	0.44
1:C:1962:ARG:HH21	1:C:1963:GLU:HA	1.83	0.44
1:C:2477:ILE:O	1:C:2477:ILE:HG13	2.16	0.44
1:D:926:GLU:H	1:D:926:GLU:HG2	1.54	0.44
1:D:1038:LEU:O	1:D:1043:LYS:HE3	2.16	0.44
1:D:2091:TYR:CE2	1:D:3639:LEU:HD13	2.52	0.44
1:D:2501:LEU:HD11	1:D:2505:ALA:HB2	1.99	0.44
1:D:4079:TYR:O	1:D:4083:VAL:HG22	2.17	0.44
1:D:4116:THR:O	1:D:4119:GLU:HG2	2.17	0.44
1:A:3860:GLN:NE2	1:A:3867:VAL:H	2.15	0.44
1:A:4108:MET:HE2	1:A:4108:MET:HB3	1.90	0.44
1:B:836:HIS:CG	1:B:841:LYS:HB3	2.52	0.44
1:B:1060:TYR:HD1	1:B:1060:TYR:N	2.08	0.44
1:C:61:ASP:HB3	1:C:64:ILE:HG12	1.99	0.44
1:C:710:GLY:H	1:C:716:ASN:HD22	1.64	0.44
1:C:821:ALA:HB3	1:C:823:TYR:CE1	2.52	0.44
1:C:2091:TYR:CE2	1:C:3639:LEU:HD13	2.52	0.44
1:C:4029:ASP:OD1	1:C:4029:ASP:N	2.48	0.44
1:C:4079:TYR:O	1:C:4083:VAL:HG22	2.17	0.44
1:C:4615:TYR:CE1	1:C:4631:ARG:HB2	2.51	0.44
1:D:626:ARG:NH2	1:D:1669:GLY:O	2.51	0.44
1:D:3876:TYR:HD1	1:D:3879:ARG:HH21	1.65	0.44
1:D:3923:ILE:HD12	1:D:3984:MET:HG2	1.99	0.44
1:A:299:HIS:HD2	1:A:302:THR:HG22	1.82	0.44
1:A:1140:PHE:HD2	1:A:1141:LYS:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HD11	1:B:214:VAL:HG21	1.99	0.44
1:B:1962:ARG:HH21	1:B:1963:GLU:HA	1.83	0.44
1:B:2206:SER:HB2	1:B:2209:ASN:HD22	1.82	0.44
1:B:4630:ASP:O	1:B:4634:ILE:HG23	2.18	0.44
1:C:24:CYS:HB3	1:C:212:TRP:CE3	2.52	0.44
1:C:675:TYR:CE1	1:C:790:PRO:HB3	2.52	0.44
1:C:1038:LEU:O	1:C:1043:LYS:HE3	2.16	0.44
1:C:3920:THR:HG22	1:C:3980:MET:HA	1.99	0.44
1:C:3923:ILE:HD12	1:C:3984:MET:HG2	1.99	0.44
1:C:4116:THR:O	1:C:4119:GLU:HG2	2.17	0.44
1:C:4122:GLU:HA	1:C:4125:LEU:HD12	1.99	0.44
1:D:661:LEU:HD22	1:D:673:TRP:NE1	2.32	0.44
1:D:710:GLY:H	1:D:716:ASN:ND2	2.15	0.44
1:D:1001:GLU:OE2	1:D:1035:TYR:HB3	2.17	0.44
1:D:1196:ASP:OD1	1:D:1196:ASP:N	2.51	0.44
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.90	0.44
1:D:1962:ARG:HH21	1:D:1963:GLU:HA	1.83	0.44
1:A:692:HIS:HB3	1:A:795:SER:HB3	1.98	0.44
1:A:1097:LYS:HA	1:A:1168:MET:HE2	2.00	0.44
1:A:3998:MET:HE3	1:A:3998:MET:HB2	1.94	0.44
1:A:4116:THR:O	1:A:4119:GLU:HG2	2.17	0.44
1:B:661:LEU:HD22	1:B:673:TRP:NE1	2.32	0.44
1:B:710:GLY:H	1:B:716:ASN:HD22	1.64	0.44
1:B:1140:PHE:HD2	1:B:1141:LYS:HD2	1.83	0.44
1:C:1190:LEU:HD11	1:C:1193:LYS:HE3	1.99	0.44
1:D:299:HIS:HD2	1:D:302:THR:HG22	1.82	0.44
1:D:1190:LEU:HD11	1:D:1193:LYS:HE3	1.99	0.44
1:D:3982:LEU:HD21	1:D:4100:LEU:HA	2.00	0.44
1:A:24:CYS:HB3	1:A:212:TRP:CE3	2.52	0.44
1:A:710:GLY:H	1:A:716:ASN:ND2	2.15	0.44
1:A:821:ALA:HB3	1:A:823:TYR:CE1	2.52	0.44
1:A:1586:ARG:NH2	1:A:1635:GLU:OE1	2.50	0.44
1:A:1680:HIS:CE1	2:G:91:VAL:HA	2.53	0.44
1:A:2501:LEU:HD11	1:A:2505:ALA:HB2	1.99	0.44
1:A:3982:LEU:HD21	1:A:4100:LEU:HA	2.00	0.44
1:A:4821:ARG:HG2	1:D:4850:PHE:CD2	2.53	0.44
1:B:626:ARG:NH2	1:B:1669:GLY:O	2.51	0.44
1:B:2091:TYR:CE2	1:B:3639:LEU:HD13	2.52	0.44
1:C:2134:GLY:H	1:C:2137:GLU:HB2	1.82	0.44
1:D:555:LEU:HD11	1:D:585:ALA:HB1	1.98	0.44
1:D:1754:LEU:HD23	1:D:1754:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HD22	1:A:526:TRP:HD1	1.83	0.44
1:A:1819:PHE:O	1:A:1823:ILE:HG12	2.18	0.44
1:A:1976:LEU:HD11	1:A:3619:PHE:CE2	2.53	0.44
1:A:4122:GLU:HA	1:A:4125:LEU:HD12	1.99	0.44
1:B:4023:LYS:HG3	1:B:4087:HIS:CG	2.53	0.44
1:B:4601:ARG:HD2	1:B:4711:VAL:HG21	1.98	0.44
2:H:58:LYS:HA	2:H:61:GLU:HG3	1.99	0.44
1:C:1097:LYS:HA	1:C:1168:MET:HE2	2.00	0.44
1:D:606:ARG:HH22	1:D:1635:GLU:HG2	1.82	0.44
1:D:821:ALA:HB3	1:D:823:TYR:CE1	2.52	0.44
1:D:2154:PHE:CD2	1:D:2205:ILE:HD11	2.52	0.44
1:D:2253:ALA:O	1:D:2315:ASN:ND2	2.40	0.44
1:D:3998:MET:HE3	1:D:3998:MET:HB2	1.94	0.44
1:D:4630:ASP:O	1:D:4634:ILE:HG23	2.18	0.44
1:A:1119:ARG:NH2	1:A:1196:ASP:OD1	2.51	0.44
1:A:1250:TRP:CH2	1:A:1644:GLU:HG3	2.53	0.44
1:A:2463:HIS:O	1:A:2467:MET:HG2	2.18	0.44
1:A:4821:ARG:HD3	1:D:4847:ILE:HA	2.00	0.44
1:B:675:TYR:CE1	1:B:790:PRO:HB3	2.52	0.44
1:B:1001:GLU:OE2	1:B:1035:TYR:HB3	2.17	0.44
1:B:1119:ARG:NH2	1:B:1196:ASP:OD1	2.51	0.44
1:B:1250:TRP:CH2	1:B:1644:GLU:HG3	2.53	0.44
1:B:1296:ASN:OD1	1:B:1296:ASN:N	2.51	0.44
1:B:1754:LEU:HD23	1:B:1754:LEU:HA	1.86	0.44
1:B:2740:TRP:CD1	1:B:2751:LYS:HE3	2.43	0.44
1:B:3923:ILE:HD12	1:B:3984:MET:HG2	1.99	0.44
1:B:4116:THR:O	1:B:4119:GLU:HG2	2.17	0.44
1:C:14:LEU:HD11	1:C:214:VAL:HG21	1.99	0.44
1:C:836:HIS:CG	1:C:841:LYS:HB3	2.53	0.44
1:C:3860:GLN:NE2	1:C:3867:VAL:H	2.15	0.44
1:C:4708:LYS:O	1:C:4712:VAL:HG13	2.18	0.44
1:D:61:ASP:HB3	1:D:64:ILE:HG12	1.99	0.44
1:D:1097:LYS:HA	1:D:1168:MET:HE2	2.00	0.44
1:D:1976:LEU:HD11	1:D:3619:PHE:CE2	2.53	0.44
1:D:3920:THR:HG22	1:D:3980:MET:HA	1.99	0.44
1:A:2320:VAL:O	1:A:2324:ILE:HG12	2.18	0.44
1:A:3727:GLN:C	1:A:3731:HIS:HD1	2.23	0.44
1:A:3923:ILE:HD12	1:A:3984:MET:HG2	1.99	0.44
1:A:4023:LYS:HG3	1:A:4087:HIS:CG	2.53	0.44
1:A:4821:ARG:O	1:D:4824:GLY:HA3	2.16	0.44
1:A:4833:PRO:HD3	1:A:4842:ARG:NE	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:58:LYS:HA	2:G:61:GLU:HG3	1.99	0.44
1:B:1346:LEU:HD23	1:B:1347:MET:O	2.18	0.44
1:B:4929:GLU:HG2	1:B:4930:THR:H	1.82	0.44
1:C:1196:ASP:OD1	1:C:1196:ASP:N	2.51	0.44
1:C:1250:TRP:CH2	1:C:1644:GLU:HG3	2.53	0.44
1:C:3950:PHE:HZ	1:C:3973:LEU:HG	1.83	0.44
1:C:4051:MET:HE3	1:C:4062:THR:HB	2.00	0.44
1:D:943:LEU:HG	1:D:999:LEU:CD1	2.46	0.44
1:D:4023:LYS:HG3	1:D:4087:HIS:CG	2.53	0.44
1:A:884:ARG:O	1:A:887:GLU:HG3	2.18	0.43
1:B:190:ARG:HB2	1:B:205:ALA:HB1	2.00	0.43
1:B:1097:LYS:HA	1:B:1168:MET:HE2	2.00	0.43
1:B:1397:UNK:HA	1:B:1412:UNK:HA	2.00	0.43
1:B:1586:ARG:NH2	1:B:1635:GLU:OE1	2.50	0.43
1:B:1680:HIS:CE1	2:H:91:VAL:HA	2.53	0.43
1:B:3982:LEU:HD21	1:B:4100:LEU:HA	2.00	0.43
1:C:626:ARG:NH2	1:C:1669:GLY:O	2.51	0.43
1:C:884:ARG:O	1:C:887:GLU:HG3	2.18	0.43
1:C:1976:LEU:HD11	1:C:3619:PHE:CE2	2.53	0.43
2:J:58:LYS:HA	2:J:61:GLU:HG3	1.99	0.43
1:A:661:LEU:HD22	1:A:673:TRP:NE1	2.32	0.43
1:A:675:TYR:CE1	1:A:790:PRO:HB3	2.52	0.43
1:A:1962:ARG:HH21	1:A:1963:GLU:HA	1.83	0.43
1:A:2741:ILE:HD12	1:A:2741:ILE:HA	1.72	0.43
1:B:20:VAL:HG22	1:B:21:VAL:N	2.33	0.43
1:B:821:ALA:HB3	1:B:823:TYR:CE1	2.52	0.43
1:B:1165:MET:HE1	1:B:1231:GLY:CA	2.42	0.43
1:B:1731:THR:O	1:B:1734:THR:OG1	2.27	0.43
1:B:1819:PHE:O	1:B:1823:ILE:HG12	2.18	0.43
1:B:2501:LEU:HD11	1:B:2505:ALA:HB2	1.99	0.43
1:C:1119:ARG:NH2	1:C:1196:ASP:OD1	2.51	0.43
1:C:2320:VAL:O	1:C:2324:ILE:HG12	2.18	0.43
1:C:2463:HIS:O	1:C:2467:MET:HG2	2.18	0.43
1:C:2501:LEU:HD11	1:C:2505:ALA:HB2	1.99	0.43
1:C:2740:TRP:CD1	1:C:2751:LYS:HE3	2.43	0.43
1:D:884:ARG:O	1:D:887:GLU:HG3	2.18	0.43
1:D:1140:PHE:HD2	1:D:1141:LYS:HD2	1.83	0.43
1:D:2463:HIS:O	1:D:2467:MET:HG2	2.18	0.43
1:D:4122:GLU:HA	1:D:4125:LEU:HD12	1.99	0.43
1:B:748:LEU:HD13	1:B:748:LEU:HA	1.77	0.43
1:B:1040:ASP:HA	1:B:1043:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3727:GLN:C	1:B:3731:HIS:HD1	2.23	0.43
1:B:3920:THR:HG22	1:B:3980:MET:HA	1.99	0.43
1:C:894:VAL:O	1:C:898:ILE:HG13	2.19	0.43
1:C:4023:LYS:HG3	1:C:4087:HIS:CG	2.53	0.43
1:D:190:ARG:HB2	1:D:205:ALA:HB1	2.00	0.43
1:D:1250:TRP:CH2	1:D:1644:GLU:HG3	2.53	0.43
1:D:1346:LEU:HD23	1:D:1347:MET:O	2.18	0.43
1:D:1712:LEU:HD22	1:D:1832:MET:SD	2.58	0.43
1:A:190:ARG:HD3	1:A:205:ALA:O	2.19	0.43
1:A:654:SER:H	1:A:841:LYS:HZ3	1.64	0.43
1:B:1190:LEU:HD11	1:B:1193:LYS:HE3	1.99	0.43
1:B:2853:LYS:HD3	1:B:2853:LYS:HA	1.68	0.43
1:B:4079:TYR:O	1:B:4083:VAL:HG22	2.17	0.43
1:B:4197:PHE:HB2	1:B:4644:TRP:HZ3	1.83	0.43
1:C:235:ARG:NH1	1:C:412:GLU:OE2	2.51	0.43
1:C:728:ASP:O	1:C:749:LEU:HG	2.19	0.43
1:C:1730:MET:SD	1:C:2106:THR:OG1	2.69	0.43
1:D:1119:ARG:NH2	1:D:1196:ASP:OD1	2.51	0.43
1:D:4108:MET:HE2	1:D:4108:MET:HB3	1.90	0.43
1:A:626:ARG:NH2	1:A:1669:GLY:O	2.51	0.43
1:A:1190:LEU:HD11	1:A:1193:LYS:HE3	2.00	0.43
1:A:1196:ASP:OD1	1:A:1196:ASP:N	2.51	0.43
1:A:1572:PHE:HZ	1:A:1587:LEU:HD11	1.82	0.43
1:A:4079:TYR:O	1:A:4083:VAL:HG22	2.17	0.43
1:B:606:ARG:HH22	1:B:1635:GLU:HG2	1.82	0.43
1:B:687:THR:OG1	1:B:1627:GLN:NE2	2.52	0.43
1:C:62:LEU:HD11	1:C:282:VAL:HG23	2.01	0.43
1:C:1346:LEU:HD23	1:C:1347:MET:O	2.18	0.43
1:C:1819:PHE:O	1:C:1823:ILE:HG12	2.18	0.43
1:D:505:LEU:HD22	1:D:526:TRP:HD1	1.83	0.43
1:D:562:LEU:HD21	1:D:600:LEU:HD22	2.00	0.43
1:D:2321:ARG:O	1:D:2325:ARG:HG2	2.18	0.43
1:A:34:LYS:HB3	1:A:34:LYS:HE3	1.92	0.43
1:A:1712:LEU:HD22	1:A:1832:MET:SD	2.58	0.43
1:A:4197:PHE:HB2	1:A:4644:TRP:HZ3	1.83	0.43
1:B:190:ARG:HD3	1:B:205:ALA:O	2.19	0.43
1:B:775:VAL:HG23	1:B:777:GLY:H	1.82	0.43
1:C:2741:ILE:HD12	1:C:2741:ILE:HA	1.72	0.43
1:C:3982:LEU:HD21	1:C:4100:LEU:HA	2.00	0.43
1:C:4197:PHE:HB2	1:C:4644:TRP:HZ3	1.83	0.43
1:C:4630:ASP:O	1:C:4634:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ARG:HH21	1:D:202:HIS:CD2	2.37	0.43
1:D:1040:ASP:HA	1:D:1043:LYS:HD2	2.01	0.43
1:D:2320:VAL:O	1:D:2324:ILE:HG12	2.18	0.43
1:D:2853:LYS:HA	1:D:2853:LYS:HD3	1.68	0.43
1:D:4051:MET:HE3	1:D:4062:THR:HB	2.00	0.43
1:A:331:PHE:HE1	1:A:363:ILE:HG22	1.84	0.43
1:A:934:GLN:OE1	1:A:935:MET:N	2.52	0.43
1:A:939:THR:O	1:A:999:LEU:HD11	2.19	0.43
1:A:3876:TYR:HD1	1:A:3879:ARG:HH21	1.66	0.43
1:B:137:ARG:HH21	1:B:202:HIS:CD2	2.37	0.43
1:B:505:LEU:HD22	1:B:526:TRP:HD1	1.83	0.43
1:B:894:VAL:O	1:B:898:ILE:HG13	2.19	0.43
1:B:934:GLN:OE1	1:B:935:MET:N	2.52	0.43
1:B:2253:ALA:O	1:B:2315:ASN:ND2	2.40	0.43
1:B:3950:PHE:HZ	1:B:3973:LEU:HG	1.83	0.43
1:C:20:VAL:HG22	1:C:21:VAL:N	2.33	0.43
1:C:190:ARG:HD3	1:C:205:ALA:O	2.19	0.43
1:C:224:ALA:HB3	1:C:227:TYR:HD2	1.84	0.43
1:C:297:LEU:HD13	1:C:297:LEU:HA	1.81	0.43
1:C:669:GLN:HB3	1:C:673:TRP:HZ2	1.83	0.43
1:C:687:THR:OG1	1:C:1627:GLN:NE2	2.52	0.43
1:C:1140:PHE:HD2	1:C:1141:LYS:HD2	1.83	0.43
1:C:3763:ALA:HA	1:C:3766:ASN:ND2	2.34	0.43
1:C:3961:SER:OG	1:C:3962:SER:N	2.52	0.43
1:D:687:THR:OG1	1:D:1627:GLN:NE2	2.52	0.43
1:D:1311:ALA:HA	1:D:1312:UNK:HA	1.50	0.43
1:D:1397:UNK:HA	1:D:1412:UNK:HA	2.00	0.43
1:D:2428:LEU:HD21	1:D:2482:PHE:CE1	2.54	0.43
1:D:3955:MET:HE2	1:D:3955:MET:HB3	1.90	0.43
1:D:4708:LYS:O	1:D:4712:VAL:HG13	2.18	0.43
1:A:137:ARG:HH21	1:A:202:HIS:CD2	2.37	0.43
1:A:235:ARG:NH1	1:A:412:GLU:OE2	2.51	0.43
1:A:669:GLN:HB3	1:A:673:TRP:HZ2	1.83	0.43
1:A:775:VAL:HG23	1:A:777:GLY:H	1.82	0.43
1:A:1826:PHE:CE1	1:A:1843:ILE:HG21	2.54	0.43
1:A:3950:PHE:HZ	1:A:3973:LEU:HG	1.83	0.43
1:A:3961:SER:OG	1:A:3962:SER:N	2.52	0.43
1:B:19:GLU:HB2	1:B:217:ILE:HB	2.01	0.43
1:B:235:ARG:NH1	1:B:412:GLU:OE2	2.51	0.43
1:B:1712:LEU:HD22	1:B:1832:MET:SD	2.58	0.43
1:B:3763:ALA:HA	1:B:3766:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:HH21	1:C:202:HIS:CD2	2.37	0.43
1:C:191:TYR:OH	1:D:2325:ARG:NH1	2.51	0.43
1:C:606:ARG:HH22	1:C:1635:GLU:HG2	1.82	0.43
1:C:1712:LEU:HD22	1:C:1832:MET:SD	2.58	0.43
1:D:331:PHE:HE1	1:D:363:ILE:HG22	1.84	0.43
1:D:728:ASP:O	1:D:749:LEU:HG	2.19	0.43
1:D:1684:PRO:HD3	2:J:42:ASP:HB3	2.00	0.43
1:D:1819:PHE:O	1:D:1823:ILE:HG12	2.18	0.43
1:D:2777:SER:OG	1:D:2843:MET:SD	2.68	0.43
1:D:3961:SER:OG	1:D:3962:SER:N	2.52	0.43
1:D:4841:TYR:O	1:D:4844:ILE:HG22	2.19	0.43
2:J:29:GLY:N	2:J:38:ASP:O	2.48	0.43
1:A:20:VAL:HG22	1:A:21:VAL:N	2.33	0.43
1:A:728:ASP:O	1:A:749:LEU:HG	2.19	0.43
1:A:1909:LEU:HD13	1:A:2061:ILE:HG12	2.01	0.43
1:A:4630:ASP:O	1:A:4634:ILE:HG23	2.18	0.43
1:A:4708:LYS:O	1:A:4712:VAL:HG13	2.18	0.43
1:B:669:GLN:HB3	1:B:673:TRP:HZ2	1.83	0.43
1:B:1196:ASP:OD1	1:B:1196:ASP:N	2.51	0.43
1:B:1572:PHE:HZ	1:B:1587:LEU:HD11	1.82	0.43
1:B:2428:LEU:HD21	1:B:2482:PHE:CE1	2.53	0.43
1:C:750:ARG:NH2	2:I:9:SER:OG	2.47	0.43
2:I:79:PRO:HB3	2:I:95:ASN:HA	2.01	0.43
2:I:93:PRO:HG2	2:I:96:ALA:HB2	2.01	0.43
1:D:14:LEU:HD11	1:D:214:VAL:HG21	1.99	0.43
1:D:62:LEU:HD11	1:D:282:VAL:HG23	2.01	0.43
1:D:1826:PHE:CE1	1:D:1843:ILE:HG21	2.54	0.43
1:D:1901:VAL:O	1:D:1905:MET:HG2	2.19	0.43
2:J:93:PRO:HG2	2:J:96:ALA:HB2	2.01	0.43
1:A:674:TYR:HE1	1:A:756:SER:HB2	1.83	0.43
1:A:1397:UNK:HA	1:A:1412:UNK:HA	2.00	0.43
1:A:1841:LYS:O	1:A:1845:GLN:HG2	2.19	0.43
2:G:83:TYR:HB3	2:G:87:GLY:HA2	2.01	0.43
1:B:62:LEU:HD11	1:B:282:VAL:HG23	2.01	0.43
1:B:167:LYS:HE2	1:B:167:LYS:HB2	1.48	0.43
1:B:562:LEU:HD21	1:B:600:LEU:HD22	2.00	0.43
