



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:57 AM UTC

PDB ID : 7VMN / pdb_00007vmn
EMDB ID : EMD-33937
Title : Structure of recombinant RyR2 (EGTA dataset, class 2, closed state)
Authors : Kobayashi, T.; Tsutsumi, A.; Kurebayashi, N.; Kodama, M.; Kikkawa, M.;
Murayama, T.; Ogawa, H.
Deposited on : 2021-10-09
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

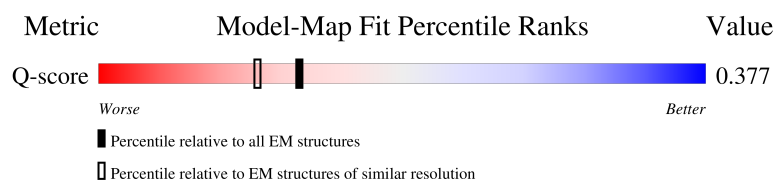
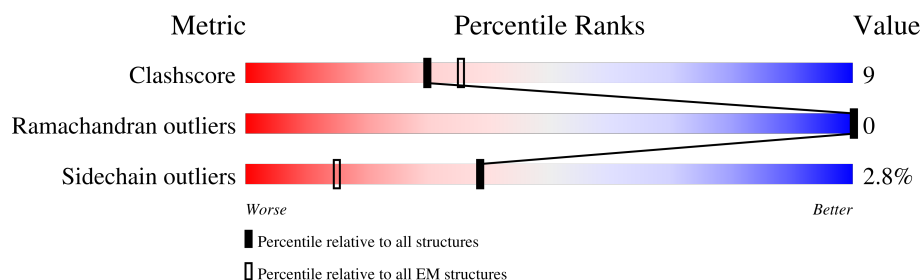
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13017 (3.02 - 4.02)

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	28% 65% 16% • 19%
1	B	4966	28% 65% 16% • 19%
1	C	4966	28% 65% 16% • 19%
1	D	4966	29% 65% 16% • 19%

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Mol	Chain	Length	Quality of chain
2	G	176	9% 45% 16% 39%
2	H	176	7% 45% 16% 39%
2	I	176	7% 45% 16% 39%
2	J	176	7% 46% 15% 39%

2 Entry composition

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

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

- Molecule 1 is a protein called Ryanodine receptor 2.

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

- 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

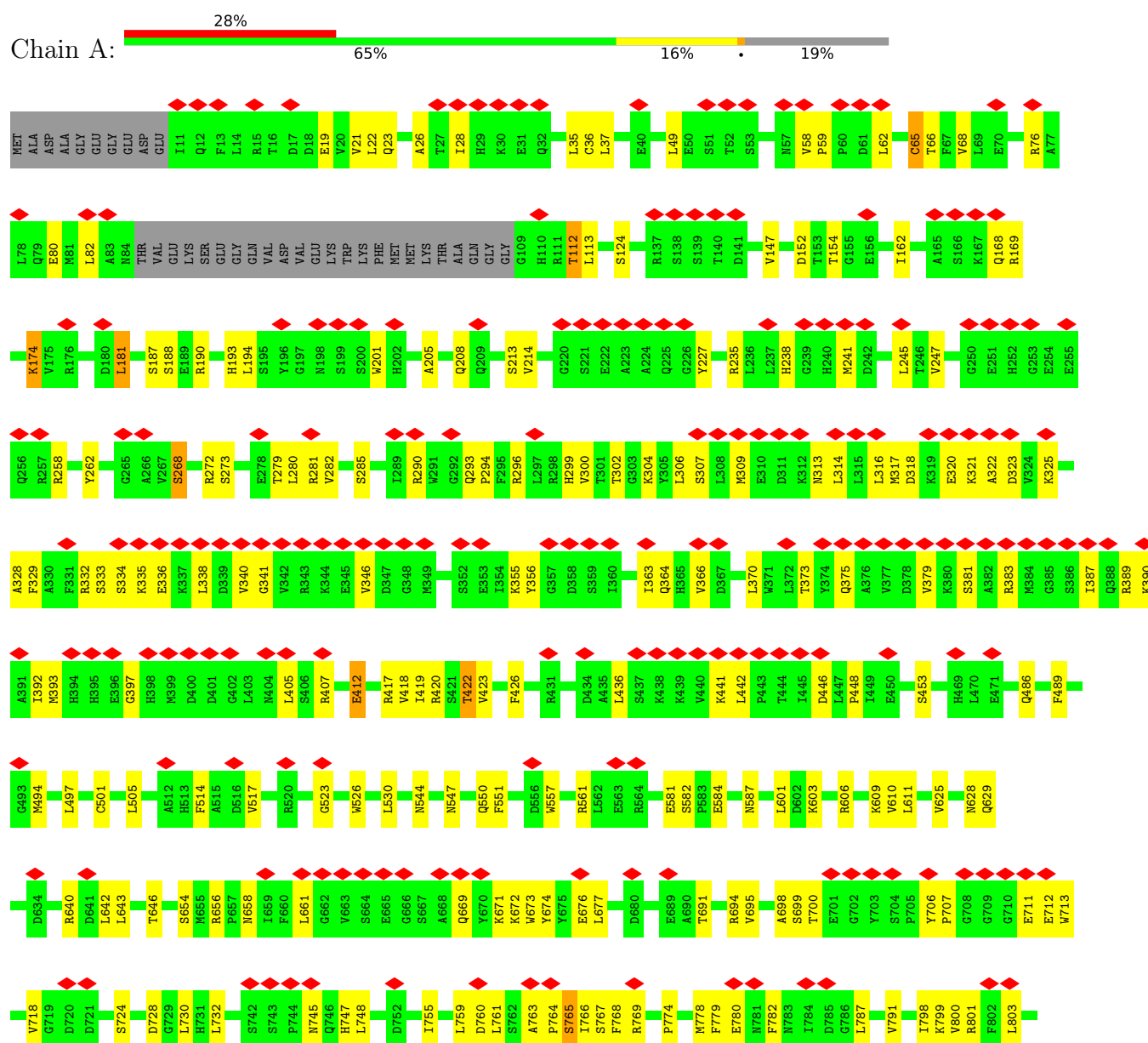
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

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

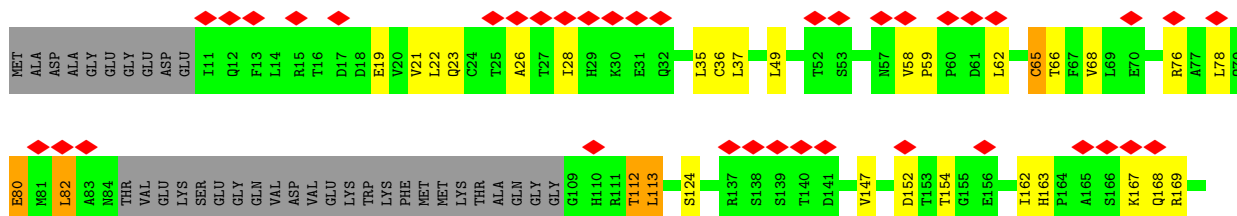
• Molecule 1: Ryanodine receptor 2









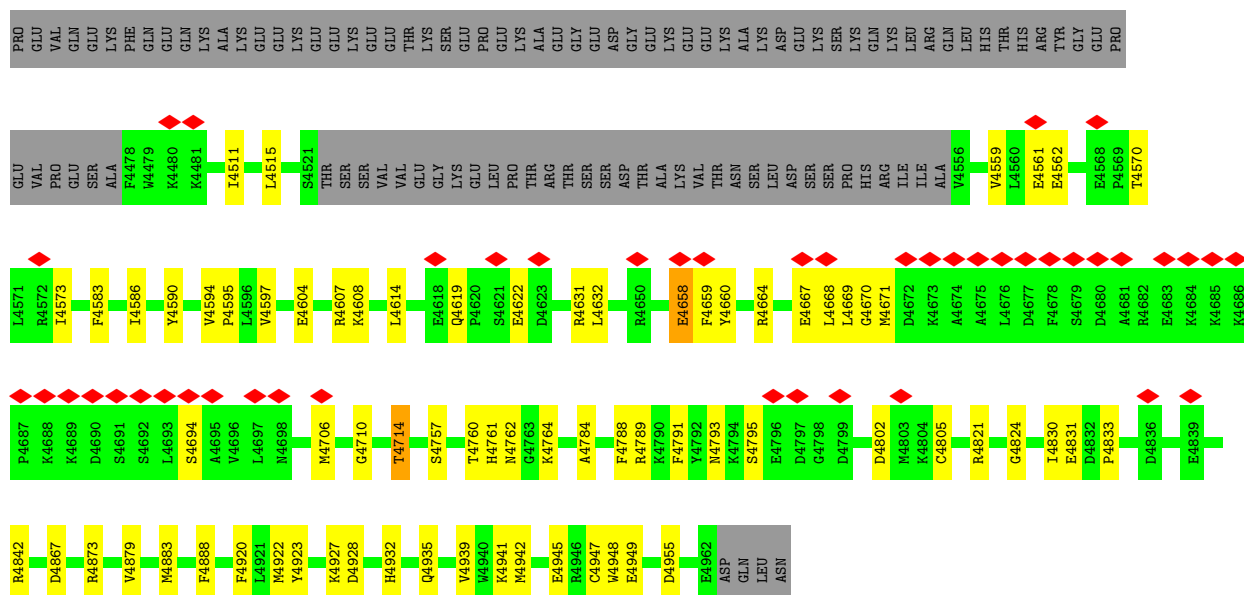




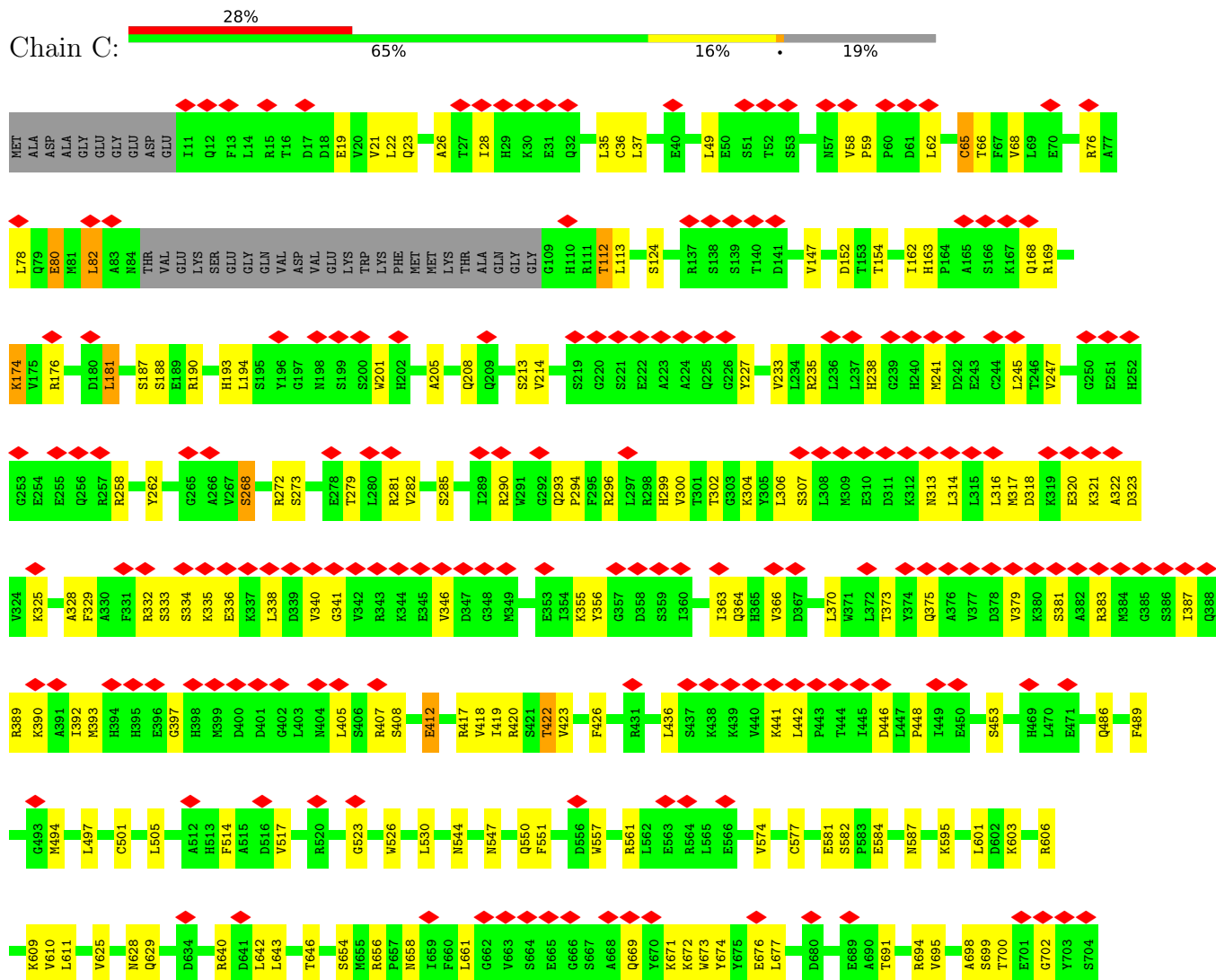








• Molecule 1: Ryanodine receptor 2

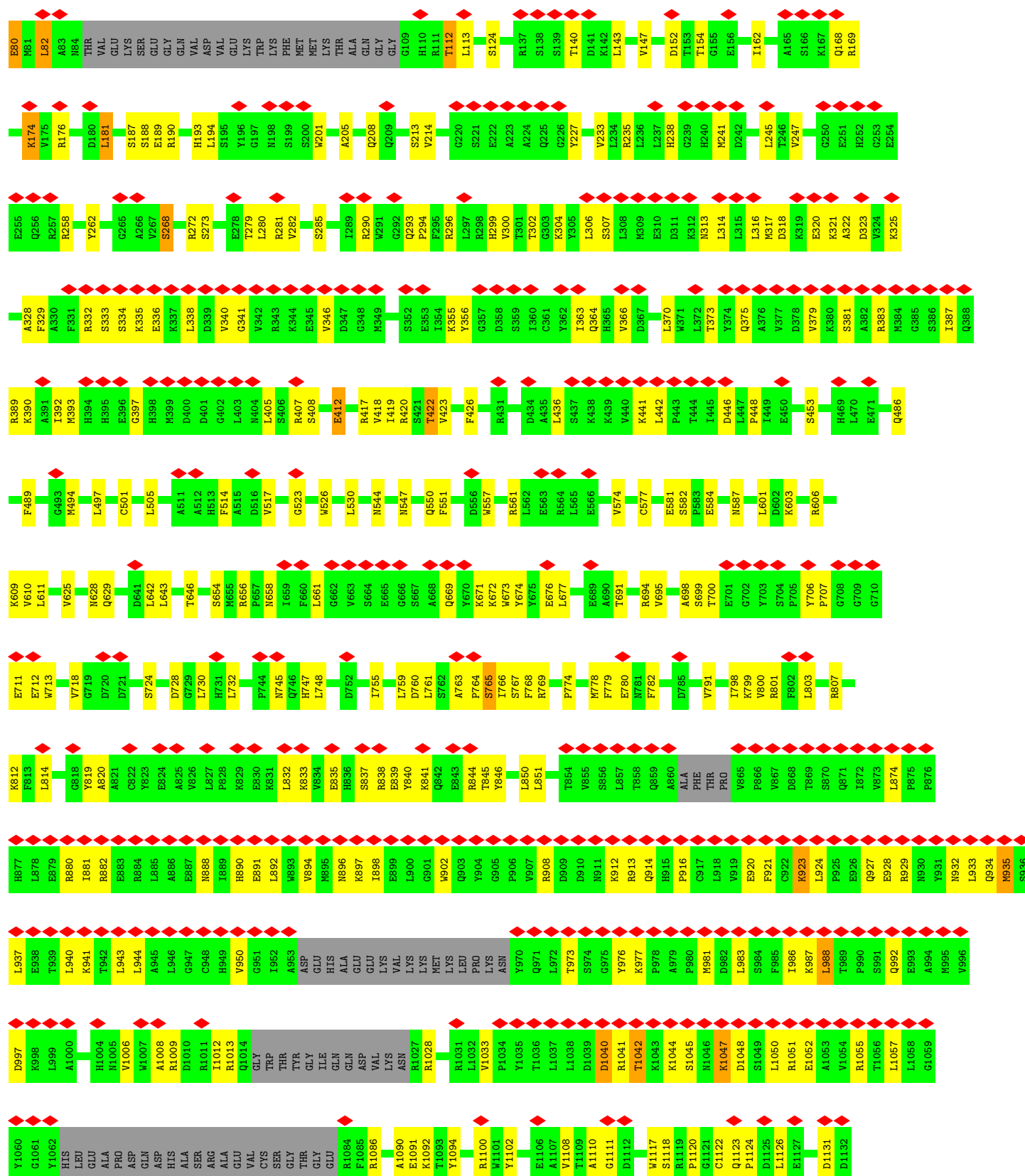


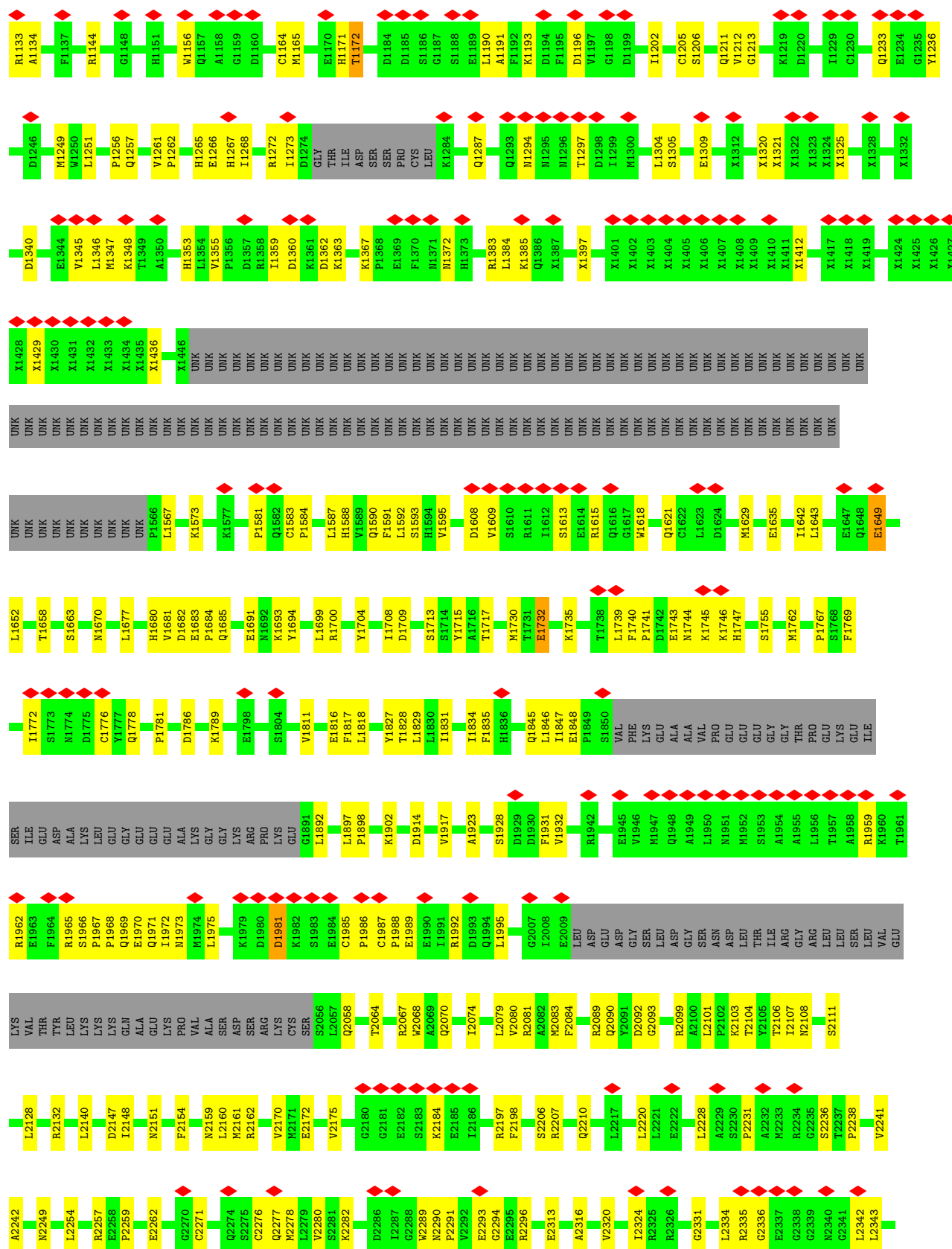






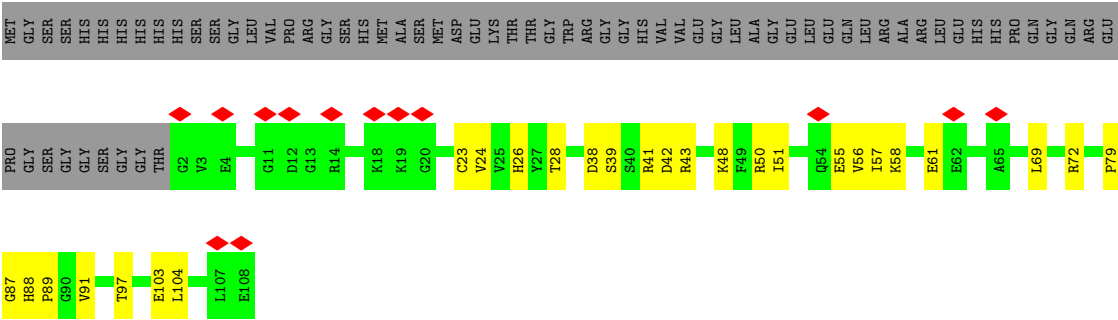




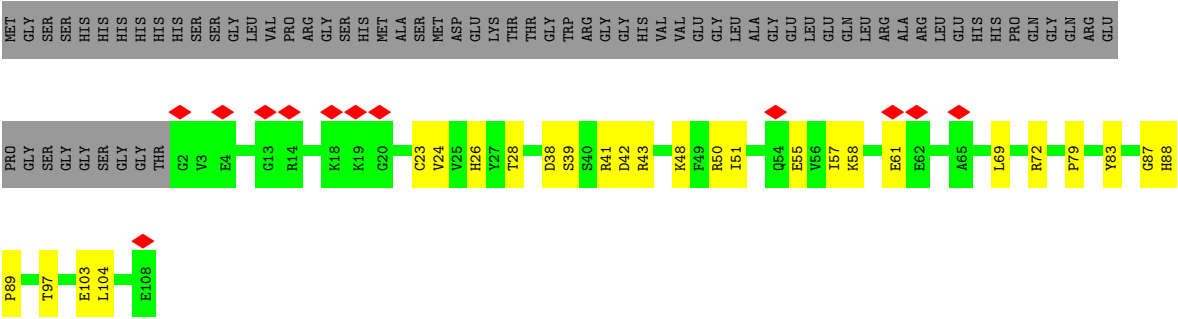


[illegible]

[illegible]



• 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	41197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.076	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.284, 1.284, 1.284	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/26895	0.36	0/36316
1	B	0.14	0/26895	0.36	0/36316
1	C	0.14	0/26895	0.36	0/36316
1	D	0.14	0/26895	0.36	0/36316
2	G	0.11	0/835	0.38	0/1123
2	H	0.11	0/835	0.38	0/1123
2	I	0.11	0/835	0.38	0/1123
2	J	0.11	0/835	0.38	0/1123
All	All	0.14	0/110920	0.36	0/149756

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30071	0	26711	523	0
1	B	30071	0	26711	523	0
1	C	30071	0	26711	524	0
1	D	30071	0	26711	529	0
2	G	819	0	821	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	819	0	821	19	0
2	I	819	0	821	20	0
2	J	819	0	821	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	123564	0	110128	2131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1772:ILE:HD11	2:J:57:ILE:HA	1.57	0.86
1:A:1233:GLN:HG3	1:B:3493:UNK:HA	1.56	0.86
1:A:4833:PRO:HB3	1:A:4842:ARG:HD3	1.61	0.82
1:C:4833:PRO:HB3	1:C:4842:ARG:HD3	1.61	0.81
1:D:76:ARG:O	1:D:80:GLU:HB2	1.81	0.81
1:D:890:HIS:HB2	1:D:932:ASN:HD22	1.46	0.81
1:B:76:ARG:O	1:B:80:GLU:HB2	1.81	0.80
1:D:4833:PRO:HB3	1:D:4842:ARG:HD3	1.61	0.80
1:B:2406:HIS:HA	1:B:2409:HIS:HB3	1.64	0.80
1:A:890:HIS:HB2	1:A:932:ASN:HD22	1.46	0.80
1:D:2406:HIS:HA	1:D:2409:HIS:HB3	1.63	0.80
1:C:76:ARG:O	1:C:80:GLU:HB2	1.81	0.80
1:A:2406:HIS:HA	1:A:2409:HIS:HB3	1.64	0.80
1:C:890:HIS:HB2	1:C:932:ASN:HD22	1.46	0.80
1:C:2406:HIS:HA	1:C:2409:HIS:HB3	1.64	0.80
1:B:4833:PRO:HB3	1:B:4842:ARG:HD3	1.61	0.79
1:B:890:HIS:HB2	1:B:932:ASN:HD22	1.46	0.79
1:A:76:ARG:O	1:A:80:GLU:HB2	1.81	0.79
1:A:1772:ILE:HD11	2:G:57:ILE:HA	1.65	0.78
1:C:1629:MET:HE3	1:C:1685:GLN:HE21	1.49	0.77
1:B:1629:MET:HE3	1:B:1685:GLN:HE21	1.49	0.77
1:A:1629:MET:HE3	1:A:1685:GLN:HE21	1.49	0.76
1:D:1629:MET:HE3	1:D:1685:GLN:HE21	1.49	0.76
1:D:1741:PRO:HB3	1:D:1746:LYS:HE3	1.68	0.75
1:A:1741:PRO:HB3	1:A:1746:LYS:HE3	1.68	0.75
1:C:1741:PRO:HB3	1:C:1746:LYS:HE3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4042:ILE:HG22	1:B:4044:LYS:H	1.53	0.73
1:D:1122:CYS:HA	1:D:1133:ARG:HD3	1.71	0.73
1:C:1122:CYS:HA	1:C:1133:ARG:HD3	1.71	0.73
1:B:1741:PRO:HB3	1:B:1746:LYS:HE3	1.68	0.73
1:C:4042:ILE:HG22	1:C:4044:LYS:H	1.53	0.73
1:A:4042:ILE:HG22	1:A:4044:LYS:H	1.53	0.73
1:D:4042:ILE:HG22	1:D:4044:LYS:H	1.53	0.72
1:B:1989:GLU:HG2	1:B:1992:ARG:HD3	1.72	0.72
1:A:1122:CYS:HA	1:A:1133:ARG:HD3	1.71	0.72
1:C:1262:PRO:HG2	1:C:1265:HIS:HB2	1.72	0.72
1:A:1262:PRO:HG2	1:A:1265:HIS:HB2	1.72	0.72
1:A:1989:GLU:HG2	1:A:1992:ARG:HD3	1.72	0.72
1:C:279:THR:HG22	1:C:281:ARG:H	1.55	0.72
1:B:1122:CYS:HA	1:B:1133:ARG:HD3	1.71	0.72
1:D:1262:PRO:HG2	1:D:1265:HIS:HB2	1.72	0.72
1:B:279:THR:HG22	1:B:281:ARG:H	1.55	0.71
1:C:1989:GLU:HG2	1:C:1992:ARG:HD3	1.72	0.71
1:B:760:ASP:HB3	1:B:764:PRO:HG2	1.73	0.71
1:D:920:GLU:HB2	1:D:923:LYS:HB2	1.73	0.71
1:A:279:THR:HG22	1:A:281:ARG:H	1.55	0.71
1:B:1262:PRO:HG2	1:B:1265:HIS:HB2	1.72	0.71
1:C:4867:ASP:OD1	1:D:4873:ARG:NH1	2.23	0.71
1:C:920:GLU:HB2	1:C:923:LYS:HB2	1.72	0.71
1:A:920:GLU:HB2	1:A:923:LYS:HB2	1.73	0.71
1:A:760:ASP:HB3	1:A:764:PRO:HG2	1.73	0.71
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.73	0.70
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.73	0.70
1:D:1989:GLU:HG2	1:D:1992:ARG:HD3	1.72	0.70
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.73	0.70
1:C:1681:VAL:HG23	1:C:1682:ASP:H	1.55	0.70
1:C:2128:LEU:HD11	1:C:2140:LEU:HD12	1.73	0.70
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.74	0.70
1:D:279:THR:HG22	1:D:281:ARG:H	1.55	0.70
1:A:162:ILE:HD11	1:A:181:LEU:HD13	1.74	0.70
1:C:4824:GLY:O	1:D:4821:ARG:NH2	2.24	0.70
1:D:2128:LEU:HD11	1:D:2140:LEU:HD12	1.73	0.70
2:J:24:VAL:HG22	2:J:48:LYS:HG2	1.74	0.70
1:A:1681:VAL:HG23	1:A:1682:ASP:H	1.55	0.70
1:A:2502:ASP:OD1	1:A:2503:THR:N	2.25	0.70
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.73	0.69
1:B:920:GLU:HB2	1:B:923:LYS:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:HD11	1:C:181:LEU:HD13	1.74	0.69
1:D:162:ILE:HD11	1:D:181:LEU:HD13	1.74	0.69
1:D:760:ASP:HB3	1:D:764:PRO:HG2	1.73	0.69
2:I:24:VAL:HG22	2:I:48:LYS:HG2	1.74	0.69
1:D:1681:VAL:HG23	1:D:1682:ASP:H	1.55	0.69
1:A:2128:LEU:HD11	1:A:2140:LEU:HD12	1.73	0.69
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.74	0.69
1:B:162:ILE:HD11	1:B:181:LEU:HD13	1.74	0.69
1:C:671:LYS:HB3	1:C:761:LEU:HB2	1.75	0.69
1:B:1233:GLN:HG3	1:C:3493:UNK:HA	1.73	0.69
1:B:671:LYS:HB3	1:B:761:LEU:HB2	1.75	0.69
1:B:1681:VAL:HG23	1:B:1682:ASP:H	1.55	0.68
1:B:2128:LEU:HD11	1:B:2140:LEU:HD12	1.73	0.68
1:A:412:GLU:OE2	1:A:412:GLU:N	2.26	0.68
1:D:671:LYS:HB3	1:D:761:LEU:HB2	1.75	0.68
1:B:2502:ASP:OD1	1:B:2503:THR:N	2.24	0.68
1:C:760:ASP:HB3	1:C:764:PRO:HG2	1.73	0.68
1:A:671:LYS:HB3	1:A:761:LEU:HB2	1.75	0.68
1:D:412:GLU:N	1:D:412:GLU:OE2	2.26	0.68
2:G:69:LEU:HA	2:G:104:LEU:HD22	1.76	0.68
1:C:412:GLU:N	1:C:412:GLU:OE2	2.26	0.67
1:B:412:GLU:N	1:B:412:GLU:OE2	2.27	0.67
2:J:69:LEU:HA	2:J:104:LEU:HD22	1.76	0.67
1:A:1044:LYS:HD2	1:A:1051:ARG:HH12	1.59	0.67
1:C:2502:ASP:OD1	1:C:2503:THR:N	2.25	0.67
1:B:1044:LYS:HD2	1:B:1051:ARG:HH12	1.59	0.67
1:D:3831:ASP:HB3	1:D:3834:PHE:HB3	1.77	0.67
1:B:908:ARG:HG2	1:B:916:PRO:HG3	1.77	0.67
1:A:486:GLN:HB3	1:A:544:ASN:HD21	1.59	0.67
1:B:486:GLN:HB3	1:B:544:ASN:HD21	1.59	0.67
1:C:3831:ASP:HB3	1:C:3834:PHE:HB3	1.77	0.66
1:D:1044:LYS:HD2	1:D:1051:ARG:HH12	1.59	0.66
1:B:1684:PRO:HD3	2:H:42:ASP:HB3	1.77	0.66
1:B:544:ASN:ND2	1:B:547:ASN:OD1	2.29	0.66
2:I:69:LEU:HA	2:I:104:LEU:HD22	1.76	0.66
1:C:486:GLN:HB3	1:C:544:ASN:HD21	1.59	0.66
1:C:1272:ARG:NH2	1:C:1584:PRO:O	2.29	0.66
1:B:1772:ILE:HD11	2:H:57:ILE:HA	1.78	0.66
1:A:544:ASN:ND2	1:A:547:ASN:OD1	2.29	0.66
1:A:940:LEU:HA	1:A:943:LEU:HD12	1.78	0.66
1:C:908:ARG:HG2	1:C:916:PRO:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:LYS:HD2	1:C:1051:ARG:HH12	1.59	0.66
1:C:2084:PHE:O	1:C:3690:TYR:OH	2.14	0.66
1:A:1272:ARG:NH2	1:A:1584:PRO:O	2.29	0.66
1:A:3831:ASP:HB3	1:A:3834:PHE:HB3	1.77	0.66
1:B:1272:ARG:NH2	1:B:1584:PRO:O	2.29	0.66
2:H:69:LEU:HA	2:H:104:LEU:HD22	1.76	0.66
1:D:908:ARG:HG2	1:D:916:PRO:HG3	1.77	0.66
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.29	0.66
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.29	0.66
1:B:2084:PHE:O	1:B:3690:TYR:OH	2.14	0.65
1:C:880:ARG:HG3	1:C:881:ILE:HD12	1.78	0.65
1:D:940:LEU:HA	1:D:943:LEU:HD12	1.78	0.65
1:A:908:ARG:HG2	1:A:916:PRO:HG3	1.77	0.65
1:B:3831:ASP:HB3	1:B:3834:PHE:HB3	1.77	0.65
1:B:4042:ILE:HG21	1:B:4047:PHE:HB2	1.79	0.65
1:A:1266:GLU:O	1:A:1267:HIS:ND1	2.30	0.65
1:C:544:ASN:ND2	1:C:547:ASN:OD1	2.29	0.65
1:C:1266:GLU:O	1:C:1267:HIS:ND1	2.30	0.65
1:D:694:ARG:HG2	1:D:728:ASP:HB3	1.78	0.65
1:A:4042:ILE:HG21	1:A:4047:PHE:HB2	1.79	0.65
1:B:1266:GLU:O	1:B:1267:HIS:ND1	2.30	0.65
1:A:4619:GLN:HE22	1:A:4631:ARG:HH12	1.43	0.65
1:D:486:GLN:HB3	1:D:544:ASN:HD21	1.59	0.65
1:D:544:ASN:ND2	1:D:547:ASN:OD1	2.29	0.65
1:B:4619:GLN:HE22	1:B:4631:ARG:HH12	1.43	0.65
1:C:694:ARG:HG2	1:C:728:ASP:HB3	1.78	0.65
1:D:880:ARG:HG3	1:D:881:ILE:HD12	1.78	0.65
1:D:1266:GLU:O	1:D:1267:HIS:ND1	2.30	0.65
1:D:2084:PHE:O	1:D:3690:TYR:OH	2.14	0.65
1:B:3954:GLN:NE2	1:B:3974:GLN:OE1	2.30	0.65
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.80	0.64
1:A:3954:GLN:NE2	1:A:3974:GLN:OE1	2.30	0.64
1:B:694:ARG:HG2	1:B:728:ASP:HB3	1.78	0.64
1:B:880:ARG:HG3	1:B:881:ILE:HD12	1.78	0.64
1:B:2074:ILE:HG21	1:B:2079:LEU:HD22	1.80	0.64
1:C:940:LEU:HA	1:C:943:LEU:HD12	1.78	0.64
1:C:4042:ILE:HG21	1:C:4047:PHE:HB2	1.79	0.64
1:B:940:LEU:HA	1:B:943:LEU:HD12	1.78	0.64
1:C:3954:GLN:NE2	1:C:3974:GLN:OE1	2.30	0.64
1:C:1684:PRO:HD3	2:I:42:ASP:HB3	1.79	0.64
1:D:1272:ARG:NH2	1:D:1584:PRO:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.29	0.64
1:D:3954:GLN:NE2	1:D:3974:GLN:OE1	2.30	0.64
1:A:3754:VAL:HA	1:A:3757:THR:HG22	1.80	0.64
1:D:1613:SER:O	1:D:1615:ARG:NH2	2.31	0.64
1:D:2074:ILE:HG21	1:D:2079:LEU:HD22	1.80	0.64
1:A:1613:SER:O	1:A:1615:ARG:NH2	2.31	0.64
1:A:2074:ILE:HG21	1:A:2079:LEU:HD22	1.80	0.64
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.79	0.64
1:D:3754:VAL:HA	1:D:3757:THR:HG22	1.80	0.64
1:A:694:ARG:HG2	1:A:728:ASP:HB3	1.78	0.64
1:A:880:ARG:HG3	1:A:881:ILE:HD12	1.78	0.64
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.29	0.64
1:A:2084:PHE:O	1:A:3690:TYR:OH	2.14	0.64
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.80	0.64
1:B:2220:LEU:HD11	1:B:2242:ALA:HB2	1.80	0.64
1:C:3754:VAL:HA	1:C:3757:THR:HG22	1.80	0.64
1:D:2502:ASP:OD1	1:D:2503:THR:N	2.24	0.64
1:C:2074:ILE:HG21	1:C:2079:LEU:HD22	1.80	0.64
1:D:4042:ILE:HG21	1:D:4047:PHE:HB2	1.79	0.64
1:C:1769:PHE:O	2:I:83:TYR:OH	2.16	0.63
1:C:4710:GLY:O	1:C:4714:THR:OG1	2.17	0.63
1:B:3754:VAL:HA	1:B:3757:THR:HG22	1.80	0.63
1:C:1902:LYS:HG3	1:C:2079:LEU:HD11	1.80	0.63
1:D:1902:LYS:HG3	1:D:2079:LEU:HD11	1.80	0.63
1:C:1092:LYS:HG2	1:C:1120:PRO:HB3	1.81	0.63
1:C:1613:SER:O	1:C:1615:ARG:NH2	2.31	0.63
1:C:2220:LEU:HD11	1:C:2242:ALA:HB2	1.80	0.63
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.80	0.63
1:C:2092:ASP:OD1	1:C:2093:GLY:N	2.31	0.63
1:C:4619:GLN:HE22	1:C:4631:ARG:HH12	1.44	0.63
1:D:2092:ASP:OD1	1:D:2093:GLY:N	2.31	0.63
1:D:4710:GLY:O	1:D:4714:THR:OG1	2.17	0.63
1:A:2220:LEU:HD11	1:A:2242:ALA:HB2	1.80	0.63
1:B:1902:LYS:HG3	1:B:2079:LEU:HD11	1.80	0.63
1:B:2092:ASP:OD1	1:B:2093:GLY:N	2.31	0.63
1:D:1092:LYS:HG2	1:D:1120:PRO:HB3	1.81	0.63
1:D:4619:GLN:HE22	1:D:4631:ARG:HH12	1.43	0.63
1:D:1359:ILE:HG13	1:D:1360:ASP:H	1.64	0.62
1:D:2099:ARG:O	1:D:2103:LYS:NZ	2.32	0.62
1:A:4710:GLY:O	1:A:4714:THR:OG1	2.16	0.62
1:B:1613:SER:O	1:B:1615:ARG:NH2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:LYS:HG2	1:A:1120:PRO:HB3	1.80	0.62
1:D:1744:ASN:HD21	1:D:1746:LYS:HE2	1.65	0.62
1:A:2335:ARG:NE	1:D:143:LEU:HD21	2.15	0.62
1:D:1588:HIS:HE1	1:D:1590:GLN:HE21	1.48	0.62
1:A:1359:ILE:HG13	1:A:1360:ASP:H	1.64	0.62
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.82	0.62
1:B:1981:ASP:OD1	1:B:1981:ASP:N	2.32	0.62
1:C:988:LEU:HD23	1:C:992:GLN:HB2	1.81	0.62
1:A:1588:HIS:HE1	1:A:1590:GLN:HE21	1.48	0.62
1:A:2092:ASP:OD1	1:A:2093:GLY:N	2.31	0.62
1:B:1730:MET:SD	1:B:2106:THR:OG1	2.58	0.62
1:B:3845:LEU:HB3	1:B:3853:PHE:CE2	2.35	0.62
1:D:1981:ASP:OD1	1:D:1981:ASP:N	2.32	0.62
1:D:3845:LEU:HB3	1:D:3853:PHE:CE2	2.35	0.62
1:A:1265:HIS:HD2	1:A:1268:ILE:HB	1.64	0.62
1:A:1902:LYS:HG3	1:A:2079:LEU:HD11	1.80	0.62
1:A:3845:LEU:HB3	1:A:3853:PHE:CE2	2.35	0.62
1:C:759:LEU:HD13	1:C:766:ILE:HG12	1.82	0.62
1:C:1359:ILE:HG13	1:C:1360:ASP:H	1.64	0.62
1:C:3845:LEU:HB3	1:C:3853:PHE:CE2	2.35	0.62
1:B:1588:HIS:HE1	1:B:1590:GLN:HE21	1.48	0.62
1:B:1297:THR:HA	1:B:1346:LEU:HD23	1.82	0.62
1:C:1171:HIS:HB2	1:C:1193:LYS:HZ2	1.64	0.62
1:C:1297:THR:HA	1:C:1346:LEU:HD23	1.82	0.62
1:D:2220:LEU:HD11	1:D:2242:ALA:HB2	1.80	0.62
1:A:4659:PHE:O	1:B:4055:LYS:NZ	2.25	0.61
1:B:759:LEU:HD13	1:B:766:ILE:HG12	1.82	0.61
1:B:4710:GLY:O	1:B:4714:THR:OG1	2.17	0.61
1:C:1588:HIS:HE1	1:C:1590:GLN:HE21	1.48	0.61
1:D:988:LEU:HD23	1:D:992:GLN:HB2	1.81	0.61
1:A:759:LEU:HD13	1:A:766:ILE:HG12	1.82	0.61
1:A:1730:MET:SD	1:A:2106:THR:OG1	2.58	0.61
1:B:2099:ARG:O	1:B:2103:LYS:NZ	2.32	0.61
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.82	0.61
1:D:4044:LYS:HB2	1:D:4075:GLU:HG2	1.82	0.61
1:B:1092:LYS:HG2	1:B:1120:PRO:HB3	1.81	0.61
1:B:1265:HIS:HD2	1:B:1268:ILE:HB	1.64	0.61
1:C:1265:HIS:HD2	1:C:1268:ILE:HB	1.64	0.61
1:C:2099:ARG:O	1:C:2103:LYS:NZ	2.32	0.61
1:C:4044:LYS:HB2	1:C:4075:GLU:HG2	1.82	0.61
1:A:4044:LYS:HB2	1:A:4075:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1744:ASN:HD21	1:B:1746:LYS:HE2	1.65	0.61
1:B:4044:LYS:HB2	1:B:4075:GLU:HG2	1.82	0.61
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.82	0.61
1:D:759:LEU:HD13	1:D:766:ILE:HG12	1.82	0.61
1:A:1684:PRO:HD3	2:G:42:ASP:HB3	1.82	0.61
1:A:1744:ASN:HD21	1:A:1746:LYS:HE2	1.65	0.61
1:B:988:LEU:HD23	1:B:992:GLN:HB2	1.82	0.61
1:B:1359:ILE:HG13	1:B:1360:ASP:H	1.64	0.61
1:D:1829:LEU:HB3	1:D:1834:ILE:HD11	1.83	0.61
1:B:235:ARG:NH1	1:B:268:SER:O	2.34	0.61
1:B:1829:LEU:HB3	1:B:1834:ILE:HD11	1.83	0.61
1:A:839:GLU:H	1:A:841:LYS:NZ	1.99	0.61
1:B:290:ARG:H	1:B:293:GLN:HE21	1.48	0.61
1:B:839:GLU:H	1:B:841:LYS:NZ	1.99	0.61
1:D:290:ARG:H	1:D:293:GLN:HE21	1.48	0.61
1:D:839:GLU:H	1:D:841:LYS:NZ	1.99	0.61
1:A:1829:LEU:HB3	1:A:1834:ILE:HD11	1.83	0.60
1:B:1847:ILE:HG23	1:B:1892:LEU:HB3	1.83	0.60
1:D:1297:THR:HA	1:D:1346:LEU:HD23	1.82	0.60
1:A:235:ARG:NH1	1:A:268:SER:O	2.34	0.60
1:A:1297:THR:HA	1:A:1346:LEU:HD23	1.82	0.60
1:B:373:THR:HG22	1:B:397:GLY:HA2	1.83	0.60
1:C:1730:MET:SD	1:C:2106:THR:OG1	2.58	0.60
1:A:375:GLN:NE2	1:A:390:LYS:O	2.34	0.60
1:C:839:GLU:H	1:C:841:LYS:NZ	1.99	0.60
1:C:1829:LEU:HB3	1:C:1834:ILE:HD11	1.83	0.60
1:D:235:ARG:NH1	1:D:268:SER:O	2.34	0.60
1:D:2228:LEU:HD22	1:D:2296:ARG:HG3	1.83	0.60
1:A:2228:LEU:HD22	1:A:2296:ARG:HG3	1.84	0.60
1:C:375:GLN:NE2	1:C:390:LYS:O	2.34	0.60
1:C:1267:HIS:HB2	1:C:1294:ASN:HB2	1.84	0.60
1:C:1744:ASN:HD21	1:C:1746:LYS:HE2	1.65	0.60
1:D:375:GLN:NE2	1:D:390:LYS:O	2.34	0.60
1:D:1265:HIS:HD2	1:D:1268:ILE:HB	1.64	0.60
1:C:3995:GLY:O	1:C:3999:VAL:HG12	2.02	0.60
1:D:1847:ILE:HG23	1:D:1892:LEU:HB3	1.83	0.60
1:A:1267:HIS:HB2	1:A:1294:ASN:HB2	1.84	0.60
1:B:1267:HIS:HB2	1:B:1294:ASN:HB2	1.84	0.60
1:B:3995:GLY:O	1:B:3999:VAL:HG12	2.02	0.60
1:C:2228:LEU:HD22	1:C:2296:ARG:HG3	1.84	0.60
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3731:HIS:O	1:D:3775:LYS:NZ	2.35	0.60
1:A:290:ARG:H	1:A:293:GLN:HE21	1.48	0.60
1:A:988:LEU:HD23	1:A:992:GLN:HB2	1.81	0.60
1:C:373:THR:HG22	1:C:397:GLY:HA2	1.83	0.60
1:D:1171:HIS:HB2	1:D:1193:LYS:HZ2	1.67	0.60
1:D:3995:GLY:O	1:D:3999:VAL:HG12	2.02	0.60
1:A:1171:HIS:HB2	1:A:1193:LYS:HZ3	1.65	0.60
1:B:375:GLN:NE2	1:B:390:LYS:O	2.34	0.60
1:C:379:VAL:HG13	1:C:381:SER:H	1.67	0.60
1:D:2064:THR:HG22	1:D:2067:ARG:HH12	1.67	0.60
1:C:235:ARG:NH1	1:C:268:SER:O	2.34	0.60
1:A:3995:GLY:O	1:A:3999:VAL:HG12	2.02	0.59
1:B:2228:LEU:HD22	1:B:2296:ARG:HG3	1.83	0.59
1:C:317:MET:HE3	1:C:322:ALA:HA	1.84	0.59
1:C:844:ARG:HE	1:C:845:THR:H	1.50	0.59
1:D:317:MET:HE3	1:D:322:ALA:HA	1.84	0.59
1:C:1847:ILE:HG23	1:C:1892:LEU:HB3	1.83	0.59
1:A:4784:ALA:HA	1:A:4788:PHE:HD2	1.68	0.59
1:B:426:PHE:HB3	1:B:497:LEU:HD21	1.85	0.59
1:D:379:VAL:HG13	1:D:381:SER:H	1.67	0.59
1:A:373:THR:HG22	1:A:397:GLY:HA2	1.83	0.59
1:A:1847:ILE:HG23	1:A:1892:LEU:HB3	1.83	0.59
1:A:2873:TYR:HA	1:A:2876:LEU:HD13	1.85	0.59
1:B:4784:ALA:HA	1:B:4788:PHE:HD2	1.68	0.59
1:D:1267:HIS:HB2	1:D:1294:ASN:HB2	1.84	0.59
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.68	0.59
1:B:2064:THR:HG22	1:B:2067:ARG:HH12	1.67	0.59
1:B:1171:HIS:HB2	1:B:1193:LYS:HZ3	1.66	0.59
1:D:373:THR:HG22	1:D:397:GLY:HA2	1.83	0.59
1:B:2873:TYR:HA	1:B:2876:LEU:HD13	1.85	0.59
1:C:418:VAL:O	1:C:422:THR:HG22	2.03	0.59
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.68	0.59
1:C:2064:THR:HG22	1:C:2067:ARG:HH12	1.67	0.59
1:D:2484:LEU:O	1:D:2488:GLU:HG2	2.03	0.59
1:A:426:PHE:HB3	1:A:497:LEU:HD21	1.85	0.59
1:A:4873:ARG:NH1	1:D:4867:ASP:OD1	2.36	0.59
1:C:290:ARG:H	1:C:293:GLN:HE21	1.48	0.59
1:D:4784:ALA:HA	1:D:4788:PHE:HD2	1.67	0.59
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.68	0.58
1:A:418:VAL:O	1:A:422:THR:HG22	2.03	0.58
1:B:418:VAL:O	1:B:422:THR:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2484:LEU:O	1:A:2488:GLU:HG2	2.03	0.58
1:B:2484:LEU:O	1:B:2488:GLU:HG2	2.03	0.58
1:A:1827:TYR:CZ	1:A:1831:ILE:HD11	2.39	0.58
1:C:426:PHE:HB3	1:C:497:LEU:HD21	1.85	0.58
1:C:3731:HIS:O	1:C:3775:LYS:NZ	2.35	0.58
1:C:4784:ALA:HA	1:C:4788:PHE:HD2	1.68	0.58
1:D:1827:TYR:CZ	1:D:1831:ILE:HD11	2.39	0.58
1:B:379:VAL:HG13	1:B:381:SER:H	1.67	0.58
1:C:2873:TYR:HA	1:C:2876:LEU:HD13	1.85	0.58
1:D:844:ARG:HE	1:D:845:THR:H	1.50	0.58
1:A:317:MET:HE3	1:A:322:ALA:HA	1.84	0.58
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.68	0.58
1:A:2064:THR:HG22	1:A:2067:ARG:HH12	1.67	0.58
1:A:3731:HIS:O	1:A:3775:LYS:NZ	2.35	0.58
1:B:844:ARG:HE	1:B:845:THR:H	1.50	0.58
1:B:3999:VAL:O	1:B:4003:VAL:HG12	2.04	0.58
2:H:39:SER:O	2:H:43:ARG:NH1	2.37	0.58
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.68	0.58
1:D:418:VAL:O	1:D:422:THR:HG22	2.03	0.58
1:B:317:MET:HE3	1:B:322:ALA:HA	1.84	0.58
1:D:426:PHE:HB3	1:D:497:LEU:HD21	1.85	0.58
1:C:36:CYS:SG	1:C:37:LEU:N	2.77	0.58
1:C:1827:TYR:CZ	1:C:1831:ILE:HD11	2.38	0.58
1:D:1044:LYS:HA	1:D:1047:LYS:HZ3	1.69	0.58
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.68	0.58
1:B:3731:HIS:O	1:B:3775:LYS:NZ	2.35	0.58
1:C:2484:LEU:O	1:C:2488:GLU:HG2	2.03	0.58
1:D:2873:TYR:HA	1:D:2876:LEU:HD13	1.84	0.58
1:A:36:CYS:SG	1:A:37:LEU:N	2.77	0.58
1:A:844:ARG:HE	1:A:845:THR:H	1.50	0.58
1:B:934:GLN:HA	1:B:937:LEU:HD12	1.85	0.58
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.86	0.58
1:C:2434:VAL:HG11	1:C:2467:MET:HE2	1.86	0.58
1:C:3999:VAL:O	1:C:4003:VAL:HG12	2.04	0.58
1:D:838:ARG:H	1:D:841:LYS:NZ	2.02	0.58
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.68	0.58
1:A:379:VAL:HG13	1:A:381:SER:H	1.67	0.57
1:A:2099:ARG:O	1:A:2103:LYS:NZ	2.32	0.57
1:B:36:CYS:SG	1:B:37:LEU:N	2.77	0.57
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.37	0.57
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:934:GLN:HA	1:D:937:LEU:HD12	1.85	0.57
1:B:1827:TYR:CZ	1:B:1831:ILE:HD11	2.38	0.57
1:C:890:HIS:HB2	1:C:932:ASN:ND2	2.19	0.57
2:I:39:SER:O	2:I:43:ARG:NH1	2.37	0.57
1:D:2408:ILE:O	1:D:2412:LYS:HB2	2.05	0.57
1:A:700:THR:HG1	1:A:787:LEU:H	1.52	0.57
1:D:36:CYS:SG	1:D:37:LEU:N	2.77	0.57
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.86	0.57
1:C:1110:ALA:HA	1:C:1156:TRP:HE1	1.69	0.57
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.86	0.57
1:D:2159:ASN:OD1	1:D:2162:ARG:NH2	2.37	0.57
1:B:2210:GLN:OE1	1:B:2249:ASN:ND2	2.38	0.57
1:A:838:ARG:H	1:A:841:LYS:NZ	2.02	0.57
1:A:1383:ARG:HE	1:A:1385:LYS:HE2	1.70	0.57
1:B:2434:VAL:HG11	1:B:2467:MET:HE2	1.86	0.57
1:B:2867:HIS:HE2	1:B:2869:LEU:HD12	1.69	0.57
1:C:838:ARG:H	1:C:841:LYS:NZ	2.02	0.57
1:C:1383:ARG:HE	1:C:1385:LYS:HE2	1.70	0.57
1:C:2408:ILE:O	1:C:2412:LYS:HB2	2.05	0.57
1:A:934:GLN:HA	1:A:937:LEU:HD12	1.85	0.57
1:A:1044:LYS:HA	1:A:1047:LYS:HZ3	1.68	0.57
1:A:1981:ASP:OD1	1:A:1981:ASP:N	2.32	0.57
1:A:2867:HIS:HE2	1:A:2869:LEU:HD12	1.70	0.57
1:B:4941:LYS:O	1:B:4945:GLU:HG2	2.05	0.57
1:C:934:GLN:HA	1:C:937:LEU:HD12	1.85	0.57
1:C:2210:GLN:OE1	1:C:2249:ASN:ND2	2.38	0.57
1:D:3999:VAL:O	1:D:4003:VAL:HG12	2.04	0.57
1:B:1383:ARG:HE	1:B:1385:LYS:HE2	1.70	0.57
1:C:2276:CYS:SG	1:C:2290:ASN:ND2	2.78	0.57
1:D:1730:MET:SD	1:D:2106:THR:OG1	2.58	0.57
1:D:2867:HIS:HE2	1:D:2869:LEU:HD12	1.70	0.57
2:J:39:SER:O	2:J:43:ARG:NH1	2.37	0.57
1:A:1110:ALA:HA	1:A:1156:TRP:HE1	1.69	0.57
1:A:3999:VAL:O	1:A:4003:VAL:HG12	2.04	0.57
1:B:2276:CYS:SG	1:B:2290:ASN:ND2	2.78	0.57
1:D:2210:GLN:OE1	1:D:2249:ASN:ND2	2.38	0.57
1:A:677:LEU:HD22	1:A:695:VAL:HG21	1.87	0.56
1:A:1190:LEU:HD11	1:A:1193:LYS:HB2	1.87	0.56
1:A:2408:ILE:O	1:A:2412:LYS:HB2	2.05	0.56
1:D:1383:ARG:HE	1:D:1385:LYS:HE2	1.70	0.56
1:B:677:LEU:HD22	1:B:695:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1190:LEU:HD11	1:B:1193:LYS:HB2	1.87	0.56
1:D:1040:ASP:OD1	1:D:1040:ASP:N	2.35	0.56
1:A:4049:LYS:HA	1:A:4052:GLU:HG2	1.87	0.56
2:G:39:SER:O	2:G:43:ARG:NH1	2.37	0.56
1:B:838:ARG:H	1:B:841:LYS:NZ	2.02	0.56
1:B:1044:LYS:HA	1:B:1047:LYS:HZ3	1.70	0.56
1:C:1772:ILE:HD11	2:I:57:ILE:HA	1.87	0.56
1:C:2159:ASN:OD1	1:C:2162:ARG:NH2	2.37	0.56
2:I:79:PRO:HD3	2:I:97:THR:HG22	1.86	0.56
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.68	0.56
1:D:2107:ILE:HG23	1:D:2108:ASN:H	1.70	0.56
1:D:2434:VAL:HG11	1:D:2467:MET:HE2	1.86	0.56
1:A:2107:ILE:HG23	1:A:2108:ASN:H	1.70	0.56
2:G:79:PRO:HD3	2:G:97:THR:HG22	1.86	0.56
1:B:1110:ALA:HA	1:B:1156:TRP:HE1	1.69	0.56
1:B:1117:TRP:HE1	1:B:1164:CYS:HB3	1.71	0.56
1:B:4049:LYS:HA	1:B:4052:GLU:HG2	1.87	0.56
1:D:227:TYR:HA	1:D:355:LYS:HA	1.88	0.56
1:D:1110:ALA:HA	1:D:1156:TRP:HE1	1.69	0.56
1:A:2210:GLN:OE1	1:A:2249:ASN:ND2	2.38	0.56
1:A:4941:LYS:O	1:A:4945:GLU:HG2	2.05	0.56