1:B:654:SER:H	1:B:841:LYS:HZ1	1.64	0.43
1:B:884:ARG:O	1:B:887:GLU:HG3	2.18	0.43
1:B:1909:LEU:HD13	1:B:2061:ILE:HG12	2.01	0.43
1:B:1976:LEU:HD11	1:B:3619:PHE:CE2	2.53	0.43
1:C:190:ARG:HB2	1:C:205:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:LEU:HD13	1:C:589:ILE:HD11	2.01	0.43
1:C:686:VAL:HG13	1:C:687:THR:N	2.34	0.43
1:C:894:VAL:HG21	1:C:976:TYR:HE2	1.83	0.43
1:D:555:LEU:HD13	1:D:589:ILE:HD11	2.01	0.43
2:J:79:PRO:HB3	2:J:95:ASN:HA	2.00	0.43
1:A:19:GLU:HG2	1:A:68:VAL:HG22	2.01	0.42
1:A:224:ALA:HB3	1:A:227:TYR:HD2	1.84	0.42
1:A:363:ILE:HG12	1:A:372:LEU:HD22	2.01	0.42
1:A:562:LEU:HD21	1:A:600:LEU:HD22	2.00	0.42
1:A:2065:MET:SD	1:A:2083:MET:HG3	2.59	0.42
1:A:2171:MET:O	1:A:2175:VAL:HG13	2.19	0.42
1:A:2224:SER:OG	1:A:2239:LEU:HB2	2.19	0.42
2:G:79:PRO:HB3	2:G:95:ASN:HA	2.01	0.42
1:B:1901:VAL:O	1:B:1905:MET:HG2	2.19	0.42
1:B:2065:MET:SD	1:B:2083:MET:HG3	2.59	0.42
1:B:2113:GLU:OE1	1:B:2113:GLU:N	2.37	0.42
1:B:2320:VAL:O	1:B:2324:ILE:HG12	2.18	0.42
1:B:2463:HIS:O	1:B:2467:MET:HG2	2.18	0.42
1:B:4841:TYR:O	1:B:4844:ILE:HG22	2.19	0.42
2:H:93:PRO:HG2	2:H:96:ALA:HB2	2.01	0.42
1:C:748:LEU:HD13	1:C:748:LEU:HA	1.77	0.42
1:C:939:THR:O	1:C:999:LEU:HD11	2.19	0.42
1:C:1397:UNK:HA	1:C:1412:UNK:HA	2.00	0.42
1:C:1704:TYR:CG	1:C:1821:PRO:HB2	2.54	0.42
1:C:2321:ARG:O	1:C:2325:ARG:HG2	2.18	0.42
1:C:3728:ALA:HA	1:C:3731:HIS:ND1	2.34	0.42
1:D:20:VAL:HG22	1:D:21:VAL:N	2.33	0.42
1:D:894:VAL:HG21	1:D:976:TYR:HE2	1.83	0.42
1:D:939:THR:O	1:D:999:LEU:HD11	2.19	0.42
1:A:190:ARG:HB2	1:A:205:ALA:HB1	2.00	0.42
1:A:2223:ASN:O	1:A:2226:VAL:HG22	2.19	0.42
2:G:27:TYR:O	2:G:40:SER:N	2.53	0.42
2:G:93:PRO:HG2	2:G:96:ALA:HB2	2.01	0.42
1:B:331:PHE:HE1	1:B:363:ILE:HG22	1.84	0.42
1:B:555:LEU:HD13	1:B:589:ILE:HD11	2.01	0.42
1:B:686:VAL:HG13	1:B:687:THR:N	2.34	0.42
1:B:2102:PRO:HD3	1:B:3624:GLU:HG3	2.01	0.42
1:B:3804:LEU:HD21	1:B:3890:TYR:HB2	2.01	0.42
2:H:79:PRO:HB3	2:H:95:ASN:HA	2.00	0.42
1:C:562:LEU:HD21	1:C:600:LEU:HD22	2.00	0.42
1:C:1909:LEU:HD13	1:C:2061:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4108:MET:HE2	1:C:4108:MET:HB3	1.90	0.42
1:D:19:GLU:HB2	1:D:217:ILE:HB	2.01	0.42
1:D:363:ILE:HG12	1:D:372:LEU:HD22	2.01	0.42
1:D:2223:ASN:O	1:D:2226:VAL:HG22	2.19	0.42
1:D:2741:ILE:HD12	1:D:2741:ILE:HA	1.72	0.42
1:D:3727:GLN:O	1:D:3731:HIS:ND1	2.41	0.42
1:D:4197:PHE:HB2	1:D:4644:TRP:HZ3	1.83	0.42
1:A:514:PHE:HD2	1:A:523:GLY:HA2	1.84	0.42
1:B:224:ALA:HB3	1:B:227:TYR:HD2	1.84	0.42
1:B:728:ASP:O	1:B:749:LEU:HG	2.19	0.42
1:B:754:VAL:HG21	1:B:812:LYS:HD3	2.01	0.42
1:B:1704:TYR:CG	1:B:1821:PRO:HB2	2.54	0.42
1:B:1826:PHE:CE1	1:B:1843:ILE:HG21	2.54	0.42
1:B:2224:SER:OG	1:B:2239:LEU:HB2	2.19	0.42
1:B:4708:LYS:O	1:B:4712:VAL:HG13	2.18	0.42
1:B:4798:GLY:HA3	1:B:4799:ASP:HA	1.85	0.42
1:C:1353:HIS:CE1	1:C:1367:LYS:HD2	2.55	0.42
1:D:224:ALA:HB3	1:D:227:TYR:HD2	1.84	0.42
1:D:489:PHE:HD2	1:D:494:MET:HG2	1.84	0.42
1:D:882:ARG:NH2	1:D:944:LEU:HD21	2.35	0.42
1:D:3860:GLN:NE2	1:D:3867:VAL:H	2.15	0.42
1:A:489:PHE:HD2	1:A:494:MET:HG2	1.84	0.42
1:A:894:VAL:O	1:A:898:ILE:HG13	2.19	0.42
1:A:894:VAL:HG21	1:A:976:TYR:HE2	1.83	0.42
1:A:1353:HIS:CE1	1:A:1367:LYS:HD2	2.55	0.42
1:A:2321:ARG:O	1:A:2325:ARG:HG2	2.18	0.42
1:A:3728:ALA:HA	1:A:3731:HIS:ND1	2.34	0.42
1:A:3804:LEU:HD21	1:A:3890:TYR:HB2	2.02	0.42
1:B:836:HIS:NE2	1:B:842:GLN:OE1	2.46	0.42
1:B:2171:MET:O	1:B:2175:VAL:HG13	2.19	0.42
2:H:83:TYR:HB3	2:H:87:GLY:HA2	2.01	0.42
1:C:836:HIS:NE2	1:C:842:GLN:OE1	2.46	0.42
1:C:1841:LYS:O	1:C:1845:GLN:HG2	2.19	0.42
1:C:2243:ALA:O	1:C:2247:MET:HB2	2.19	0.42
1:C:4841:TYR:O	1:C:4844:ILE:HG22	2.19	0.42
1:D:894:VAL:O	1:D:898:ILE:HG13	2.19	0.42
1:D:1170:GLU:N	1:D:1170:GLU:CD	2.77	0.42
1:D:2102:PRO:HD3	1:D:3624:GLU:HG3	2.01	0.42
1:A:156:GLU:H	1:A:156:GLU:CD	2.28	0.42
1:A:687:THR:OG1	1:A:1627:GLN:NE2	2.52	0.42
1:A:982:ASP:OD1	1:A:982:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:TYR:HD1	1:A:1060:TYR:N	2.08	0.42
1:A:1346:LEU:HD23	1:A:1347:MET:O	2.18	0.42
1:A:2279:LEU:HB3	1:A:2284:TYR:HB2	2.01	0.42
1:A:2428:LEU:HD21	1:A:2482:PHE:CE1	2.54	0.42
1:A:2507:SER:O	1:A:2507:SER:OG	2.34	0.42
1:B:489:PHE:HD2	1:B:494:MET:HG2	1.84	0.42
1:B:2000:GLU:O	1:B:2004:THR:HG23	2.20	0.42
1:B:2321:ARG:O	1:B:2325:ARG:HG2	2.18	0.42
2:H:26:HIS:CE1	2:H:41:ARG:HG2	2.55	0.42
1:C:495:ILE:O	1:C:499:LEU:HG	2.20	0.42
1:C:674:TYR:HE1	1:C:756:SER:HB2	1.83	0.42
1:C:882:ARG:NH2	1:C:944:LEU:HD21	2.35	0.42
1:C:2238:PRO:O	1:C:2241:VAL:HG12	2.20	0.42
1:C:3727:GLN:O	1:C:3731:HIS:ND1	2.41	0.42
1:C:3804:LEU:HD21	1:C:3890:TYR:HB2	2.02	0.42
2:I:26:HIS:CE1	2:I:41:ARG:HG2	2.54	0.42
1:D:190:ARG:HD3	1:D:205:ALA:O	2.19	0.42
1:D:235:ARG:NH1	1:D:412:GLU:OE2	2.51	0.42
1:D:669:GLN:HB3	1:D:673:TRP:HZ2	1.83	0.42
1:D:674:TYR:HE1	1:D:756:SER:HB2	1.83	0.42
1:D:754:VAL:HG21	1:D:812:LYS:HD3	2.01	0.42
1:D:1704:TYR:CG	1:D:1821:PRO:HB2	2.54	0.42
1:D:2238:PRO:O	1:D:2241:VAL:HG12	2.20	0.42
1:D:3763:ALA:HA	1:D:3766:ASN:ND2	2.34	0.42
1:D:3804:LEU:HD21	1:D:3890:TYR:HB2	2.02	0.42
1:D:3950:PHE:HZ	1:D:3973:LEU:HG	1.83	0.42
1:A:1040:ASP:HA	1:A:1043:LYS:HD2	2.01	0.42
1:A:1270:VAL:HG21	1:A:1589:VAL:HG21	2.02	0.42
1:A:2900:TYR:HD1	1:A:2900:TYR:HA	1.74	0.42
1:A:4051:MET:HE3	1:A:4062:THR:HB	2.00	0.42
2:G:29:GLY:N	2:G:38:ASP:O	2.48	0.42
1:B:156:GLU:H	1:B:156:GLU:CD	2.28	0.42
1:B:514:PHE:HD2	1:B:523:GLY:HA2	1.84	0.42
1:B:939:THR:O	1:B:999:LEU:HD11	2.19	0.42
1:B:982:ASP:OD1	1:B:982:ASP:C	2.63	0.42
1:B:1270:VAL:HG21	1:B:1589:VAL:HG21	2.02	0.42
1:B:1353:HIS:CE1	1:B:1367:LYS:HD2	2.55	0.42
1:B:4058:THR:HG22	1:B:4061:GLU:HG3	2.02	0.42
2:H:27:TYR:O	2:H:40:SER:N	2.53	0.42
1:C:19:GLU:HG2	1:C:68:VAL:HG22	2.01	0.42
1:C:331:PHE:HE1	1:C:363:ILE:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ILE:HG12	1:C:372:LEU:HD22	2.02	0.42
1:C:934:GLN:OE1	1:C:935:MET:N	2.52	0.42
1:C:1040:ASP:HA	1:C:1043:LYS:HD2	2.01	0.42
1:C:1682:ASP:HB2	1:C:1685:GLN:CB	2.49	0.42
1:C:3876:TYR:HD1	1:C:3879:ARG:HH21	1.66	0.42
1:D:19:GLU:HG2	1:D:68:VAL:HG22	2.01	0.42
1:D:1128:LEU:HG	1:D:1136:ALA:HB2	2.02	0.42
1:D:2065:MET:SD	1:D:2083:MET:HG3	2.59	0.42
1:A:2243:ALA:O	1:A:2247:MET:HB2	2.19	0.42
1:A:2290:ASN:ND2	1:A:2293:GLU:OE1	2.53	0.42
1:A:2776:GLU:O	1:A:2780:THR:HG23	2.20	0.42
1:B:363:ILE:HG12	1:B:372:LEU:HD22	2.01	0.42
1:B:882:ARG:NH2	1:B:944:LEU:HD21	2.35	0.42
1:B:1841:LYS:O	1:B:1845:GLN:HG2	2.19	0.42
1:B:2325:ARG:HA	1:B:2325:ARG:HD3	1.82	0.42
1:B:3961:SER:OG	1:B:3962:SER:N	2.52	0.42
1:C:505:LEU:HD22	1:C:526:TRP:HD1	1.83	0.42
1:C:2144:GLY:O	1:C:2148:ILE:HG12	2.20	0.42
1:C:4058:THR:HG22	1:C:4061:GLU:HG3	2.02	0.42
1:D:296:ARG:HH21	1:D:324:VAL:HB	1.85	0.42
1:D:495:ILE:O	1:D:499:LEU:HG	2.20	0.42
1:D:1841:LYS:O	1:D:1845:GLN:HG2	2.19	0.42
1:D:3728:ALA:HA	1:D:3731:HIS:ND1	2.34	0.42
2:J:26:HIS:CE1	2:J:41:ARG:HG2	2.54	0.42
2:J:27:TYR:O	2:J:40:SER:N	2.53	0.42
1:A:1901:VAL:O	1:A:1905:MET:HG2	2.19	0.42
1:B:152:ASP:OD1	1:B:152:ASP:N	2.52	0.42
1:B:439:LYS:HE2	1:B:439:LYS:HB3	1.59	0.42
1:B:674:TYR:HE1	1:B:756:SER:HB2	1.83	0.42
1:B:2238:PRO:O	1:B:2241:VAL:HG12	2.20	0.42
1:B:3728:ALA:HA	1:B:3731:HIS:ND1	2.35	0.42
1:B:4051:MET:HE3	1:B:4062:THR:HB	2.00	0.42
1:C:514:PHE:HD2	1:C:523:GLY:HA2	1.84	0.42
1:C:2065:MET:SD	1:C:2083:MET:HG3	2.59	0.42
1:C:2223:ASN:O	1:C:2226:VAL:HG22	2.19	0.42
1:C:2224:SER:OG	1:C:2239:LEU:HB2	2.20	0.42
1:C:2253:ALA:O	1:C:2315:ASN:ND2	2.40	0.42
2:I:83:TYR:HB3	2:I:87:GLY:HA2	2.01	0.42
1:D:387:ILE:O	1:D:388:GLN:NE2	2.53	0.42
1:D:946:LEU:H	1:D:946:LEU:HG	1.56	0.42
1:D:1909:LEU:HD13	1:D:2061:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2144:GLY:O	1:D:2148:ILE:HG12	2.20	0.42
1:A:62:LEU:HD11	1:A:282:VAL:HG23	2.01	0.42
1:A:296:ARG:HH21	1:A:324:VAL:HB	1.85	0.42
1:A:2102:PRO:HD3	1:A:3624:GLU:HG3	2.01	0.42
1:A:4841:TYR:O	1:A:4844:ILE:HG22	2.19	0.42
1:B:296:ARG:HH21	1:B:324:VAL:HB	1.85	0.42
1:B:1643:LEU:HD22	1:B:1694:TYR:O	2.20	0.42
1:B:2223:ASN:O	1:B:2226:VAL:HG22	2.19	0.42
1:C:845:THR:HG23	1:C:847:THR:H	1.85	0.42
1:C:926:GLU:H	1:C:926:GLU:HG2	1.54	0.42
1:C:1270:VAL:HG21	1:C:1589:VAL:HG21	2.02	0.42
1:C:1363:LYS:HE2	1:C:1365:THR:HG22	2.01	0.42
1:C:2428:LEU:HD21	1:C:2482:PHE:CE1	2.54	0.42
1:C:4044:LYS:NZ	1:C:4069:ALA:HB1	2.35	0.42
1:D:2325:ARG:HA	1:D:2325:ARG:HD3	1.82	0.42
1:D:4058:THR:HG22	1:D:4061:GLU:HG3	2.02	0.42
1:D:4833:PRO:HD3	1:D:4842:ARG:NE	2.25	0.42
1:A:555:LEU:HD13	1:A:589:ILE:HD11	2.01	0.42
1:A:1643:LEU:HD22	1:A:1694:TYR:O	2.20	0.42
1:A:4633:VAL:HG11	1:A:4707:TRP:HB2	2.02	0.42
2:G:26:HIS:CE1	2:G:41:ARG:HG2	2.55	0.42
1:B:1128:LEU:HG	1:B:1136:ALA:HB2	2.02	0.42
1:B:2290:ASN:ND2	1:B:2293:GLU:OE1	2.53	0.42
1:B:2507:SER:O	1:B:2507:SER:OG	2.35	0.42
1:C:19:GLU:HB2	1:C:217:ILE:HB	2.01	0.42
1:C:1395:UNK:HA	1:C:1415:UNK:HA	2.02	0.42
1:C:2000:GLU:O	1:C:2004:THR:HG23	2.20	0.42
1:C:2279:LEU:HB3	1:C:2284:TYR:HB2	2.01	0.42
1:C:4701:ASP:OD1	1:C:4701:ASP:N	2.45	0.42
1:D:574:VAL:HA	1:D:577:CYS:SG	2.60	0.42
1:D:934:GLN:OE1	1:D:935:MET:N	2.52	0.42
1:D:1353:HIS:CE1	1:D:1367:LYS:HD2	2.55	0.42
1:D:1363:LYS:HE2	1:D:1365:THR:HG22	2.01	0.42
1:D:1832:MET:HE3	1:D:1832:MET:HB2	1.97	0.42
1:D:2243:ALA:O	1:D:2247:MET:HB2	2.19	0.42
1:D:2290:ASN:ND2	1:D:2293:GLU:OE1	2.53	0.42
1:D:4633:VAL:HG11	1:D:4707:TRP:HB2	2.02	0.42
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.93	0.41
1:A:574:VAL:HA	1:A:577:CYS:SG	2.60	0.41
1:A:2238:PRO:O	1:A:2241:VAL:HG12	2.20	0.41
1:A:3763:ALA:HA	1:A:3766:ASN:ND2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLU:HG2	1:B:68:VAL:HG22	2.01	0.41
1:B:113:LEU:HD23	1:B:175:VAL:HG21	2.01	0.41
1:B:1686:LEU:HD11	1:B:1710:ILE:HD11	2.02	0.41
1:B:2144:GLY:O	1:B:2148:ILE:HG12	2.20	0.41
1:C:156:GLU:H	1:C:156:GLU:CD	2.28	0.41
1:C:489:PHE:HD2	1:C:494:MET:HG2	1.84	0.41
1:C:1138:ASP:OD1	1:C:1139:GLY:N	2.53	0.41
1:C:1686:LEU:HD11	1:C:1710:ILE:HD11	2.02	0.41
1:C:2102:PRO:HD3	1:C:3624:GLU:HG3	2.01	0.41
1:C:2290:ASN:ND2	1:C:2293:GLU:OE1	2.53	0.41
1:D:514:PHE:HD2	1:D:523:GLY:HA2	1.84	0.41
1:D:1092:LYS:HE3	1:D:1092:LYS:HB2	1.93	0.41
1:D:2171:MET:O	1:D:2175:VAL:HG13	2.19	0.41
2:J:83:TYR:HB3	2:J:87:GLY:HA2	2.01	0.41
1:A:19:GLU:HB2	1:A:217:ILE:HB	2.01	0.41
1:A:686:VAL:HG13	1:A:687:THR:N	2.34	0.41
1:A:822:CYS:HA	1:A:825:ALA:HB3	2.03	0.41
1:A:946:LEU:H	1:A:946:LEU:HG	1.56	0.41
1:A:1031:ARG:HA	1:A:1031:ARG:HD3	1.88	0.41
1:A:1138:ASP:OD1	1:A:1139:GLY:N	2.53	0.41
1:A:1704:TYR:CG	1:A:1821:PRO:HB2	2.54	0.41
1:B:894:VAL:HG21	1:B:976:TYR:HE2	1.83	0.41
1:B:1395:UNK:HA	1:B:1415:UNK:HA	2.02	0.41
1:B:2776:GLU:O	1:B:2780:THR:HG23	2.20	0.41
1:C:1901:VAL:O	1:C:1905:MET:HG2	2.19	0.41
1:C:2423:ARG:HH21	1:C:2475:TYR:HA	1.85	0.41
1:D:686:VAL:HG13	1:D:687:THR:N	2.34	0.41
1:D:1138:ASP:OD1	1:D:1139:GLY:N	2.53	0.41
1:D:4044:LYS:NZ	1:D:4069:ALA:HB1	2.35	0.41
1:A:18:ASP:N	1:A:18:ASP:OD1	2.54	0.41
1:A:227:TYR:CD1	1:A:352:SER:HB3	2.56	0.41
1:A:2405:MET:H	1:A:2405:MET:HG3	1.48	0.41
1:B:495:ILE:O	1:B:499:LEU:HG	2.20	0.41
1:B:1031:ARG:HA	1:B:1031:ARG:HD3	1.88	0.41
1:B:1363:LYS:HE2	1:B:1365:THR:HG22	2.01	0.41
1:B:2243:ALA:O	1:B:2247:MET:HB2	2.19	0.41
1:B:3812:LYS:HE2	1:B:3812:LYS:HB3	1.83	0.41
1:C:281:ARG:NH1	1:C:346:VAL:O	2.38	0.41
1:C:1826:PHE:CE1	1:C:1843:ILE:HG21	2.54	0.41
1:D:747:HIS:CD2	1:D:750:ARG:HG2	2.55	0.41
1:D:982:ASP:OD1	1:D:982:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1270:VAL:HG21	1:D:1589:VAL:HG21	2.02	0.41
1:D:1680:HIS:CE1	2:J:91:VAL:HA	2.55	0.41
1:D:2000:GLU:O	1:D:2004:THR:HG23	2.20	0.41
1:D:2224:SER:OG	1:D:2239:LEU:HB2	2.19	0.41
1:D:2279:LEU:HB3	1:D:2284:TYR:HB2	2.01	0.41
1:A:113:LEU:HD23	1:A:175:VAL:HG21	2.01	0.41
1:A:747:HIS:CD2	1:A:750:ARG:HG2	2.55	0.41
1:A:1128:LEU:HG	1:A:1136:ALA:HB2	2.02	0.41
1:A:2000:GLU:O	1:A:2004:THR:HG23	2.20	0.41
1:B:18:ASP:N	1:B:18:ASP:OD1	2.54	0.41
1:B:227:TYR:CD1	1:B:352:SER:HB3	2.56	0.41
1:B:4633:VAL:HG11	1:B:4707:TRP:HB2	2.02	0.41
1:C:189:GLU:OE2	1:D:2321:ARG:NH1	2.53	0.41
1:C:754:VAL:HG21	1:C:812:LYS:HD3	2.01	0.41
1:C:822:CYS:HA	1:C:825:ALA:HB3	2.03	0.41