1:C:677:LEU:HD22	1:C:695:VAL:HG21	1.88	0.56
1:D:677:LEU:HD22	1:D:695:VAL:HG21	1.87	0.56
1:D:2147:ASP:O	1:D:2151:ASN:ND2	2.39	0.56
1:D:3729:ARG:O	1:D:3733:ARG:NH1	2.39	0.56
1:B:2408:ILE:O	1:B:2412:LYS:HB2	2.05	0.56
1:C:3891:TYR:O	1:C:3956:LYS:NZ	2.39	0.56
1:D:2276:CYS:SG	1:D:2290:ASN:ND2	2.78	0.56
1:D:2289:TRP:CZ2	1:D:2387:ILE:HD12	2.41	0.56
2:J:79:PRO:HD3	2:J:97:THR:HG22	1.86	0.56
1:A:1117:TRP:HE1	1:A:1164:CYS:HB3	1.71	0.56
1:C:1044:LYS:HA	1:C:1047:LYS:HZ3	1.71	0.56
1:A:2434:VAL:HG11	1:A:2467:MET:HE2	1.86	0.56
1:A:3729:ARG:O	1:A:3733:ARG:NH1	2.39	0.56
1:A:3891:TYR:O	1:A:3956:LYS:NZ	2.39	0.56
1:B:676:GLU:HB2	1:B:803:LEU:HB2	1.86	0.56
1:C:2289:TRP:CZ2	1:C:2387:ILE:HD12	2.41	0.56
1:C:2867:HIS:HE2	1:C:2869:LEU:HD12	1.69	0.56
1:D:1190:LEU:HD11	1:D:1193:LYS:HB2	1.88	0.56
1:A:2276:CYS:SG	1:A:2290:ASN:ND2	2.78	0.56
1:B:1131:ASP:HB3	1:B:1133:ARG:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2107:ILE:HG23	1:B:2108:ASN:H	1.70	0.56
1:B:2147:ASP:O	1:B:2151:ASN:ND2	2.39	0.56
1:C:2107:ILE:HG23	1:C:2108:ASN:H	1.70	0.56
1:D:890:HIS:HB2	1:D:932:ASN:ND2	2.19	0.56
1:D:3891:TYR:O	1:D:3956:LYS:NZ	2.39	0.56
1:A:227:TYR:HA	1:A:355:LYS:HA	1.87	0.55
1:C:718:VAL:HG11	1:C:791:VAL:HG13	1.88	0.55
1:C:1123:GLN:HB2	1:C:1126:LEU:HB2	1.88	0.55
1:D:1117:TRP:HE1	1:D:1164:CYS:HB3	1.71	0.55
1:D:4941:LYS:O	1:D:4945:GLU:HG2	2.05	0.55
1:A:2147:ASP:O	1:A:2151:ASN:ND2	2.39	0.55
1:B:718:VAL:HG11	1:B:791:VAL:HG13	1.88	0.55
1:B:4142:LYS:NZ	1:B:4955:ASP:OD2	2.39	0.55
1:C:4941:LYS:O	1:C:4945:GLU:HG2	2.05	0.55
1:B:168:GLN:HG3	1:B:169:ARG:HG3	1.88	0.55
1:B:4079:TYR:O	1:B:4083:VAL:HG23	2.07	0.55
2:H:79:PRO:HD3	2:H:97:THR:HG22	1.86	0.55
1:C:1131:ASP:HB3	1:C:1133:ARG:HG2	1.89	0.55
1:D:769:ARG:HA	1:D:774:PRO:HA	1.89	0.55
1:A:1123:GLN:HB2	1:A:1126:LEU:HB2	1.88	0.55
1:A:1131:ASP:HB3	1:A:1133:ARG:HG2	1.88	0.55
1:A:2289:TRP:CZ2	1:A:2387:ILE:HD12	2.41	0.55
1:A:4079:TYR:O	1:A:4083:VAL:HG23	2.07	0.55
1:B:1123:GLN:HB2	1:B:1126:LEU:HB2	1.88	0.55
1:C:3729:ARG:O	1:C:3733:ARG:NH1	2.39	0.55
1:D:4079:TYR:O	1:D:4083:VAL:HG23	2.07	0.55
1:A:890:HIS:HB2	1:A:932:ASN:ND2	2.19	0.55
1:A:2335:ARG:HE	1:D:143:LEU:HD21	1.72	0.55
1:B:1009:ARG:O	1:B:1013:ARG:NH1	2.40	0.55
1:C:1321:UNK:HA	1:C:1436:UNK:HA	1.89	0.55
1:C:4079:TYR:O	1:C:4083:VAL:HG23	2.07	0.55
1:D:281:ARG:NH1	1:D:346:VAL:O	2.30	0.55
1:D:3796:MET:HE1	1:D:3869:ILE:HG23	1.89	0.55
1:A:844:ARG:HE	1:A:845:THR:HG22	1.72	0.55
1:A:4789:ARG:NH2	1:A:4805:CYS:SG	2.80	0.55
1:C:1190:LEU:HD11	1:C:1193:LYS:HB2	1.88	0.55
1:C:2147:ASP:O	1:C:2151:ASN:ND2	2.39	0.55
1:D:247:VAL:O	1:D:272:ARG:NH1	2.40	0.55
1:D:4789:ARG:NH2	1:D:4805:CYS:SG	2.80	0.55
1:A:168:GLN:HG3	1:A:169:ARG:HG3	1.88	0.55
1:B:227:TYR:HA	1:B:355:LYS:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:O	1:B:272:ARG:NH1	2.40	0.55
1:C:1709:ASP:HA	1:C:1713:SER:HB3	1.89	0.55
1:D:1584:PRO:HD2	1:D:1587:LEU:HD23	1.89	0.55
1:A:247:VAL:O	1:A:272:ARG:NH1	2.40	0.55
1:A:2337:GLU:HG3	1:D:140:THR:O	2.06	0.55
1:A:4867:ASP:OD1	1:B:4873:ARG:NH1	2.40	0.55
1:B:1709:ASP:HA	1:B:1713:SER:HB3	1.89	0.55
1:B:2289:TRP:CZ2	1:B:2387:ILE:HD12	2.41	0.55
1:D:4049:LYS:HA	1:D:4052:GLU:HG2	1.88	0.55
1:D:4757:SER:O	1:D:4761:HIS:HB2	2.07	0.55
1:A:4142:LYS:NZ	1:A:4955:ASP:OD2	2.39	0.55
1:C:247:VAL:O	1:C:272:ARG:NH1	2.40	0.55
1:D:4142:LYS:NZ	1:D:4955:ASP:OD2	2.39	0.55
1:A:718:VAL:HG11	1:A:791:VAL:HG13	1.88	0.55
1:B:2277:GLN:HA	1:B:2280:VAL:HG22	1.89	0.55
1:B:2721:ASN:C	1:B:2721:ASN:HD22	2.15	0.55
1:B:3729:ARG:O	1:B:3733:ARG:NH1	2.39	0.55
1:B:4757:SER:O	1:B:4761:HIS:HB2	2.07	0.55
1:C:3796:MET:HE1	1:C:3869:ILE:HG23	1.89	0.55
1:D:1131:ASP:HB3	1:D:1133:ARG:HG2	1.89	0.55
1:A:4757:SER:O	1:A:4761:HIS:HB2	2.07	0.54
1:B:1321:UNK:HA	1:B:1436:UNK:HA	1.89	0.54
1:C:227:TYR:HA	1:C:355:LYS:HA	1.88	0.54
1:C:2721:ASN:C	1:C:2721:ASN:HD22	2.15	0.54
1:D:1321:UNK:HA	1:D:1436:UNK:HA	1.89	0.54
1:A:769:ARG:HA	1:A:774:PRO:HA	1.89	0.54
1:A:1584:PRO:HD2	1:A:1587:LEU:HD23	1.89	0.54
1:A:1709:ASP:HA	1:A:1713:SER:HB3	1.89	0.54
1:D:844:ARG:HE	1:D:845:THR:HG22	1.72	0.54
1:B:844:ARG:HE	1:B:845:THR:HG22	1.72	0.54
1:B:4789:ARG:NH2	1:B:4805:CYS:SG	2.80	0.54
1:C:4789:ARG:NH2	1:C:4805:CYS:SG	2.80	0.54
1:D:168:GLN:HG3	1:D:169:ARG:HG3	1.88	0.54
1:A:629:GLN:HE21	1:A:1670:ASN:HD22	1.56	0.54
1:B:4659:PHE:O	1:C:4055:LYS:NZ	2.39	0.54
1:C:769:ARG:HA	1:C:774:PRO:HA	1.89	0.54
1:C:1117:TRP:HE1	1:C:1164:CYS:HB3	1.71	0.54
1:D:486:GLN:CB	1:D:544:ASN:HD21	2.20	0.54
1:D:1709:ASP:HA	1:D:1713:SER:HB3	1.89	0.54
1:B:1769:PHE:O	2:H:83:TYR:OH	2.25	0.54
1:C:844:ARG:HE	1:C:845:THR:HG22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1009:ARG:O	1:C:1013:ARG:NH1	2.40	0.54
1:C:4049:LYS:HA	1:C:4052:GLU:HG2	1.88	0.54
1:D:1123:GLN:HB2	1:D:1126:LEU:HB2	1.88	0.54
1:D:1249:MET:HA	1:D:1249:MET:HE3	1.90	0.54
1:C:168:GLN:HG3	1:C:169:ARG:HG3	1.88	0.54
1:C:838:ARG:H	1:C:841:LYS:HZ1	1.54	0.54
1:D:718:VAL:HG11	1:D:791:VAL:HG13	1.88	0.54
1:A:1249:MET:HA	1:A:1249:MET:HE3	1.90	0.54
1:B:3796:MET:HE1	1:B:3869:ILE:HG23	1.89	0.54
1:C:1249:MET:HA	1:C:1249:MET:HE3	1.90	0.54
1:A:1009:ARG:O	1:A:1013:ARG:NH1	2.40	0.54
1:A:4160:GLU:OE1	1:A:4160:GLU:N	2.41	0.54
1:C:1932:VAL:HG21	1:C:3616:VAL:HA	1.90	0.54
1:D:1009:ARG:O	1:D:1013:ARG:NH1	2.40	0.54
1:D:2277:GLN:HA	1:D:2280:VAL:HG22	1.89	0.54
1:D:4046:ASP:OD1	1:D:4046:ASP:N	2.40	0.54
1:D:4160:GLU:N	1:D:4160:GLU:OE1	2.41	0.54
1:A:1040:ASP:OD1	1:A:1040:ASP:N	2.35	0.54
1:B:629:GLN:HE21	1:B:1670:ASN:HD22	1.56	0.54
1:C:4046:ASP:OD1	1:C:4046:ASP:N	2.40	0.54
1:D:1677:LEU:HA	1:D:1680:HIS:HB2	1.89	0.54
1:A:2721:ASN:HD22	1:A:2721:ASN:C	2.15	0.54
1:B:769:ARG:HA	1:B:774:PRO:HA	1.89	0.54
1:B:1584:PRO:HD2	1:B:1587:LEU:HD23	1.89	0.54
1:D:1932:VAL:HG21	1:D:3616:VAL:HA	1.90	0.54
1:D:2271:CYS:SG	1:D:2294:GLY:N	2.81	0.54
1:D:2747:SER:O	1:D:2753:GLN:NE2	2.39	0.54
1:A:486:GLN:CB	1:A:544:ASN:HD21	2.20	0.53
1:A:838:ARG:H	1:A:841:LYS:HZ1	1.55	0.53
1:C:1397:UNK:HA	1:C:1412:UNK:HA	1.90	0.53
1:C:2271:CYS:SG	1:C:2294:GLY:N	2.81	0.53
1:C:4757:SER:O	1:C:4761:HIS:HB2	2.07	0.53
1:D:1397:UNK:HA	1:D:1412:UNK:HA	1.90	0.53
1:A:1629:MET:HE2	1:A:1642:ILE:HD13	1.89	0.53
1:B:1249:MET:HA	1:B:1249:MET:HE3	1.90	0.53
1:C:4160:GLU:OE1	1:C:4160:GLU:N	2.41	0.53
2:I:58:LYS:HA	2:I:61:GLU:HG2	1.90	0.53
1:A:582:SER:HB2	1:A:584:GLU:OE2	2.09	0.53
1:A:1321:UNK:HA	1:A:1436:UNK:HA	1.89	0.53
1:A:2325:ARG:NH2	1:D:189:GLU:O	2.39	0.53
1:A:4830:ILE:HG22	1:A:4831:GLU:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:GLN:CB	1:C:544:ASN:HD21	2.20	0.53
1:D:334:SER:OG	1:D:335:LYS:N	2.41	0.53
1:D:2721:ASN:HD22	1:D:2721:ASN:C	2.15	0.53
1:A:2271:CYS:SG	1:A:2294:GLY:N	2.81	0.53
1:A:2747:SER:O	1:A:2753:GLN:NE2	2.38	0.53
1:A:3796:MET:HE1	1:A:3869:ILE:HG23	1.89	0.53
1:B:1397:UNK:HA	1:B:1412:UNK:HA	1.90	0.53
1:B:1932:VAL:HG21	1:B:3616:VAL:HA	1.90	0.53
1:C:1677:LEU:HA	1:C:1680:HIS:HB2	1.89	0.53
1:D:582:SER:HB2	1:D:584:GLU:OE2	2.09	0.53
1:A:1677:LEU:HA	1:A:1680:HIS:HB2	1.89	0.53
1:B:1629:MET:HE2	1:B:1642:ILE:HD13	1.90	0.53
1:B:2455:MET:HG3	1:B:2457:ALA:H	1.74	0.53
1:C:2277:GLN:HA	1:C:2280:VAL:HG22	1.89	0.53
1:B:59:PRO:HB3	1:B:296:ARG:HH12	1.74	0.53
1:B:4160:GLU:OE1	1:B:4160:GLU:N	2.41	0.53
1:B:4276:LYS:NZ	1:B:4562:GLU:OE1	2.42	0.53
1:C:4051:MET:HE1	1:C:4065:LEU:HB2	1.91	0.53
1:A:59:PRO:HB3	1:A:296:ARG:HH12	1.74	0.53
1:B:486:GLN:CB	1:B:544:ASN:HD21	2.20	0.53
1:D:2383:MET:O	1:D:2387:ILE:HG12	2.09	0.53
1:A:1914:ASP:OD1	1:A:2089:ARG:NH1	2.40	0.53
1:A:1932:VAL:HG21	1:A:3616:VAL:HA	1.89	0.53
1:A:2277:GLN:HA	1:A:2280:VAL:HG22	1.89	0.53
1:B:2747:SER:O	1:B:2753:GLN:NE2	2.38	0.53
1:B:3891:TYR:O	1:B:3956:LYS:NZ	2.39	0.53
2:H:58:LYS:HA	2:H:61:GLU:HG2	1.90	0.53
1:C:1584:PRO:HD2	1:C:1587:LEU:HD23	1.89	0.53
1:C:2254:LEU:O	1:C:3809:ARG:HD3	2.09	0.53
2:J:58:LYS:HA	2:J:61:GLU:HG2	1.90	0.53
1:B:300:VAL:O	1:B:420:ARG:NH1	2.37	0.53
1:B:2271:CYS:SG	1:B:2294:GLY:N	2.81	0.53
1:B:4830:ILE:HG22	1:B:4831:GLU:H	1.74	0.53
1:C:672:LYS:HB3	1:C:819:TYR:HA	1.91	0.53
1:C:4276:LYS:NZ	1:C:4562:GLU:OE1	2.42	0.53
1:A:4276:LYS:NZ	1:A:4562:GLU:OE1	2.42	0.53
1:A:4824:GLY:O	1:B:4821:ARG:NH2	2.42	0.53
1:B:1677:LEU:HA	1:B:1680:HIS:HB2	1.89	0.53
1:B:2867:HIS:CD2	1:B:2869:LEU:HB2	2.44	0.53
1:C:2455:MET:HG3	1:C:2457:ALA:H	1.74	0.53
1:C:2867:HIS:CD2	1:C:2869:LEU:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4830:ILE:HG22	1:C:4831:GLU:H	1.74	0.53
1:D:59:PRO:HB3	1:D:296:ARG:HH12	1.74	0.53
1:D:1629:MET:HE2	1:D:1642:ILE:HD13	1.89	0.53
1:A:1397:UNK:HA	1:A:1412:UNK:HA	1.90	0.52
1:B:2383:MET:O	1:B:2387:ILE:HG12	2.09	0.52
1:B:4051:MET:HE1	1:B:4065:LEU:HB2	1.91	0.52
1:C:1972:ILE:HA	1:C:1975:LEU:HG	1.91	0.52
1:C:2383:MET:O	1:C:2387:ILE:HG12	2.09	0.52
1:D:2254:LEU:O	1:D:3809:ARG:HD3	2.09	0.52
1:A:2383:MET:O	1:A:2387:ILE:HG12	2.09	0.52
1:A:4051:MET:HE1	1:A:4065:LEU:HB2	1.91	0.52
1:C:629:GLN:HE21	1:C:1670:ASN:HD22	1.56	0.52
1:C:640:ARG:HH22	2:I:91:VAL:HG13	1.74	0.52
1:C:1981:ASP:OD1	1:C:1981:ASP:N	2.32	0.52
1:D:838:ARG:H	1:D:841:LYS:HZ1	1.55	0.52
1:D:4830:ILE:HG22	1:D:4831:GLU:H	1.74	0.52
2:J:50:ARG:N	2:J:55:GLU:OE2	2.41	0.52
1:A:2148:ILE:HA	1:A:2151:ASN:HD22	1.73	0.52
1:A:2867:HIS:CD2	1:A:2869:LEU:HB2	2.44	0.52
1:B:1040:ASP:OD1	1:B:1040:ASP:N	2.35	0.52
1:C:874:LEU:HD21	1:C:941:LYS:HD3	1.92	0.52
1:C:1629:MET:HE2	1:C:1642:ILE:HD13	1.89	0.52
1:C:2081:ARG:HG3	1:C:3686:LEU:HD22	1.92	0.52
1:D:1972:ILE:HA	1:D:1975:LEU:HG	1.92	0.52
1:A:334:SER:OG	1:A:335:LYS:N	2.41	0.52
1:B:838:ARG:H	1:B:841:LYS:HZ1	1.56	0.52
1:D:629:GLN:HE21	1:D:1670:ASN:HD22	1.56	0.52
1:A:281:ARG:NH1	1:A:346:VAL:O	2.30	0.52
1:A:874:LEU:HD21	1:A:941:LYS:HD3	1.92	0.52
1:A:2455:MET:HG3	1:A:2457:ALA:H	1.74	0.52
1:B:340:VAL:HG23	1:B:341:GLY:H	1.75	0.52
1:B:582:SER:HB2	1:B:584:GLU:OE2	2.09	0.52
1:B:672:LYS:HB3	1:B:819:TYR:HA	1.91	0.52
1:B:874:LEU:HD21	1:B:941:LYS:HD3	1.92	0.52
1:B:3954:GLN:NE2	1:B:3971:MET:SD	2.83	0.52
1:C:3961:SER:OG	1:C:3962:SER:N	2.43	0.52
1:D:874:LEU:HD21	1:D:941:LYS:HD3	1.92	0.52
1:A:2254:LEU:O	1:A:3809:ARG:HD3	2.09	0.52
1:B:2148:ILE:HA	1:B:2151:ASN:HD22	1.73	0.52
1:D:672:LYS:HB3	1:D:819:TYR:HA	1.91	0.52
1:D:711:GLU:O	1:D:712:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3640:ILE:HD12	1:D:3697:SER:HB2	1.92	0.52
1:D:3954:GLN:NE2	1:D:3971:MET:SD	2.83	0.52
1:D:4276:LYS:NZ	1:D:4562:GLU:OE1	2.42	0.52
1:A:927:GLN:HG3	1:A:928:GLU:HG3	1.92	0.52
1:B:489:PHE:HD1	1:B:494:MET:SD	2.33	0.52
1:C:3954:GLN:NE2	1:C:3971:MET:SD	2.83	0.52
1:D:375:GLN:HE22	1:D:392:ILE:H	1.58	0.52
1:A:3954:GLN:NE2	1:A:3971:MET:SD	2.83	0.52
2:G:58:LYS:HA	2:G:61:GLU:HG2	1.91	0.52
1:C:4928:ASP:O	1:C:4932:HIS:NE2	2.43	0.52
1:D:340:VAL:HG23	1:D:341:GLY:H	1.75	0.52
1:D:2148:ILE:HA	1:D:2151:ASN:HD22	1.73	0.52
1:D:2455:MET:HG3	1:D:2457:ALA:H	1.74	0.52
1:A:672:LYS:HB3	1:A:819:TYR:HA	1.91	0.52
1:C:334:SER:OG	1:C:335:LYS:N	2.41	0.52
1:C:375:GLN:HE22	1:C:392:ILE:H	1.58	0.52
1:D:4928:ASP:O	1:D:4932:HIS:NE2	2.43	0.52
1:A:2335:ARG:HH21	1:D:143:LEU:HD11	1.73	0.52
1:A:4928:ASP:O	1:A:4932:HIS:NE2	2.43	0.52
1:B:2081:ARG:HG3	1:B:3686:LEU:HD22	1.92	0.52
1:A:489:PHE:HD1	1:A:494:MET:SD	2.33	0.51
1:C:1715:TYR:CZ	1:C:1762:MET:HB3	2.45	0.51
1:C:2148:ILE:HA	1:C:2151:ASN:HD22	1.73	0.51
1:C:2775:LYS:O	1:C:2779:LYS:HG3	2.10	0.51
1:C:2858:GLU:O	1:C:2862:LYS:HG2	2.10	0.51
1:D:2867:HIS:CD2	1:D:2869:LEU:HB2	2.44	0.51
1:A:3961:SER:OG	1:A:3962:SER:N	2.43	0.51
2:G:50:ARG:N	2:G:55:GLU:OE2	2.41	0.51
2:H:50:ARG:N	2:H:55:GLU:OE2	2.41	0.51
1:C:927:GLN:HG3	1:C:928:GLU:HG3	1.92	0.51
1:C:2342:LEU:HB2	1:C:2430:ASP:OD2	2.11	0.51
1:D:1042:THR:O	1:D:1045:SER:OG	2.28	0.51
1:D:1265:HIS:CD2	1:D:1268:ILE:HB	2.45	0.51
1:D:1715:TYR:CZ	1:D:1762:MET:HB3	2.45	0.51
1:A:711:GLU:O	1:A:712:GLU:HG2	2.10	0.51
1:A:3640:ILE:HD12	1:A:3697:SER:HB2	1.91	0.51
1:B:26:ALA:HB2	1:B:194:LEU:HD21	1.93	0.51
1:B:927:GLN:HG3	1:B:928:GLU:HG3	1.92	0.51
1:B:1914:ASP:OD1	1:B:2089:ARG:NH1	2.40	0.51
1:B:2342:LEU:HB2	1:B:2430:ASP:OD2	2.11	0.51
1:B:2775:LYS:O	1:B:2779:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3640:ILE:HD12	1:B:3697:SER:HB2	1.92	0.51
1:C:711:GLU:O	1:C:712:GLU:HG2	2.10	0.51
1:C:4142:LYS:NZ	1:C:4955:ASP:OD2	2.39	0.51
1:D:26:ALA:HB2	1:D:194:LEU:HD21	1.93	0.51
1:B:2254:LEU:O	1:B:3809:ARG:HD3	2.09	0.51
1:C:340:VAL:HG23	1:C:341:GLY:H	1.75	0.51
1:C:489:PHE:HD1	1:C:494:MET:SD	2.33	0.51
1:D:2081:ARG:HG3	1:D:3686:LEU:HD22	1.92	0.51
1:D:4051:MET:HE1	1:D:4065:LEU:HB2	1.91	0.51
1:A:26:ALA:HB2	1:A:194:LEU:HD21	1.93	0.51
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.93	0.51
1:B:763:ALA:HB3	1:B:764:PRO:HD3	1.93	0.51
1:C:59:PRO:HB3	1:C:296:ARG:HH12	1.74	0.51
1:C:582:SER:HB2	1:C:584:GLU:OE2	2.09	0.51
1:A:1845:GLN:HA	1:A:1848:GLU:HG2	1.93	0.51
1:A:2343:LEU:O	1:A:2347:GLU:HG2	2.11	0.51
1:B:4928:ASP:O	1:B:4932:HIS:NE2	2.43	0.51
1:C:26:ALA:HB2	1:C:194:LEU:HD21	1.93	0.51
1:C:763:ALA:HB3	1:C:764:PRO:HD3	1.93	0.51
1:C:2343:LEU:O	1:C:2347:GLU:HG2	2.11	0.51
1:C:3640:ILE:HD12	1:C:3697:SER:HB2	1.92	0.51
2:I:50:ARG:N	2:I:55:GLU:OE2	2.41	0.51
1:D:489:PHE:HD1	1:D:494:MET:SD	2.33	0.51
1:D:927:GLN:HG3	1:D:928:GLU:HG3	1.92	0.51
1:D:2343:LEU:O	1:D:2347:GLU:HG2	2.11	0.51
1:D:2858:GLU:O	1:D:2862:LYS:HG2	2.10	0.51
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.18	0.51
1:B:1265:HIS:CD2	1:B:1268:ILE:HB	2.45	0.51
1:C:1102:TYR:HA	1:C:1164:CYS:O	2.11	0.51
1:D:1845:GLN:HA	1:D:1848:GLU:HG2	1.93	0.51
1:A:375:GLN:HE22	1:A:392:ILE:H	1.58	0.51
1:A:1715:TYR:CZ	1:A:1762:MET:HB3	2.45	0.51
1:B:1845:GLN:HA	1:B:1848:GLU:HG2	1.93	0.51
1:B:4046:ASP:N	1:B:4046:ASP:OD1	2.40	0.51
1:C:238:HIS:HB2	1:C:241:MET:HB2	1.93	0.51
1:D:1914:ASP:OD1	1:D:2089:ARG:NH1	2.40	0.51
1:D:2740:TRP:HB3	1:D:2756:MET:HG3	1.93	0.51
1:D:2775:LYS:O	1:D:2779:LYS:HG3	2.10	0.51
1:A:1042:THR:O	1:A:1045:SER:OG	2.28	0.51
1:A:1972:ILE:HA	1:A:1975:LEU:HG	1.92	0.51
1:A:2081:ARG:HG3	1:A:3686:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.18	0.51
1:B:711:GLU:O	1:B:712:GLU:HG2	2.10	0.51
1:B:1811:VAL:HB	1:B:1818:LEU:HD13	1.93	0.51
1:B:1972:ILE:HA	1:B:1975:LEU:HG	1.92	0.51
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.18	0.51
1:A:640:ARG:HH22	2:G:91:VAL:HG13	1.74	0.51
1:A:732:LEU:HB3	1:A:779:PHE:CZ	2.46	0.51
1:A:2108:ASN:HD21	1:A:2111:SER:HB3	1.76	0.51
1:A:2291:PRO:HB3	1:A:2387:ILE:HD13	1.93	0.51
1:A:2740:TRP:HB3	1:A:2756:MET:HG3	1.93	0.51
1:A:2775:LYS:O	1:A:2779:LYS:HG3	2.10	0.51
1:B:1715:TYR:CZ	1:B:1762:MET:HB3	2.45	0.51
1:B:2291:PRO:HB3	1:B:2387:ILE:HD13	1.93	0.51
1:B:2740:TRP:HB3	1:B:2756:MET:HG3	1.93	0.51
1:C:765:SER:OG	1:C:780:GLU:HA	2.11	0.51
1:C:2291:PRO:HB3	1:C:2387:ILE:HD13	1.93	0.51
1:C:2498:ALA:O	1:C:2501:LEU:HD23	2.11	0.51
1:D:2291:PRO:HB3	1:D:2387:ILE:HD13	1.93	0.51
1:A:340:VAL:HG23	1:A:341:GLY:H	1.75	0.50
1:B:732:LEU:HB3	1:B:779:PHE:CZ	2.46	0.50
1:B:1102:TYR:HA	1:B:1164:CYS:O	2.11	0.50
1:C:1743:GLU:CD	1:C:1744:ASN:HD22	2.20	0.50
1:C:2278:MET:N	1:C:2278:MET:SD	2.84	0.50
1:D:763:ALA:HB3	1:D:764:PRO:HD3	1.93	0.50
1:A:2342:LEU:HB2	1:A:2430:ASP:OD2	2.10	0.50
1:A:2858:GLU:O	1:A:2862:LYS:HG2	2.10	0.50
1:B:2498:ALA:O	1:B:2501:LEU:HD23	2.11	0.50
1:C:28:ILE:HG21	1:C:201:TRP:HH2	1.77	0.50
1:A:238:HIS:HB2	1:A:241:MET:HB2	1.94	0.50
1:A:765:SER:OG	1:A:780:GLU:HA	2.11	0.50
1:B:765:SER:OG	1:B:780:GLU:HA	2.11	0.50
1:B:890:HIS:HB2	1:B:932:ASN:ND2	2.19	0.50
1:C:2716:LEU:O	1:C:2720:ILE:HG12	2.12	0.50
1:C:2740:TRP:HB3	1:C:2756:MET:HG3	1.93	0.50
1:D:765:SER:OG	1:D:780:GLU:HA	2.11	0.50
1:D:839:GLU:H	1:D:841:LYS:HZ1	1.58	0.50
1:D:3961:SER:OG	1:D:3962:SER:N	2.43	0.50
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.45	0.50
1:A:2278:MET:N	1:A:2278:MET:SD	2.84	0.50
1:B:28:ILE:HG21	1:B:201:TRP:HH2	1.77	0.50
1:B:839:GLU:H	1:B:841:LYS:HZ1	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:THR:O	1:B:1045:SER:OG	2.28	0.50
1:B:2108:ASN:HD21	1:B:2111:SER:HB3	1.76	0.50
1:B:2716:LEU:O	1:B:2720:ILE:HG12	2.12	0.50
1:C:281:ARG:NH1	1:C:346:VAL:O	2.30	0.50
1:C:732:LEU:HB3	1:C:779:PHE:CZ	2.46	0.50
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.45	0.50
1:C:1811:VAL:HB	1:C:1818:LEU:HD13	1.93	0.50
1:C:2206:SER:OG	1:C:2207:ARG:N	2.44	0.50
1:C:4866:ILE:HD12	1:D:4866:ILE:HD13	1.93	0.50
1:D:238:HIS:HB2	1:D:241:MET:HB2	1.94	0.50
1:A:281:ARG:O	1:A:285:SER:OG	2.26	0.50
1:A:300:VAL:O	1:A:420:ARG:NH1	2.37	0.50
1:A:2716:LEU:O	1:A:2720:ILE:HG12	2.12	0.50
1:B:281:ARG:O	1:B:285:SER:OG	2.26	0.50
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.44	0.50
1:B:2858:GLU:O	1:B:2862:LYS:HG2	2.10	0.50
1:C:2070:GLN:O	1:C:3659:ARG:NH1	2.44	0.50
1:A:1102:TYR:HB2	1:A:1165:MET:HG3	1.94	0.50
1:A:4942:MET:HE1	1:A:4949:GLU:HB2	1.93	0.50
1:C:1845:GLN:HA	1:C:1848:GLU:HG2	1.93	0.50
1:C:1914:ASP:OD1	1:C:2089:ARG:NH1	2.40	0.50
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.94	0.50
1:D:2498:ALA:O	1:D:2501:LEU:HD23	2.11	0.50
1:A:851:LEU:HB3	1:A:1212:VAL:HG12	1.94	0.50
1:A:1985:CYS:SG	1:A:1992:ARG:HD2	2.52	0.50
1:A:2498:ALA:O	1:A:2501:LEU:HD23	2.11	0.50
1:B:281:ARG:NH1	1:B:346:VAL:O	2.30	0.50
1:B:851:LEU:HB3	1:B:1212:VAL:HG12	1.94	0.50
1:B:2206:SER:OG	1:B:2207:ARG:N	2.44	0.50
1:B:3961:SER:OG	1:B:3962:SER:N	2.43	0.50
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.18	0.50
1:C:1985:CYS:SG	1:C:1992:ARG:HD2	2.52	0.50
1:C:2108:ASN:HD21	1:C:2111:SER:HB3	1.76	0.50
1:D:28:ILE:HG21	1:D:201:TRP:HH2	1.77	0.50
1:D:2108:ASN:HD21	1:D:2111:SER:HB3	1.76	0.50
1:D:2278:MET:SD	1:D:2278:MET:N	2.84	0.50
1:A:839:GLU:H	1:A:841:LYS:HZ1	1.59	0.50
1:A:1265:HIS:CD2	1:A:1268:ILE:HB	2.45	0.50
1:B:375:GLN:HE22	1:B:392:ILE:H	1.58	0.50
1:B:640:ARG:HH22	2:H:91:VAL:HG13	1.76	0.50
1:B:1986:PRO:HB2	1:B:1988:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2343:LEU:O	1:B:2347:GLU:HG2	2.11	0.50
1:C:1102:TYR:HB2	1:C:1165:MET:HG3	1.94	0.50
1:A:28:ILE:HG21	1:A:201:TRP:HH2	1.77	0.50
1:A:1008:ALA:O	1:A:1012:ILE:HG23	2.12	0.50
1:A:1102:TYR:HA	1:A:1164:CYS:O	2.11	0.50
1:A:1743:GLU:CD	1:A:1744:ASN:HD22	2.20	0.50
1:B:238:HIS:HB2	1:B:241:MET:HB2	1.93	0.50
1:B:1345:VAL:HG13	1:B:1347:MET:SD	2.52	0.50
1:B:4942:MET:HE1	1:B:4949:GLU:HB2	1.93	0.50
1:C:851:LEU:HB3	1:C:1212:VAL:HG12	1.94	0.50
1:C:1986:PRO:HB2	1:C:1988:PRO:HD2	1.94	0.50
1:A:1629:MET:CE	1:A:1685:GLN:HE21	2.22	0.49
1:A:1789:LYS:HZ1	1:A:1835:PHE:H	1.60	0.49
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.94	0.49
1:B:1743:GLU:CD	1:B:1744:ASN:HD22	2.20	0.49
1:B:2278:MET:N	1:B:2278:MET:SD	2.84	0.49
1:B:2894:PHE:HA	1:B:2897:ILE:HG12	1.94	0.49
1:D:851:LEU:HB3	1:D:1212:VAL:HG12	1.94	0.49
1:D:1102:TYR:HA	1:D:1164:CYS:O	2.11	0.49
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.45	0.49
1:D:1359:ILE:HG12	1:D:1363:LYS:HD2	1.94	0.49
1:D:1811:VAL:HB	1:D:1818:LEU:HD13	1.93	0.49
1:D:1986:PRO:HB2	1:D:1988:PRO:HD2	1.94	0.49
1:D:4942:MET:HE1	1:D:4949:GLU:HB2	1.93	0.49
1:A:1345:VAL:HG13	1:A:1347:MET:SD	2.52	0.49
1:C:23:GLN:HG3	1:C:213:SER:HB3	1.94	0.49
1:C:2334:LEU:HD13	1:C:2342:LEU:HD12	1.95	0.49
1:C:4942:MET:HE1	1:C:4949:GLU:HB2	1.93	0.49
1:D:2206:SER:OG	1:D:2207:ARG:N	2.44	0.49
1:D:2334:LEU:HD13	1:D:2342:LEU:HD12	1.95	0.49
1:C:1040:ASP:N	1:C:1040:ASP:OD1	2.35	0.49
1:C:2080:VAL:HG13	1:C:3669:LEU:HD22	1.94	0.49
1:C:2747:SER:O	1:C:2753:GLN:NE2	2.38	0.49
1:C:4570:THR:HA	1:C:4573:ILE:HG12	1.95	0.49
1:D:1102:TYR:HB2	1:D:1165:MET:HG3	1.94	0.49
1:D:1743:GLU:CD	1:D:1744:ASN:HD22	2.19	0.49
1:A:441:LYS:HG2	1:A:442:LEU:HD23	1.94	0.49
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.94	0.49
1:B:2080:VAL:HG13	1:B:3669:LEU:HD22	1.94	0.49
1:C:1345:VAL:HG13	1:C:1347:MET:SD	2.52	0.49
1:D:1008:ALA:O	1:D:1012:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2342:LEU:HB2	1:D:2430:ASP:OD2	2.11	0.49
1:A:1811:VAL:HB	1:A:1818:LEU:HD13	1.93	0.49
1:B:1359:ILE:HG12	1:B:1363:LYS:HD2	1.94	0.49