1:C:2171:MET:O	1:C:2175:VAL:HG13	2.19	0.41
1:C:2776:GLU:O	1:C:2780:THR:HG23	2.20	0.41
1:C:3955:MET:HE2	1:C:3955:MET:HB3	1.90	0.41
1:D:18:ASP:OD1	1:D:18:ASP:N	2.54	0.41
1:D:200:SER:O	1:D:200:SER:OG	2.36	0.41
1:D:1642:ILE:HG23	1:D:1643:LEU:HD23	2.02	0.41
1:A:387:ILE:O	1:A:388:GLN:NE2	2.53	0.41
1:A:1157:GLN:N	1:A:1160:ASP:OD2	2.41	0.41
1:A:1274:ASP:HB3	1:A:1286:THR:HA	2.03	0.41
1:A:1395:UNK:HA	1:A:1415:UNK:HA	2.02	0.41
1:A:4044:LYS:NZ	1:A:4069:ALA:HB1	2.35	0.41
1:B:200:SER:O	1:B:200:SER:OG	2.36	0.41
1:B:2159:ASN:HD22	1:B:2162:ARG:NH2	2.19	0.41
1:B:3731:HIS:CD2	1:B:3772:VAL:HG22	2.55	0.41
1:B:3955:MET:HE2	1:B:3955:MET:HB3	1.90	0.41
1:C:982:ASP:OD1	1:C:982:ASP:C	2.62	0.41
1:C:3731:HIS:CD2	1:C:3772:VAL:HG22	2.55	0.41
1:C:4759:VAL:HG23	1:C:4865:ILE:HD13	2.03	0.41
1:D:1035:TYR:O	1:D:1043:LYS:HE2	2.21	0.41
1:D:1395:UNK:HA	1:D:1415:UNK:HA	2.02	0.41
1:A:672:LYS:NZ	1:A:760:ASP:OD2	2.39	0.41
1:A:1092:LYS:HE3	1:A:1092:LYS:HB2	1.93	0.41
1:A:1363:LYS:HE2	1:A:1365:THR:HG22	2.01	0.41
1:A:1609:VAL:HG12	1:A:1620:VAL:HG23	2.03	0.41
1:A:1752:ILE:HA	1:A:1837:ASN:ND2	2.36	0.41
1:A:1967:PRO:HD2	1:A:1970:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2159:ASN:HD22	1:A:2162:ARG:NH2	2.19	0.41
1:A:2739:GLY:O	1:A:2751:LYS:HE2	2.21	0.41
1:A:3940:TRP:HA	1:A:3943:VAL:HG12	2.02	0.41
1:A:4798:GLY:HA3	1:A:4799:ASP:HA	1.85	0.41
1:B:237:LEU:HD23	1:B:404:ASN:O	2.21	0.41
1:B:387:ILE:O	1:B:388:GLN:NE2	2.53	0.41
1:B:1752:ILE:HA	1:B:1837:ASN:ND2	2.36	0.41
1:B:2423:ARG:HH21	1:B:2475:TYR:HA	1.85	0.41
1:B:4044:LYS:NZ	1:B:4069:ALA:HB1	2.35	0.41
1:B:4759:VAL:HG23	1:B:4865:ILE:HD13	2.03	0.41
1:C:237:LEU:HD23	1:C:404:ASN:O	2.21	0.41
1:C:1060:TYR:HD1	1:C:1060:TYR:N	2.08	0.41
1:C:3802:LEU:HB2	1:C:3883:SER:HB2	2.03	0.41
1:D:297:LEU:HD13	1:D:297:LEU:HA	1.81	0.41
1:D:433:LEU:HD12	1:D:433:LEU:HA	1.93	0.41
1:A:237:LEU:HD23	1:A:404:ASN:O	2.21	0.41
1:B:1274:ASP:HB3	1:B:1286:THR:HA	2.03	0.41
1:B:1642:ILE:HG23	1:B:1643:LEU:HD23	2.02	0.41
1:B:3761:GLY:O	1:B:3764:ILE:HG22	2.21	0.41
1:C:296:ARG:HH21	1:C:324:VAL:HB	1.85	0.41
1:C:747:HIS:CD2	1:C:750:ARG:HG2	2.55	0.41
1:C:747:HIS:HD2	1:C:750:ARG:HG2	1.85	0.41
1:C:1967:PRO:HD2	1:C:1970:GLU:OE2	2.21	0.41
1:C:3940:TRP:HA	1:C:3943:VAL:HG12	2.02	0.41
1:C:4633:VAL:HG11	1:C:4707:TRP:HB2	2.02	0.41
1:C:4663:ASP:OD1	1:C:4663:ASP:N	2.54	0.41
1:C:4857:LEU:O	1:C:4861:ILE:HG13	2.21	0.41
2:I:12:ASP:C	2:I:12:ASP:OD1	2.64	0.41
1:D:822:CYS:HA	1:D:825:ALA:HB3	2.03	0.41
1:D:1967:PRO:HD2	1:D:1970:GLU:OE2	2.21	0.41
1:D:2739:GLY:O	1:D:2751:LYS:HE2	2.21	0.41
1:D:2776:GLU:O	1:D:2780:THR:HG23	2.20	0.41
1:D:3731:HIS:CD2	1:D:3772:VAL:HG22	2.55	0.41
1:D:4098:ALA:HB1	1:D:4125:LEU:HD23	2.03	0.41
1:D:4759:VAL:HG23	1:D:4865:ILE:HD13	2.03	0.41
1:A:281:ARG:NH1	1:A:346:VAL:O	2.38	0.41
1:A:495:ILE:O	1:A:499:LEU:HG	2.20	0.41
1:A:992:GLN:HA	1:A:995:MET:SD	2.61	0.41
1:A:1209:VAL:O	1:A:1211:GLN:NE2	2.54	0.41
1:A:4496:ASN:HD22	1:A:4499:ASN:HD22	1.69	0.41
1:A:4651:LYS:HB2	1:A:4651:LYS:HE3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4759:VAL:HG23	1:A:4865:ILE:HD13	2.03	0.41
1:B:459:LEU:HD12	1:B:459:LEU:HA	1.95	0.41
1:B:747:HIS:HD2	1:B:750:ARG:HG2	1.85	0.41
1:B:1138:ASP:OD1	1:B:1139:GLY:N	2.53	0.41
1:B:4098:ALA:HB1	1:B:4125:LEU:HD23	2.03	0.41
2:H:12:ASP:OD1	2:H:12:ASP:C	2.64	0.41
1:C:387:ILE:O	1:C:388:GLN:NE2	2.53	0.41
1:C:1035:TYR:O	1:C:1043:LYS:HE2	2.21	0.41
1:C:1610:SER:C	1:C:1612:ILE:H	2.29	0.41
1:C:1643:LEU:HD22	1:C:1694:TYR:O	2.20	0.41
1:C:1752:ILE:HA	1:C:1837:ASN:ND2	2.36	0.41
1:C:1754:LEU:HD23	1:C:1754:LEU:HA	1.86	0.41
1:C:4601:ARG:HD3	1:C:4707:TRP:HZ2	1.86	0.41
1:D:113:LEU:HD23	1:D:175:VAL:HG21	2.01	0.41
1:D:156:GLU:H	1:D:156:GLU:CD	2.28	0.41
1:D:992:GLN:HA	1:D:995:MET:SD	2.61	0.41
1:A:747:HIS:HD2	1:A:750:ARG:HG2	1.85	0.41
1:A:754:VAL:HG21	1:A:812:LYS:HD3	2.01	0.41
1:A:845:THR:HG23	1:A:847:THR:H	1.85	0.41
1:A:882:ARG:HH21	1:A:944:LEU:HD21	1.86	0.41
1:A:2144:GLY:O	1:A:2148:ILE:HG12	2.20	0.41
1:A:3765:LEU:HB3	1:A:3844:LEU:HB3	2.03	0.41
1:A:3923:ILE:HG13	1:A:3983:SER:HB3	2.03	0.41
1:A:4065:LEU:HD13	1:A:4065:LEU:HA	1.95	0.41
1:A:4843:ILE:HG13	1:A:4844:ILE:N	2.36	0.41
1:B:191:TYR:N	1:B:206:ALA:O	2.54	0.41
1:B:538:ALA:HB1	1:B:542:ARG:HH21	1.86	0.41
1:B:747:HIS:CD2	1:B:750:ARG:HG2	2.55	0.41
1:B:822:CYS:HA	1:B:825:ALA:HB3	2.03	0.41
1:B:845:THR:HG23	1:B:847:THR:H	1.85	0.41
1:B:1035:TYR:O	1:B:1043:LYS:HE2	2.21	0.41
1:B:2084:PHE:CZ	1:B:3666:LEU:HB2	2.56	0.41
1:B:2279:LEU:HB3	1:B:2284:TYR:HB2	2.01	0.41
1:B:4496:ASN:HD22	1:B:4499:ASN:HD22	1.69	0.41
1:C:113:LEU:HD23	1:C:175:VAL:HG21	2.01	0.41
1:C:1128:LEU:HG	1:C:1136:ALA:HB2	2.02	0.41
1:C:1170:GLU:N	1:C:1170:GLU:CD	2.77	0.41
1:C:1965:ARG:O	1:C:1966:SER:OG	2.35	0.41
1:C:2755:LEU:HD13	1:C:2764:GLU:OE2	2.21	0.41
1:D:306:LEU:HG	1:D:314:LEU:HD23	2.03	0.41
1:D:403:LEU:HD23	1:D:403:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:747:HIS:HD2	1:D:750:ARG:HG2	1.85	0.41
1:D:1609:VAL:HG12	1:D:1620:VAL:HG23	2.03	0.41
1:D:2159:ASN:HD22	1:D:2162:ARG:NH2	2.19	0.41
1:D:2755:LEU:HD13	1:D:2764:GLU:OE2	2.21	0.41
1:D:3765:LEU:HB3	1:D:3844:LEU:HB3	2.03	0.41
1:D:3940:TRP:HA	1:D:3943:VAL:HG12	2.02	0.41
1:A:274:LEU:HD22	1:A:408:SER:OG	2.21	0.41
1:A:882:ARG:NH2	1:A:944:LEU:HD21	2.35	0.41
1:A:988:LEU:HD21	1:A:1054:VAL:HG23	2.03	0.41
1:A:1610:SER:C	1:A:1612:ILE:H	2.29	0.41
2:G:12:ASP:OD1	2:G:12:ASP:C	2.64	0.41
1:B:712:GLU:OE1	1:B:838:ARG:HB3	2.21	0.41
1:B:988:LEU:HD21	1:B:1054:VAL:HG23	2.03	0.41
1:B:2230:SER:O	1:B:2230:SER:OG	2.39	0.41
1:B:3765:LEU:HB3	1:B:3844:LEU:HB3	2.03	0.41
1:B:3940:TRP:HA	1:B:3943:VAL:HG12	2.02	0.41
1:B:4047:PHE:O	1:B:4051:MET:HG2	2.21	0.41
1:C:82:LEU:HD11	1:C:156:GLU:HB3	2.03	0.41
1:C:244:CYS:SG	1:C:273:SER:HB2	2.61	0.41
1:C:1609:VAL:HG12	1:C:1620:VAL:HG23	2.03	0.41
1:C:1642:ILE:HG23	1:C:1643:LEU:HD23	2.02	0.41
1:C:2159:ASN:HD22	1:C:2162:ARG:NH2	2.19	0.41
1:D:227:TYR:CD1	1:D:352:SER:HB3	2.56	0.41
1:D:237:LEU:HD23	1:D:404:ASN:O	2.21	0.41
1:D:882:ARG:NH1	1:D:937:LEU:HG	2.36	0.41
1:D:2113:GLU:OE1	1:D:2113:GLU:N	2.37	0.41
1:D:4047:PHE:O	1:D:4051:MET:HG2	2.21	0.41
1:D:4601:ARG:HD3	1:D:4707:TRP:HZ2	1.86	0.41
1:A:306:LEU:HG	1:A:314:LEU:HD23	2.03	0.40
1:A:748:LEU:HD13	1:A:748:LEU:HA	1.77	0.40
1:A:941:LYS:HA	1:A:944:LEU:HG	2.03	0.40
1:A:1035:TYR:O	1:A:1043:LYS:HE2	2.21	0.40
1:A:1686:LEU:HD11	1:A:1710:ILE:HD11	2.02	0.40
1:A:4058:THR:HG22	1:A:4061:GLU:HG3	2.02	0.40
1:A:4098:ALA:HB1	1:A:4125:LEU:HD23	2.03	0.40
1:B:244:CYS:SG	1:B:273:SER:HB2	2.61	0.40
1:B:926:GLU:H	1:B:926:GLU:HG2	1.54	0.40
1:B:1610:SER:C	1:B:1612:ILE:H	2.29	0.40
1:B:2334:LEU:HD13	1:B:2342:LEU:HB2	2.03	0.40
1:B:4833:PRO:HD3	1:B:4842:ARG:NE	2.25	0.40
2:H:29:GLY:N	2:H:38:ASP:O	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:TYR:CD1	1:C:352:SER:HB3	2.56	0.40
1:C:274:LEU:HD22	1:C:408:SER:OG	2.21	0.40
1:C:1111:GLY:HA3	1:C:1211:GLN:HE22	1.87	0.40
1:C:3765:LEU:HB3	1:C:3844:LEU:HB3	2.03	0.40
1:D:191:TYR:N	1:D:206:ALA:O	2.54	0.40
1:D:237:LEU:HD23	1:D:237:LEU:H	1.87	0.40
1:D:314:LEU:HD11	1:D:393:MET:HG3	2.03	0.40
1:D:836:HIS:NE2	1:D:842:GLN:OE1	2.46	0.40
1:D:845:THR:HG23	1:D:847:THR:H	1.85	0.40
1:D:1274:ASP:HB3	1:D:1286:THR:HA	2.03	0.40
1:D:3761:GLY:O	1:D:3764:ILE:HG22	2.21	0.40
1:D:3923:ILE:HG13	1:D:3983:SER:HB3	2.03	0.40
1:D:4857:LEU:O	1:D:4861:ILE:HG13	2.21	0.40
1:A:1962:ARG:NH2	1:A:1963:GLU:HA	2.36	0.40
1:A:2755:LEU:HD13	1:A:2764:GLU:OE2	2.21	0.40
1:A:4649:LYS:HA	1:A:4669:LEU:HD21	2.04	0.40
1:B:2157:HIS:O	1:B:2161:MET:HG2	2.22	0.40
1:C:574:VAL:HA	1:C:577:CYS:SG	2.60	0.40
1:C:730:LEU:HD21	2:I:6:GLU:OE2	2.21	0.40
1:C:882:ARG:NH1	1:C:937:LEU:HG	2.37	0.40
1:C:992:GLN:HA	1:C:995:MET:SD	2.61	0.40
1:C:1776:CYS:O	1:C:1778:GLN:HG3	2.22	0.40
1:C:2084:PHE:CZ	1:C:3666:LEU:HB2	2.56	0.40
1:C:4047:PHE:O	1:C:4051:MET:HG2	2.21	0.40
2:I:27:TYR:O	2:I:40:SER:N	2.53	0.40
1:D:274:LEU:HD22	1:D:408:SER:OG	2.21	0.40
1:D:654:SER:H	1:D:841:LYS:HZ1	1.66	0.40
1:D:1643:LEU:HD22	1:D:1694:TYR:O	2.20	0.40
1:D:1776:CYS:O	1:D:1778:GLN:HG3	2.22	0.40
1:D:1962:ARG:NH2	1:D:1963:GLU:HA	2.36	0.40
1:D:3934:LEU:HD23	1:D:3939:LEU:HD22	2.03	0.40
1:D:4496:ASN:HD22	1:D:4499:ASN:HD22	1.69	0.40
2:J:12:ASP:OD1	2:J:12:ASP:C	2.64	0.40
1:A:882:ARG:NH1	1:A:937:LEU:HG	2.36	0.40
1:A:1719:ARG:HD3	1:A:1832:MET:HA	2.04	0.40
1:A:2325:ARG:HA	1:A:2325:ARG:HD3	1.82	0.40
1:A:3731:HIS:CD2	1:A:3772:VAL:HG22	2.55	0.40
1:A:4847:ILE:HA	1:B:4821:ARG:HD3	2.02	0.40
1:B:304:LYS:HB2	1:B:316:LEU:HD23	2.03	0.40
1:B:882:ARG:NH1	1:B:937:LEU:HG	2.36	0.40
1:B:882:ARG:HH21	1:B:944:LEU:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:941:LYS:HA	1:B:944:LEU:HG	2.03	0.40
1:B:1962:ARG:NH2	1:B:1963:GLU:HA	2.37	0.40
1:B:3878:LEU:HD22	1:B:3938:ARG:HE	1.86	0.40
1:B:4895:ASP:OD1	1:B:4895:ASP:N	2.54	0.40
1:B:4929:GLU:HA	1:B:4932:HIS:CD2	2.57	0.40
1:C:191:TYR:N	1:C:206:ALA:O	2.54	0.40
1:C:237:LEU:HD23	1:C:237:LEU:H	1.86	0.40
1:C:387:ILE:HD11	1:C:389:ARG:NH1	2.37	0.40
1:C:538:ALA:HB1	1:C:542:ARG:HH21	1.86	0.40
1:C:1843:ILE:O	1:C:1846:LEU:HG	2.21	0.40
1:C:2230:SER:O	1:C:2230:SER:OG	2.39	0.40
1:C:3878:LEU:HD22	1:C:3938:ARG:HE	1.85	0.40
1:C:4098:ALA:HB1	1:C:4125:LEU:HD23	2.03	0.40
1:C:4483:ILE:O	1:C:4486:GLN:HG3	2.22	0.40
1:D:244:CYS:SG	1:D:273:SER:HB2	2.61	0.40
1:D:398:HIS:HB3	1:D:400:ASP:OD1	2.22	0.40
1:D:1089:ARG:HB3	1:D:1204:VAL:HG23	2.03	0.40
1:D:1111:GLY:HA3	1:D:1211:GLN:HE22	1.87	0.40
1:D:1610:SER:C	1:D:1612:ILE:H	2.28	0.40
1:D:3868:ASN:HB3	1:D:3871:ILE:HB	2.03	0.40
1:A:1170:GLU:N	1:A:1170:GLU:CD	2.77	0.40
1:A:1642:ILE:HG23	1:A:1643:LEU:HD23	2.02	0.40
1:A:1783:PHE:HE2	1:A:1788:LEU:HB2	1.87	0.40
1:A:1843:ILE:O	1:A:1846:LEU:HG	2.21	0.40
1:A:3761:GLY:O	1:A:3764:ILE:HG22	2.21	0.40
1:A:4042:ILE:O	1:A:4076:THR:HA	2.22	0.40
1:A:4601:ARG:HD3	1:A:4707:TRP:HZ2	1.86	0.40
1:B:227:TYR:CE1	1:B:352:SER:HB3	2.57	0.40
1:B:314:LEU:HD11	1:B:393:MET:HG3	2.03	0.40
1:B:627:SER:O	1:B:631:LEU:HG	2.22	0.40
1:B:992:GLN:HA	1:B:995:MET:SD	2.61	0.40
1:B:1170:GLU:N	1:B:1170:GLU:CD	2.77	0.40
1:B:1719:ARG:HD3	1:B:1832:MET:HA	2.04	0.40
1:B:2755:LEU:HD13	1:B:2764:GLU:OE2	2.21	0.40
1:B:4601:ARG:HD3	1:B:4707:TRP:HZ2	1.86	0.40
1:C:2071:GLU:O	1:C:3659:ARG:NH1	2.55	0.40
1:D:1686:LEU:HD11	1:D:1710:ILE:HD11	2.02	0.40
1:D:1719:ARG:HD3	1:D:1832:MET:HA	2.04	0.40
1:D:3878:LEU:HD22	1:D:3938:ARG:HE	1.86	0.40
1:D:4649:LYS:HA	1:D:4669:LEU:HD21	2.04	0.40
1:A:640:ARG:HB3	1:A:645:GLN:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:GLY:HA3	1:A:1211:GLN:HE22	1.87	0.40
1:A:2230:SER:O	1:A:2230:SER:OG	2.39	0.40
1:A:2889:GLN:O	1:A:2893:LYS:HG3	2.22	0.40
1:A:3854:GLN:HB3	1:A:3930:ASN:HD21	1.87	0.40
1:A:3934:LEU:HD23	1:A:3939:LEU:HD22	2.04	0.40
1:B:34:LYS:HB3	1:B:34:LYS:HE3	1.92	0.40
1:B:191:TYR:HE2	1:C:2325:ARG:HD2	1.86	0.40
1:B:403:LEU:HD23	1:B:403:LEU:HA	1.90	0.40
1:B:548:CYS:HB2	1:B:582:SER:HB2	2.04	0.40
1:B:912:LYS:N	1:B:912:LYS:HD3	2.37	0.40
1:B:1609:VAL:HG12	1:B:1620:VAL:HG23	2.03	0.40
1:B:1783:PHE:HE2	1:B:1788:LEU:HB2	1.87	0.40
1:B:2351:LYS:HD2	1:B:2351:LYS:C	2.47	0.40
1:C:66:THR:HG23	1:C:124:SER:OG	2.21	0.40
1:C:709:GLY:N	1:C:721:ASP:OD2	2.55	0.40
1:C:712:GLU:OE1	1:C:838:ARG:HB3	2.21	0.40
1:C:1165:MET:HE1	1:C:1231:GLY:CA	2.42	0.40
1:C:2113:GLU:OE1	1:C:2113:GLU:N	2.37	0.40
1:D:66:THR:HG23	1:D:124:SER:OG	2.21	0.40
1:D:82:LEU:HD11	1:D:156:GLU:HB3	2.03	0.40
1:D:227:TYR:CE1	1:D:352:SER:HB3	2.57	0.40
1:D:2084:PHE:CZ	1:D:3666:LEU:HB2	2.56	0.40
1:D:2157:HIS:O	1:D:2161:MET:HG2	2.22	0.40
1:D:4107:HIS:O	1:D:4109:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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%)	2688 (95%)	139 (5%)	22	48
1	B	2827/3387 (84%)	2687 (95%)	140 (5%)	22	48
1	C	1938/3387 (57%)	1832 (94%)	106 (6%)	19	46
1	D	1728/3387 (51%)	1656 (96%)	72 (4%)	26	52
2	G	88/140 (63%)	84 (96%)	4 (4%)	24	50
2	H	88/140 (63%)	84 (96%)	4 (4%)	24	50
2	J	88/140 (63%)	84 (96%)	4 (4%)	24	50
All	All	9584/13968 (69%)	9115 (95%)	469 (5%)	24	48

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	34	LYS
1	A	56	LYS
1	A	61	ASP
1	A	62	LEU
1	A	153	THR
1	A	166	SER
1	A	167	LYS
1	A	173	GLU
1	A	175	VAL
1	A	225	GLN
1	A	233	VAL
1	A	285	SER
1	A	297	LEU
1	A	302	THR
1	A	310	GLU
1	A	347	ASP
1	A	378	ASP
1	A	400	ASP
1	A	415	THR
1	A	439	LYS
1	A	450	GLU
1	A	473	GLU
1	A	501	CYS
1	A	516	ASP
1	A	524	GLU
1	A	528	SER
1	A	649	VAL
1	A	677	LEU

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Mol	Chain	Res	Type
1	A	695	VAL
1	A	711	GLU
1	A	748	LEU
1	A	770	ILE
1	A	778	MET
1	A	804	LEU
1	A	830	GLU
1	A	867	VAL
1	A	887	GLU
1	A	893	TRP
1	A	894	VAL
1	A	914	GLN
1	A	919	VAL
1	A	920	GLU
1	A	922	CYS
1	A	926	GLU
1	A	927	GLN
1	A	935	MET
1	A	936	SER
1	A	944	LEU
1	A	946	LEU
1	A	952	ILE
1	A	971	GLN
1	A	972	LEU
1	A	982	ASP
1	A	986	ILE
1	A	987	LYS
1	A	999	LEU
1	A	1006	VAL
1	A	1047	LYS
1	A	1057	LEU
1	A	1060	TYR
1	A	1161	VAL
1	A	1170	GLU
1	A	1186	SER
1	A	1261	VAL
1	A	1271	THR
1	A	1359	ILE
1	A	1373	HIS
1	A	1598	SER
1	A	1691	GLU
1	A	1738	THR