1:B:2717:GLU:HA	1:B:2720:ILE:HG12	1.95	0.49
1:B:3728:ALA:HA	1:B:3731:HIS:ND1	2.28	0.49
1:D:732:LEU:HB3	1:D:779:PHE:CZ	2.46	0.49
1:D:1345:VAL:HG13	1:D:1347:MET:SD	2.52	0.49
1:A:2070:GLN:O	1:A:3659:ARG:NH1	2.44	0.49
1:A:3493:UNK:HA	1:D:1233:GLN:HG3	1.95	0.49
1:B:4079:TYR:HA	1:B:4082:PHE:HB3	1.95	0.49
1:C:1700:ARG:NH1	1:C:1817:PHE:O	2.46	0.49
1:A:436:LEU:HD21	1:A:517:VAL:HG12	1.95	0.49
1:A:1700:ARG:NH1	1:A:1817:PHE:O	2.46	0.49
1:A:1986:PRO:HB2	1:A:1988:PRO:HD2	1.94	0.49
1:B:441:LYS:HG2	1:B:442:LEU:HD23	1.94	0.49
1:B:1102:TYR:HB2	1:B:1165:MET:HG3	1.94	0.49
1:C:1042:THR:O	1:C:1045:SER:OG	2.28	0.49
1:C:2894:PHE:HA	1:C:2897:ILE:HG12	1.94	0.49
1:D:1266:GLU:OE1	1:D:1267:HIS:HB3	2.12	0.49
1:D:1985:CYS:SG	1:D:1992:ARG:HD2	2.52	0.49
1:D:4660:TYR:HB3	1:D:4664:ARG:HH21	1.78	0.49
1:A:2717:GLU:HA	1:A:2720:ILE:HG12	1.95	0.49
1:B:1970:GLU:HA	1:B:1973:ASN:HB2	1.95	0.49
1:C:658:ASN:HD22	1:C:833:LYS:H	1.61	0.49
1:C:1266:GLU:OE1	1:C:1267:HIS:HB3	2.12	0.49
1:C:2183:SER:O	1:C:2183:SER:OG	2.31	0.49
1:D:658:ASN:HD22	1:D:833:LYS:H	1.61	0.49
1:D:4757:SER:HA	1:D:4760:THR:HG22	1.95	0.49
1:A:1266:GLU:OE1	1:A:1267:HIS:HB3	2.12	0.49
1:A:2334:LEU:HD13	1:A:2342:LEU:HD12	1.95	0.49
1:A:4079:TYR:HA	1:A:4082:PHE:HB3	1.95	0.49
1:A:4757:SER:HA	1:A:4760:THR:HG22	1.95	0.49
1:B:699:SER:OG	1:B:700:THR:N	2.46	0.49
1:B:1266:GLU:OE1	1:B:1267:HIS:HB3	2.12	0.49
1:B:1985:CYS:SG	1:B:1992:ARG:HD2	2.52	0.49
1:B:4660:TYR:HB3	1:B:4664:ARG:HH21	1.78	0.49
1:C:300:VAL:O	1:C:420:ARG:NH1	2.37	0.49
1:C:4079:TYR:HA	1:C:4082:PHE:HB3	1.95	0.49
1:A:23:GLN:HG3	1:A:213:SER:HB3	1.94	0.49
1:A:2206:SER:OG	1:A:2207:ARG:N	2.44	0.49
1:B:112:THR:HG21	1:B:174:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1649:GLU:HA	1:B:1649:GLU:OE2	2.13	0.49
1:C:1359:ILE:HG12	1:C:1363:LYS:HD2	1.94	0.49
1:C:3728:ALA:HA	1:C:3731:HIS:ND1	2.28	0.49
1:A:2080:VAL:HG13	1:A:3669:LEU:HD22	1.94	0.48
1:A:4570:THR:HA	1:A:4573:ILE:HG12	1.95	0.48
1:B:1008:ALA:O	1:B:1012:ILE:HG23	2.12	0.48
1:B:2334:LEU:HD13	1:B:2342:LEU:HD12	1.95	0.48
1:C:700:THR:HG1	1:C:787:LEU:H	1.59	0.48
1:C:1970:GLU:HA	1:C:1973:ASN:HB2	1.95	0.48
1:C:4608:LYS:HG3	1:C:4614:LEU:HB2	1.95	0.48
1:D:329:PHE:HB3	1:D:363:ILE:HD11	1.95	0.48
1:D:2717:GLU:HA	1:D:2720:ILE:HG12	1.95	0.48
1:A:890:HIS:O	1:A:894:VAL:HG23	2.13	0.48
1:D:23:GLN:HG3	1:D:213:SER:HB3	1.94	0.48
1:D:2070:GLN:O	1:D:3659:ARG:NH1	2.44	0.48
1:D:2716:LEU:O	1:D:2720:ILE:HG12	2.12	0.48
1:D:2894:PHE:HA	1:D:2897:ILE:HG12	1.94	0.48
1:D:3728:ALA:HA	1:D:3731:HIS:ND1	2.28	0.48
1:A:112:THR:HG21	1:A:174:LYS:HD3	1.95	0.48
1:A:1241:VAL:HG21	1:B:3539:UNK:HA	1.94	0.48
1:A:1359:ILE:HG12	1:A:1363:LYS:HD2	1.94	0.48
1:A:2894:PHE:HA	1:A:2897:ILE:HG12	1.94	0.48
1:A:3728:ALA:HA	1:A:3731:HIS:ND1	2.28	0.48
1:B:4608:LYS:HG3	1:B:4614:LEU:HB2	1.95	0.48
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.94	0.48
1:C:3636:GLU:HG2	1:C:3696:LYS:HE3	1.94	0.48
1:D:4570:THR:HA	1:D:4573:ILE:HG12	1.95	0.48
2:J:88:HIS:HD2	2:J:89:PRO:HD2	1.78	0.48
1:A:1649:GLU:HA	1:A:1649:GLU:OE2	2.13	0.48
1:C:890:HIS:O	1:C:894:VAL:HG23	2.13	0.48
1:C:1649:GLU:HA	1:C:1649:GLU:OE2	2.13	0.48
1:C:2717:GLU:HA	1:C:2720:ILE:HG12	1.95	0.48
2:I:72:ARG:HG2	2:I:103:GLU:HB2	1.95	0.48
1:D:19:GLU:HG2	1:D:68:VAL:HG22	1.96	0.48
1:D:1567:LEU:HD22	1:D:1581:PRO:HB3	1.95	0.48
1:A:699:SER:OG	1:A:700:THR:N	2.46	0.48
1:A:4046:ASP:OD1	1:A:4046:ASP:N	2.40	0.48
1:B:258:ARG:NH1	1:B:316:LEU:O	2.47	0.48
1:B:334:SER:OG	1:B:335:LYS:N	2.41	0.48
1:B:730:LEU:HD23	1:B:748:LEU:HD23	1.96	0.48
1:B:4273:MET:HE3	1:B:4273:MET:HB2	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:ARG:HG2	2:H:103:GLU:HB2	1.95	0.48
2:H:88:HIS:HD2	2:H:89:PRO:HD2	1.79	0.48
1:C:112:THR:HG21	1:C:174:LYS:HD3	1.95	0.48
1:C:329:PHE:HB3	1:C:363:ILE:HD11	1.95	0.48
1:C:1567:LEU:HD22	1:C:1581:PRO:HB3	1.95	0.48
1:D:112:THR:HG21	1:D:174:LYS:HD3	1.95	0.48
1:D:1649:GLU:HA	1:D:1649:GLU:OE2	2.13	0.48
1:D:1700:ARG:NH1	1:D:1817:PHE:O	2.46	0.48
1:D:2080:VAL:HG13	1:D:3669:LEU:HD22	1.94	0.48
1:D:4079:TYR:HA	1:D:4082:PHE:HB3	1.95	0.48
2:J:72:ARG:HG2	2:J:103:GLU:HB2	1.95	0.48
1:B:1165:MET:HB3	1:B:1236:TYR:CE2	2.49	0.48
1:B:1700:ARG:NH1	1:B:1817:PHE:O	2.46	0.48
1:B:2070:GLN:O	1:B:3659:ARG:NH1	2.44	0.48
1:C:1090:ALA:HB3	1:C:1202:ILE:HD11	1.95	0.48
1:C:1968:PRO:HA	1:C:1971:GLN:HB3	1.96	0.48
1:A:19:GLU:HG2	1:A:68:VAL:HG22	1.96	0.48
1:A:1567:LEU:HD22	1:A:1581:PRO:HB3	1.95	0.48
1:A:1970:GLU:HA	1:A:1973:ASN:HB2	1.95	0.48
1:A:3923:ILE:HD13	1:A:3934:LEU:HD12	1.96	0.48
1:B:658:ASN:HD22	1:B:833:LYS:H	1.61	0.48
1:B:3636:GLU:HG2	1:B:3696:LYS:HE3	1.94	0.48
1:B:4570:THR:HA	1:B:4573:ILE:HG12	1.95	0.48
1:C:1165:MET:HB3	1:C:1236:TYR:CE2	2.49	0.48
1:C:1642:ILE:HD11	1:C:1699:LEU:HD23	1.96	0.48
1:D:258:ARG:NH1	1:D:316:LEU:O	2.47	0.48
1:D:932:ASN:OD1	1:D:933:LEU:N	2.47	0.48
1:A:329:PHE:HB3	1:A:363:ILE:HD11	1.95	0.48
1:B:329:PHE:HB3	1:B:363:ILE:HD11	1.95	0.48
1:B:1567:LEU:HD22	1:B:1581:PRO:HB3	1.95	0.48
1:C:839:GLU:H	1:C:841:LYS:HZ1	1.60	0.48
1:D:882:ARG:HD2	1:D:937:LEU:HD23	1.96	0.48
1:D:3636:GLU:HG2	1:D:3696:LYS:HE3	1.94	0.48
1:A:932:ASN:OD1	1:A:933:LEU:N	2.47	0.48
1:A:3636:GLU:HG2	1:A:3696:LYS:HE3	1.94	0.48
2:G:72:ARG:HG2	2:G:103:GLU:HB2	1.96	0.48
1:C:258:ARG:NH1	1:C:316:LEU:O	2.47	0.48
1:D:436:LEU:HD21	1:D:517:VAL:HG12	1.95	0.48
1:D:1118:SER:HA	1:D:1134:ALA:HA	1.96	0.48
1:A:730:LEU:HD23	1:A:748:LEU:HD23	1.96	0.48
1:A:4660:TYR:HB3	1:A:4664:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLN:HG3	1:B:213:SER:HB3	1.94	0.48
1:B:642:LEU:HD12	1:B:643:LEU:HA	1.96	0.48
1:B:4757:SER:HA	1:B:4760:THR:HG22	1.95	0.48
1:C:436:LEU:HD21	1:C:517:VAL:HG12	1.95	0.48
1:C:441:LYS:HG2	1:C:442:LEU:HD23	1.94	0.48
1:C:1008:ALA:O	1:C:1012:ILE:HG23	2.12	0.48
1:C:1257:GLN:HA	1:C:1384:LEU:HD22	1.95	0.48
1:C:1273:ILE:HD11	1:C:1287:GLN:HB2	1.95	0.48
1:C:4290:PHE:HZ	1:C:4573:ILE:HD11	1.79	0.48
1:D:2784:TRP:HH2	1:D:2846:ASN:HB2	1.78	0.48
1:A:1090:ALA:HB3	1:A:1202:ILE:HD11	1.95	0.47
1:A:4029:ASP:OD1	1:A:4029:ASP:N	2.47	0.47
1:B:3923:ILE:HD13	1:B:3934:LEU:HD12	1.96	0.47
1:D:706:TYR:HA	1:D:838:ARG:HG2	1.97	0.47
1:D:890:HIS:O	1:D:894:VAL:HG23	2.13	0.47
1:D:1052:GLU:HA	1:D:1055:ARG:HB2	1.96	0.47
1:A:1257:GLN:HA	1:A:1384:LEU:HD22	1.95	0.47
1:A:4608:LYS:HG3	1:A:4614:LEU:HB2	1.95	0.47
1:B:606:ARG:NH2	1:B:1635:GLU:OE1	2.34	0.47
1:B:713:TRP:NE1	1:B:841:LYS:HG2	2.30	0.47
1:B:1052:GLU:HA	1:B:1055:ARG:HB2	1.96	0.47
1:B:2784:TRP:HH2	1:B:2846:ASN:HB2	1.79	0.47
1:C:3728:ALA:HA	1:C:3731:HIS:CE1	2.49	0.47
1:C:4757:SER:HA	1:C:4760:THR:HG22	1.95	0.47
1:C:4863:GLY:CA	1:D:4866:ILE:HG12	2.44	0.47
2:I:88:HIS:HD2	2:I:89:PRO:HD2	1.79	0.47
1:D:441:LYS:HG2	1:D:442:LEU:HD23	1.94	0.47
1:D:4608:LYS:HG3	1:D:4614:LEU:HB2	1.95	0.47
1:A:258:ARG:NH1	1:A:316:LEU:O	2.47	0.47
1:A:658:ASN:HD22	1:A:833:LYS:H	1.61	0.47
1:A:807:ARG:O	1:A:1615:ARG:NE	2.46	0.47
1:B:19:GLU:HG2	1:B:68:VAL:HG22	1.96	0.47
1:B:1642:ILE:HD11	1:B:1699:LEU:HD23	1.96	0.47
1:C:713:TRP:NE1	1:C:841:LYS:HG2	2.30	0.47
1:C:4029:ASP:OD1	1:C:4029:ASP:N	2.47	0.47
1:D:1642:ILE:HD11	1:D:1699:LEU:HD23	1.96	0.47
1:D:1970:GLU:HA	1:D:1973:ASN:HB2	1.95	0.47
1:D:1972:ILE:HD12	1:D:1975:LEU:HD11	1.96	0.47
1:A:882:ARG:HD2	1:A:937:LEU:HD23	1.96	0.47
1:A:1273:ILE:HD11	1:A:1287:GLN:HB2	1.95	0.47
1:A:2784:TRP:HH2	1:A:2846:ASN:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2485:HIS:O	1:B:2489:VAL:HG12	2.14	0.47
1:B:4290:PHE:HZ	1:B:4573:ILE:HD11	1.79	0.47
1:B:4694:SER:O	1:B:4694:SER:OG	2.32	0.47
1:C:19:GLU:HG2	1:C:68:VAL:HG22	1.96	0.47
1:C:606:ARG:NH2	1:C:1635:GLU:OE1	2.34	0.47
1:C:1265:HIS:CD2	1:C:1268:ILE:HB	2.45	0.47
1:C:2776:GLU:O	1:C:2780:THR:HG22	2.15	0.47
1:D:713:TRP:NE1	1:D:841:LYS:HG2	2.29	0.47
1:D:4762:ASN:O	1:D:4764:LYS:N	2.48	0.47
1:A:606:ARG:NH2	1:A:1635:GLU:OE1	2.34	0.47
1:A:706:TYR:HA	1:A:838:ARG:HG2	1.96	0.47
1:A:2197:ARG:HB3	1:A:2236:SER:OG	2.15	0.47
1:A:4290:PHE:HZ	1:A:4573:ILE:HD11	1.79	0.47
1:B:1100:ARG:HB3	1:B:1236:TYR:CD2	2.49	0.47
1:B:1118:SER:HA	1:B:1134:ALA:HA	1.96	0.47
1:B:1968:PRO:HA	1:B:1971:GLN:HB3	1.96	0.47
1:C:1118:SER:HA	1:C:1134:ALA:HA	1.96	0.47
1:C:3923:ILE:HD13	1:C:3934:LEU:HD12	1.96	0.47
1:D:921:PHE:HE1	1:D:932:ASN:HD21	1.63	0.47
1:D:3728:ALA:HA	1:D:3731:HIS:CE1	2.49	0.47
1:A:642:LEU:HD12	1:A:643:LEU:HA	1.96	0.47
2:G:88:HIS:HD2	2:G:89:PRO:HD2	1.78	0.47
1:B:882:ARG:HD2	1:B:937:LEU:HD23	1.96	0.47
1:B:932:ASN:OD1	1:B:933:LEU:N	2.47	0.47
1:B:1652:LEU:HD12	1:B:1699:LEU:HD13	1.97	0.47
1:B:3728:ALA:HA	1:B:3731:HIS:CE1	2.49	0.47
1:C:730:LEU:HD23	1:C:748:LEU:HD23	1.96	0.47
1:C:1100:ARG:HB3	1:C:1236:TYR:CD2	2.49	0.47
1:D:1100:ARG:HB3	1:D:1236:TYR:CD2	2.49	0.47
1:D:1273:ILE:HD11	1:D:1287:GLN:HB2	1.95	0.47
1:D:1629:MET:CE	1:D:1685:GLN:HE21	2.22	0.47
1:D:2231:PRO:HD3	1:D:2381:ILE:HD11	1.96	0.47
1:D:4290:PHE:HZ	1:D:4573:ILE:HD11	1.79	0.47
1:A:336:GLU:HG3	1:A:338:LEU:HD22	1.97	0.47
1:A:713:TRP:NE1	1:A:841:LYS:HG2	2.30	0.47
1:A:921:PHE:HE1	1:A:932:ASN:HD21	1.63	0.47
1:A:1165:MET:HB3	1:A:1236:TYR:CE2	2.49	0.47
1:A:1972:ILE:HD12	1:A:1975:LEU:HD11	1.96	0.47
1:A:2780:THR:HG21	1:A:2846:ASN:ND2	2.30	0.47
1:A:4830:ILE:HB	1:A:4842:ARG:NH2	2.30	0.47
1:B:486:GLN:HB3	1:B:544:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:PHE:HE1	1:B:932:ASN:HD21	1.63	0.47
1:B:1090:ALA:HB3	1:B:1202:ILE:HD11	1.95	0.47
1:B:1273:ILE:HD11	1:B:1287:GLN:HB2	1.95	0.47
1:B:2197:ARG:HB3	1:B:2236:SER:OG	2.15	0.47
1:B:4830:ILE:HB	1:B:4842:ARG:NH2	2.30	0.47
1:C:642:LEU:HD12	1:C:643:LEU:HA	1.96	0.47
1:C:699:SER:OG	1:C:700:THR:N	2.46	0.47
1:C:921:PHE:HE1	1:C:932:ASN:HD21	1.63	0.47
1:C:932:ASN:OD1	1:C:933:LEU:N	2.47	0.47
1:C:1052:GLU:HA	1:C:1055:ARG:HB2	1.96	0.47
1:C:2784:TRP:HH2	1:C:2846:ASN:HB2	1.78	0.47
1:C:4660:TYR:HB3	1:C:4664:ARG:HH21	1.78	0.47
1:C:4863:GLY:HA2	1:D:4866:ILE:HG12	1.97	0.47
1:D:699:SER:OG	1:D:700:THR:N	2.46	0.47
1:D:1257:GLN:HA	1:D:1384:LEU:HD22	1.95	0.47
2:J:26:HIS:CE1	2:J:41:ARG:HG2	2.50	0.47
1:A:1052:GLU:HA	1:A:1055:ARG:HB2	1.96	0.47
1:A:1100:ARG:HB3	1:A:1236:TYR:CD2	2.49	0.47
1:A:3728:ALA:HA	1:A:3731:HIS:CE1	2.49	0.47
1:A:3805:ASN:OD1	1:A:3806:ALA:N	2.48	0.47
1:B:436:LEU:HD21	1:B:517:VAL:HG12	1.95	0.47
1:B:888:ASN:O	1:B:892:LEU:HG	2.15	0.47
1:B:1257:GLN:HA	1:B:1384:LEU:HD22	1.95	0.47
1:C:706:TYR:HA	1:C:838:ARG:HG2	1.97	0.47
2:I:26:HIS:CE1	2:I:41:ARG:HG2	2.50	0.47
1:D:2776:GLU:O	1:D:2780:THR:HG22	2.15	0.47
1:A:2485:HIS:O	1:A:2489:VAL:HG12	2.14	0.47
1:B:2506:LEU:HD23	1:B:2506:LEU:H	1.80	0.47
1:B:4029:ASP:OD1	1:B:4029:ASP:N	2.48	0.47
1:C:888:ASN:O	1:C:892:LEU:HG	2.15	0.47
1:D:730:LEU:HD23	1:D:748:LEU:HD23	1.96	0.47
1:D:1165:MET:HB3	1:D:1236:TYR:CE2	2.49	0.47
1:D:2197:ARG:HB3	1:D:2236:SER:OG	2.15	0.47
1:D:3923:ILE:HD13	1:D:3934:LEU:HD12	1.96	0.47
1:A:2068:TRP:HE3	1:A:2083:MET:HE2	1.80	0.47
1:A:2101:LEU:O	1:A:2104:THR:HG22	2.15	0.47
1:A:2231:PRO:HD3	1:A:2381:ILE:HD11	1.96	0.47
1:B:890:HIS:O	1:B:894:VAL:HG23	2.13	0.47
1:C:235:ARG:NH1	1:C:273:SER:OG	2.48	0.47
1:C:2780:THR:HG21	1:C:2846:ASN:ND2	2.30	0.47
1:D:888:ASN:O	1:D:892:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1090:ALA:HB3	1:D:1202:ILE:HD11	1.95	0.47
1:D:1305:SER:OG	1:D:1588:HIS:O	2.33	0.47
1:A:1287:GLN:HG2	1:A:1355:VAL:HG13	1.97	0.46
1:A:1652:LEU:HD12	1:A:1699:LEU:HD13	1.97	0.46
1:A:2058:GLN:HA	1:A:2090:GLN:HE21	1.81	0.46
1:B:2776:GLU:O	1:B:2780:THR:HG22	2.15	0.46
1:B:2780:THR:HG21	1:B:2846:ASN:ND2	2.30	0.46
1:B:3761:GLY:HA2	1:B:3764:ILE:HG22	1.97	0.46
1:B:3805:ASN:OD1	1:B:3806:ALA:N	2.48	0.46
1:C:336:GLU:HG3	1:C:338:LEU:HD22	1.97	0.46
1:C:2485:HIS:O	1:C:2489:VAL:HG12	2.14	0.46
1:C:4883:MET:HE1	1:C:4888:PHE:HD1	1.80	0.46
1:D:1968:PRO:HA	1:D:1971:GLN:HB3	1.96	0.46
1:D:2506:LEU:HD23	1:D:2506:LEU:H	1.80	0.46
1:A:486:GLN:HB3	1:A:544:ASN:ND2	2.30	0.46
1:A:973:THR:OG1	1:A:976:TYR:O	2.19	0.46
1:A:1118:SER:HA	1:A:1134:ALA:HA	1.96	0.46
1:A:1642:ILE:HD11	1:A:1699:LEU:HD23	1.96	0.46
1:A:1713:SER:O	1:A:1717:THR:HG23	2.16	0.46
1:A:2257:ARG:HG3	1:A:2259:PRO:HD3	1.97	0.46
1:B:235:ARG:NH1	1:B:273:SER:OG	2.48	0.46
1:B:2346:MET:HE2	1:B:2346:MET:HB2	1.85	0.46
1:D:300:VAL:O	1:D:420:ARG:NH1	2.37	0.46
1:D:2780:THR:HG21	1:D:2846:ASN:ND2	2.30	0.46
1:D:4830:ILE:HB	1:D:4842:ARG:NH2	2.30	0.46
1:A:1305:SER:OG	1:A:1588:HIS:O	2.33	0.46
1:A:2506:LEU:HD23	1:A:2506:LEU:H	1.80	0.46
1:B:706:TYR:HA	1:B:838:ARG:HG2	1.96	0.46
1:B:921:PHE:O	1:B:929:ARG:NH1	2.45	0.46
1:B:1287:GLN:HG2	1:B:1355:VAL:HG13	1.97	0.46
1:B:2058:GLN:HA	1:B:2090:GLN:HE21	1.81	0.46
1:C:629:GLN:NE2	1:C:1670:ASN:HD22	2.13	0.46
1:C:1629:MET:CE	1:C:1685:GLN:HE21	2.22	0.46
1:C:2231:PRO:HD3	1:C:2381:ILE:HD11	1.96	0.46
1:C:4830:ILE:HB	1:C:4842:ARG:NH2	2.30	0.46
1:D:235:ARG:NH1	1:D:273:SER:OG	2.48	0.46
1:D:1684:PRO:HD3	2:J:42:ASP:HB3	1.98	0.46
1:D:2485:HIS:O	1:D:2489:VAL:HG12	2.14	0.46
1:A:2776:GLU:O	1:A:2780:THR:HG22	2.15	0.46
1:A:4883:MET:HE1	1:A:4888:PHE:HD1	1.80	0.46
2:G:38:ASP:OD1	2:G:39:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLU:HG3	1:B:338:LEU:HD22	1.97	0.46
1:C:882:ARG:HD2	1:C:937:LEU:HD23	1.96	0.46
1:C:4193:GLU:OE2	1:C:4943:TYR:OH	2.28	0.46
1:D:642:LEU:HD12	1:D:643:LEU:HA	1.96	0.46
1:D:1287:GLN:HG2	1:D:1355:VAL:HG13	1.97	0.46
1:D:4294:LEU:HA	1:D:4297:VAL:HG12	1.97	0.46
1:A:547:ASN:O	1:A:551:PHE:HD1	1.99	0.46
1:A:4193:GLU:OE2	1:A:4943:TYR:OH	2.28	0.46
1:B:587:ASN:OD1	1:B:2132:ARG:NH1	2.49	0.46
1:B:629:GLN:NE2	1:B:1670:ASN:HD22	2.13	0.46
1:B:2101:LEU:O	1:B:2104:THR:HG22	2.15	0.46
1:C:547:ASN:O	1:C:551:PHE:HD1	1.99	0.46
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.98	0.46
1:C:2068:TRP:HE3	1:C:2083:MET:HE2	1.80	0.46
1:D:547:ASN:O	1:D:551:PHE:HD1	1.99	0.46
1:D:587:ASN:OD1	1:D:2132:ARG:NH1	2.49	0.46
1:D:2346:MET:HE2	1:D:2346:MET:HB2	1.85	0.46
1:A:1968:PRO:HA	1:A:1971:GLN:HB3	1.96	0.46
1:B:547:ASN:O	1:B:551:PHE:HD1	1.99	0.46
1:B:1969:GLN:O	1:B:1973:ASN:ND2	2.49	0.46
2:H:38:ASP:OD1	2:H:39:SER:N	2.49	0.46
1:C:193:HIS:CE1	1:C:208:GLN:HE21	2.34	0.46
1:C:1287:GLN:HG2	1:C:1355:VAL:HG13	1.97	0.46
1:C:4947:CYS:SG	1:C:4948:TRP:N	2.89	0.46
1:D:629:GLN:NE2	1:D:1670:ASN:HD22	2.13	0.46
1:D:812:LYS:O	1:D:812:LYS:NZ	2.35	0.46
1:D:1969:GLN:O	1:D:1973:ASN:ND2	2.49	0.46
1:D:2068:TRP:HE3	1:D:2083:MET:HE2	1.80	0.46
1:A:235:ARG:NH1	1:A:273:SER:OG	2.48	0.46
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.98	0.46
1:B:654:SER:HB2	1:B:837:SER:OG	2.16	0.46
1:B:981:MET:HG3	1:B:983:LEU:HG	1.98	0.46
1:B:1124:PRO:HD2	1:B:1595:VAL:HG23	1.98	0.46
1:B:2068:TRP:HE3	1:B:2083:MET:HE2	1.80	0.46
2:H:26:HIS:CE1	2:H:41:ARG:HG2	2.50	0.46
1:C:1972:ILE:HD12	1:C:1975:LEU:HD11	1.96	0.46
1:C:2058:GLN:HA	1:C:2090:GLN:HE21	1.81	0.46
1:C:2197:ARG:HB3	1:C:2236:SER:OG	2.15	0.46
1:D:2058:GLN:HA	1:D:2090:GLN:HE21	1.81	0.46
1:A:888:ASN:O	1:A:892:LEU:HG	2.14	0.46
1:A:1969:GLN:O	1:A:1973:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:26:HIS:CE1	2:G:41:ARG:HG2	2.50	0.46
1:B:1241:VAL:HG21	1:C:3539:UNK:HA	1.98	0.46
1:B:4947:CYS:SG	1:B:4948:TRP:N	2.89	0.46
2:H:28:THR:O	2:H:28:THR:OG1	2.34	0.46
1:C:281:ARG:O	1:C:285:SER:OG	2.26	0.46
1:C:587:ASN:OD1	1:C:2132:ARG:NH1	2.49	0.46
1:A:21:VAL:HG13	1:A:65:CYS:O	2.16	0.46
1:A:700:THR:HA	1:A:707:PRO:HB3	1.98	0.46
1:A:3898:ASP:OD1	1:A:3898:ASP:N	2.46	0.46
1:A:4294:LEU:HA	1:A:4297:VAL:HG12	1.97	0.46
1:B:530:LEU:HD23	1:B:530:LEU:HA	1.78	0.46
1:B:1967:PRO:HD2	1:B:1970:GLU:OE1	2.16	0.46
1:B:3986:GLU:O	1:B:4935:GLN:NE2	2.49	0.46
1:B:4294:LEU:HA	1:B:4297:VAL:HG12	1.97	0.46
1:C:486:GLN:HB3	1:C:544:ASN:ND2	2.30	0.46
1:C:1305:SER:OG	1:C:1588:HIS:O	2.33	0.46
1:C:1969:GLN:O	1:C:1973:ASN:ND2	2.49	0.46
1:C:2346:MET:HE2	1:C:2346:MET:HB2	1.85	0.46
1:D:2492:LEU:N	1:D:2493:PRO:HD2	2.31	0.46
1:D:3986:GLU:O	1:D:4935:GLN:NE2	2.49	0.46
1:D:4115:GLN:O	1:D:4119:GLU:HG3	2.16	0.46
1:A:193:HIS:CE1	1:A:208:GLN:HE21	2.34	0.46
1:A:629:GLN:NE2	1:A:1670:ASN:HD22	2.13	0.46
1:A:2334:LEU:HD13	1:A:2342:LEU:CD1	2.46	0.46
1:A:2732:SER:O	1:A:2735:LYS:HG3	2.16	0.46
1:B:2231:PRO:HD3	1:B:2381:ILE:HD11	1.96	0.46
1:B:4883:MET:HE1	1:B:4888:PHE:HD1	1.80	0.46
1:C:505:LEU:HD22	1:C:526:TRP:HD1	1.81	0.46
1:C:1713:SER:O	1:C:1717:THR:HG23	2.16	0.46
1:C:2506:LEU:HD23	1:C:2506:LEU:H	1.80	0.46
2:I:28:THR:O	2:I:28:THR:OG1	2.34	0.46
1:D:700:THR:HA	1:D:707:PRO:HB3	1.98	0.46
1:D:981:MET:HG3	1:D:983:LEU:HG	1.98	0.46
1:D:1786:ASP:O	1:D:1789:LYS:HG2	2.16	0.46
1:D:2101:LEU:O	1:D:2104:THR:HG22	2.15	0.46
1:D:4883:MET:HE1	1:D:4888:PHE:HD1	1.80	0.46
1:A:3761:GLY:HA2	1:A:3764:ILE:HG22	1.98	0.45
1:A:4632:LEU:H	1:A:4632:LEU:HD23	1.81	0.45
1:B:706:TYR:HA	1:B:838:ARG:CG	2.46	0.45
1:B:2732:SER:O	1:B:2735:LYS:HG3	2.16	0.45
1:B:4632:LEU:HD23	1:B:4632:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4762:ASN:O	1:B:4764:LYS:N	2.48	0.45
1:C:671:LYS:HA	1:C:761:LEU:HD12	1.99	0.45
1:C:2101:LEU:O	1:C:2104:THR:HG22	2.15	0.45
1:C:3805:ASN:OD1	1:C:3806:ALA:N	2.48	0.45
1:C:4632:LEU:HD23	1:C:4632:LEU:H	1.81	0.45
1:D:21:VAL:HG13	1:D:65:CYS:O	2.16	0.45
1:D:3761:GLY:HA2	1:D:3764:ILE:HG22	1.97	0.45
1:D:4632:LEU:HD23	1:D:4632:LEU:H	1.81	0.45
2:J:38:ASP:OD1	2:J:39:SER:N	2.49	0.45
1:A:654:SER:HB2	1:A:837:SER:OG	2.16	0.45
1:A:706:TYR:HA	1:A:838:ARG:CG	2.46	0.45
1:A:1786:ASP:O	1:A:1789:LYS:HG2	2.16	0.45
1:A:2385:ASN:HA	1:A:2388:MET:HE3	1.98	0.45
1:A:4304:PHE:O	1:A:4308:VAL:HG22	2.16	0.45
1:B:1362:ASP:OD1	1:B:1362:ASP:N	2.49	0.45
1:B:1713:SER:O	1:B:1717:THR:HG23	2.16	0.45
1:C:318:ASP:OD1	1:C:318:ASP:N	2.50	0.45
1:C:1362:ASP:N	1:C:1362:ASP:OD1	2.49	0.45
1:C:2257:ARG:HG3	1:C:2259:PRO:HD3	1.97	0.45
1:C:2732:SER:HA	1:C:2735:LYS:HG3	1.99	0.45
1:D:2732:SER:O	1:D:2735:LYS:HG3	2.16	0.45
1:A:603:LYS:HG2	1:A:1573:LYS:HZ1	1.81	0.45
1:A:3986:GLU:O	1:A:4935:GLN:NE2	2.49	0.45
1:A:4115:GLN:O	1:A:4119:GLU:HG3	2.16	0.45
1:B:505:LEU:HD22	1:B:526:TRP:HD1	1.81	0.45
1:B:1972:ILE:HD12	1:B:1975:LEU:HD11	1.96	0.45
1:B:2206:SER:HG	1:B:2209:ASN:H	1.61	0.45
1:B:4115:GLN:O	1:B:4119:GLU:HG3	2.16	0.45
1:B:4304:PHE:O	1:B:4308:VAL:HG22	2.16	0.45
1:C:700:THR:HA	1:C:707:PRO:HB3	1.98	0.45
1:C:1124:PRO:HD2	1:C:1595:VAL:HG23	1.98	0.45
1:C:1652:LEU:HD12	1:C:1699:LEU:HD13	1.97	0.45
1:C:1967:PRO:HD2	1:C:1970:GLU:OE1	2.16	0.45
1:C:2732:SER:O	1:C:2735:LYS:HG3	2.16	0.45
1:C:4304:PHE:O	1:C:4308:VAL:HG22	2.16	0.45
1:D:281:ARG:O	1:D:285:SER:OG	2.26	0.45
1:D:1652:LEU:HD12	1:D:1699:LEU:HD13	1.97	0.45
1:D:3805:ASN:OD1	1:D:3806:ALA:N	2.48	0.45
1:D:4304:PHE:O	1:D:4308:VAL:HG22	2.16	0.45
1:D:4947:CYS:SG	1:D:4948:TRP:N	2.89	0.45
1:A:1767:PRO:HG3	1:A:1781:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:HIS:CE1	1:B:208:GLN:HE21	2.34	0.45
1:B:1359:ILE:HG13	1:B:1360:ASP:N	2.31	0.45
1:B:4070:GLU:OE1	1:B:4070:GLU:N	2.47	0.45
1:C:3761:GLY:HA2	1:C:3764:ILE:HG22	1.97	0.45
1:C:3845:LEU:HD13	1:C:3853:PHE:CZ	2.52	0.45
1:D:336:GLU:HG3	1:D:338:LEU:HD22	1.97	0.45
1:D:973:THR:OG1	1:D:976:TYR:O	2.19	0.45
1:D:2385:ASN:HA	1:D:2388:MET:HE3	1.98	0.45
1:A:2346:MET:HE2	1:A:2346:MET:HB2	1.84	0.45
1:A:2732:SER:HA	1:A:2735:LYS:HG3	1.99	0.45
1:B:1305:SER:OG	1:B:1588:HIS:O	2.33	0.45
1:B:1608:ASP:OD1	1:B:1608:ASP:N	2.49	0.45
1:C:706:TYR:CD1	1:C:838:ARG:HB3	2.52	0.45
2:I:38:ASP:OD1	2:I:39:SER:N	2.49	0.45
1:D:2320:VAL:O	1:D:2324:ILE:HG12	2.17	0.45
1:A:4947:CYS:SG	1:A:4948:TRP:N	2.89	0.45
1:B:700:THR:HA	1:B:707:PRO:HB3	1.98	0.45
1:B:745:ASN:O	1:B:747:HIS:ND1	2.47	0.45
1:B:1629:MET:CE	1:B:1685:GLN:HE21	2.22	0.45
1:B:2257:ARG:HG3	1:B:2259:PRO:HD3	1.97	0.45
1:B:2334:LEU:HD13	1:B:2342:LEU:CD1	2.46	0.45
1:C:603:LYS:HG2	1:C:1573:LYS:HZ1	1.82	0.45
1:C:981:MET:HG3	1:C:983:LEU:HG	1.98	0.45
1:D:486:GLN:HB3	1:D:544:ASN:ND2	2.29	0.45
1:D:530:LEU:HD23	1:D:530:LEU:HA	1.78	0.45
1:D:706:TYR:CD1	1:D:838:ARG:HB3	2.52	0.45
1:D:1713:SER:O	1:D:1717:THR:HG23	2.16	0.45
1:D:1967:PRO:HD2	1:D:1970:GLU:OE1	2.16	0.45