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Mol	Chain	Res	Type
1	A	1755	SER
1	A	1772	ILE
1	A	1814	THR
1	A	1838	GLU
1	A	1896	LYS
1	A	1953	SER
1	A	1956	LEU
1	A	1961	THR
1	A	1997	ASP
1	A	2060	LEU
1	A	2098	VAL
1	A	2131	VAL
1	A	2245	SER
1	A	2246	VAL
1	A	2265	VAL
1	A	2389	THR
1	A	2405	MET
1	A	2408	ILE
1	A	2414	GLU
1	A	2436	SER
1	A	2441	MET
1	A	2479	VAL
1	A	2489	VAL
1	A	2715	LYS
1	A	2725	GLU
1	A	2727	SER
1	A	2729	ASP
1	A	2736	LEU
1	A	2738	ASN
1	A	2741	ILE
1	A	2768	GLU
1	A	2769	ILE
1	A	2774	ILE
1	A	2777	SER
1	A	2779	LYS
1	A	2839	MET
1	A	2858	GLU
1	A	2880	GLU
1	A	2883	LYS
1	A	2884	ASP
1	A	2900	TYR
1	A	3620	LEU

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Mol	Chain	Res	Type
1	A	3692	ASP
1	A	3717	GLU
1	A	3800	SER
1	A	3824	SER
1	A	3885	SER
1	A	3899	GLU
1	A	3928	THR
1	A	3937	SER
1	A	3949	VAL
1	A	3962	SER
1	A	4017	ASP
1	A	4066	LEU
1	A	4080	GLU
1	A	4112	THR
1	A	4116	THR
1	A	4152	SER
1	A	4167	SER
1	A	4559	VAL
1	A	4561	GLU
1	A	4697	LEU
1	A	4776	VAL
1	A	4783	VAL
1	A	4797	ASP
1	A	4836	ASP
1	A	4884	GLU
1	A	4955	ASP
2	G	7	THR
2	G	22	THR
2	G	68	SER
2	G	69	LEU
1	B	22	LEU
1	B	34	LYS
1	B	56	LYS
1	B	61	ASP
1	B	62	LEU
1	B	153	THR
1	B	166	SER
1	B	167	LYS
1	B	173	GLU
1	B	175	VAL
1	B	225	GLN
1	B	233	VAL

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Mol	Chain	Res	Type
1	B	285	SER
1	B	297	LEU
1	B	302	THR
1	B	310	GLU
1	B	347	ASP
1	B	378	ASP
1	B	400	ASP
1	B	415	THR
1	B	439	LYS
1	B	450	GLU
1	B	473	GLU
1	B	501	CYS
1	B	516	ASP
1	B	524	GLU
1	B	528	SER
1	B	649	VAL
1	B	677	LEU
1	B	695	VAL
1	B	711	GLU
1	B	748	LEU
1	B	770	ILE
1	B	778	MET
1	B	804	LEU
1	B	830	GLU
1	B	867	VAL
1	B	887	GLU
1	B	893	TRP
1	B	894	VAL
1	B	914	GLN
1	B	919	VAL
1	B	920	GLU
1	B	922	CYS
1	B	926	GLU
1	B	927	GLN
1	B	935	MET
1	B	936	SER
1	B	944	LEU
1	B	946	LEU
1	B	952	ILE
1	B	971	GLN
1	B	972	LEU
1	B	982	ASP

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Mol	Chain	Res	Type
1	B	986	ILE
1	B	987	LYS
1	B	999	LEU
1	B	1006	VAL
1	B	1047	LYS
1	B	1057	LEU
1	B	1060	TYR
1	B	1161	VAL
1	B	1170	GLU
1	B	1186	SER
1	B	1261	VAL
1	B	1271	THR
1	B	1359	ILE
1	B	1373	HIS
1	B	1598	SER
1	B	1691	GLU
1	B	1738	THR
1	B	1755	SER
1	B	1772	ILE
1	B	1814	THR
1	B	1838	GLU
1	B	1896	LYS
1	B	1953	SER
1	B	1956	LEU
1	B	1961	THR
1	B	1997	ASP
1	B	2060	LEU
1	B	2098	VAL
1	B	2131	VAL
1	B	2245	SER
1	B	2246	VAL
1	B	2265	VAL
1	B	2389	THR
1	B	2405	MET
1	B	2408	ILE
1	B	2414	GLU
1	B	2436	SER
1	B	2441	MET
1	B	2479	VAL
1	B	2489	VAL
1	B	2715	LYS
1	B	2725	GLU

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Mol	Chain	Res	Type
1	B	2727	SER
1	B	2729	ASP
1	B	2736	LEU
1	B	2738	ASN
1	B	2741	ILE
1	B	2768	GLU
1	B	2769	ILE
1	B	2774	ILE
1	B	2777	SER
1	B	2779	LYS
1	B	2839	MET
1	B	2858	GLU
1	B	2870	LEU
1	B	2880	GLU
1	B	2883	LYS
1	B	2884	ASP
1	B	2900	TYR
1	B	3620	LEU
1	B	3692	ASP
1	B	3717	GLU
1	B	3800	SER
1	B	3824	SER
1	B	3885	SER
1	B	3899	GLU
1	B	3928	THR
1	B	3937	SER
1	B	3949	VAL
1	B	3962	SER
1	B	4017	ASP
1	B	4066	LEU
1	B	4080	GLU
1	B	4112	THR
1	B	4116	THR
1	B	4152	SER
1	B	4167	SER
1	B	4559	VAL
1	B	4561	GLU
1	B	4697	LEU
1	B	4776	VAL
1	B	4783	VAL
1	B	4797	ASP
1	B	4836	ASP

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Mol	Chain	Res	Type
1	B	4884	GLU
1	B	4955	ASP
2	H	7	THR
2	H	22	THR
2	H	68	SER
2	H	69	LEU
1	C	22	LEU
1	C	34	LYS
1	C	56	LYS
1	C	61	ASP
1	C	62	LEU
1	C	153	THR
1	C	166	SER
1	C	167	LYS
1	C	173	GLU
1	C	175	VAL
1	C	225	GLN
1	C	233	VAL
1	C	285	SER
1	C	297	LEU
1	C	302	THR
1	C	310	GLU
1	C	347	ASP
1	C	378	ASP
1	C	400	ASP
1	C	415	THR
1	C	439	LYS
1	C	450	GLU
1	C	473	GLU
1	C	501	CYS
1	C	516	ASP
1	C	524	GLU
1	C	528	SER
1	C	649	VAL
1	C	677	LEU
1	C	695	VAL
1	C	711	GLU
1	C	748	LEU
1	C	770	ILE
1	C	778	MET
1	C	804	LEU
1	C	830	GLU

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Mol	Chain	Res	Type
1	C	867	VAL
1	C	887	GLU
1	C	893	TRP
1	C	894	VAL
1	C	914	GLN
1	C	919	VAL
1	C	920	GLU
1	C	922	CYS
1	C	926	GLU
1	C	927	GLN
1	C	935	MET
1	C	936	SER
1	C	944	LEU
1	C	946	LEU
1	C	952	ILE
1	C	971	GLN
1	C	972	LEU
1	C	982	ASP
1	C	986	ILE
1	C	987	LYS
1	C	999	LEU
1	C	1006	VAL
1	C	1047	LYS
1	C	1057	LEU
1	C	1060	TYR
1	C	1161	VAL
1	C	1170	GLU
1	C	1186	SER
1	C	1261	VAL
1	C	1271	THR
1	C	1359	ILE
1	C	1373	HIS
1	C	1598	SER
1	C	1691	GLU
1	C	1738	THR
1	C	1755	SER
1	C	1772	ILE
1	C	1814	THR
1	C	1838	GLU
1	C	1896	LYS
1	C	1953	SER
1	C	1956	LEU

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Mol	Chain	Res	Type
1	C	1961	THR
1	C	1997	ASP
1	C	2060	LEU
1	C	2098	VAL
1	C	2131	VAL
1	C	2245	SER
1	C	2246	VAL
1	C	2265	VAL
1	C	2436	SER
1	C	2441	MET
1	C	2479	VAL
1	C	2489	VAL
1	C	2715	LYS
1	C	2725	GLU
1	C	2727	SER
1	C	2729	ASP
1	C	2736	LEU
1	C	2738	ASN
1	C	2741	ILE
1	C	2768	GLU
1	C	2769	ILE
1	C	2774	ILE
1	C	2777	SER
1	C	2779	LYS
1	C	2900	TYR
1	C	3620	LEU
1	C	3692	ASP
1	C	3717	GLU
1	D	914	GLN
1	D	972	LEU
1	D	982	ASP
1	D	1006	VAL
1	D	1047	LYS
1	D	1057	LEU
1	D	1060	TYR
1	D	1261	VAL
1	D	1271	THR
1	D	1359	ILE
1	D	1373	HIS
1	D	1598	SER
1	D	1691	GLU
1	D	1738	THR

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Mol	Chain	Res	Type
1	D	1896	LYS
1	D	2098	VAL
1	D	2245	SER
1	D	2246	VAL
1	D	2265	VAL
1	D	2389	THR
1	D	2405	MET
1	D	2408	ILE
1	D	2414	GLU
1	D	2436	SER
1	D	2441	MET
1	D	2479	VAL
1	D	2489	VAL
1	D	2715	LYS
1	D	2725	GLU
1	D	2727	SER
1	D	2729	ASP
1	D	2736	LEU
1	D	2738	ASN
1	D	2741	ILE
1	D	2768	GLU
1	D	2769	ILE
1	D	2774	ILE
1	D	2777	SER
1	D	2779	LYS
1	D	2839	MET
1	D	2858	GLU
1	D	2880	GLU
1	D	2883	LYS
1	D	2884	ASP
1	D	2900	TYR
1	D	3620	LEU
1	D	3692	ASP
1	D	3717	GLU
1	D	3800	SER
1	D	3824	SER
1	D	3885	SER
1	D	3899	GLU
1	D	3928	THR
1	D	3937	SER
1	D	3949	VAL
1	D	3962	SER

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Mol	Chain	Res	Type
1	D	4017	ASP
1	D	4066	LEU
1	D	4080	GLU
1	D	4112	THR
1	D	4116	THR
1	D	4152	SER
1	D	4167	SER
1	D	4559	VAL
1	D	4561	GLU
1	D	4697	LEU
1	D	4776	VAL
1	D	4783	VAL
1	D	4797	ASP
1	D	4836	ASP
1	D	4884	GLU
1	D	4955	ASP
2	J	7	THR
2	J	22	THR
2	J	68	SER
2	J	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	54	ASN
1	A	79	GLN
1	A	123	HIS
1	A	150	GLN
1	A	288	HIS
1	A	299	HIS
1	A	394	HIS
1	A	410	HIS
1	A	472	HIS
1	A	476	GLN
1	A	487	ASN
1	A	496	ASN
1	A	576	HIS
1	A	593	HIS
1	A	629	GLN
1	A	635	ASN
1	A	650	ASN

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Mol	Chain	Res	Type
1	A	651	HIS
1	A	669	GLN
1	A	731	HIS
1	A	781	ASN
1	A	1002	ASN
1	A	1005	ASN
1	A	1123	GLN
1	A	1244	ASN
1	A	1257	GLN
1	A	1265	HIS
1	A	1353	HIS
1	A	1590	GLN
1	A	1627	GLN
1	A	1685	GLN
1	A	1711	HIS
1	A	1806	HIS
1	A	1938	ASN
1	A	1944	ASN
1	A	1999	HIS
1	A	2159	ASN
1	A	2317	ASN
1	A	2382	HIS
1	A	2728	HIS
1	A	2866	ASN
1	A	2867	HIS
1	A	3721	GLN
1	A	3860	GLN
1	A	3868	ASN
1	A	3881	GLN
1	A	3932	GLN
1	A	3959	GLN
1	A	3974	GLN
1	A	4096	ASN
1	A	4170	GLN
1	A	4491	ASN
1	A	4496	ASN
1	A	4628	GLN
1	A	4637	GLN
1	A	4642	ASN
1	A	4716	ASN
1	A	4862	GLN
1	A	4960	GLN

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Mol	Chain	Res	Type
2	G	32	GLN
1	B	12	GLN
1	B	54	ASN
1	B	79	GLN
1	B	123	HIS
1	B	150	GLN
1	B	288	HIS
1	B	299	HIS
1	B	394	HIS
1	B	410	HIS
1	B	472	HIS
1	B	476	GLN
1	B	487	ASN
1	B	496	ASN
1	B	576	HIS
1	B	593	HIS
1	B	629	GLN
1	B	635	ASN
1	B	650	ASN
1	B	651	HIS
1	B	669	GLN
1	B	681	HIS
1	B	731	HIS
1	B	781	ASN
1	B	888	ASN
1	B	1002	ASN
1	B	1005	ASN
1	B	1123	GLN
1	B	1244	ASN
1	B	1257	GLN
1	B	1265	HIS
1	B	1353	HIS
1	B	1590	GLN
1	B	1627	GLN
1	B	1685	GLN
1	B	1711	HIS
1	B	1806	HIS
1	B	1836	HIS
1	B	1936	GLN
1	B	1938	ASN
1	B	1944	ASN
1	B	1999	HIS

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Continued from previous page...

Mol	Chain	Res	Type
1	B	2159	ASN
1	B	2317	ASN
1	B	2382	HIS
1	B	2728	HIS
1	B	2866	ASN
1	B	2867	HIS
1	B	3721	GLN
1	B	3805	ASN
1	B	3860	GLN
1	B	3868	ASN
1	B	3881	GLN
1	B	3930	ASN
1	B	3932	GLN
1	B	3959	GLN
1	B	3974	GLN
1	B	4096	ASN
1	B	4170	GLN
1	B	4491	ASN
1	B	4496	ASN
1	B	4642	ASN
1	B	4716	ASN
1	B	4786	ASN
1	B	4960	GLN
2	H	32	GLN
1	C	12	GLN
1	C	54	ASN
1	C	79	GLN
1	C	123	HIS
1	C	150	GLN
1	C	288	HIS
1	C	299	HIS
1	C	394	HIS
1	C	410	HIS
1	C	472	HIS
1	C	476	GLN
1	C	487	ASN
1	C	496	ASN
1	C	576	HIS
1	C	593	HIS
1	C	629	GLN
1	C	635	ASN
1	C	650	ASN

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Mol	Chain	Res	Type
1	C	651	HIS
1	C	669	GLN
1	C	681	HIS
1	C	692	HIS
1	C	731	HIS
1	C	746	GLN
1	C	781	ASN
1	C	888	ASN
1	C	1002	ASN
1	C	1005	ASN
1	C	1123	GLN
1	C	1244	ASN
1	C	1257	GLN
1	C	1265	HIS
1	C	1353	HIS
1	C	1590	GLN
1	C	1627	GLN
1	C	1685	GLN
1	C	1711	HIS
1	C	1806	HIS
1	C	1944	ASN
1	C	1999	HIS
1	C	2159	ASN
1	C	2317	ASN
1	C	3721	GLN
1	D	1005	ASN
1	D	1244	ASN
1	D	1257	GLN
1	D	1265	HIS
1	D	1353	HIS
1	D	1590	GLN
1	D	1627	GLN
1	D	1685	GLN
1	D	1711	HIS
1	D	2159	ASN
1	D	2317	ASN
1	D	2382	HIS
1	D	2728	HIS
1	D	2866	ASN
1	D	2867	HIS
1	D	3721	GLN
1	D	3766	ASN

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Mol	Chain	Res	Type
1	D	3860	GLN
1	D	3868	ASN
1	D	3881	GLN
1	D	3932	GLN
1	D	3959	GLN
1	D	3974	GLN
1	D	4096	ASN
1	D	4170	GLN
1	D	4491	ASN
1	D	4496	ASN
1	D	4637	GLN
1	D	4642	ASN
1	D	4716	ASN
1	D	4786	ASN
1	D	4894	ASN
1	D	4932	HIS
1	D	4960	GLN
2	J	32	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

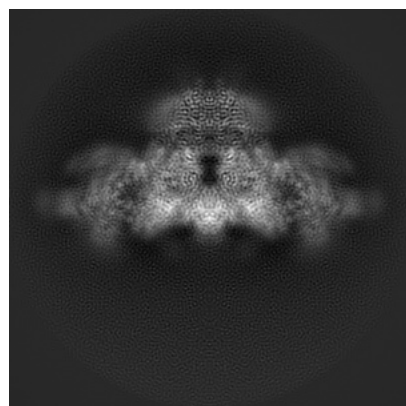
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33939. These allow visual inspection of the internal detail of the map and identification of artifacts.

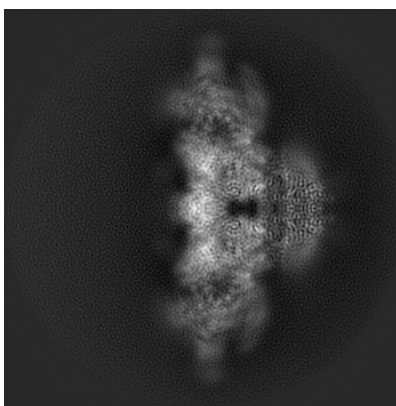
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

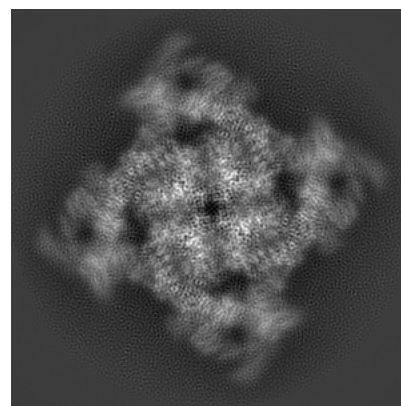
6.1.1 Primary map



X

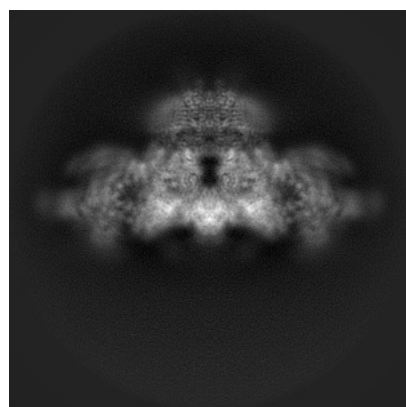


Y

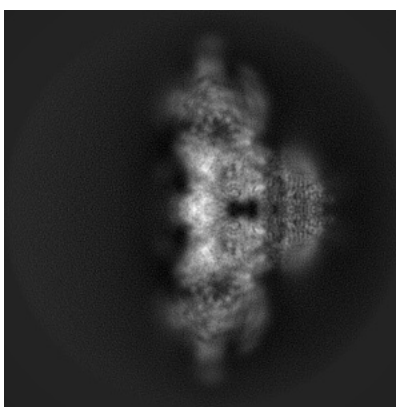


Z

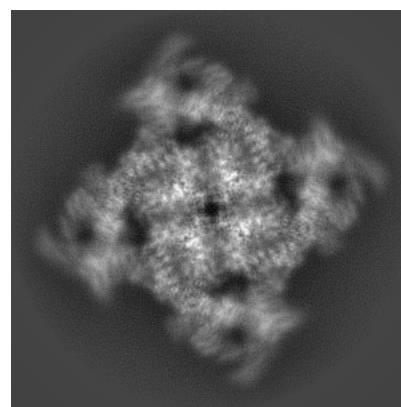
6.1.2 Raw map



X



Y

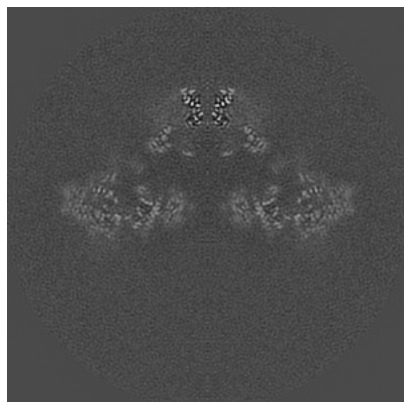


Z

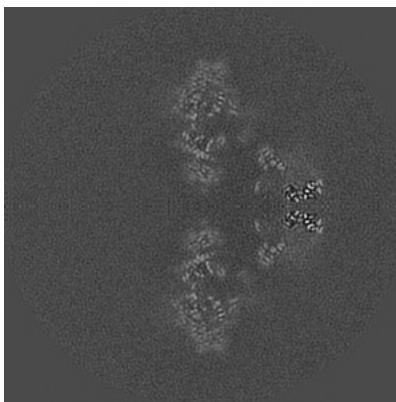
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

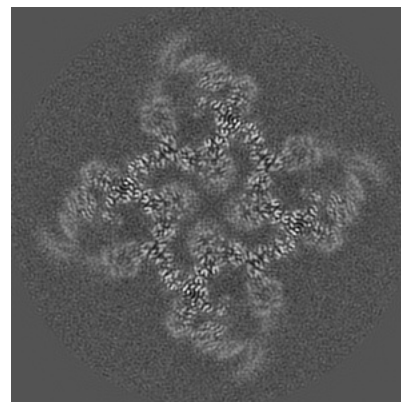
6.2.1 Primary map



X Index: 170

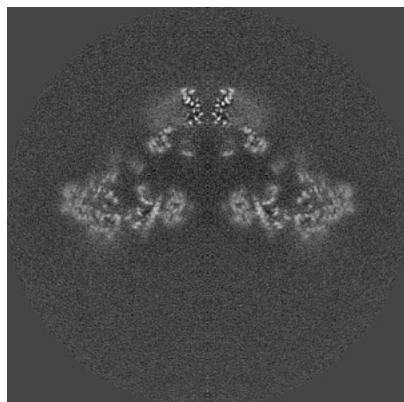


Y Index: 170

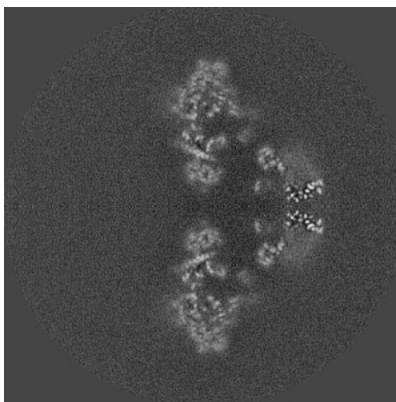


Z Index: 170

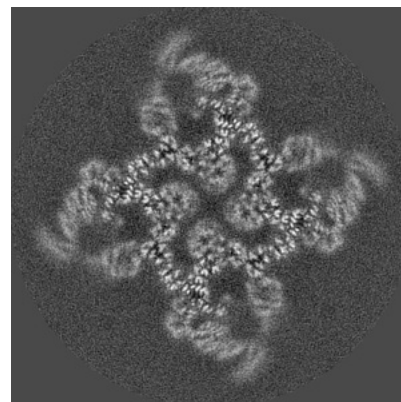
6.2.2 Raw map



X Index: 170



Y Index: 170

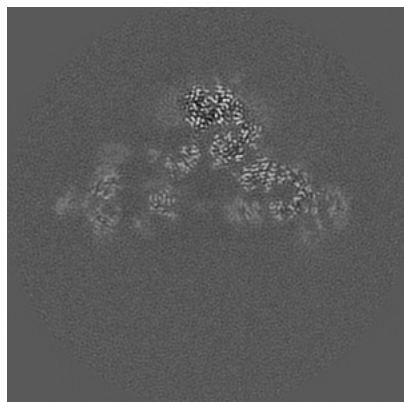


Z Index: 170

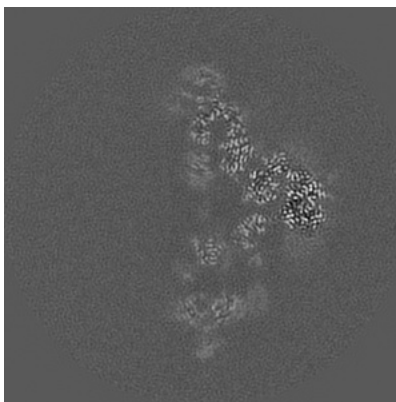
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

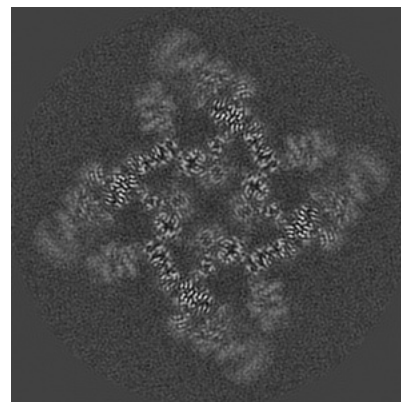
6.3.1 Primary map



X Index: 182

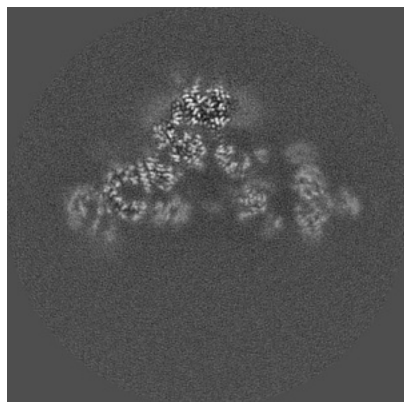


Y Index: 158

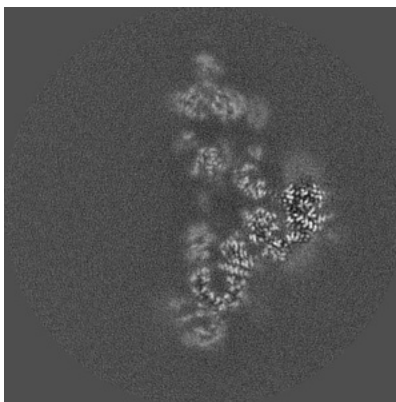


Z Index: 174

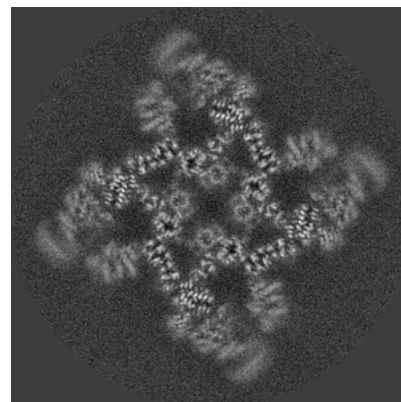
6.3.2 Raw map



X Index: 158



Y Index: 182

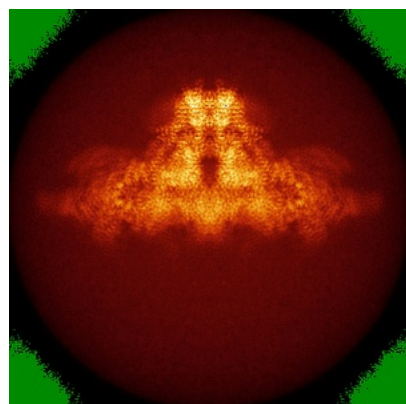


Z Index: 174

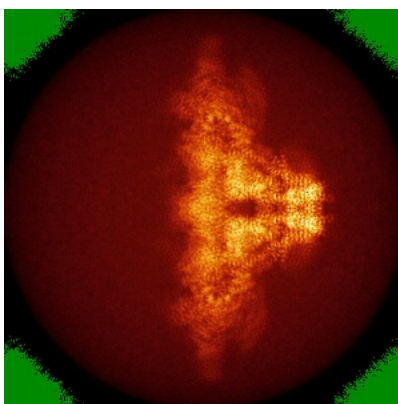
The images above show the largest variance slices of the map in three orthogonal directions.