1:D:2058:GLN:HG3	1:D:2090:GLN:NE2	2.32	0.45
1:D:2732:SER:HA	1:D:2735:LYS:HG3	1.99	0.45
1:A:587:ASN:OD1	1:A:2132:ARG:NH1	2.49	0.45
1:A:669:GLN:HB3	1:A:673:TRP:HZ2	1.82	0.45
1:A:4670:GLY:O	1:A:4671:MET:HG2	2.17	0.45
1:B:21:VAL:HG13	1:B:65:CYS:O	2.16	0.45
1:B:671:LYS:HA	1:B:761:LEU:HD12	1.99	0.45
1:B:2058:GLN:HG3	1:B:2090:GLN:NE2	2.32	0.45
1:B:2320:VAL:O	1:B:2324:ILE:HG12	2.17	0.45
1:B:4670:GLY:O	1:B:4671:MET:HG2	2.17	0.45
1:C:1786:ASP:O	1:C:1789:LYS:HG2	2.16	0.45
1:C:4294:LEU:HA	1:C:4297:VAL:HG12	1.97	0.45
1:D:299:HIS:HD2	1:D:302:THR:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:GLN:HB3	1:D:673:TRP:HZ2	1.82	0.45
1:D:671:LYS:HA	1:D:761:LEU:HD12	1.99	0.45
1:D:2257:ARG:HG3	1:D:2259:PRO:HD3	1.97	0.45
1:A:981:MET:HG3	1:A:983:LEU:HG	1.98	0.45
1:A:1967:PRO:HD2	1:A:1970:GLU:OE1	2.16	0.45
1:B:318:ASP:OD1	1:B:318:ASP:N	2.50	0.45
1:B:1086:ARG:HH21	1:B:1251:LEU:HD13	1.82	0.45
1:C:812:LYS:O	1:C:812:LYS:NZ	2.35	0.45
1:C:1086:ARG:HH21	1:C:1251:LEU:HD13	1.82	0.45
1:C:4115:GLN:O	1:C:4119:GLU:HG3	2.16	0.45
1:D:193:HIS:CE1	1:D:208:GLN:HE21	2.34	0.45
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.98	0.45
1:D:654:SER:HB2	1:D:837:SER:OG	2.16	0.45
1:D:706:TYR:HA	1:D:838:ARG:CG	2.46	0.45
1:D:1608:ASP:OD1	1:D:1608:ASP:N	2.49	0.45
1:A:299:HIS:HD2	1:A:302:THR:H	1.65	0.45
1:A:1608:ASP:OD1	1:A:1608:ASP:N	2.49	0.45
1:A:2762:LEU:HD22	1:A:2766:GLU:O	2.17	0.45
1:A:3845:LEU:HD13	1:A:3853:PHE:CZ	2.52	0.45
1:A:4762:ASN:O	1:A:4764:LYS:N	2.48	0.45
1:B:603:LYS:HG2	1:B:1573:LYS:HZ1	1.81	0.45
1:B:2257:ARG:CG	1:B:2259:PRO:HD3	2.47	0.45
1:B:2732:SER:HA	1:B:2735:LYS:HG3	1.99	0.45
1:C:654:SER:HB2	1:C:837:SER:OG	2.16	0.45
1:C:669:GLN:HB3	1:C:673:TRP:HZ2	1.82	0.45
1:C:976:TYR:O	1:C:977:LYS:HD2	2.17	0.45
1:C:2320:VAL:O	1:C:2324:ILE:HG12	2.17	0.45
1:C:2385:ASN:HA	1:C:2388:MET:HE3	1.98	0.45
1:D:1124:PRO:HD2	1:D:1595:VAL:HG23	1.98	0.45
1:D:2334:LEU:HD13	1:D:2342:LEU:CD1	2.46	0.45
1:D:3845:LEU:HD13	1:D:3853:PHE:CZ	2.52	0.45
1:A:845:THR:OG1	1:A:846:TYR:N	2.50	0.45
1:A:2257:ARG:CG	1:A:2259:PRO:HD3	2.47	0.45
1:A:2405:MET:SD	1:A:2407:LEU:HB2	2.57	0.45
1:B:656:ARG:NH2	1:B:835:GLU:OE2	2.50	0.45
1:B:2172:GLU:HA	1:B:2175:VAL:HG12	1.99	0.45
1:B:2405:MET:SD	1:B:2407:LEU:HB2	2.57	0.45
1:C:924:LEU:HB2	1:C:929:ARG:HD3	1.99	0.45
1:C:1320:UNK:HA	1:C:1325:UNK:HA	1.99	0.45
1:C:1359:ILE:HG13	1:C:1360:ASP:N	2.31	0.45
1:C:3986:GLU:O	1:C:4935:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4594:VAL:HA	1:C:4597:VAL:HG12	1.99	0.45
1:D:1320:UNK:HA	1:D:1325:UNK:HA	1.99	0.45
1:D:1629:MET:HG3	1:D:1642:ILE:HG21	1.99	0.45
1:A:671:LYS:HA	1:A:761:LEU:HD12	1.98	0.44
1:A:745:ASN:O	1:A:747:HIS:ND1	2.47	0.44
1:A:1353:HIS:CE1	1:A:1367:LYS:HE3	2.52	0.44
1:B:706:TYR:OH	1:B:851:LEU:HD11	2.18	0.44
1:B:1353:HIS:CE1	1:B:1367:LYS:HE3	2.52	0.44
1:B:1767:PRO:HG3	1:B:1781:PRO:HB3	1.98	0.44
1:B:4594:VAL:HA	1:B:4597:VAL:HG12	1.99	0.44
1:C:807:ARG:O	1:C:1615:ARG:NE	2.46	0.44
1:C:1353:HIS:CE1	1:C:1367:LYS:HE3	2.52	0.44
1:C:1591:PHE:CZ	1:C:1593:SER:HB2	2.52	0.44
1:C:1629:MET:HG3	1:C:1642:ILE:HG21	1.98	0.44
1:C:2405:MET:SD	1:C:2407:LEU:HB2	2.57	0.44
1:D:976:TYR:O	1:D:977:LYS:HD2	2.17	0.44
1:D:1362:ASP:OD1	1:D:1362:ASP:N	2.49	0.44
1:D:1591:PHE:CZ	1:D:1593:SER:HB2	2.52	0.44
1:D:1677:LEU:O	1:D:1681:VAL:HG22	2.18	0.44
1:D:1789:LYS:HZ1	1:D:1835:PHE:H	1.65	0.44
1:D:4176:VAL:HG11	1:D:4879:VAL:HA	1.99	0.44
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.98	0.44
1:A:706:TYR:CD1	1:A:838:ARG:HB3	2.52	0.44
1:A:706:TYR:OH	1:A:851:LEU:HD11	2.18	0.44
1:A:921:PHE:O	1:A:929:ARG:NH1	2.45	0.44
1:A:1124:PRO:HD2	1:A:1595:VAL:HG23	1.98	0.44
1:A:1196:ASP:OD1	1:A:1196:ASP:N	2.50	0.44
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.49	0.44
1:A:2172:GLU:HA	1:A:2175:VAL:HG12	1.99	0.44
1:B:674:TYR:N	1:B:820:ALA:O	2.51	0.44
1:B:1629:MET:HG3	1:B:1642:ILE:HG21	1.99	0.44
1:B:2492:LEU:N	1:B:2493:PRO:HD2	2.31	0.44
2:H:83:TYR:HB3	2:H:87:GLY:HA2	2.00	0.44
1:C:299:HIS:HD2	1:C:302:THR:H	1.65	0.44
1:C:674:TYR:N	1:C:820:ALA:O	2.51	0.44
1:C:706:TYR:HA	1:C:838:ARG:CG	2.46	0.44
1:C:2257:ARG:CG	1:C:2259:PRO:HD3	2.47	0.44
1:C:3898:ASP:OD1	1:C:3898:ASP:N	2.46	0.44
1:C:4273:MET:HE3	1:C:4273:MET:HB2	1.73	0.44
1:D:656:ARG:NH2	1:D:835:GLU:OE2	2.50	0.44
1:D:845:THR:OG1	1:D:846:TYR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1767:PRO:HG3	1:D:1781:PRO:HB3	1.99	0.44
1:A:896:ASN:OD1	1:A:897:LYS:N	2.51	0.44
1:A:2492:LEU:N	1:A:2493:PRO:HD2	2.31	0.44
1:A:4594:VAL:HA	1:A:4597:VAL:HG12	1.99	0.44
1:C:845:THR:OG1	1:C:846:TYR:N	2.50	0.44
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.83	0.44
1:D:924:LEU:HB2	1:D:929:ARG:HD3	1.99	0.44
1:D:2405:MET:SD	1:D:2407:LEU:HB2	2.57	0.44
1:D:4594:VAL:HA	1:D:4597:VAL:HG12	1.99	0.44
1:A:66:THR:HG1	1:A:124:SER:HG	1.61	0.44
1:A:318:ASP:OD1	1:A:318:ASP:N	2.50	0.44
1:A:924:LEU:HB2	1:A:929:ARG:HD3	1.99	0.44
1:A:2058:GLN:HG3	1:A:2090:GLN:NE2	2.32	0.44
1:A:2320:VAL:O	1:A:2324:ILE:HG12	2.17	0.44
1:B:706:TYR:CD1	1:B:838:ARG:HB3	2.52	0.44
1:B:1591:PHE:CZ	1:B:1593:SER:HB2	2.52	0.44
1:B:1786:ASP:O	1:B:1789:LYS:HG2	2.16	0.44
1:B:2731:TRP:CE2	1:B:2762:LEU:HD12	2.53	0.44
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.87	0.44
1:C:2058:GLN:HG3	1:C:2090:GLN:NE2	2.32	0.44
1:C:2334:LEU:HD13	1:C:2342:LEU:CD1	2.46	0.44
1:C:2492:LEU:N	1:C:2493:PRO:HD2	2.31	0.44
1:D:2316:ALA:O	1:D:2320:VAL:HG23	2.18	0.44
1:A:888:ASN:O	1:A:891:GLU:HG2	2.18	0.44
1:A:1256:PRO:HG2	1:A:1592:LEU:HD21	1.99	0.44
2:G:83:TYR:HB3	2:G:87:GLY:HA2	2.00	0.44
1:B:669:GLN:HB3	1:B:673:TRP:HZ2	1.82	0.44
1:B:888:ASN:O	1:B:891:GLU:HG2	2.18	0.44
1:B:2282:LYS:HA	1:B:2282:LYS:HD2	1.89	0.44
1:B:2385:ASN:HA	1:B:2388:MET:HE3	1.98	0.44
1:C:850:LEU:HD23	1:C:1213:GLY:O	2.18	0.44
1:D:807:ARG:O	1:D:1615:ARG:NE	2.46	0.44
1:D:888:ASN:O	1:D:891:GLU:HG2	2.18	0.44
1:D:4670:GLY:O	1:D:4671:MET:HG2	2.17	0.44
2:J:83:TYR:HB3	2:J:87:GLY:HA2	2.00	0.44
1:A:976:TYR:O	1:A:977:LYS:HD2	2.17	0.44
1:A:1086:ARG:HH21	1:A:1251:LEU:HD13	1.82	0.44
1:A:2160:LEU:HB3	1:A:2161:MET:HE2	2.00	0.44
1:A:2316:ALA:O	1:A:2320:VAL:HG23	2.18	0.44
1:B:896:ASN:OD1	1:B:897:LYS:N	2.51	0.44
1:B:935:MET:HE1	1:B:1050:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1196:ASP:N	1:B:1196:ASP:OD1	2.50	0.44
1:B:2316:ALA:O	1:B:2320:VAL:HG23	2.18	0.44
1:B:2331:GLY:HA3	1:B:2391:TYR:HE1	1.83	0.44
1:C:21:VAL:HG13	1:C:65:CYS:O	2.16	0.44
1:C:611:LEU:HD11	1:C:643:LEU:HD21	2.00	0.44
1:C:1767:PRO:HG3	1:C:1781:PRO:HB3	1.98	0.44
1:C:2731:TRP:CE2	1:C:2762:LEU:HD12	2.53	0.44
1:C:4670:GLY:O	1:C:4671:MET:HG2	2.17	0.44
1:D:603:LYS:HG2	1:D:1573:LYS:HZ1	1.83	0.44
1:D:674:TYR:N	1:D:820:ALA:O	2.51	0.44
1:D:4044:LYS:HE2	1:D:4044:LYS:HB3	1.81	0.44
1:A:674:TYR:N	1:A:820:ALA:O	2.51	0.44
2:G:23:CYS:SG	2:G:51:ILE:HD11	2.58	0.44
1:B:850:LEU:HD23	1:B:1213:GLY:O	2.18	0.44
1:C:896:ASN:OD1	1:C:897:LYS:N	2.51	0.44
2:I:23:CYS:SG	2:I:51:ILE:HD11	2.58	0.44
1:D:706:TYR:OH	1:D:851:LEU:HD11	2.18	0.44
1:D:1048:ASP:OD1	1:D:1051:ARG:NH1	2.48	0.44
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.83	0.44
1:A:1591:PHE:CZ	1:A:1593:SER:HB2	2.52	0.44
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.84	0.44
1:B:2892:PHE:O	1:B:2896:GLN:HG2	2.18	0.44
1:C:557:TRP:CE2	1:C:561:ARG:HG3	2.53	0.44
1:C:4762:ASN:O	1:C:4764:LYS:N	2.48	0.44
2:J:23:CYS:SG	2:J:51:ILE:HD11	2.58	0.44
1:A:1359:ILE:HG13	1:A:1360:ASP:N	2.31	0.44
1:A:1677:LEU:O	1:A:1681:VAL:HG22	2.18	0.44
1:A:2731:TRP:CE2	1:A:2762:LEU:HD12	2.53	0.44
1:B:924:LEU:HB2	1:B:929:ARG:HD3	1.99	0.44
1:B:1028:ARG:O	1:B:1028:ARG:HD3	2.18	0.44
1:B:1677:LEU:O	1:B:1681:VAL:HG22	2.18	0.44
1:B:2160:LEU:HB3	1:B:2161:MET:HE2	2.00	0.44
1:B:2762:LEU:HD22	1:B:2766:GLU:O	2.17	0.44
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.83	0.44
1:C:1608:ASP:OD1	1:C:1608:ASP:N	2.49	0.44
1:C:2331:GLY:HA3	1:C:2391:TYR:HE1	1.83	0.44
1:C:2404:GLU:HG3	1:C:2405:MET:H	1.83	0.44
2:I:83:TYR:HB3	2:I:87:GLY:HA2	2.00	0.44
1:D:505:LEU:HD22	1:D:526:TRP:HD1	1.81	0.44
1:D:1086:ARG:HH21	1:D:1251:LEU:HD13	1.82	0.44
1:D:1196:ASP:OD1	1:D:1196:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1304:LEU:HD12	1:D:1340:ASP:HB2	2.00	0.44
1:A:712:GLU:HB3	1:A:713:TRP:CE3	2.53	0.43
1:A:850:LEU:HD23	1:A:1213:GLY:O	2.18	0.43
1:A:997:ASP:HB2	1:A:1047:LYS:HD3	2.00	0.43
1:A:1304:LEU:HD12	1:A:1340:ASP:HB2	2.00	0.43
1:A:1629:MET:HG3	1:A:1642:ILE:HG21	1.99	0.43
1:A:1704:TYR:O	1:A:1708:ILE:HG12	2.18	0.43
1:A:2733:MET:O	1:A:2736:LEU:HG	2.18	0.43
1:A:3719:GLU:HA	1:A:3722:LYS:HG2	2.00	0.43
1:B:2183:SER:O	1:B:2183:SER:OG	2.31	0.43
2:H:23:CYS:SG	2:H:51:ILE:HD11	2.58	0.43
1:C:712:GLU:HB3	1:C:713:TRP:CE3	2.53	0.43
1:C:1028:ARG:O	1:C:1028:ARG:HD3	2.18	0.43
1:C:1256:PRO:HG2	1:C:1592:LEU:HD21	1.99	0.43
1:C:1747:HIS:O	1:C:1747:HIS:ND1	2.51	0.43
1:D:557:TRP:CE2	1:D:561:ARG:HG3	2.53	0.43
1:D:707:PRO:HD2	1:D:838:ARG:HD2	2.00	0.43
1:D:712:GLU:HB3	1:D:713:TRP:CE3	2.53	0.43
1:D:986:ILE:O	1:D:1055:ARG:NH1	2.51	0.43
1:D:1172:THR:HB	1:D:1190:LEU:HD12	2.00	0.43
1:D:1747:HIS:ND1	1:D:1747:HIS:O	2.51	0.43
1:A:4594:VAL:N	1:A:4595:PRO:HD2	2.33	0.43
1:B:986:ILE:O	1:B:1055:ARG:NH1	2.51	0.43
1:B:1320:UNK:HA	1:B:1325:UNK:HA	1.99	0.43
1:B:2715:LYS:HG3	1:B:2900:TYR:OH	2.17	0.43
1:B:3845:LEU:HD13	1:B:3853:PHE:CZ	2.52	0.43
1:B:4594:VAL:N	1:B:4595:PRO:HD2	2.33	0.43
1:C:656:ARG:NH2	1:C:835:GLU:OE2	2.50	0.43
1:C:1704:TYR:O	1:C:1708:ILE:HG12	2.18	0.43
1:C:2101:LEU:HD13	1:C:3624:GLU:HB3	2.00	0.43
1:D:1353:HIS:CE1	1:D:1367:LYS:HE3	2.52	0.43
1:A:611:LEU:HD11	1:A:643:LEU:HD21	2.00	0.43
1:A:986:ILE:O	1:A:1055:ARG:NH1	2.51	0.43
1:A:2892:PHE:O	1:A:2896:GLN:HG2	2.18	0.43
1:B:544:ASN:O	1:B:581:GLU:HG2	2.19	0.43
1:B:845:THR:OG1	1:B:846:TYR:N	2.50	0.43
1:B:976:TYR:O	1:B:977:LYS:HD2	2.17	0.43
1:B:2101:LEU:HD13	1:B:3624:GLU:HB3	2.00	0.43
1:B:2404:GLU:HG3	1:B:2405:MET:H	1.83	0.43
1:B:2733:MET:O	1:B:2736:LEU:HG	2.18	0.43
1:C:233:VAL:O	1:C:408:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ASN:CG	1:C:392:ILE:HD13	2.44	0.43
1:C:888:ASN:O	1:C:891:GLU:HG2	2.18	0.43
1:C:2172:GLU:HA	1:C:2175:VAL:HG12	1.99	0.43
1:C:2240:ASP:OD1	1:C:2296:ARG:NH2	2.43	0.43
1:C:2316:ALA:O	1:C:2320:VAL:HG23	2.18	0.43
1:C:2715:LYS:HG3	1:C:2900:TYR:OH	2.17	0.43
1:C:2733:MET:O	1:C:2736:LEU:HG	2.18	0.43
1:C:4294:LEU:HA	1:C:4294:LEU:HD12	1.88	0.43
1:C:4590:TYR:HA	1:C:4594:VAL:CG2	2.49	0.43
1:D:646:THR:OG1	1:D:1685:GLN:NE2	2.52	0.43
1:D:745:ASN:O	1:D:747:HIS:ND1	2.47	0.43
1:D:850:LEU:HD23	1:D:1213:GLY:O	2.18	0.43
1:D:896:ASN:OD1	1:D:897:LYS:N	2.51	0.43
1:D:1928:SER:OG	1:D:3616:VAL:HG23	2.19	0.43
1:D:2172:GLU:HA	1:D:2175:VAL:HG12	1.99	0.43
1:D:2257:ARG:CG	1:D:2259:PRO:HD3	2.47	0.43
1:D:2715:LYS:HG3	1:D:2900:TYR:OH	2.17	0.43
1:D:4594:VAL:N	1:D:4595:PRO:HD2	2.33	0.43
1:A:290:ARG:H	1:A:293:GLN:NE2	2.16	0.43
1:A:707:PRO:HD2	1:A:838:ARG:HD2	2.00	0.43
1:A:2715:LYS:HG3	1:A:2900:TYR:OH	2.17	0.43
1:B:1304:LEU:HD12	1:B:1340:ASP:HB2	2.00	0.43
1:B:1747:HIS:ND1	1:B:1747:HIS:O	2.51	0.43
1:B:1789:LYS:HZ1	1:B:1835:PHE:H	1.66	0.43
1:B:2335:ARG:HD3	1:B:2336:GLY:N	2.34	0.43
1:C:544:ASN:O	1:C:581:GLU:HG2	2.19	0.43
1:C:1677:LEU:O	1:C:1681:VAL:HG22	2.18	0.43
1:D:544:ASN:O	1:D:581:GLU:HG2	2.19	0.43
1:D:3719:GLU:HA	1:D:3722:LYS:HG2	2.00	0.43
1:A:505:LEU:HD22	1:A:526:TRP:HD1	1.82	0.43
1:A:544:ASN:O	1:A:581:GLU:HG2	2.19	0.43
1:A:557:TRP:CE2	1:A:561:ARG:HG3	2.53	0.43
1:A:2331:GLY:HA3	1:A:2391:TYR:HE1	1.83	0.43
1:B:4273:MET:HE2	1:B:4273:MET:N	2.34	0.43
1:B:4793:ASN:O	1:B:4795:SER:N	2.50	0.43
1:C:4273:MET:N	1:C:4273:MET:HE2	2.34	0.43
1:D:152:ASP:OD2	1:D:154:THR:OG1	2.37	0.43
1:D:407:ARG:HH21	1:D:3864:ASN:HB3	1.84	0.43
1:D:611:LEU:HD11	1:D:643:LEU:HD21	2.00	0.43
1:D:1028:ARG:O	1:D:1028:ARG:HD3	2.18	0.43
1:D:2355:ASP:OD2	1:D:2357:SER:OG	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LEU:HG	1:A:642:LEU:HD21	2.00	0.43
1:A:656:ARG:NH2	1:A:835:GLU:OE2	2.50	0.43
1:A:4176:VAL:HG11	1:A:4879:VAL:HA	1.99	0.43
1:A:4273:MET:HE2	1:A:4273:MET:N	2.34	0.43
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.83	0.43
1:B:313:ASN:CG	1:B:392:ILE:HD13	2.44	0.43
1:B:557:TRP:CE2	1:B:561:ARG:HG3	2.53	0.43
1:B:1987:CYS:N	1:B:1988:PRO:HD2	2.34	0.43
1:B:4176:VAL:HG11	1:B:4879:VAL:HA	1.99	0.43
1:C:646:THR:OG1	1:C:1685:GLN:NE2	2.52	0.43
1:C:986:ILE:O	1:C:1055:ARG:NH1	2.51	0.43
1:C:1928:SER:OG	1:C:3616:VAL:HG23	2.19	0.43
1:C:2762:LEU:HD22	1:C:2766:GLU:O	2.17	0.43
1:C:4594:VAL:N	1:C:4595:PRO:HD2	2.33	0.43
1:D:921:PHE:O	1:D:929:ARG:NH1	2.45	0.43
1:D:1704:TYR:O	1:D:1708:ILE:HG12	2.18	0.43
1:D:2731:TRP:CE2	1:D:2762:LEU:HD12	2.53	0.43
1:D:2762:LEU:HD22	1:D:2766:GLU:O	2.17	0.43
1:D:2892:PHE:O	1:D:2896:GLN:HG2	2.18	0.43
1:D:4830:ILE:HG22	1:D:4831:GLU:N	2.34	0.43
1:A:1172:THR:HB	1:A:1190:LEU:HD12	2.00	0.43
1:A:1320:UNK:HA	1:A:1325:UNK:HA	1.99	0.43
1:B:407:ARG:HH21	1:B:3864:ASN:HB3	1.84	0.43
1:B:712:GLU:HB3	1:B:713:TRP:CE3	2.53	0.43
1:B:997:ASP:HB2	1:B:1047:LYS:HD3	2.00	0.43
1:B:1256:PRO:HG2	1:B:1592:LEU:HD21	1.99	0.43
1:B:1733:GLU:O	1:B:1736:SER:OG	2.30	0.43
1:B:4019:PHE:CD1	1:B:4086:PHE:HB3	2.54	0.43
1:B:4867:ASP:OD1	1:C:4873:ARG:NH1	2.51	0.43
1:C:1172:THR:HB	1:C:1190:LEU:HD12	2.00	0.43
1:D:233:VAL:O	1:D:408:SER:OG	2.36	0.43
1:D:1256:PRO:HG2	1:D:1592:LEU:HD21	1.99	0.43
1:D:1769:PHE:O	2:J:83:TYR:OH	2.33	0.43
1:D:4273:MET:HE2	1:D:4273:MET:N	2.34	0.43
1:A:765:SER:HB3	1:A:782:PHE:CE1	2.54	0.43
1:A:778:MET:HG3	1:A:780:GLU:OE2	2.19	0.43
1:A:2712:ILE:HG21	1:A:2717:GLU:OE2	2.19	0.43
1:B:299:HIS:HD2	1:B:302:THR:H	1.65	0.43
1:B:698:ALA:HA	1:B:724:SER:HA	2.01	0.43
1:C:765:SER:HB3	1:C:782:PHE:CE1	2.54	0.43
1:C:4176:VAL:HG11	1:C:4879:VAL:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:765:SER:HB3	1:D:782:PHE:CE1	2.54	0.43
1:D:2160:LEU:HB3	1:D:2161:MET:HE2	2.00	0.43
1:D:3715:GLU:OE2	1:D:3716:LYS:NZ	2.52	0.43
1:D:4590:TYR:HA	1:D:4594:VAL:CG2	2.49	0.43
1:A:245:LEU:HD13	1:A:262:TYR:CE1	2.54	0.43
1:A:1028:ARG:O	1:A:1028:ARG:HD3	2.18	0.43
1:A:1789:LYS:HB2	1:A:1835:PHE:CE1	2.54	0.43
1:A:4830:ILE:HG22	1:A:4831:GLU:N	2.33	0.43
1:B:1704:TYR:O	1:B:1708:ILE:HG12	2.18	0.43
1:C:152:ASP:OD2	1:C:154:THR:OG1	2.37	0.43
1:C:1205:CYS:SG	1:C:1206:SER:N	2.92	0.43
1:C:1789:LYS:HB2	1:C:1835:PHE:CE1	2.54	0.43
1:C:2154:PHE:HA	1:C:2161:MET:HE3	2.01	0.43
1:C:2712:ILE:HG21	1:C:2717:GLU:OE2	2.19	0.43
1:C:2892:PHE:O	1:C:2896:GLN:HG2	2.18	0.43
1:C:3715:GLU:OE2	1:C:3716:LYS:NZ	2.52	0.43
1:C:3719:GLU:HA	1:C:3722:LYS:HG2	2.00	0.43
1:D:997:ASP:HB2	1:D:1047:LYS:HD3	2.00	0.43
1:D:1789:LYS:HB2	1:D:1835:PHE:CE1	2.54	0.43
1:D:3898:ASP:OD1	1:D:3898:ASP:N	2.46	0.43
1:D:4019:PHE:CD1	1:D:4086:PHE:HB3	2.54	0.43
1:D:4200:GLN:HE21	1:D:4922:MET:HE3	1.84	0.43
1:A:1205:CYS:SG	1:A:1206:SER:N	2.92	0.43
1:A:4694:SER:O	1:A:4694:SER:OG	2.32	0.43
1:B:643:LEU:HD13	1:B:1658:THR:HG23	2.01	0.43
1:B:765:SER:HB3	1:B:782:PHE:CE1	2.54	0.43
1:B:1172:THR:HB	1:B:1190:LEU:HD12	2.00	0.43
1:B:2753:GLN:HB2	1:B:2756:MET:HG2	2.01	0.43
1:B:3719:GLU:HA	1:B:3722:LYS:HG2	2.00	0.43
1:C:706:TYR:OH	1:C:851:LEU:HD11	2.18	0.43
1:C:935:MET:HE1	1:C:1050:LEU:HD13	2.00	0.43
1:C:983:LEU:O	1:C:1055:ARG:HD2	2.19	0.43
1:C:1304:LEU:HD12	1:C:1340:ASP:HB2	2.00	0.43
1:C:4019:PHE:CD1	1:C:4086:PHE:HB3	2.54	0.43
1:C:4830:ILE:HG22	1:C:4831:GLU:N	2.34	0.43
1:C:4923:TYR:CZ	1:C:4927:LYS:HD2	2.54	0.43
1:D:245:LEU:HD13	1:D:262:TYR:CE1	2.54	0.43
1:D:601:LEU:HG	1:D:642:LEU:HD21	2.00	0.43
1:D:935:MET:HE1	1:D:1050:LEU:HD13	2.00	0.43
1:D:2282:LYS:HA	1:D:2282:LYS:HD2	1.89	0.43
1:D:2712:ILE:HG21	1:D:2717:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3943:VAL:HG13	1:D:4001:MET:HE3	2.01	0.43
1:D:4294:LEU:HA	1:D:4294:LEU:HD12	1.88	0.43
1:A:983:LEU:O	1:A:1055:ARG:HD2	2.19	0.42
1:A:1771:SER:HA	2:G:56:VAL:HA	2.00	0.42
1:A:2101:LEU:HD13	1:A:3624:GLU:HB3	2.00	0.42
1:A:2154:PHE:HA	1:A:2161:MET:HE3	2.01	0.42
1:A:4019:PHE:CD1	1:A:4086:PHE:HB3	2.54	0.42
1:A:4200:GLN:HE21	1:A:4922:MET:HE3	1.84	0.42
1:A:4793:ASN:O	1:A:4795:SER:N	2.50	0.42
1:B:58:VAL:HG12	1:B:320:GLU:HA	2.01	0.42
1:B:245:LEU:HD13	1:B:262:TYR:CE1	2.54	0.42
1:B:294:PRO:HA	1:B:329:PHE:O	2.19	0.42
1:B:799:LYS:HG2	1:B:1621:GLN:NE2	2.34	0.42
1:B:812:LYS:O	1:B:812:LYS:NZ	2.35	0.42
1:B:1928:SER:OG	1:B:3616:VAL:HG23	2.19	0.42
1:C:245:LEU:HD13	1:C:262:TYR:CE1	2.54	0.42
1:C:245:LEU:HD13	1:C:262:TYR:HE1	1.84	0.42
1:C:2335:ARG:HD3	1:C:2336:GLY:N	2.34	0.42
1:C:2768:GLU:OE2	1:C:2771:ARG:HD2	2.19	0.42
1:C:3943:VAL:HG13	1:C:4001:MET:HE3	2.01	0.42
1:C:4200:GLN:HE21	1:C:4922:MET:HE3	1.84	0.42
1:D:1205:CYS:SG	1:D:1206:SER:N	2.92	0.42
1:D:1359:ILE:HG13	1:D:1360:ASP:N	2.31	0.42
1:A:58:VAL:HG12	1:A:320:GLU:HA	2.01	0.42
1:A:245:LEU:HD13	1:A:262:TYR:HE1	1.84	0.42
1:A:407:ARG:HH21	1:A:3864:ASN:HB3	1.84	0.42
1:A:646:THR:OG1	1:A:1685:GLN:NE2	2.52	0.42
1:A:1309:GLU:H	1:A:1309:GLU:CD	2.27	0.42
1:A:4273:MET:HE3	1:A:4273:MET:HB2	1.73	0.42
1:B:2712:ILE:HG21	1:B:2717:GLU:OE2	2.19	0.42
1:B:4830:ILE:HG22	1:B:4831:GLU:N	2.33	0.42
1:C:66:THR:OG1	1:C:124:SER:OG	2.33	0.42
1:C:745:ASN:O	1:C:747:HIS:ND1	2.47	0.42
1:C:778:MET:HG3	1:C:780:GLU:OE2	2.19	0.42
1:C:1309:GLU:H	1:C:1309:GLU:CD	2.27	0.42
1:C:1987:CYS:N	1:C:1988:PRO:HD2	2.34	0.42
1:C:2753:GLN:HB2	1:C:2756:MET:HG2	2.01	0.42
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.87	0.42
1:D:1309:GLU:CD	1:D:1309:GLU:H	2.27	0.42
1:D:2154:PHE:HA	1:D:2161:MET:HE3	2.01	0.42
1:D:2404:GLU:HG3	1:D:2405:MET:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2768:GLU:OE2	1:D:2771:ARG:HD2	2.19	0.42
1:D:4923:TYR:CZ	1:D:4927:LYS:HD2	2.54	0.42
1:A:294:PRO:HA	1:A:329:PHE:O	2.19	0.42
1:A:313:ASN:CG	1:A:392:ILE:HD13	2.44	0.42
1:A:3822:GLU:HB2	1:A:3826:GLU:HA	2.01	0.42
1:A:4590:TYR:HA	1:A:4594:VAL:CG2	2.49	0.42
1:B:245:LEU:HD13	1:B:262:TYR:HE1	1.84	0.42
1:B:601:LEU:HG	1:B:642:LEU:HD21	2.00	0.42
1:B:755:ILE:HD11	1:B:768:PHE:HB3	2.01	0.42
1:B:801:ARG:HA	1:B:1618:TRP:O	2.20	0.42
1:B:1643:LEU:HD22	1:B:1694:TYR:O	2.19	0.42
1:B:1732:GLU:OE2	1:B:1735:LYS:HB2	2.20	0.42
1:B:3943:VAL:HG13	1:B:4001:MET:HE3	2.01	0.42
1:B:4294:LEU:HA	1:B:4294:LEU:HD12	1.88	0.42
1:B:4590:TYR:HA	1:B:4594:VAL:CG2	2.49	0.42
1:C:707:PRO:HD2	1:C:838:ARG:HD2	2.00	0.42
1:C:799:LYS:HG2	1:C:1621:GLN:NE2	2.34	0.42
1:C:1771:SER:HA	2:I:56:VAL:HA	2.01	0.42
1:C:1959:ARG:HH21	1:C:1962:ARG:HH12	1.67	0.42
1:C:2160:LEU:HB3	1:C:2161:MET:HE2	2.00	0.42
1:D:313:ASN:CG	1:D:392:ILE:HD13	2.44	0.42
1:D:983:LEU:O	1:D:1055:ARG:HD2	2.19	0.42
1:D:2733:MET:O	1:D:2736:LEU:HG	2.18	0.42
1:D:4070:GLU:OE1	1:D:4070:GLU:N	2.47	0.42
1:D:4694:SER:O	1:D:4694:SER:OG	2.32	0.42
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.52	0.42
1:A:530:LEU:HA	1:A:530:LEU:HD23	1.78	0.42
1:A:661:LEU:HD13	1:A:673:TRP:CD1	2.55	0.42
1:A:935:MET:HE1	1:A:1050:LEU:HD13	2.00	0.42
1:A:1928:SER:OG	1:A:3616:VAL:HG23	2.19	0.42
1:A:2404:GLU:HG3	1:A:2405:MET:H	1.83	0.42
1:A:3715:GLU:OE2	1:A:3716:LYS:NZ	2.52	0.42
1:A:3919:LEU:O	1:A:3923:ILE:HG12	2.20	0.42
1:A:3943:VAL:HG13	1:A:4001:MET:HE3	2.01	0.42
1:B:66:THR:OG1	1:B:124:SER:OG	2.32	0.42
1:B:290:ARG:H	1:B:293:GLN:NE2	2.16	0.42
1:B:611:LEU:HD11	1:B:643:LEU:HD21	2.00	0.42
1:B:4668:LEU:HG	1:B:4669:LEU:HD12	2.02	0.42
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.52	0.42
1:C:601:LEU:HG	1:C:642:LEU:HD21	2.00	0.42
1:C:997:ASP:HB2	1:C:1047:LYS:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1196:ASP:N	1:C:1196:ASP:OD1	2.50	0.42
1:C:2313:GLU:OE1	1:C:3812:LYS:HE2	2.20	0.42
1:C:4051:MET:HE2	1:C:4062:THR:HG22	2.02	0.42
1:D:940:LEU:O	1:D:944:LEU:HG	2.20	0.42
1:D:2331:GLY:HA3	1:D:2391:TYR:HE1	1.83	0.42
1:D:3964:ILE:HG13	1:D:3965:GLU:OE1	2.20	0.42
1:A:152:ASP:OD2	1:A:154:THR:OG1	2.37	0.42
1:A:190:ARG:HD3	1:A:205:ALA:O	2.20	0.42
1:A:309:MET:HE3	1:A:309:MET:HB3	1.91	0.42