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

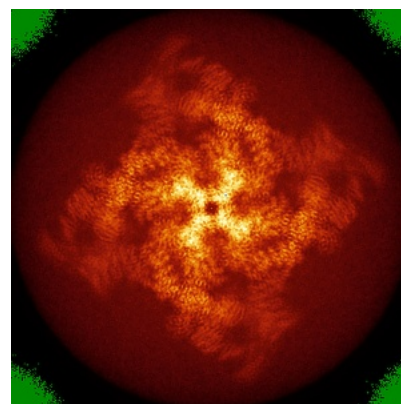
6.4.1 Primary map



X

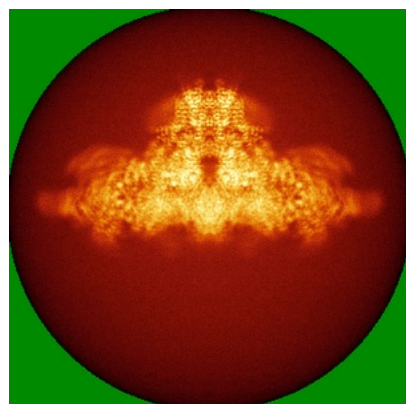


Y

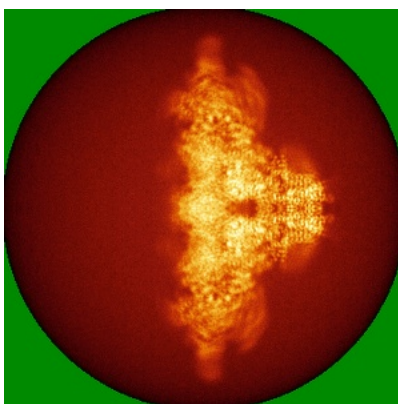


Z

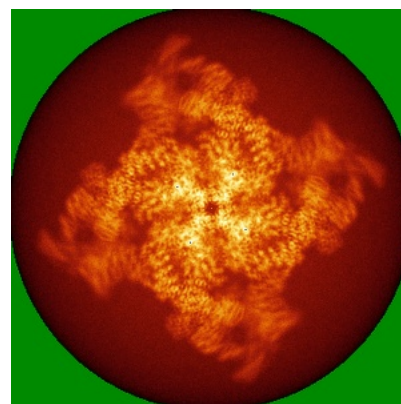
6.4.2 Raw map



X



Y

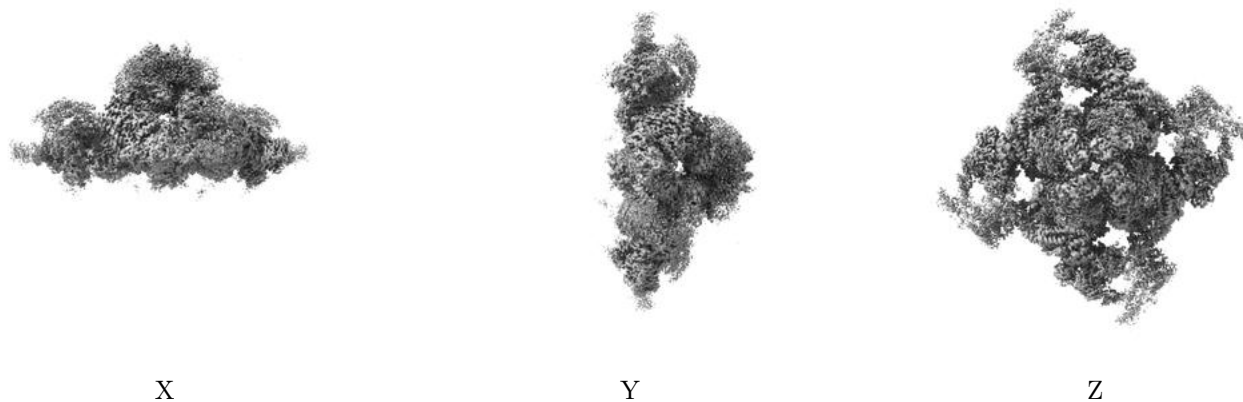


Z

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

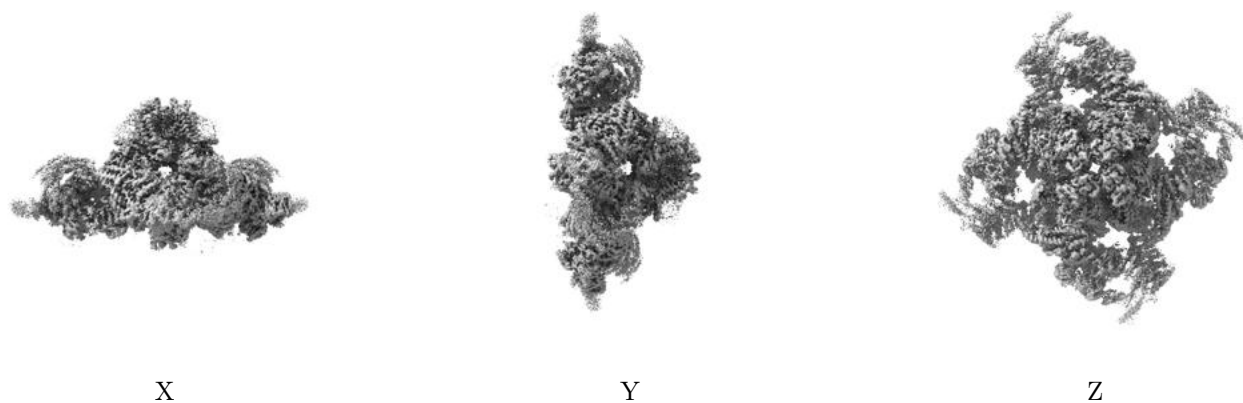
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

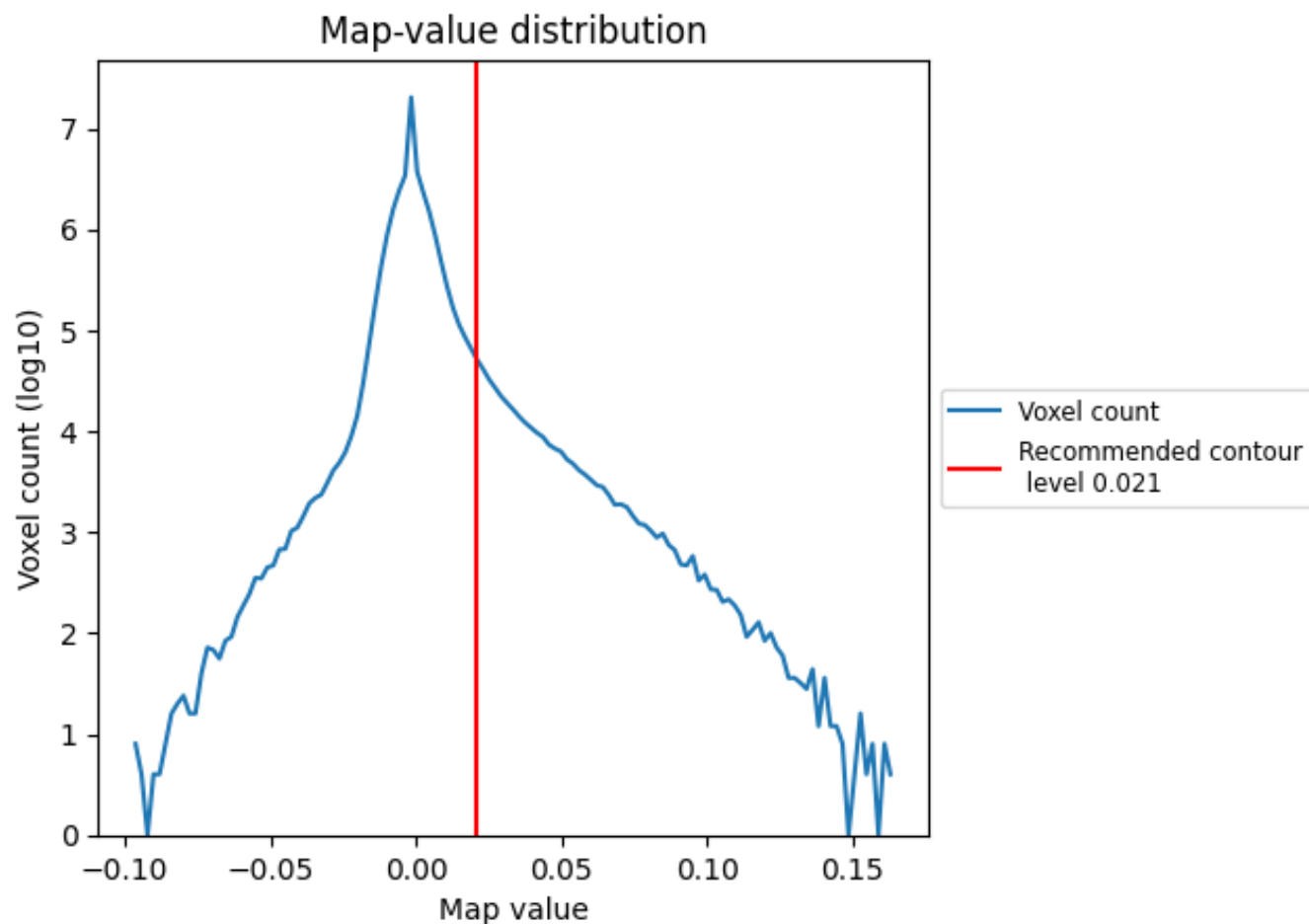
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

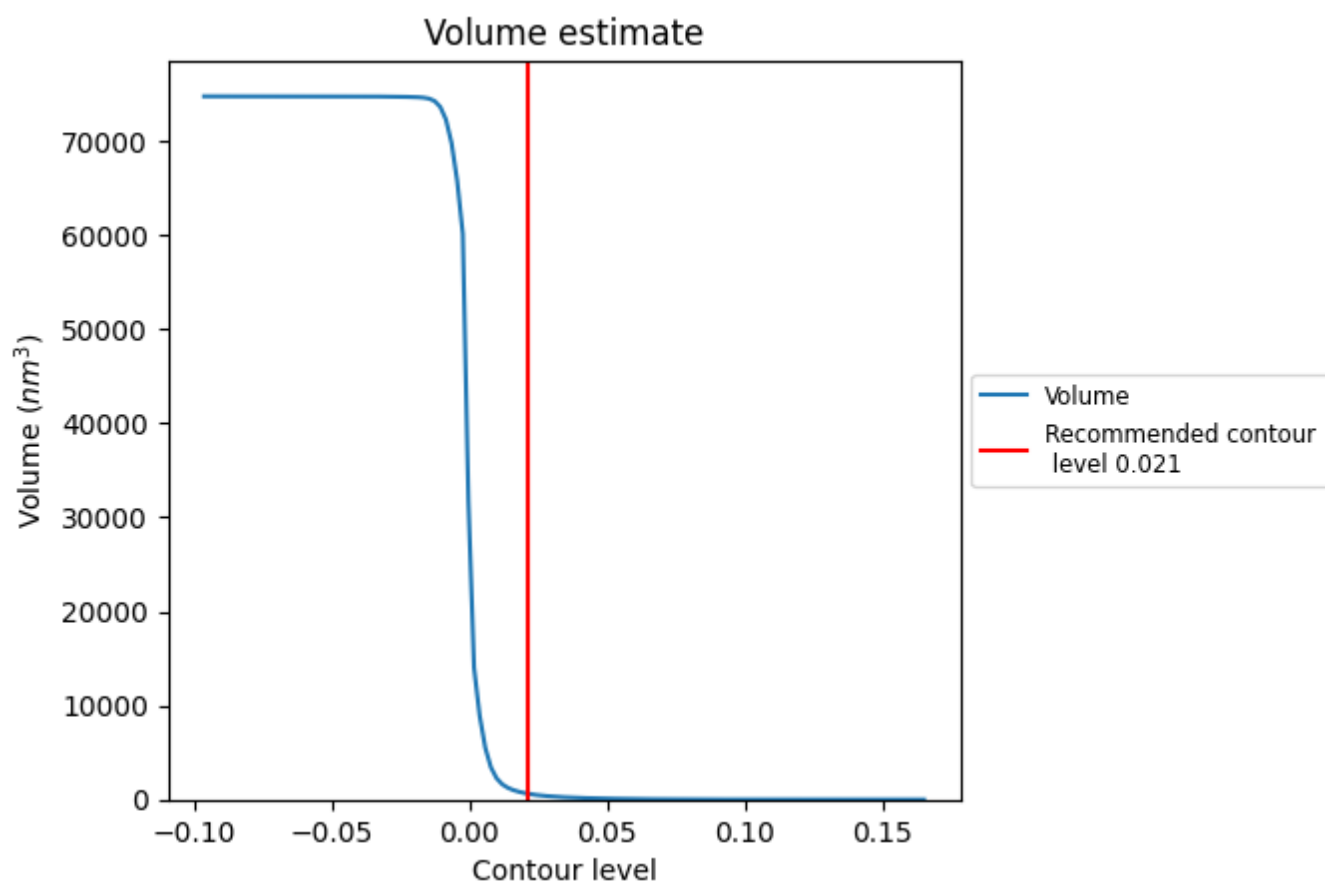
This section contains the results of statistical analysis of the map.

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.

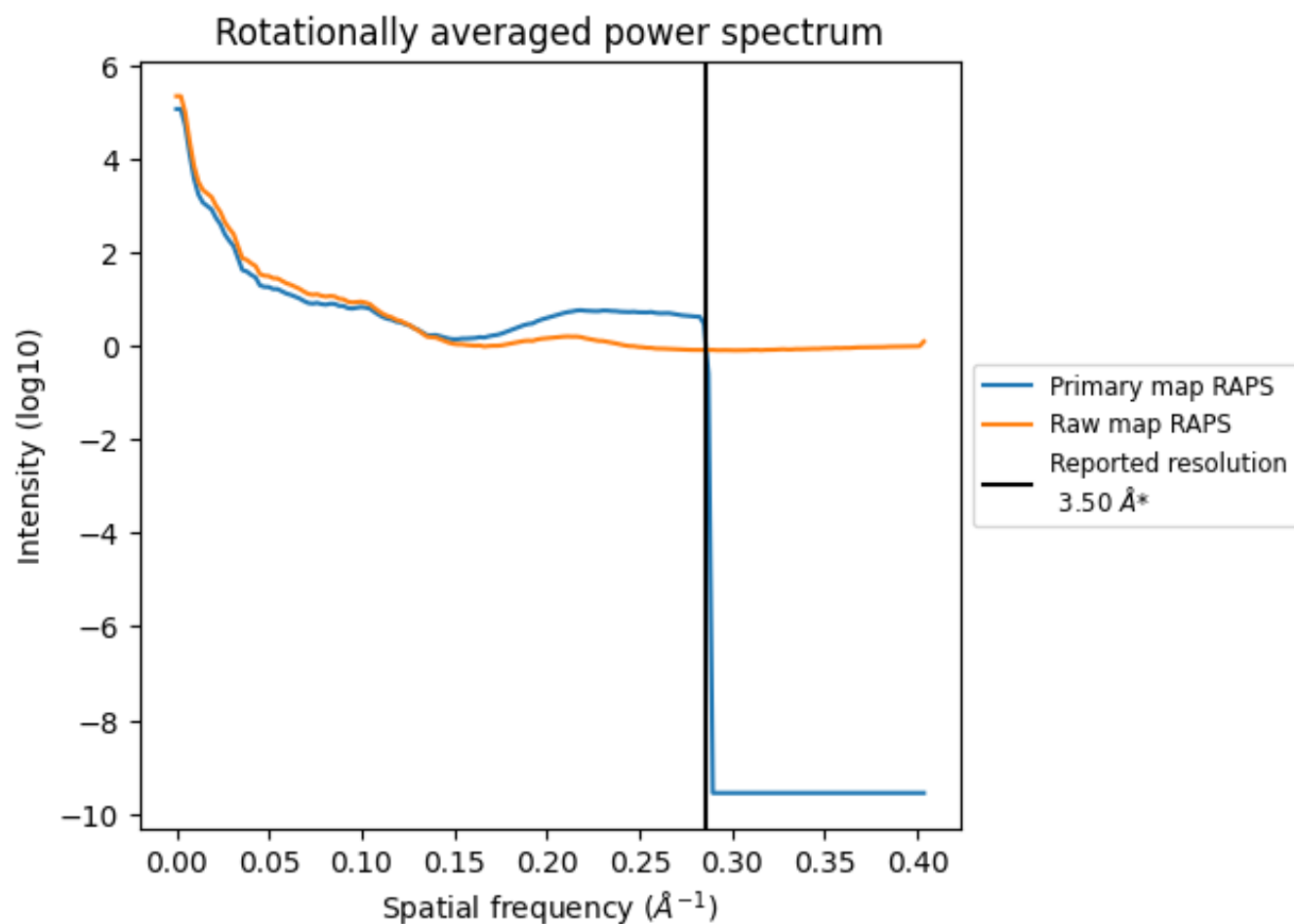
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm³; this corresponds to an approximate mass of 576 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 ⓘ

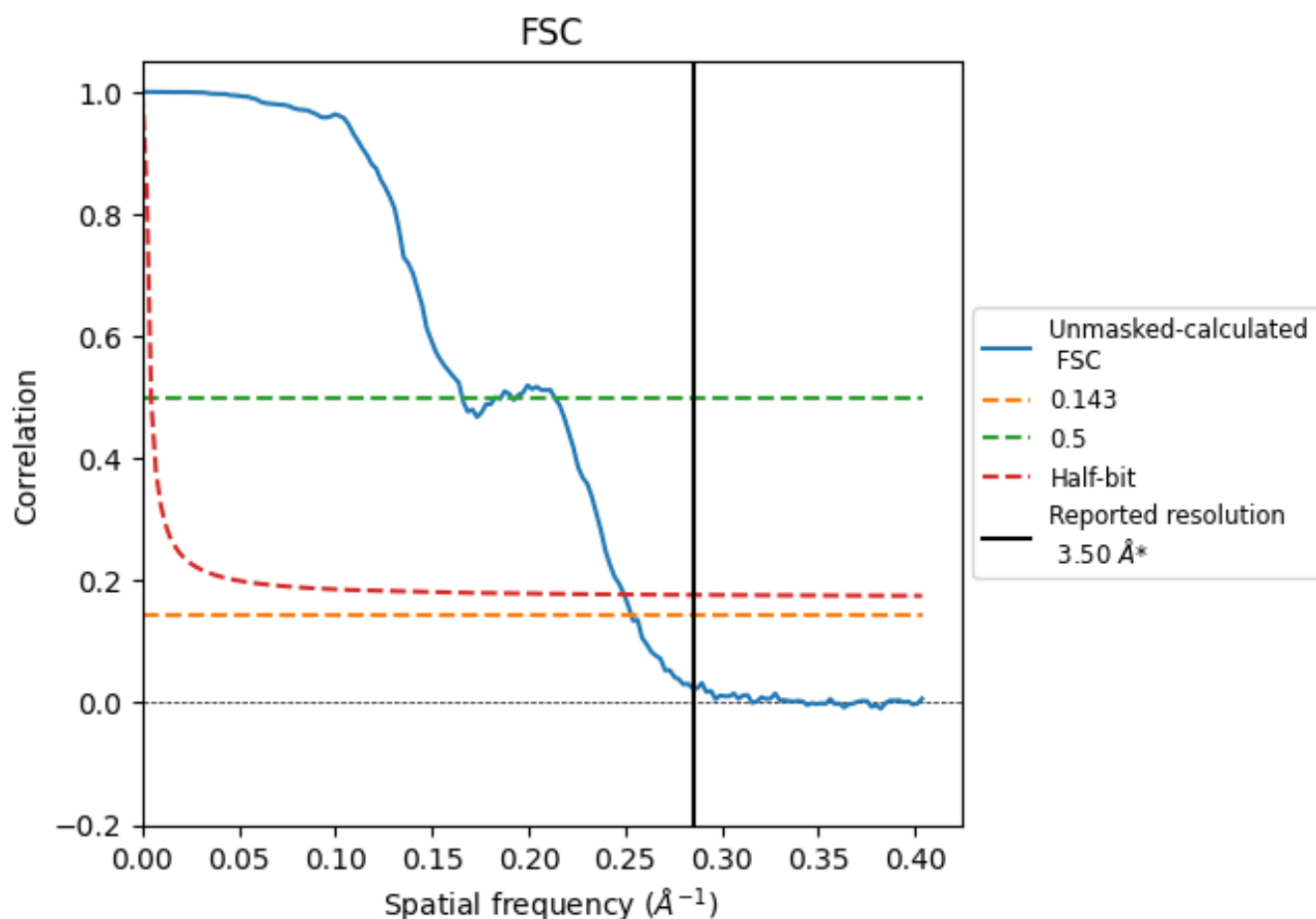


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

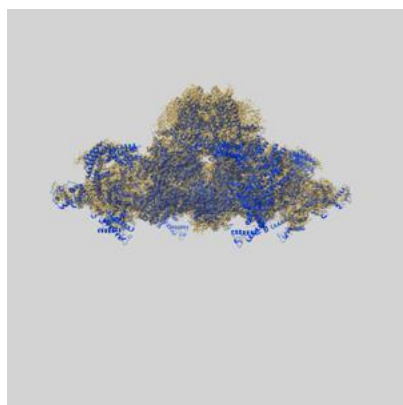
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	6.04	4.01

*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 3.95 differs from the reported value 3.5 by more than 10 %

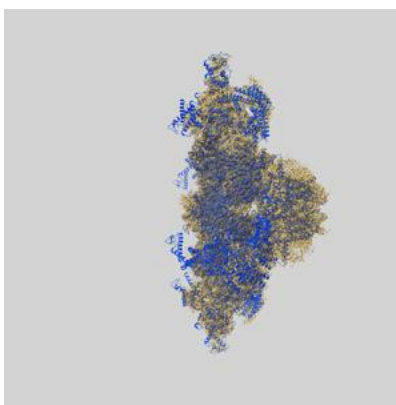
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33939 and PDB model 7VMP. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

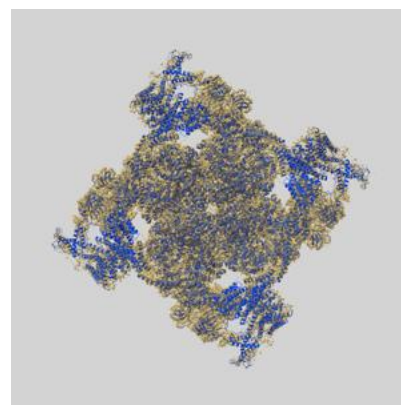
9.1 Map-model overlay [i](#)



X



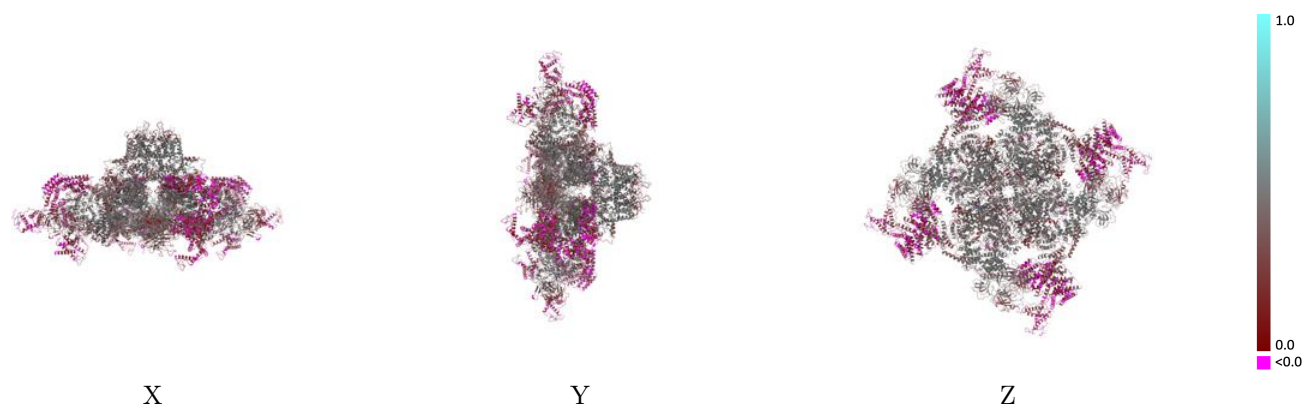
Y



Z

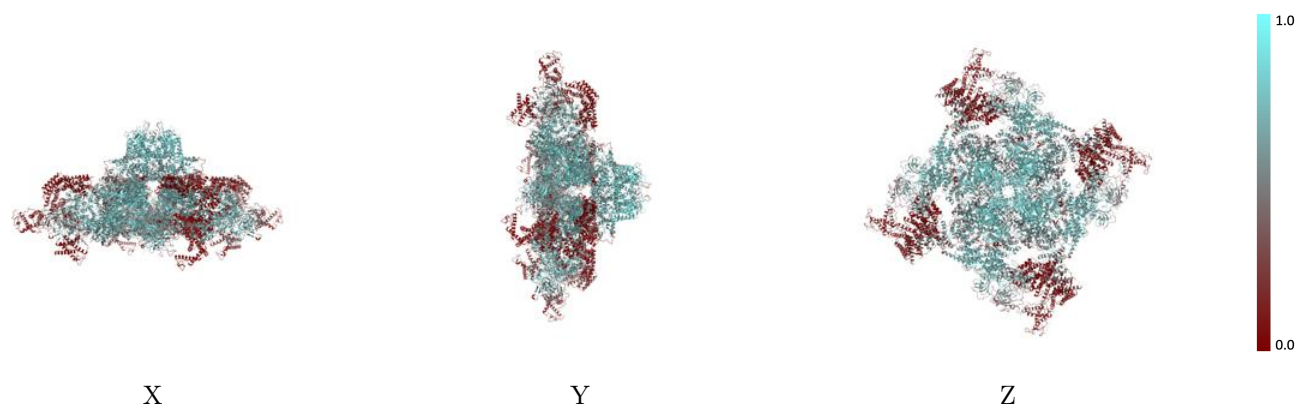
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



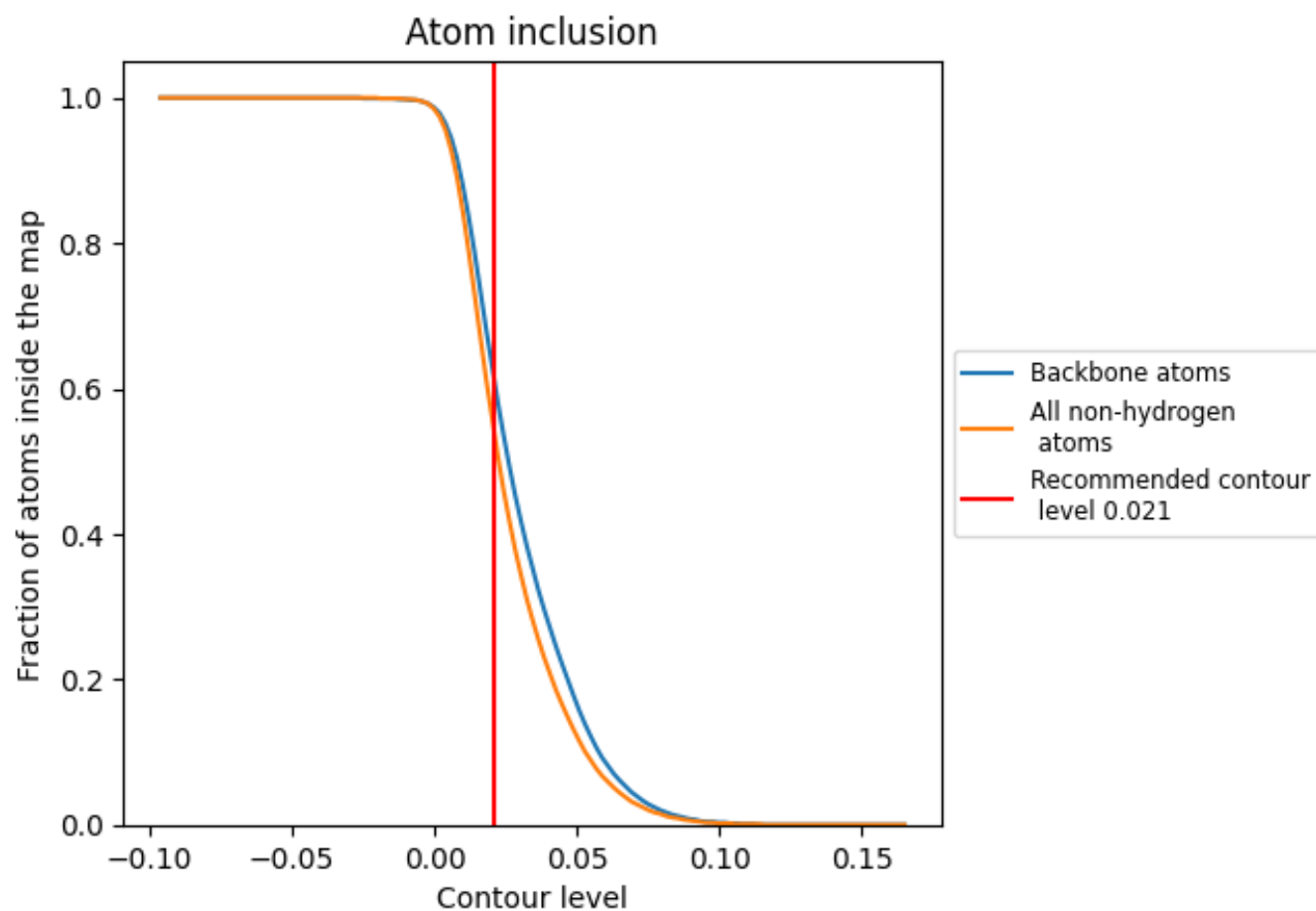
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.5370	0.3360
A	0.5360	0.3340
B	0.5370	0.3380
C	0.5330	0.3330
D	0.5350	0.3310
G	0.6070	0.4090
H	0.6100	0.4110
I	0.6050	0.4090
J	0.6130	0.4090

1.0

0.0

<0.0