1:A:4070:GLU:OE1	1:A:4070:GLU:N	2.47	0.42
1:A:4923:TYR:CZ	1:A:4927:LYS:HD2	2.54	0.42
2:G:28:THR:O	2:G:28:THR:OG1	2.34	0.42
1:B:514:PHE:HD2	1:B:523:GLY:HA2	1.84	0.42
1:B:707:PRO:HD2	1:B:838:ARG:HD2	2.00	0.42
1:B:1959:ARG:HH21	1:B:1962:ARG:HH12	1.67	0.42
1:B:2768:GLU:OE2	1:B:2771:ARG:HD2	2.19	0.42
1:B:3919:LEU:O	1:B:3923:ILE:HG12	2.20	0.42
1:C:328:ALA:HB3	1:C:366:VAL:HG11	2.02	0.42
1:C:940:LEU:O	1:C:944:LEU:HG	2.20	0.42
1:C:2355:ASP:OD2	1:C:2357:SER:OG	2.30	0.42
1:C:4791:PHE:HE1	1:C:4833:PRO:HA	1.84	0.42
1:D:66:THR:OG1	1:D:124:SER:OG	2.33	0.42
1:D:778:MET:HG3	1:D:780:GLU:OE2	2.19	0.42
1:D:799:LYS:HG2	1:D:1621:GLN:NE2	2.34	0.42
1:D:1111:GLY:HA3	1:D:1211:GLN:CD	2.45	0.42
1:D:1643:LEU:HD22	1:D:1694:TYR:O	2.19	0.42
1:D:2101:LEU:HD13	1:D:3624:GLU:HB3	2.00	0.42
1:D:2335:ARG:HD3	1:D:2336:GLY:N	2.34	0.42
1:A:625:VAL:HG23	1:A:628:ASN:HB2	2.02	0.42
1:A:643:LEU:HD13	1:A:1658:THR:HG23	2.01	0.42
1:A:1111:GLY:HA3	1:A:1211:GLN:CD	2.45	0.42
1:A:2716:LEU:HG	1:A:2900:TYR:HE2	1.84	0.42
1:A:2733:MET:HE3	1:D:1429:UNK:O	2.18	0.42
1:B:28:ILE:HG21	1:B:201:TRP:CH2	2.55	0.42
1:B:328:ALA:HB3	1:B:366:VAL:HG11	2.02	0.42
1:B:661:LEU:HD13	1:B:673:TRP:CD1	2.55	0.42
1:B:1776:CYS:SG	1:B:1778:GLN:HB2	2.60	0.42
1:B:3715:GLU:OE2	1:B:3716:LYS:NZ	2.52	0.42
1:C:28:ILE:HG21	1:C:201:TRP:CH2	2.55	0.42
1:C:1372:ASN:OD1	1:C:1372:ASN:N	2.53	0.42
1:C:2428:LEU:O	1:C:2432:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3817:GLY:C	1:C:3818:MET:HE2	2.44	0.42
1:C:4070:GLU:OE1	1:C:4070:GLU:N	2.47	0.42
2:I:28:THR:HA	2:I:39:SER:HA	2.02	0.42
1:D:698:ALA:HA	1:D:724:SER:HA	2.01	0.42
1:D:1987:CYS:N	1:D:1988:PRO:HD2	2.34	0.42
1:D:2428:LEU:O	1:D:2432:VAL:HG23	2.20	0.42
1:A:514:PHE:HD2	1:A:523:GLY:HA2	1.84	0.42
1:A:1732:GLU:OE2	1:A:1735:LYS:HB2	2.20	0.42
1:A:1747:HIS:ND1	1:A:1747:HIS:O	2.51	0.42
1:A:2753:GLN:HB2	1:A:2756:MET:HG2	2.01	0.42
1:A:3817:GLY:C	1:A:3818:MET:HE2	2.44	0.42
1:A:3964:ILE:HG13	1:A:3965:GLU:OE1	2.20	0.42
1:B:317:MET:HB2	1:B:321:LYS:HE3	2.01	0.42
1:B:840:TYR:CE2	1:B:850:LEU:HA	2.55	0.42
1:B:1205:CYS:SG	1:B:1206:SER:N	2.92	0.42
1:B:1789:LYS:HB2	1:B:1835:PHE:CE1	2.54	0.42
1:B:2154:PHE:HA	1:B:2161:MET:HE3	2.01	0.42
1:B:4200:GLN:HE21	1:B:4922:MET:HE3	1.84	0.42
2:H:28:THR:HA	2:H:39:SER:HA	2.02	0.42
1:C:290:ARG:H	1:C:293:GLN:NE2	2.16	0.42
1:C:514:PHE:HD2	1:C:523:GLY:HA2	1.84	0.42
1:C:801:ARG:HA	1:C:1618:TRP:O	2.20	0.42
1:C:1111:GLY:HA3	1:C:1211:GLN:CD	2.45	0.42
1:C:2238:PRO:O	1:C:2241:VAL:HG12	2.19	0.42
1:C:2716:LEU:HG	1:C:2900:TYR:HE2	1.85	0.42
1:D:28:ILE:HG21	1:D:201:TRP:CH2	2.55	0.42
1:D:318:ASP:OD1	1:D:318:ASP:N	2.50	0.42
1:D:1732:GLU:OE2	1:D:1735:LYS:HB2	2.20	0.42
1:D:3817:GLY:C	1:D:3818:MET:HE2	2.44	0.42
1:A:799:LYS:HG2	1:A:1621:GLN:NE2	2.34	0.42
1:A:1009:ARG:O	1:A:1012:ILE:HG12	2.20	0.42
1:A:1643:LEU:HD22	1:A:1694:TYR:O	2.19	0.42
1:A:2313:GLU:OE1	1:A:3812:LYS:HE2	2.20	0.42
1:B:233:VAL:O	1:B:408:SER:OG	2.36	0.42
1:B:778:MET:HG3	1:B:780:GLU:OE2	2.19	0.42
1:B:1771:SER:HA	2:H:56:VAL:HA	2.01	0.42
1:B:4051:MET:HE2	1:B:4062:THR:HG22	2.02	0.42
1:B:4791:PHE:HE1	1:B:4833:PRO:HA	1.84	0.42
1:C:1643:LEU:HD22	1:C:1694:TYR:O	2.19	0.42
1:C:1683:GLU:HB3	2:I:42:ASP:HB3	2.01	0.42
1:D:370:LEU:HB2	1:D:393:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:661:LEU:HD13	1:D:673:TRP:CD1	2.55	0.42
1:D:3940:TRP:HA	1:D:3943:VAL:HG12	2.01	0.42
1:A:417:ARG:NH1	1:A:420:ARG:HH22	2.18	0.42
1:A:2335:ARG:HD3	1:A:2336:GLY:N	2.34	0.42
1:A:2768:GLU:OE2	1:A:2771:ARG:HD2	2.20	0.42
1:B:280:LEU:H	1:B:280:LEU:HD12	1.85	0.42
1:B:370:LEU:HB2	1:B:393:MET:HB2	2.02	0.42
1:B:1979:LYS:HD3	1:B:1979:LYS:HA	1.95	0.42
1:B:2238:PRO:O	1:B:2241:VAL:HG12	2.19	0.42
1:C:417:ARG:NH1	1:C:420:ARG:HH22	2.18	0.42
1:C:4026:THR:O	1:C:4031:PHE:HB3	2.20	0.42
1:D:328:ALA:HB3	1:D:366:VAL:HG11	2.02	0.42
1:D:417:ARG:NH1	1:D:420:ARG:HH22	2.18	0.42
1:D:419:ILE:O	1:D:423:VAL:HG13	2.20	0.42
1:D:514:PHE:HD2	1:D:523:GLY:HA2	1.84	0.42
1:D:1009:ARG:O	1:D:1012:ILE:HG12	2.20	0.42
1:D:2716:LEU:HG	1:D:2900:TYR:HE2	1.85	0.42
1:D:4791:PHE:HE1	1:D:4833:PRO:HA	1.84	0.42
1:A:446:ASP:O	1:A:448:PRO:HD3	2.20	0.42
1:A:1048:ASP:HA	1:A:1051:ARG:HD2	2.02	0.42
1:A:1769:PHE:O	2:G:83:TYR:OH	2.37	0.42
1:A:1979:LYS:HD3	1:A:1979:LYS:HA	1.95	0.42
1:A:1987:CYS:N	1:A:1988:PRO:HD2	2.34	0.42
1:B:307:SER:OG	1:B:317:MET:HG2	2.20	0.42
1:B:1048:ASP:HA	1:B:1051:ARG:HD2	2.02	0.42
1:B:3817:GLY:C	1:B:3818:MET:HE2	2.44	0.42
1:B:4923:TYR:CZ	1:B:4927:LYS:HD2	2.54	0.42
1:C:307:SER:OG	1:C:317:MET:HG2	2.20	0.42
1:C:370:LEU:HB2	1:C:393:MET:HB2	2.02	0.42
1:C:407:ARG:HH21	1:C:3864:ASN:HB3	1.84	0.42
1:D:4273:MET:HE3	1:D:4273:MET:HB2	1.73	0.42
1:A:28:ILE:HG21	1:A:201:TRP:CH2	2.55	0.41
1:A:419:ILE:O	1:A:423:VAL:HG13	2.20	0.41
1:A:698:ALA:HA	1:A:724:SER:HA	2.01	0.41
1:A:841:LYS:HE2	1:A:841:LYS:HB2	1.79	0.41
1:A:1776:CYS:SG	1:A:1778:GLN:HB2	2.60	0.41
1:A:4026:THR:O	1:A:4031:PHE:HB3	2.20	0.41
1:B:152:ASP:OD2	1:B:154:THR:OG1	2.37	0.41
1:B:417:ARG:NH1	1:B:420:ARG:HH22	2.18	0.41
1:B:419:ILE:O	1:B:423:VAL:HG13	2.20	0.41
1:B:798:ILE:HG13	1:B:800:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2716:LEU:HG	1:B:2900:TYR:HE2	1.85	0.41
1:C:62:LEU:HA	1:C:65:CYS:SG	2.60	0.41
1:C:698:ALA:HA	1:C:724:SER:HA	2.01	0.41
1:D:446:ASP:O	1:D:448:PRO:HD3	2.20	0.41
1:D:2278:MET:O	1:D:2282:LYS:HG2	2.20	0.41
1:D:2464:LYS:HE3	1:D:2464:LYS:HB3	1.93	0.41
1:A:801:ARG:HA	1:A:1618:TRP:O	2.20	0.41
1:A:890:HIS:NE2	1:A:924:LEU:HD11	2.35	0.41
1:A:2166:MET:HE3	1:A:2166:MET:HB2	1.86	0.41
1:A:2238:PRO:O	1:A:2241:VAL:HG12	2.19	0.41
2:G:28:THR:HA	2:G:39:SER:HA	2.02	0.41
1:B:983:LEU:O	1:B:1055:ARG:HD2	2.19	0.41
1:C:661:LEU:HD13	1:C:673:TRP:CD1	2.55	0.41
1:C:1740:PHE:CD1	1:C:1923:ALA:HB1	2.56	0.41
1:C:3822:GLU:HB2	1:C:3826:GLU:HA	2.01	0.41
1:D:1372:ASN:OD1	1:D:1372:ASN:N	2.53	0.41
1:D:3822:GLU:HB2	1:D:3826:GLU:HA	2.01	0.41
1:D:4668:LEU:HG	1:D:4669:LEU:HD12	2.02	0.41
2:J:28:THR:HA	2:J:39:SER:HA	2.02	0.41
1:A:328:ALA:HB3	1:A:366:VAL:HG11	2.02	0.41
1:A:1931:PHE:CE1	1:A:1995:LEU:HB2	2.55	0.41
1:A:2278:MET:O	1:A:2282:LYS:HG2	2.20	0.41
1:A:4583:PHE:HA	1:A:4586:ILE:HG22	2.02	0.41
1:A:4791:PHE:HE1	1:A:4833:PRO:HA	1.84	0.41
1:B:1309:GLU:CD	1:B:1309:GLU:H	2.27	0.41
1:B:4511:ILE:O	1:B:4515:LEU:HG	2.20	0.41
1:C:294:PRO:HA	1:C:329:PHE:O	2.19	0.41
1:C:643:LEU:HD13	1:C:1658:THR:HG23	2.01	0.41
1:C:973:THR:OG1	1:C:976:TYR:O	2.19	0.41
1:C:1776:CYS:SG	1:C:1778:GLN:HB2	2.60	0.41
1:D:190:ARG:HD3	1:D:205:ALA:O	2.20	0.41
1:D:317:MET:HB2	1:D:321:LYS:HE3	2.01	0.41
1:D:755:ILE:HD11	1:D:768:PHE:HB3	2.01	0.41
1:D:801:ARG:HA	1:D:1618:TRP:O	2.20	0.41
1:D:1776:CYS:SG	1:D:1778:GLN:HB2	2.60	0.41
1:D:3919:LEU:O	1:D:3923:ILE:HG12	2.20	0.41
1:D:4029:ASP:OD1	1:D:4029:ASP:N	2.47	0.41
1:A:940:LEU:O	1:A:944:LEU:HG	2.20	0.41
1:A:2742:TYR:OH	1:A:2744:GLU:OE2	2.33	0.41
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.52	0.41
1:B:646:THR:OG1	1:B:1685:GLN:NE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:VAL:HA	1:B:999:LEU:HD12	2.02	0.41
1:B:1111:GLY:HA3	1:B:1211:GLN:CD	2.45	0.41
1:B:1931:PHE:CE1	1:B:1995:LEU:HB2	2.55	0.41
1:B:3940:TRP:HA	1:B:3943:VAL:HG12	2.01	0.41
1:B:4026:THR:O	1:B:4031:PHE:HB3	2.20	0.41
1:B:4583:PHE:HA	1:B:4586:ILE:HG22	2.03	0.41
1:C:190:ARG:HD3	1:C:205:ALA:O	2.20	0.41
1:C:317:MET:HB2	1:C:321:LYS:HE3	2.01	0.41
1:C:658:ASN:HB2	1:C:832:LEU:HD12	2.03	0.41
1:C:890:HIS:NE2	1:C:924:LEU:HD11	2.36	0.41
1:C:3940:TRP:HA	1:C:3943:VAL:HG12	2.01	0.41
1:C:4165:LYS:HE3	1:C:4165:LYS:HB2	1.84	0.41
1:C:4583:PHE:HA	1:C:4586:ILE:HG22	2.03	0.41
1:C:4668:LEU:HG	1:C:4669:LEU:HD12	2.02	0.41
1:C:4793:ASN:O	1:C:4795:SER:N	2.50	0.41
1:D:606:ARG:NH2	1:D:1635:GLU:OE1	2.34	0.41
1:D:643:LEU:HD13	1:D:1658:THR:HG23	2.01	0.41
1:D:1048:ASP:HA	1:D:1051:ARG:HD2	2.02	0.41
1:D:1091:GLU:HB3	1:D:1094:TYR:CD2	2.53	0.41
1:D:1931:PHE:CE1	1:D:1995:LEU:HB2	2.55	0.41
1:D:2313:GLU:OE1	1:D:3812:LYS:HE2	2.20	0.41
1:D:2753:GLN:HB2	1:D:2756:MET:HG2	2.01	0.41
1:D:4026:THR:O	1:D:4031:PHE:HB3	2.20	0.41
1:A:62:LEU:HA	1:A:65:CYS:SG	2.60	0.41
1:A:755:ILE:HD11	1:A:768:PHE:HB3	2.01	0.41
1:A:840:TYR:CE2	1:A:850:LEU:HA	2.55	0.41
1:A:1959:ARG:HH21	1:A:1962:ARG:HH12	1.67	0.41
1:B:190:ARG:HD3	1:B:205:ALA:O	2.20	0.41
1:B:3822:GLU:HB2	1:B:3826:GLU:HA	2.01	0.41
1:C:58:VAL:HG12	1:C:320:GLU:HA	2.01	0.41
1:C:530:LEU:HA	1:C:530:LEU:HD23	1.77	0.41
1:C:912:LYS:O	1:C:914:GLN:HG3	2.21	0.41
1:C:1009:ARG:O	1:C:1012:ILE:HG12	2.20	0.41
1:C:1048:ASP:HA	1:C:1051:ARG:HD2	2.02	0.41
1:C:1732:GLU:OE2	1:C:1735:LYS:HB2	2.20	0.41
1:C:3727:GLN:C	1:C:3731:HIS:HD1	2.29	0.41
1:D:245:LEU:HD13	1:D:262:TYR:HE1	1.84	0.41
1:D:294:PRO:HA	1:D:329:PHE:O	2.19	0.41
1:D:840:TYR:CE2	1:D:850:LEU:HA	2.55	0.41
1:D:898:ILE:HD13	1:D:973:THR:HB	2.02	0.41
1:D:1959:ARG:HH21	1:D:1962:ARG:HH12	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3762:ILE:HD12	1:D:3840:ARG:HG3	2.01	0.41
1:D:3857:LEU:HD23	1:D:3857:LEU:HA	1.94	0.41
1:D:4511:ILE:O	1:D:4515:LEU:HG	2.21	0.41
1:A:798:ILE:HG13	1:A:800:VAL:HG23	2.02	0.41
1:A:3762:ILE:HD12	1:A:3840:ARG:HG3	2.01	0.41
1:A:3964:ILE:HG21	1:A:4085:ARG:HH11	1.86	0.41
1:A:4051:MET:HE2	1:A:4062:THR:HG22	2.01	0.41
1:B:625:VAL:HG23	1:B:628:ASN:HB2	2.02	0.41
1:B:890:HIS:NE2	1:B:924:LEU:HD11	2.36	0.41
1:C:446:ASP:O	1:C:448:PRO:HD3	2.20	0.41
1:C:755:ILE:HD11	1:C:768:PHE:HB3	2.01	0.41
1:C:798:ILE:HG13	1:C:800:VAL:HG23	2.03	0.41
1:C:1100:ARG:HB2	1:C:1236:TYR:HA	2.03	0.41
1:C:1931:PHE:CE1	1:C:1995:LEU:HB2	2.55	0.41
1:C:2125:ILE:HD13	1:C:2125:ILE:HA	1.91	0.41
1:C:2238:PRO:HA	1:C:2241:VAL:HG12	2.03	0.41
1:C:3782:GLU:OE2	1:C:3783:LYS:HG3	2.21	0.41
1:D:58:VAL:HG12	1:D:320:GLU:HA	2.01	0.41
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.52	0.41
1:D:1740:PHE:CD1	1:D:1923:ALA:HB1	2.55	0.41
1:D:4165:LYS:HE3	1:D:4165:LYS:HB2	1.84	0.41
1:A:898:ILE:HD13	1:A:973:THR:HB	2.02	0.41
1:A:1683:GLU:HB3	2:G:42:ASP:HB3	2.02	0.41
1:A:2238:PRO:HA	1:A:2241:VAL:HG12	2.03	0.41
1:A:2428:LEU:O	1:A:2432:VAL:HG23	2.20	0.41
1:A:3940:TRP:HA	1:A:3943:VAL:HG12	2.01	0.41
1:B:304:LYS:HB2	1:B:316:LEU:HD12	2.03	0.41
1:B:1372:ASN:OD1	1:B:1372:ASN:N	2.53	0.41
1:B:2278:MET:O	1:B:2282:LYS:HG2	2.20	0.41
1:B:2313:GLU:OE1	1:B:3812:LYS:HE2	2.19	0.41
1:B:2867:HIS:ND1	1:B:2868:PRO:HD2	2.36	0.41
1:B:3905:PHE:O	1:B:3909:ILE:HG12	2.21	0.41
1:C:304:LYS:HB2	1:C:316:LEU:HD12	2.03	0.41
1:C:595:LYS:HE2	1:C:595:LYS:HB3	1.89	0.41
1:C:802:PHE:HB2	1:C:1618:TRP:HB2	2.02	0.41
1:C:3762:ILE:HD12	1:C:3840:ARG:HG3	2.01	0.41
1:C:3919:LEU:O	1:C:3923:ILE:HG12	2.20	0.41
1:D:356:TYR:HA	1:D:405:LEU:HB2	2.03	0.41
1:D:383:ARG:HH21	1:D:387:ILE:HD12	1.86	0.41
1:D:584:GLU:H	1:D:584:GLU:CD	2.29	0.41
1:D:625:VAL:HG23	1:D:628:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4051:MET:HE2	1:D:4062:THR:HG22	2.02	0.41
1:D:4193:GLU:OE2	1:D:4943:TYR:OH	2.28	0.41
1:A:307:SER:OG	1:A:317:MET:HG2	2.20	0.41
1:A:323:ASP:OD2	1:A:325:LYS:HB2	2.21	0.41
1:A:912:LYS:O	1:A:914:GLN:HG3	2.21	0.41
1:A:1740:PHE:CD1	1:A:1923:ALA:HB1	2.55	0.41
1:A:2431:LEU:HD23	1:A:2467:MET:HE3	2.03	0.41
1:A:3842:LEU:HD23	1:A:3842:LEU:HA	1.96	0.41
1:A:4668:LEU:HG	1:A:4669:LEU:HD12	2.02	0.41
1:B:62:LEU:HA	1:B:65:CYS:SG	2.60	0.41
1:B:309:MET:HE3	1:B:309:MET:HB3	1.91	0.41
1:B:898:ILE:HD13	1:B:973:THR:HB	2.02	0.41
1:B:3762:ILE:HD12	1:B:3840:ARG:HG3	2.01	0.41
1:C:78:LEU:O	1:C:82:LEU:HB2	2.21	0.41
1:C:323:ASP:OD2	1:C:325:LYS:HB2	2.21	0.41
1:C:419:ILE:O	1:C:423:VAL:HG13	2.20	0.41
1:C:840:TYR:CE2	1:C:850:LEU:HA	2.55	0.41
1:C:4044:LYS:HE2	1:C:4044:LYS:HB3	1.81	0.41
1:D:304:LYS:HB2	1:D:316:LEU:HD12	2.03	0.41
1:D:306:LEU:HD22	1:D:314:LEU:HD13	2.02	0.41
1:D:658:ASN:HB2	1:D:832:LEU:HD12	2.03	0.41
1:D:2238:PRO:HA	1:D:2241:VAL:HG12	2.03	0.41
1:D:4583:PHE:HA	1:D:4586:ILE:HG22	2.02	0.41
1:A:304:LYS:HB2	1:A:316:LEU:HD12	2.03	0.41
1:A:306:LEU:HD22	1:A:314:LEU:HD13	2.02	0.41
1:A:317:MET:HB2	1:A:321:LYS:HE3	2.02	0.41
1:A:370:LEU:HB2	1:A:393:MET:HB2	2.02	0.41
1:A:3905:PHE:O	1:A:3909:ILE:HG12	2.21	0.41
1:A:4294:LEU:HA	1:A:4294:LEU:HD12	1.88	0.41
1:A:4511:ILE:O	1:A:4515:LEU:HG	2.20	0.41
1:A:4658:GLU:OE1	1:A:4659:PHE:N	2.54	0.41
1:B:169:ARG:HH12	1:B:176:ARG:NH1	2.19	0.41
1:B:802:PHE:HB2	1:B:1618:TRP:HB2	2.02	0.41
1:B:912:LYS:O	1:B:914:GLN:HG3	2.21	0.41
1:B:940:LEU:O	1:B:944:LEU:HG	2.20	0.41
1:B:1009:ARG:O	1:B:1012:ILE:HG12	2.20	0.41
1:B:1100:ARG:HB2	1:B:1236:TYR:HA	2.03	0.41
1:B:2408:ILE:O	1:B:2412:LYS:CB	2.69	0.41
1:B:3964:ILE:HG13	1:B:3965:GLU:OE1	2.20	0.41
1:B:4658:GLU:OE1	1:B:4659:PHE:N	2.54	0.41
1:C:921:PHE:O	1:C:929:ARG:NH1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1294:ASN:O	1:C:1348:LYS:HE3	2.21	0.41
1:C:1595:VAL:O	1:C:1595:VAL:HG13	2.21	0.41
1:C:1691:GLU:OE2	1:C:1693:LYS:NZ	2.54	0.41
1:C:2278:MET:O	1:C:2282:LYS:HG2	2.20	0.41
1:C:3964:ILE:HG13	1:C:3965:GLU:OE1	2.20	0.41
1:C:4301:CYS:SG	1:C:4302:ARG:HG3	2.61	0.41
1:D:78:LEU:O	1:D:82:LEU:HB2	2.21	0.41
1:D:307:SER:OG	1:D:317:MET:HG2	2.20	0.41
1:D:323:ASP:OD2	1:D:325:LYS:HB2	2.21	0.41
1:D:798:ILE:HG13	1:D:800:VAL:HG23	2.02	0.41
1:D:912:LYS:O	1:D:914:GLN:HG3	2.21	0.41
1:D:3782:GLU:OE2	1:D:3783:LYS:HG3	2.21	0.41
1:D:3905:PHE:O	1:D:3909:ILE:HG12	2.21	0.41
1:A:2847:TYR:OH	1:A:2891:ILE:HD13	2.21	0.41
1:A:4608:LYS:HG2	1:A:4614:LEU:HD22	2.03	0.41
1:B:306:LEU:HD22	1:B:314:LEU:HD13	2.02	0.41
1:B:356:TYR:HA	1:B:405:LEU:HB2	2.03	0.41
1:B:658:ASN:HB2	1:B:832:LEU:HD12	2.03	0.41
1:B:1294:ASN:O	1:B:1348:LYS:HE3	2.21	0.41
1:B:2428:LEU:O	1:B:2432:VAL:HG23	2.20	0.41
1:C:306:LEU:HD22	1:C:314:LEU:HD13	2.02	0.41
1:C:356:TYR:HA	1:C:405:LEU:HB2	2.03	0.41
1:C:383:ARG:HH21	1:C:387:ILE:HD12	1.86	0.41
1:C:574:VAL:HA	1:C:577:CYS:SG	2.61	0.41
1:C:996:VAL:HA	1:C:999:LEU:HD12	2.02	0.41
1:C:1898:PRO:O	1:C:1902:LYS:HG2	2.21	0.41
1:C:4608:LYS:HG2	1:C:4614:LEU:HD22	2.03	0.41
1:D:574:VAL:HA	1:D:577:CYS:SG	2.61	0.41
1:D:755:ILE:HD12	1:D:769:ARG:O	2.21	0.41
1:D:1595:VAL:HG13	1:D:1595:VAL:O	2.21	0.41
1:D:1691:GLU:OE2	1:D:1693:LYS:NZ	2.54	0.41
1:D:1897:LEU:HA	1:D:1898:PRO:HD3	1.97	0.41
1:D:4301:CYS:SG	1:D:4302:ARG:HG3	2.61	0.41
1:D:4608:LYS:HG2	1:D:4614:LEU:HD22	2.03	0.41
1:A:280:LEU:HD12	1:A:280:LEU:H	1.85	0.40
1:A:383:ARG:HH21	1:A:387:ILE:HD12	1.86	0.40
1:A:658:ASN:HB2	1:A:832:LEU:HD12	2.03	0.40
1:A:812:LYS:O	1:A:812:LYS:NZ	2.35	0.40
1:A:987:LYS:HA	1:A:987:LYS:HD2	1.90	0.40
1:A:1294:ASN:O	1:A:1348:LYS:HE3	2.21	0.40
1:A:1372:ASN:OD1	1:A:1372:ASN:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2184:LYS:HZ3	1:A:2184:LYS:HG2	1.71	0.40
1:B:446:ASP:O	1:B:448:PRO:HD3	2.20	0.40
1:B:574:VAL:HA	1:B:577:CYS:SG	2.61	0.40
1:B:1100:ARG:NH1	1:B:1234:GLU:O	2.54	0.40
1:B:1740:PHE:CD1	1:B:1923:ALA:HB1	2.56	0.40
1:B:4824:GLY:O	1:C:4821:ARG:NH2	2.54	0.40
1:C:169:ARG:HH12	1:C:176:ARG:NH1	2.19	0.40
1:C:4511:ILE:O	1:C:4515:LEU:HG	2.20	0.40
1:C:4559:VAL:HG22	1:C:4561:GLU:HG2	2.03	0.40
1:C:4658:GLU:OE1	1:C:4659:PHE:N	2.54	0.40
1:D:62:LEU:HA	1:D:65:CYS:SG	2.60	0.40
1:D:902:TRP:HA	1:D:913:ARG:O	2.21	0.40
1:D:1965:ARG:O	1:D:1966:SER:OG	2.38	0.40
1:D:2238:PRO:O	1:D:2241:VAL:HG12	2.19	0.40
1:D:2271:CYS:SG	1:D:2293:GLU:HB2	2.61	0.40
1:D:2836:LEU:HD13	1:D:2836:LEU:HA	1.97	0.40
1:A:1190:LEU:HD21	1:A:1193:LYS:HB2	2.03	0.40
1:A:1898:PRO:O	1:A:1902:LYS:HG2	2.22	0.40
1:A:1970:GLU:O	1:A:1974:MET:HG2	2.22	0.40
1:A:3782:GLU:OE2	1:A:3783:LYS:HG3	2.21	0.40
1:A:4046:ASP:O	1:A:4049:LYS:HG3	2.22	0.40
1:B:78:LEU:O	1:B:82:LEU:HB2	2.21	0.40
1:B:755:ILE:HD12	1:B:769:ARG:O	2.22	0.40
1:B:1572:PHE:HE1	1:B:1587:LEU:HD21	1.87	0.40
1:B:1898:PRO:O	1:B:1902:LYS:HG2	2.22	0.40
1:B:2331:GLY:HA3	1:B:2391:TYR:CE1	2.57	0.40
1:B:2355:ASP:OD2	1:B:2357:SER:OG	2.30	0.40
1:B:4301:CYS:SG	1:B:4302:ARG:HG3	2.61	0.40
1:B:4559:VAL:HG22	1:B:4561:GLU:HG2	2.03	0.40
1:C:2262:GLU:OE1	1:C:2262:GLU:N	2.48	0.40
1:C:3964:ILE:HG21	1:C:4085:ARG:HH11	1.86	0.40
1:D:280:LEU:H	1:D:280:LEU:HD12	1.85	0.40
1:D:313:ASN:HD21	1:D:392:ILE:HA	1.87	0.40
1:D:799:LYS:HG2	1:D:1621:GLN:HE22	1.86	0.40
1:D:2262:GLU:OE1	1:D:2262:GLU:N	2.48	0.40
1:D:4501:ARG:HH12	1:D:4720:TYR:HE2	1.69	0.40
1:A:313:ASN:HD21	1:A:392:ILE:HA	1.87	0.40
1:A:356:TYR:HA	1:A:405:LEU:HB2	2.03	0.40
1:A:1691:GLU:OE2	1:A:1693:LYS:NZ	2.54	0.40
1:A:2271:CYS:SG	1:A:2293:GLU:HB2	2.61	0.40
1:A:4009:VAL:HA	1:A:4012:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:TRP:HA	1:B:913:ARG:O	2.22	0.40
1:B:1048:ASP:OD1	1:B:1051:ARG:NH1	2.48	0.40
1:B:1683:GLU:HB3	1:B:1684:PRO:HD3	2.04	0.40
1:B:1917:VAL:HG21	1:B:2089:ARG:HH21	1.86	0.40
1:B:2136:GLU:O	1:B:2140:LEU:HG	2.21	0.40
1:B:3727:GLN:C	1:B:3731:HIS:HD1	2.29	0.40
1:B:3782:GLU:OE2	1:B:3783:LYS:HG3	2.21	0.40
1:B:3964:ILE:HG21	1:B:4085:ARG:HH11	1.86	0.40
1:B:4009:VAL:HA	1:B:4012:ILE:HG12	2.03	0.40
1:C:625:VAL:HG23	1:C:628:ASN:HB2	2.02	0.40
1:C:799:LYS:HG2	1:C:1621:GLN:HE22	1.87	0.40
1:C:898:ILE:HD13	1:C:973:THR:HB	2.02	0.40
1:C:2136:GLU:O	1:C:2140:LEU:HG	2.21	0.40
1:C:4501:ARG:NH1	1:C:4720:TYR:HE2	2.19	0.40
1:C:4830:ILE:HB	1:C:4842:ARG:HH21	1.87	0.40
1:D:940:LEU:HD11	1:D:950:VAL:HG11	2.04	0.40
1:D:1898:PRO:O	1:D:1902:LYS:HG2	2.22	0.40
1:D:1917:VAL:HG21	1:D:2089:ARG:HH21	1.86	0.40
1:D:2170:VAL:HG21	1:D:2198:PHE:CD2	2.57	0.40
1:D:3727:GLN:C	1:D:3731:HIS:HD1	2.29	0.40
1:A:755:ILE:HD12	1:A:769:ARG:O	2.22	0.40
1:A:1100:ARG:NH1	1:A:1234:GLU:O	2.55	0.40
1:A:4301:CYS:SG	1:A:4302:ARG:HG3	2.61	0.40
1:B:167:LYS:HA	1:B:167:LYS:HD3	1.97	0.40
1:B:799:LYS:HG2	1:B:1621:GLN:HE22	1.86	0.40
1:B:2271:CYS:SG	1:B:2293:GLU:HB2	2.61	0.40
1:C:162:ILE:O	1:C:163:HIS:ND1	2.55	0.40
1:C:755:ILE:HD12	1:C:769:ARG:O	2.22	0.40
1:C:1048:ASP:OD1	1:C:1051:ARG:NH1	2.48	0.40
1:C:2867:HIS:ND1	1:C:2868:PRO:HD2	2.36	0.40
1:D:674:TYR:HB2	1:D:819:TYR:HB3	2.04	0.40
1:D:890:HIS:NE2	1:D:924:LEU:HD11	2.36	0.40
1:D:1100:ARG:HB2	1:D:1236:TYR:HA	2.03	0.40
1:D:1190:LEU:HD21	1:D:1193:LYS:HB2	2.03	0.40
1:D:2847:TYR:OH	1:D:2891:ILE:HD13	2.21	0.40
1:D:4501:ARG:NH1	1:D:4720:TYR:HE2	2.19	0.40
1:D:4609:LEU:HD23	1:D:4609:LEU:HA	1.96	0.40
1:D:4793:ASN:O	1:D:4795:SER:N	2.50	0.40
1:A:1668:LEU:HD23	1:A:2131:VAL:HG22	2.04	0.40
1:A:1917:VAL:HG21	1:A:2089:ARG:HH21	1.86	0.40
1:A:2170:VAL:HG21	1:A:2198:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2331:GLY:HA3	1:A:2391:TYR:CE1	2.57	0.40
1:A:3818:MET:HE2	1:A:3818:MET:N	2.37	0.40
1:B:162:ILE:O	1:B:163:HIS:ND1	2.55	0.40
1:B:940:LEU:HD11	1:B:950:VAL:HG11	2.04	0.40
1:B:1595:VAL:O	1:B:1595:VAL:HG13	2.21	0.40
1:B:1691:GLU:OE2	1:B:1693:LYS:NZ	2.54	0.40
1:B:1970:GLU:O	1:B:1974:MET:HG2	2.22	0.40
1:C:332:ARG:HH21	1:C:340:VAL:HG12	1.87	0.40
1:C:702:GLY:O	1:C:786:GLY:HA2	2.22	0.40
1:C:1683:GLU:HB3	1:C:1684:PRO:HD3	2.04	0.40
1:C:2271:CYS:SG	1:C:2293:GLU:HB2	2.61	0.40
1:D:169:ARG:HH12	1:D:176:ARG:NH1	2.19	0.40
1:D:1683:GLU:HB3	2:J:42:ASP:HB3	2.04	0.40
1:D:4046:ASP:O	1:D:4049:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100	100
1	B	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100	100
1	C	3255/4966 (66%)	3046 (94%)	209 (6%)	0	100	100
1	D	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100	100
2	G	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	H	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	I	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	J	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
All	All	13440/20568 (65%)	12595 (94%)	845 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2862/3387 (84%)	2779 (97%)	83 (3%)	37	60
1	B	2862/3387 (84%)	2778 (97%)	84 (3%)	37	60
1	C	2862/3387 (84%)	2778 (97%)	84 (3%)	37	60
1	D	2862/3387 (84%)	2777 (97%)	85 (3%)	36	60
2	G	88/140 (63%)	88 (100%)	0	100	100
2	H	88/140 (63%)	88 (100%)	0	100	100
2	I	88/140 (63%)	88 (100%)	0	100	100
2	J	88/140 (63%)	88 (100%)	0	100	100
All	All	11800/14108 (84%)	11464 (97%)	336 (3%)	38	61

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

Mol	Chain	Res	Type
1	A	22	LEU
1	A	65	CYS
1	A	82	LEU
1	A	112	THR
1	A	113	LEU
1	A	147	VAL
1	A	174	LYS
1	A	181	LEU
1	A	187	SER
1	A	214	VAL
1	A	268	SER
1	A	282	VAL
1	A	333	SER
1	A	412	GLU
1	A	422	THR
1	A	453	SER

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Mol	Chain	Res	Type
1	A	501	CYS
1	A	550	GLN
1	A	609	LYS
1	A	691	THR
1	A	765	SER
1	A	767	SER
1	A	814	LEU
1	A	923	LYS
1	A	935	MET
1	A	987	LYS
1	A	988	LEU
1	A	1006	VAL
1	A	1033	VAL
1	A	1040	ASP
1	A	1041	ARG
1	A	1042	THR
1	A	1047	LYS
1	A	1057	LEU
1	A	1108	VAL
1	A	1172	THR
1	A	1261	VAL
1	A	1348	LYS
1	A	1609	VAL
1	A	1649	GLU
1	A	1663	SER
1	A	1732	GLU
1	A	1739	LEU
1	A	1745	LYS
1	A	1755	SER
1	A	1816	GLU
1	A	1846	LEU
1	A	1981	ASP
1	A	2184	LYS
1	A	2471	LEU
1	A	2479	VAL
1	A	2492	LEU
1	A	2715	LYS
1	A	2733	MET
1	A	2768	GLU
1	A	2776	GLU
1	A	2777	SER
1	A	2778	LEU

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Mol	Chain	Res	Type
1	A	2779	LYS
1	A	2780	THR
1	A	2857	LEU
1	A	2871	VAL
1	A	3782	GLU
1	A	3851	SER
1	A	3861	THR
1	A	3965	GLU
1	A	3999	VAL
1	A	4003	VAL
1	A	4033	GLU
1	A	4041	VAL
1	A	4076	THR
1	A	4081	GLU
1	A	4273	MET
1	A	4280	LEU
1	A	4284	SER
1	A	4288	SER
1	A	4604	GLU
1	A	4622	GLU
1	A	4658	GLU
1	A	4667	GLU
1	A	4706	MET
1	A	4714	THR
1	A	4802	ASP
1	B	22	LEU
1	B	65	CYS
1	B	80	GLU
1	B	82	LEU
1	B	112	THR
1	B	113	LEU
1	B	147	VAL
1	B	174	LYS
1	B	181	LEU
1	B	187	SER
1	B	214	VAL
1	B	268	SER
1	B	282	VAL
1	B	333	SER
1	B	412	GLU
1	B	422	THR
1	B	453	SER

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Mol	Chain	Res	Type
1	B	501	CYS
1	B	550	GLN
1	B	609	LYS
1	B	691	THR
1	B	765	SER
1	B	767	SER
1	B	814	LEU
1	B	923	LYS
1	B	935	MET
1	B	987	LYS
1	B	988	LEU
1	B	1006	VAL
1	B	1033	VAL
1	B	1040	ASP
1	B	1041	ARG
1	B	1042	THR
1	B	1047	LYS
1	B	1057	LEU
1	B	1108	VAL
1	B	1172	THR
1	B	1261	VAL
1	B	1348	LYS
1	B	1609	VAL
1	B	1649	GLU
1	B	1663	SER
1	B	1732	GLU
1	B	1739	LEU
1	B	1745	LYS
1	B	1755	SER
1	B	1816	GLU
1	B	1846	LEU
1	B	1981	ASP
1	B	2184	LYS
1	B	2471	LEU
1	B	2479	VAL
1	B	2492	LEU
1	B	2715	LYS
1	B	2733	MET
1	B	2768	GLU
1	B	2776	GLU
1	B	2777	SER
1	B	2778	LEU

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Mol	Chain	Res	Type
1	B	2779	LYS
1	B	2780	THR
1	B	2857	LEU
1	B	2871	VAL
1	B	3782	GLU
1	B	3851	SER
1	B	3861	THR
1	B	3965	GLU
1	B	3999	VAL
1	B	4003	VAL
1	B	4033	GLU
1	B	4041	VAL
1	B	4076	THR
1	B	4081	GLU
1	B	4273	MET
1	B	4280	LEU
1	B	4284	SER
1	B	4288	SER
1	B	4604	GLU
1	B	4622	GLU
1	B	4658	GLU
1	B	4667	GLU
1	B	4706	MET
1	B	4714	THR
1	B	4802	ASP
1	C	22	LEU
1	C	65	CYS
1	C	80	GLU
1	C	82	LEU
1	C	112	THR
1	C	113	LEU
1	C	147	VAL
1	C	174	LYS
1	C	181	LEU
1	C	187	SER
1	C	214	VAL
1	C	268	SER
1	C	282	VAL
1	C	333	SER
1	C	412	GLU
1	C	422	THR
1	C	453	SER

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Mol	Chain	Res	Type
1	C	501	CYS
1	C	550	GLN
1	C	609	LYS
1	C	691	THR
1	C	765	SER
1	C	767	SER
1	C	814	LEU
1	C	923	LYS
1	C	935	MET
1	C	987	LYS
1	C	988	LEU
1	C	1006	VAL
1	C	1033	VAL
1	C	1040	ASP
1	C	1041	ARG
1	C	1042	THR
1	C	1047	LYS
1	C	1057	LEU
1	C	1108	VAL
1	C	1172	THR
1	C	1261	VAL
1	C	1348	LYS
1	C	1609	VAL
1	C	1649	GLU
1	C	1663	SER
1	C	1732	GLU
1	C	1739	LEU
1	C	1745	LYS
1	C	1755	SER
1	C	1816	GLU
1	C	1846	LEU
1	C	1981	ASP
1	C	2184	LYS
1	C	2471	LEU
1	C	2479	VAL
1	C	2492	LEU
1	C	2715	LYS
1	C	2733	MET
1	C	2768	GLU
1	C	2776	GLU
1	C	2777	SER
1	C	2778	LEU

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Mol	Chain	Res	Type
1	C	2779	LYS
1	C	2780	THR
1	C	2857	LEU
1	C	2871	VAL
1	C	3782	GLU
1	C	3851	SER
1	C	3861	THR
1	C	3965	GLU
1	C	3999	VAL
1	C	4003	VAL
1	C	4033	GLU
1	C	4041	VAL
1	C	4076	THR
1	C	4081	GLU
1	C	4273	MET
1	C	4280	LEU
1	C	4284	SER
1	C	4288	SER
1	C	4604	GLU
1	C	4622	GLU
1	C	4658	GLU
1	C	4667	GLU
1	C	4706	MET
1	C	4714	THR
1	C	4802	ASP
1	D	22	LEU
1	D	65	CYS
1	D	80	GLU
1	D	82	LEU
1	D	112	THR
1	D	113	LEU
1	D	147	VAL
1	D	174	LYS
1	D	181	LEU
1	D	187	SER
1	D	214	VAL
1	D	268	SER
1	D	282	VAL
1	D	333	SER
1	D	412	GLU
1	D	422	THR
1	D	453	SER

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Mol	Chain	Res	Type
1	D	501	CYS
1	D	550	GLN
1	D	609	LYS
1	D	691	THR
1	D	765	SER
1	D	767	SER
1	D	814	LEU
1	D	923	LYS
1	D	935	MET
1	D	987	LYS
1	D	988	LEU
1	D	1006	VAL
1	D	1033	VAL
1	D	1040	ASP
1	D	1041	ARG
1	D	1042	THR
1	D	1047	LYS
1	D	1057	LEU
1	D	1108	VAL
1	D	1172	THR
1	D	1261	VAL
1	D	1348	LYS
1	D	1609	VAL
1	D	1649	GLU
1	D	1663	SER
1	D	1732	GLU
1	D	1739	LEU
1	D	1745	LYS
1	D	1755	SER
1	D	1816	GLU
1	D	1846	LEU
1	D	1981	ASP
1	D	2184	LYS
1	D	2471	LEU
1	D	2479	VAL
1	D	2492	LEU
1	D	2715	LYS
1	D	2733	MET
1	D	2768	GLU
1	D	2776	GLU
1	D	2777	SER
1	D	2778	LEU

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Mol	Chain	Res	Type
1	D	2779	LYS
1	D	2780	THR
1	D	2857	LEU
1	D	2871	VAL
1	D	3782	GLU
1	D	3851	SER
1	D	3861	THR
1	D	3965	GLU
1	D	3999	VAL
1	D	4003	VAL
1	D	4033	GLU
1	D	4041	VAL
1	D	4076	THR
1	D	4081	GLU
1	D	4273	MET
1	D	4280	LEU
1	D	4284	SER
1	D	4288	SER
1	D	4604	GLU
1	D	4622	GLU
1	D	4658	GLU
1	D	4667	GLU
1	D	4706	MET
1	D	4714	THR
1	D	4797	ASP
1	D	4802	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (259) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	123	HIS
1	A	150	GLN
1	A	193	HIS
1	A	270	HIS
1	A	293	GLN
1	A	299	HIS
1	A	487	ASN
1	A	544	ASN
1	A	547	ASN
1	A	593	HIS
1	A	645	GLN

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Mol	Chain	Res	Type
1	A	650	ASN
1	A	651	HIS
1	A	658	ASN
1	A	669	GLN
1	A	808	HIS
1	A	888	ASN
1	A	890	HIS
1	A	934	GLN
1	A	971	GLN
1	A	992	GLN
1	A	1169	ASN
1	A	1178	ASN
1	A	1265	HIS
1	A	1590	GLN
1	A	1621	GLN
1	A	1670	ASN
1	A	1685	GLN
1	A	1711	HIS
1	A	1744	ASN
1	A	1944	ASN
1	A	1951	ASN
1	A	1973	ASN
1	A	2090	GLN
1	A	2150	ASN
1	A	2151	ASN
1	A	2277	GLN
1	A	2317	ASN
1	A	2721	ASN
1	A	2728	HIS
1	A	2837	HIS
1	A	2846	ASN
1	A	3613	HIS
1	A	3665	GLN
1	A	3952	HIS
1	A	3954	GLN
1	A	3959	GLN
1	A	3974	GLN
1	A	4008	ASN
1	A	4200	GLN
1	A	4295	HIS
1	A	4487	GLN
1	A	4491	ASN

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Mol	Chain	Res	Type
1	A	4496	ASN
1	A	4578	HIS
1	A	4619	GLN
1	A	4641	ASN
1	A	4642	ASN
1	A	4735	ASN
1	A	4765	GLN
1	A	4786	ASN
1	A	4894	ASN
1	A	4935	GLN
1	A	4960	GLN
2	G	32	GLN
2	G	88	HIS
1	B	12	GLN
1	B	123	HIS
1	B	150	GLN
1	B	193	HIS
1	B	270	HIS
1	B	293	GLN
1	B	299	HIS
1	B	487	ASN
1	B	544	ASN
1	B	547	ASN
1	B	593	HIS
1	B	645	GLN
1	B	650	ASN
1	B	658	ASN
1	B	669	GLN
1	B	681	HIS
1	B	746	GLN
1	B	808	HIS
1	B	888	ASN
1	B	934	GLN
1	B	971	GLN
1	B	992	GLN
1	B	1169	ASN
1	B	1178	ASN
1	B	1265	HIS
1	B	1590	GLN
1	B	1670	ASN
1	B	1685	GLN
1	B	1711	HIS

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Mol	Chain	Res	Type
1	B	1744	ASN
1	B	1944	ASN
1	B	1951	ASN
1	B	1973	ASN
1	B	2090	GLN
1	B	2150	ASN
1	B	2151	ASN
1	B	2317	ASN
1	B	2721	ASN
1	B	2728	HIS
1	B	2837	HIS
1	B	2846	ASN
1	B	3665	GLN
1	B	3952	HIS
1	B	3954	GLN
1	B	3959	GLN
1	B	3974	GLN
1	B	4008	ASN
1	B	4200	GLN
1	B	4295	HIS
1	B	4487	GLN
1	B	4491	ASN
1	B	4496	ASN
1	B	4578	HIS
1	B	4619	GLN
1	B	4641	ASN
1	B	4642	ASN
1	B	4735	ASN
1	B	4765	GLN
1	B	4786	ASN
1	B	4894	ASN
1	B	4935	GLN
1	B	4960	GLN
2	H	32	GLN
2	H	88	HIS
1	C	12	GLN
1	C	123	HIS
1	C	150	GLN
1	C	193	HIS
1	C	293	GLN
1	C	299	HIS
1	C	487	ASN

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Mol	Chain	Res	Type
1	C	544	ASN
1	C	593	HIS
1	C	645	GLN
1	C	650	ASN
1	C	651	HIS
1	C	658	ASN
1	C	669	GLN
1	C	746	GLN
1	C	808	HIS
1	C	888	ASN
1	C	890	HIS
1	C	934	GLN
1	C	971	GLN
1	C	992	GLN
1	C	1169	ASN
1	C	1178	ASN
1	C	1265	HIS
1	C	1590	GLN
1	C	1670	ASN
1	C	1685	GLN
1	C	1711	HIS
1	C	1744	ASN
1	C	1944	ASN
1	C	1951	ASN
1	C	1973	ASN
1	C	2090	GLN
1	C	2150	ASN
1	C	2151	ASN
1	C	2317	ASN
1	C	2721	ASN
1	C	2726	HIS
1	C	2728	HIS
1	C	2837	HIS
1	C	3613	HIS
1	C	3665	GLN
1	C	3952	HIS
1	C	3954	GLN
1	C	3959	GLN
1	C	3974	GLN
1	C	4008	ASN
1	C	4200	GLN
1	C	4295	HIS

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Mol	Chain	Res	Type
1	C	4487	GLN
1	C	4491	ASN
1	C	4496	ASN
1	C	4578	HIS
1	C	4619	GLN
1	C	4637	GLN
1	C	4641	ASN
1	C	4642	ASN
1	C	4735	ASN
1	C	4786	ASN
1	C	4894	ASN
1	C	4935	GLN
1	C	4960	GLN
2	I	32	GLN
2	I	88	HIS
1	D	12	GLN
1	D	123	HIS
1	D	150	GLN
1	D	193	HIS
1	D	270	HIS
1	D	293	GLN
1	D	299	HIS
1	D	487	ASN
1	D	544	ASN
1	D	547	ASN
1	D	593	HIS
1	D	645	GLN
1	D	650	ASN
1	D	651	HIS
1	D	658	ASN
1	D	669	GLN
1	D	746	GLN
1	D	808	HIS
1	D	888	ASN
1	D	890	HIS
1	D	934	GLN
1	D	971	GLN
1	D	992	GLN
1	D	1169	ASN
1	D	1178	ASN
1	D	1265	HIS
1	D	1590	GLN

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Mol	Chain	Res	Type
1	D	1621	GLN
1	D	1670	ASN
1	D	1685	GLN
1	D	1711	HIS
1	D	1744	ASN
1	D	1944	ASN
1	D	1951	ASN
1	D	1973	ASN
1	D	2090	GLN
1	D	2150	ASN
1	D	2151	ASN
1	D	2317	ASN
1	D	2728	HIS
1	D	2837	HIS
1	D	3613	HIS
1	D	3665	GLN
1	D	3952	HIS
1	D	3954	GLN
1	D	3959	GLN
1	D	3974	GLN
1	D	4008	ASN
1	D	4200	GLN
1	D	4295	HIS
1	D	4487	GLN
1	D	4491	ASN
1	D	4496	ASN
1	D	4578	HIS
1	D	4619	GLN
1	D	4641	ASN
1	D	4642	ASN
1	D	4735	ASN
1	D	4786	ASN
1	D	4894	ASN
1	D	4935	GLN
1	D	4960	GLN
2	J	32	GLN
2	J	88	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

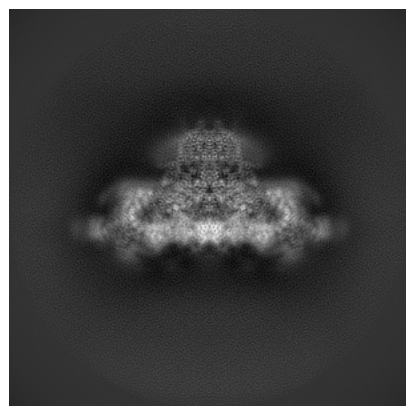
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33937. These allow visual inspection of the internal detail of the map and identification of artifacts.

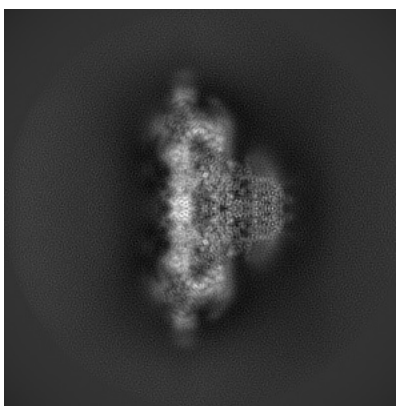
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

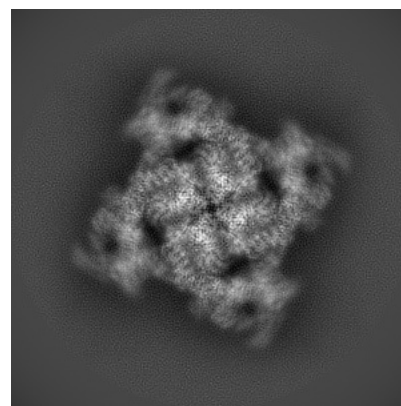
6.1.1 Primary map



X

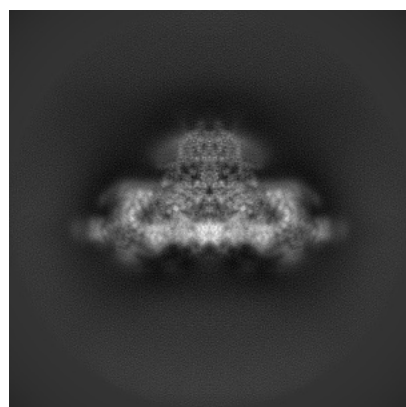


Y

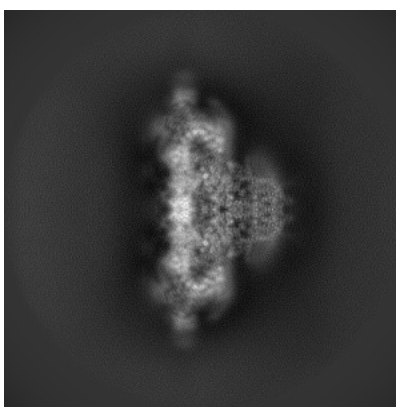


Z

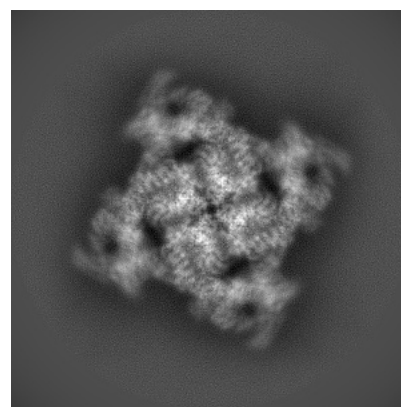
6.1.2 Raw map



X



Y

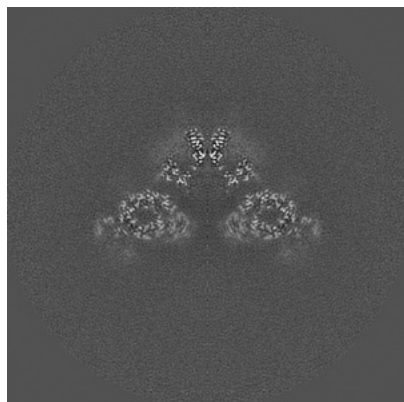


Z

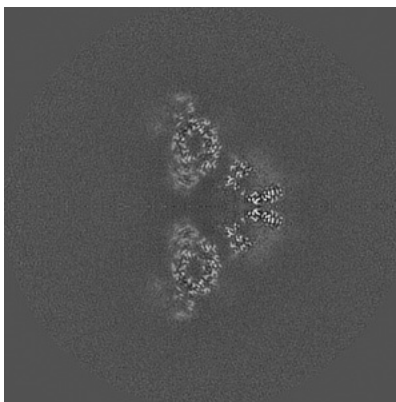
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

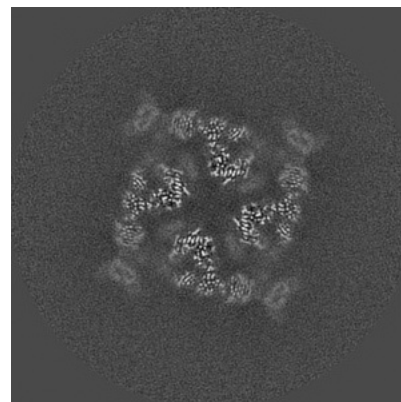
6.2.1 Primary map



X Index: 200

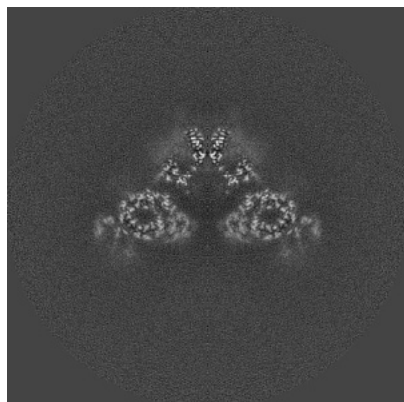


Y Index: 200

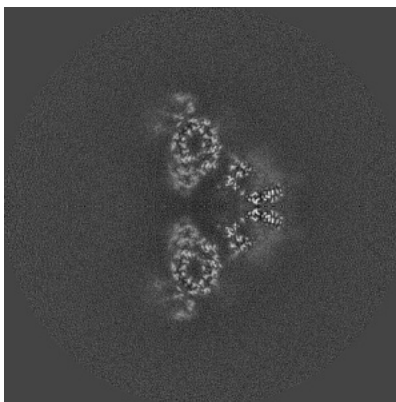


Z Index: 200

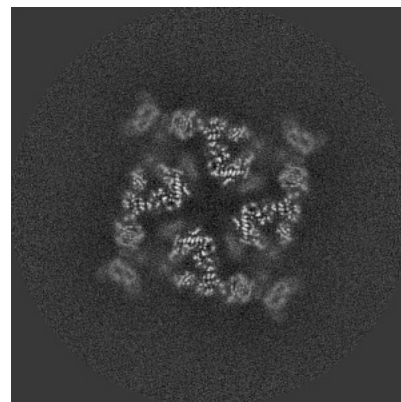
6.2.2 Raw map



X Index: 200



Y Index: 200

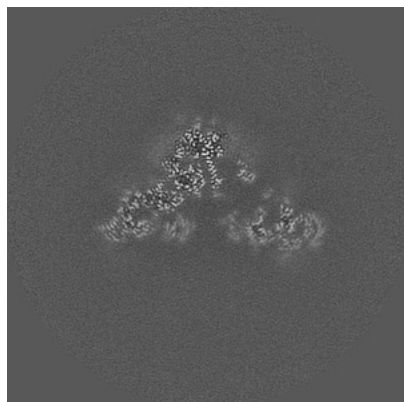


Z Index: 200

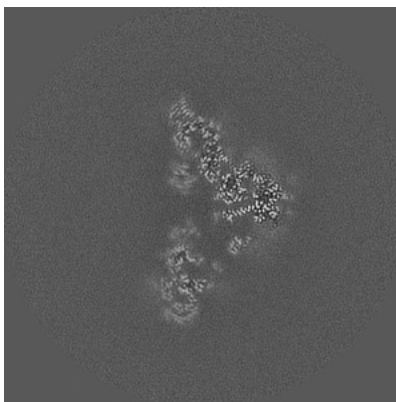
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

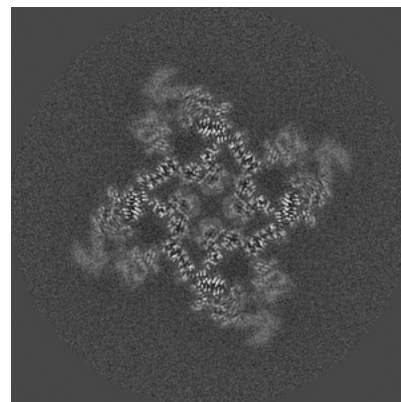
6.3.1 Primary map



X Index: 193

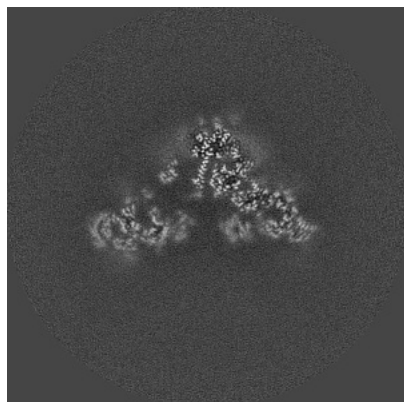


Y Index: 193

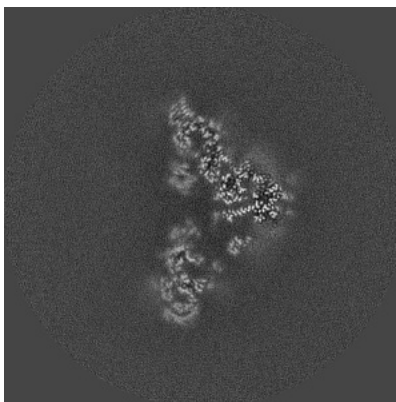


Z Index: 183

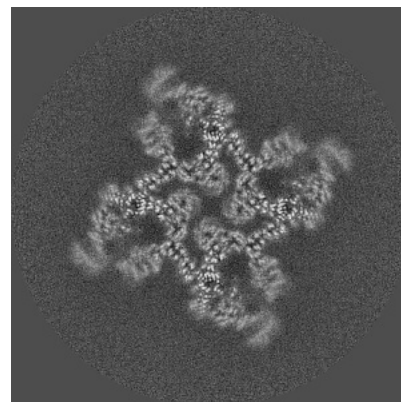
6.3.2 Raw map



X Index: 207



Y Index: 193

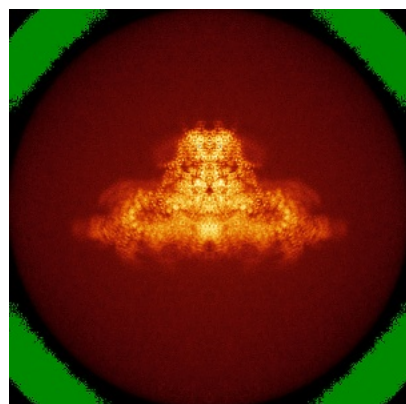


Z Index: 180

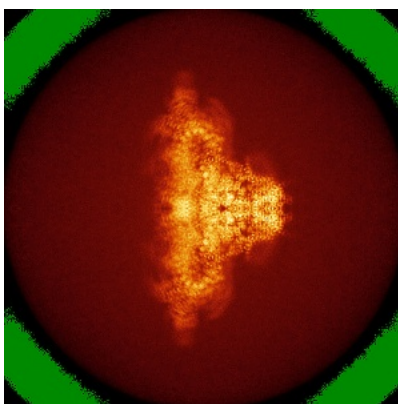
The images above show the largest variance slices of the map in three orthogonal directions.

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

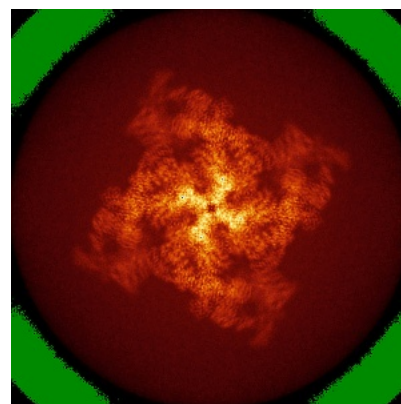
6.4.1 Primary map



X

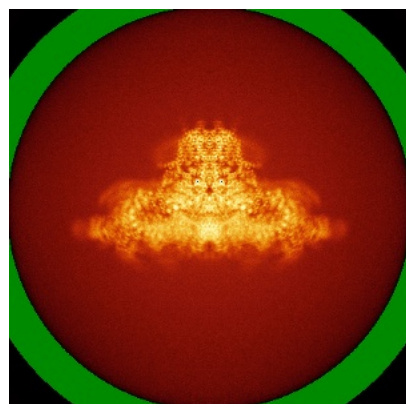


Y

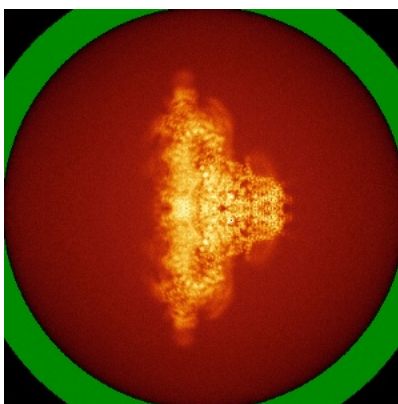


Z

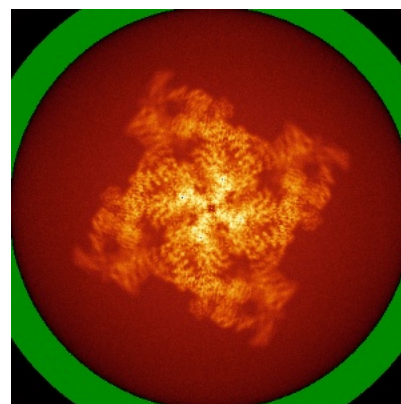
6.4.2 Raw map



X



Y

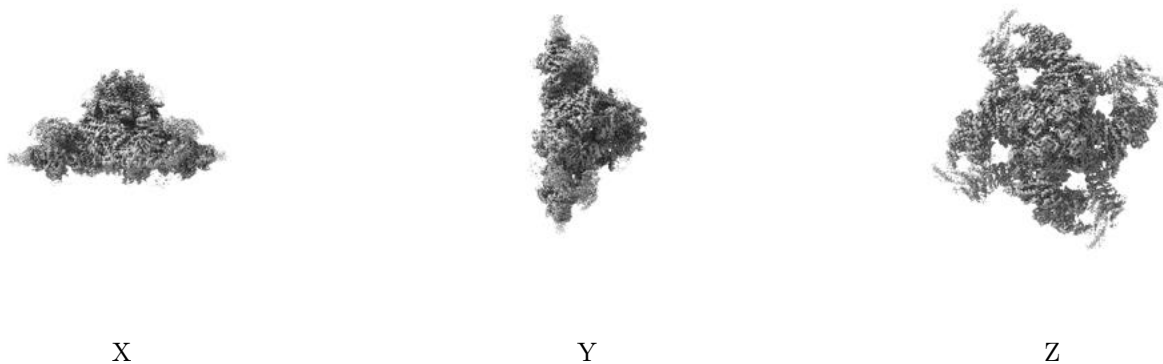


Z

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.

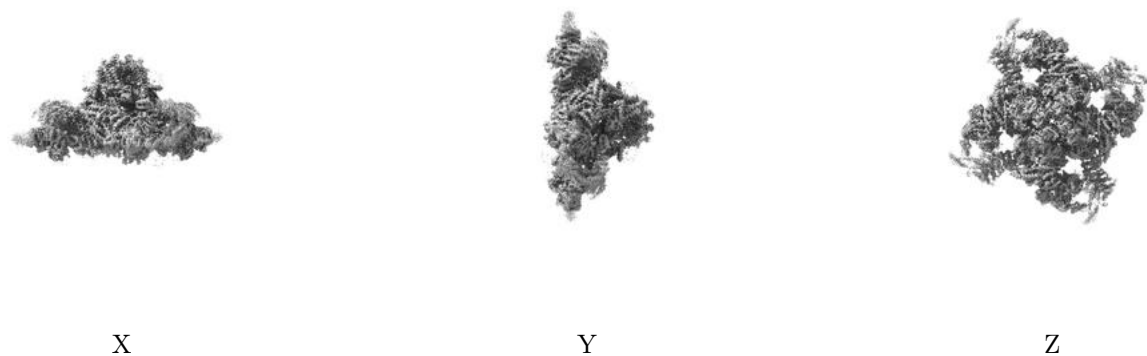
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

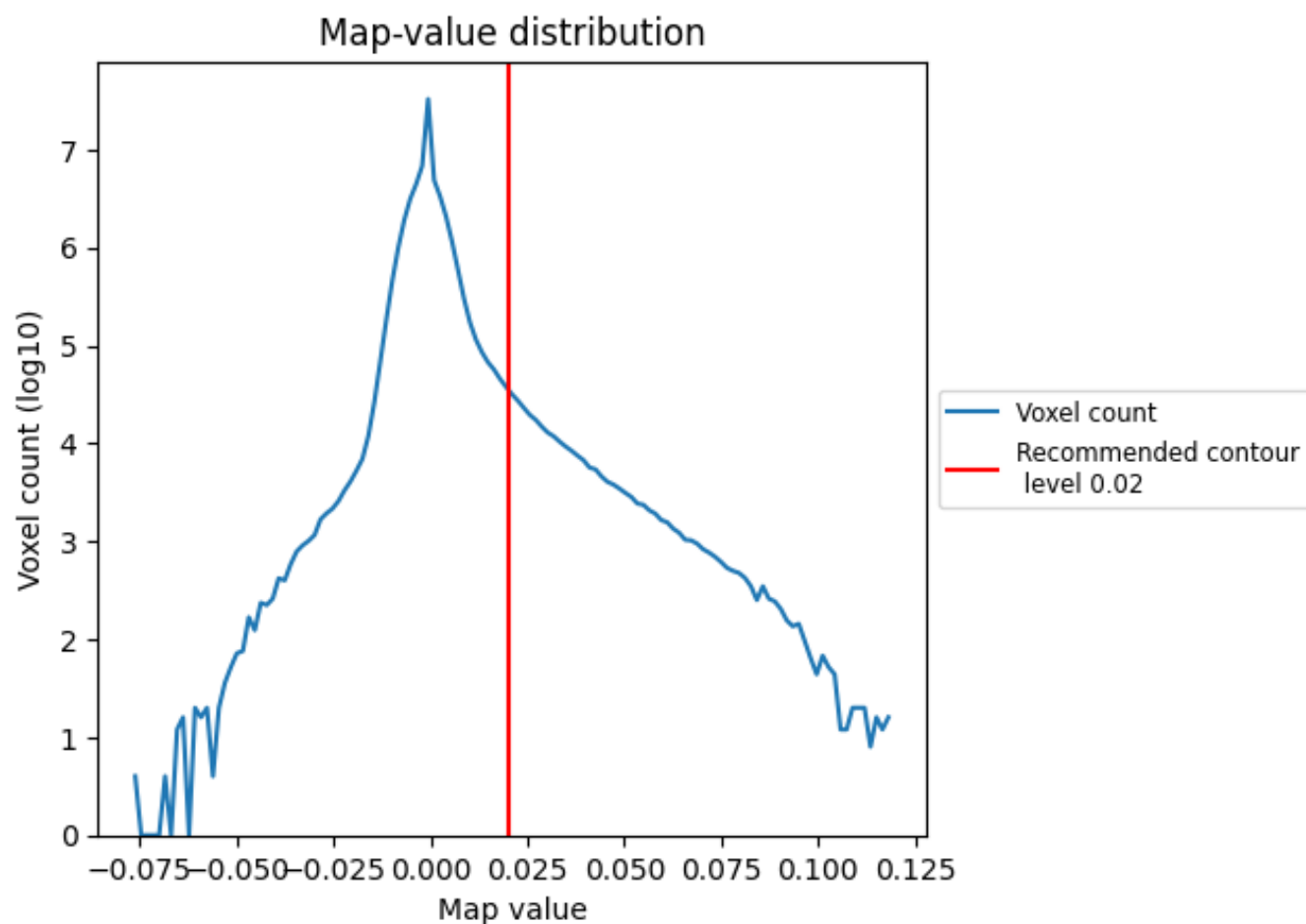
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

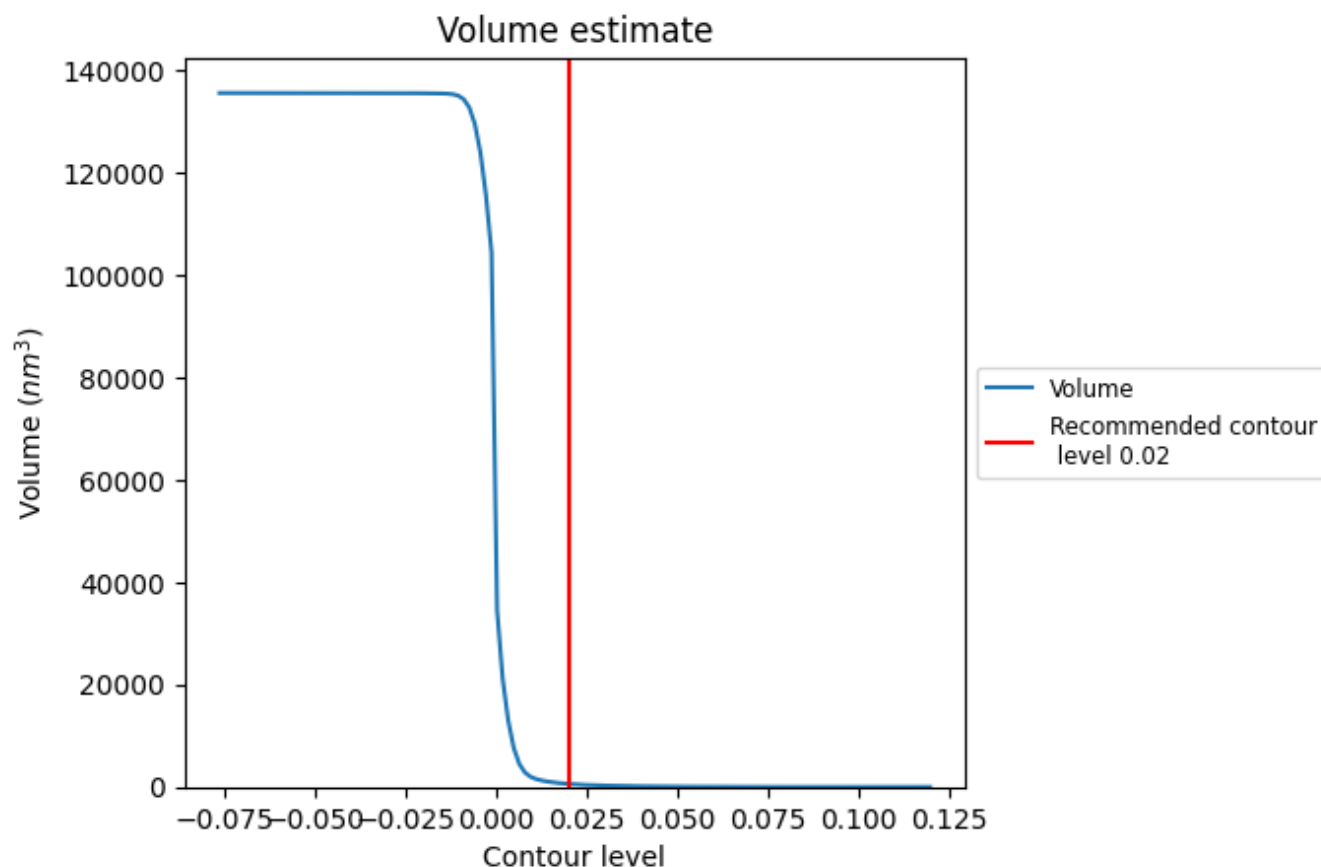
This section contains the results of statistical analysis of the map.

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.

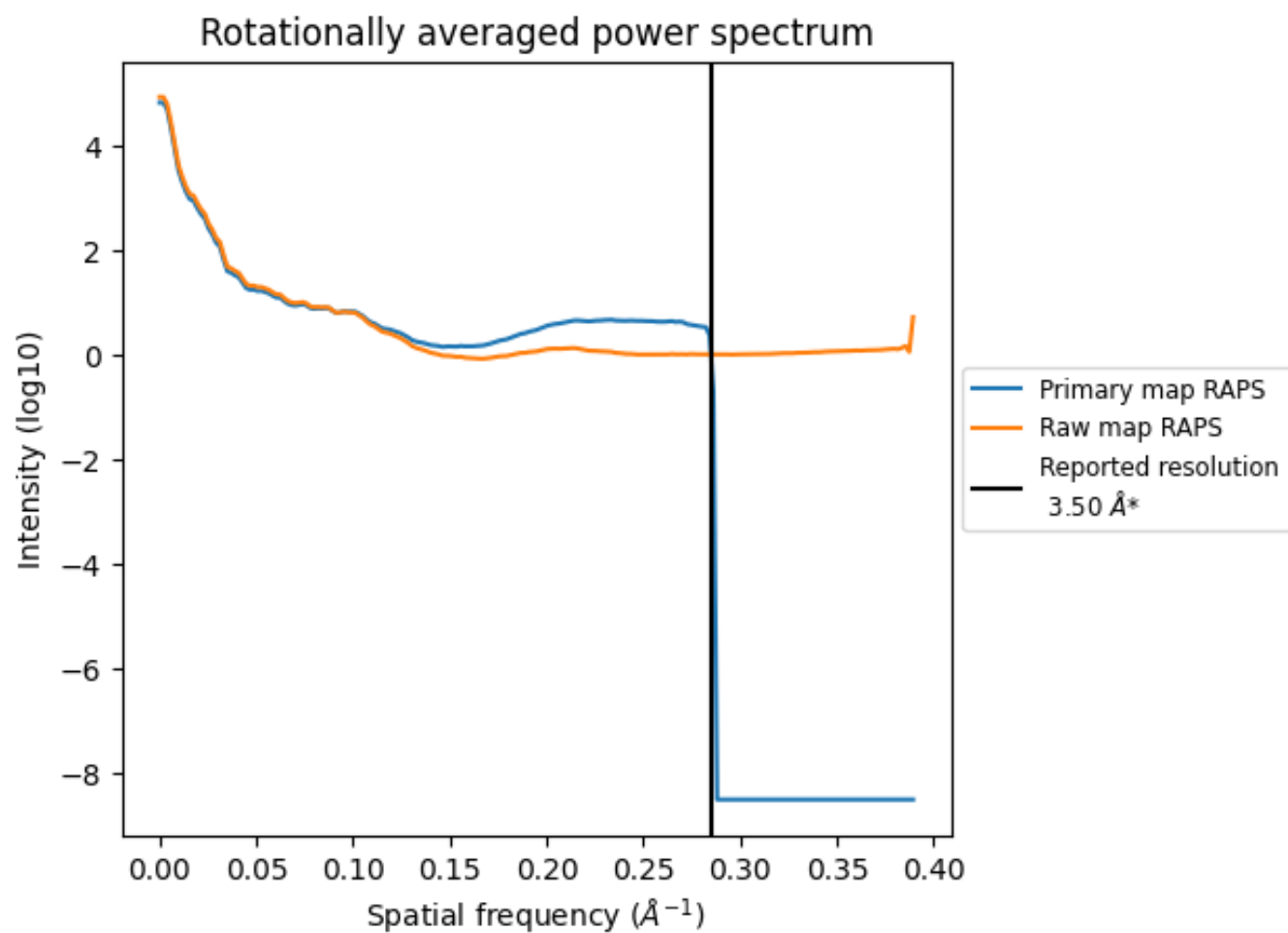
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 601 nm³; this corresponds to an approximate mass of 542 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 ⓘ

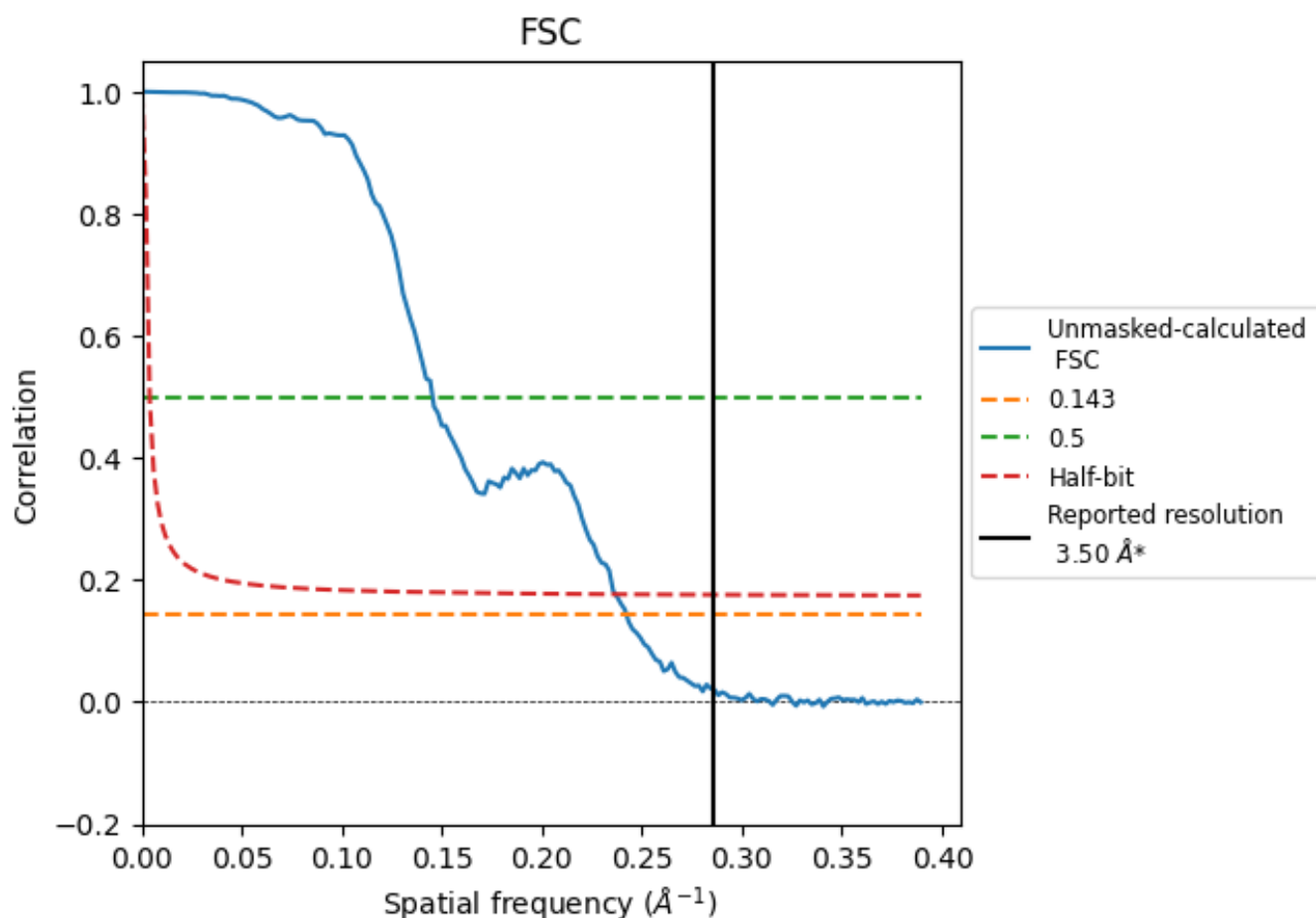


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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](#)

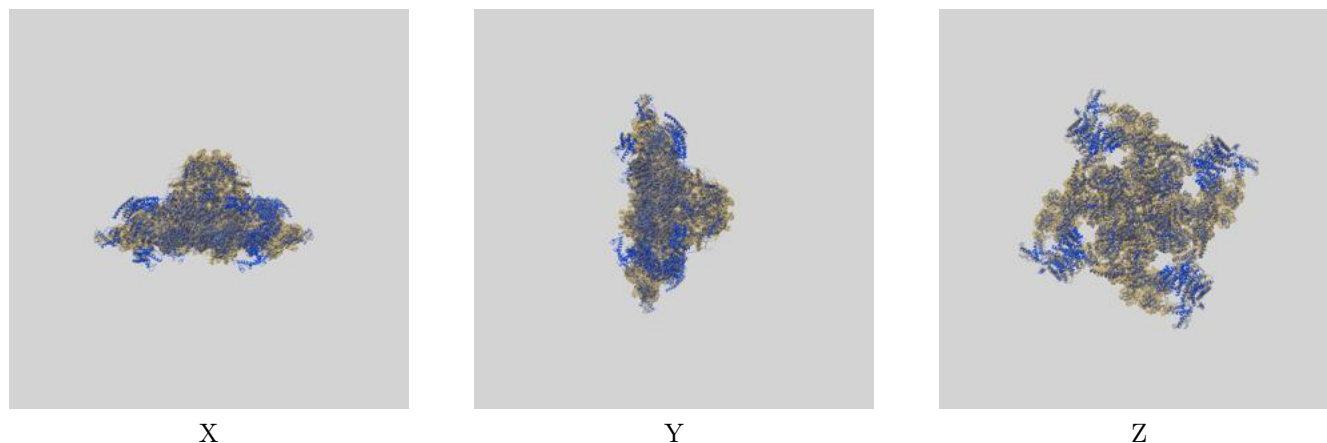
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	6.88	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

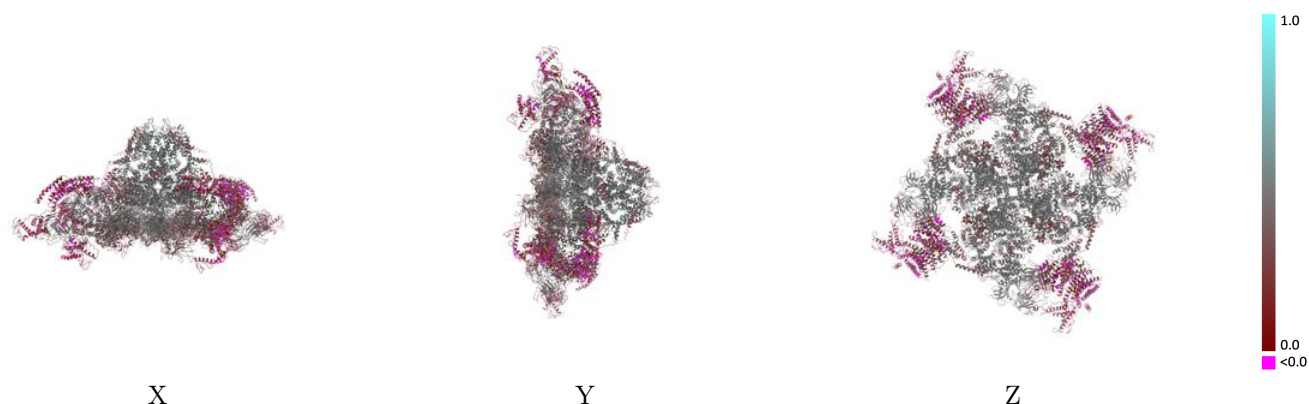
This section contains information regarding the fit between EMDB map EMD-33937 and PDB model 7VMN. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



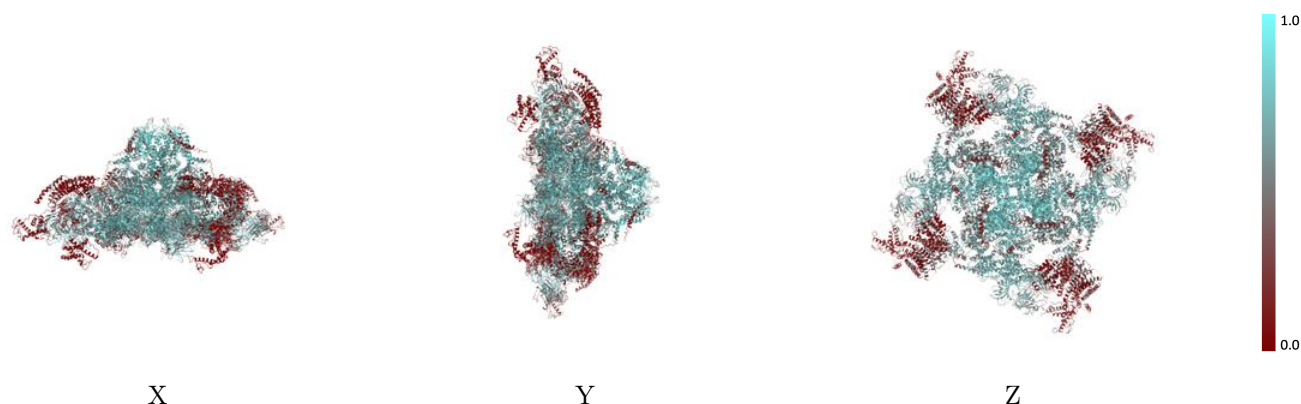
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



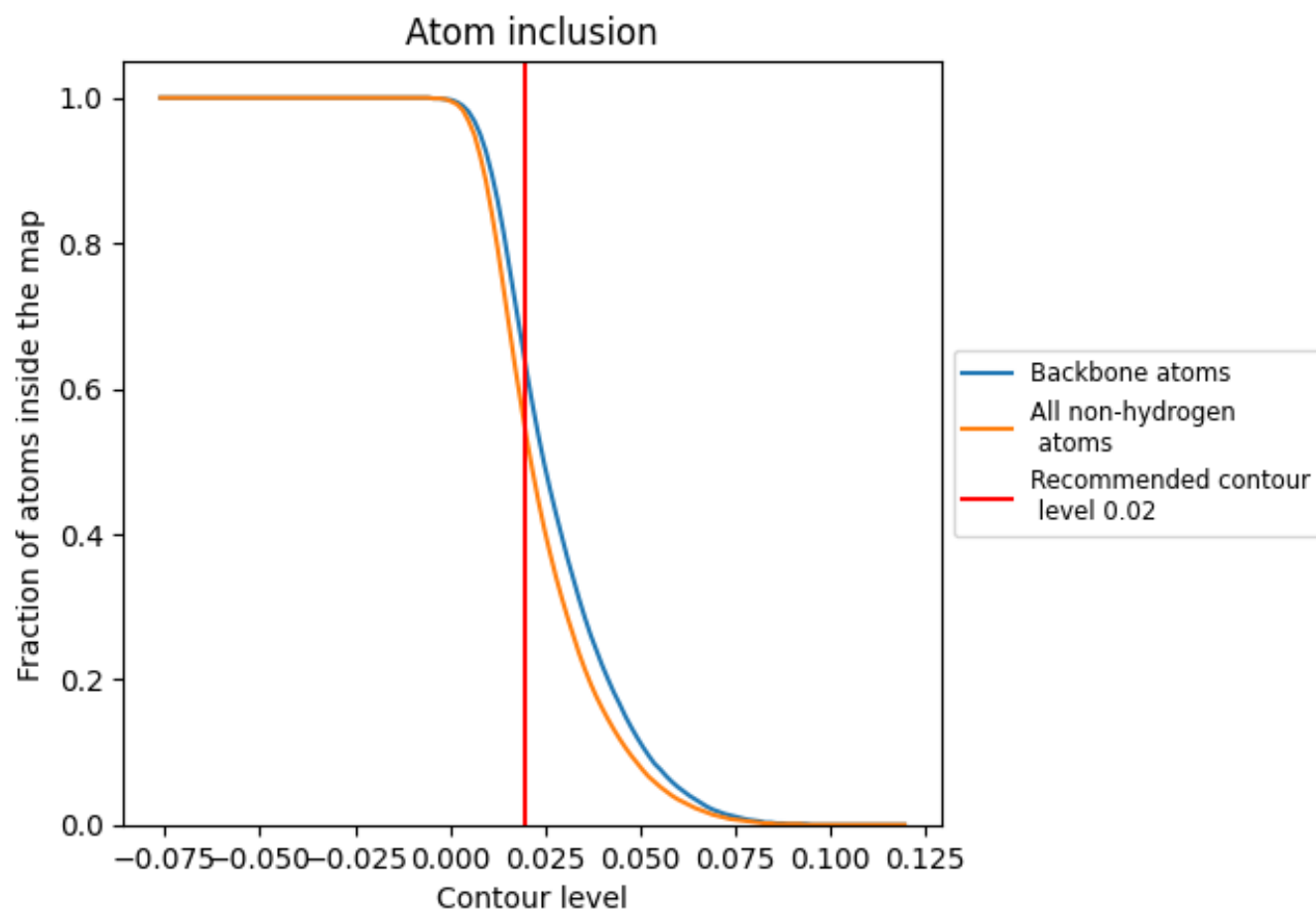
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5380	0.3770
A	0.5350	0.3750
B	0.5370	0.3760
C	0.5360	0.3760
D	0.5360	0.3740
G	0.6290	0.4370
H	0.6310	0.4350
I	0.6320	0.4300
J	0.6290	0.4350

1.0

0.0

<0.0