



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:43 PM UTC

PDB ID : 7VMM / pdb_00007vmm
EMDB ID : EMD-33936
Title : Structure of recombinant RyR2 (EGTA dataset, class 1, closed state)
Authors : Kobayashi, T.; Tsutsumi, A.; Kurebayashi, N.; Kodama, M.; Kikkawa, M.;
Murayama, T.; Ogawa, H.
Deposited on : 2021-10-09
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

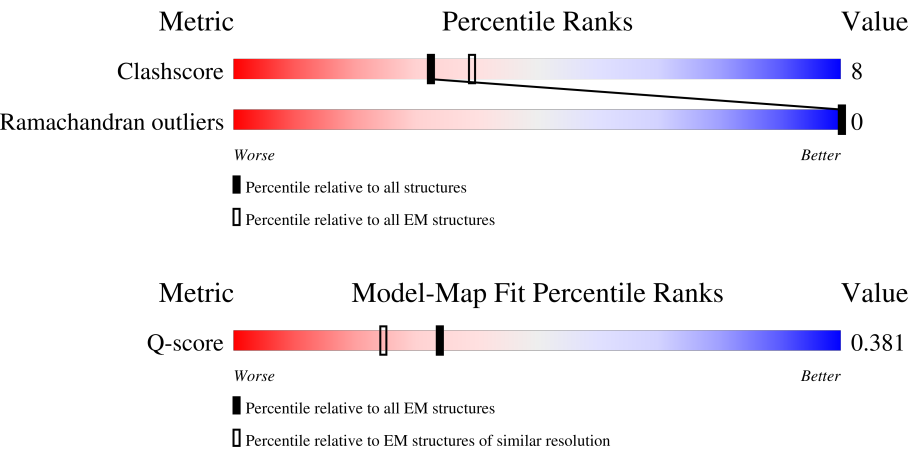
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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	-
Q-score	-	25397	13600 (2.99 - 3.99)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4966	26% 66% 15% 19%
1	B	4966	26% 66% 15% 19%
1	C	4966	26% 66% 15% 19%
1	D	4966	26% 66% 15% 19%
2	G	176	44% 17% 39%

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Mol	Chain	Length	Quality of chain
2	H	176	44%16%39%
2	I	176	43%18%39%
2	J	176	44%16%39%

2 Entry composition

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

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
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

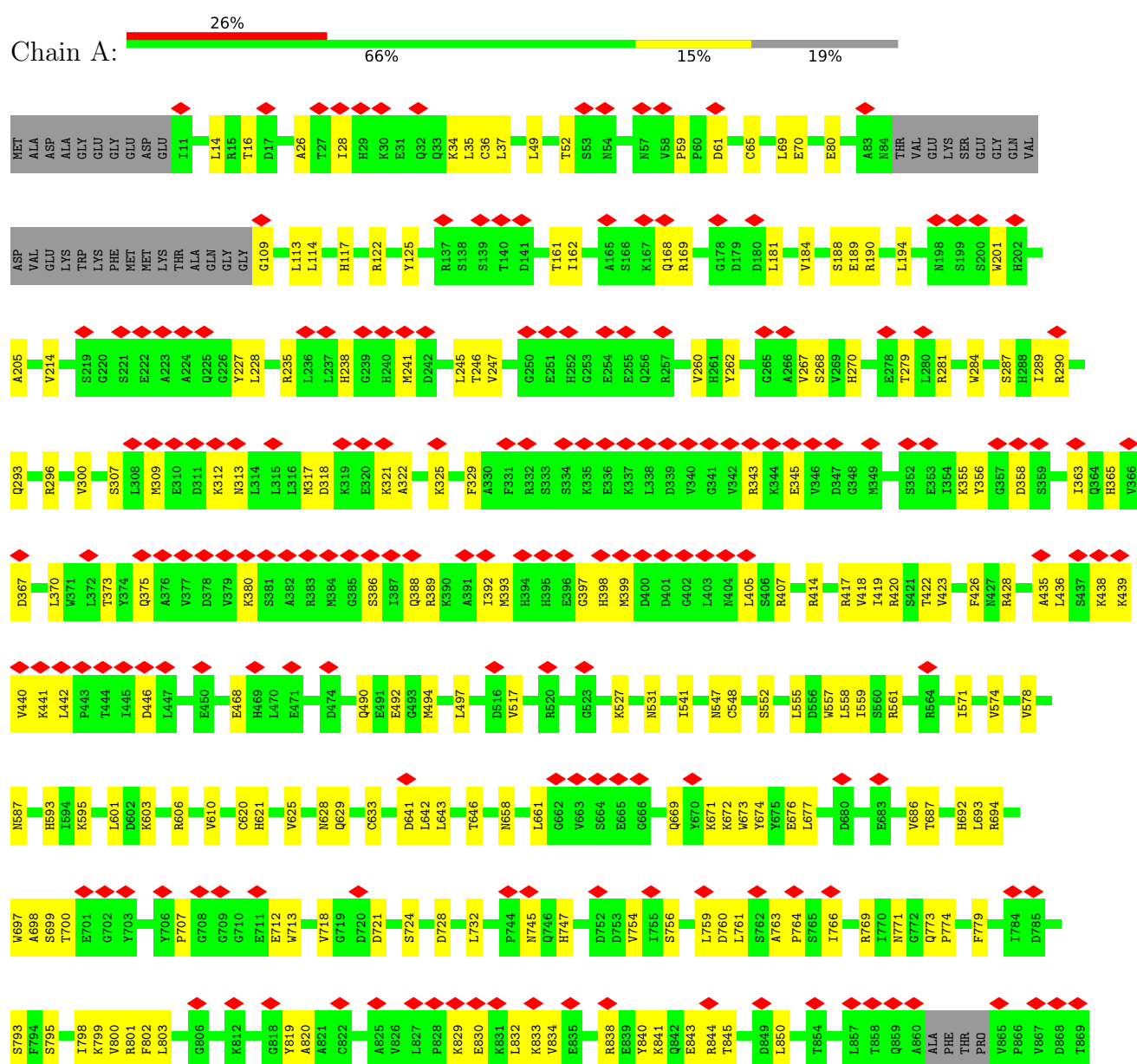
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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







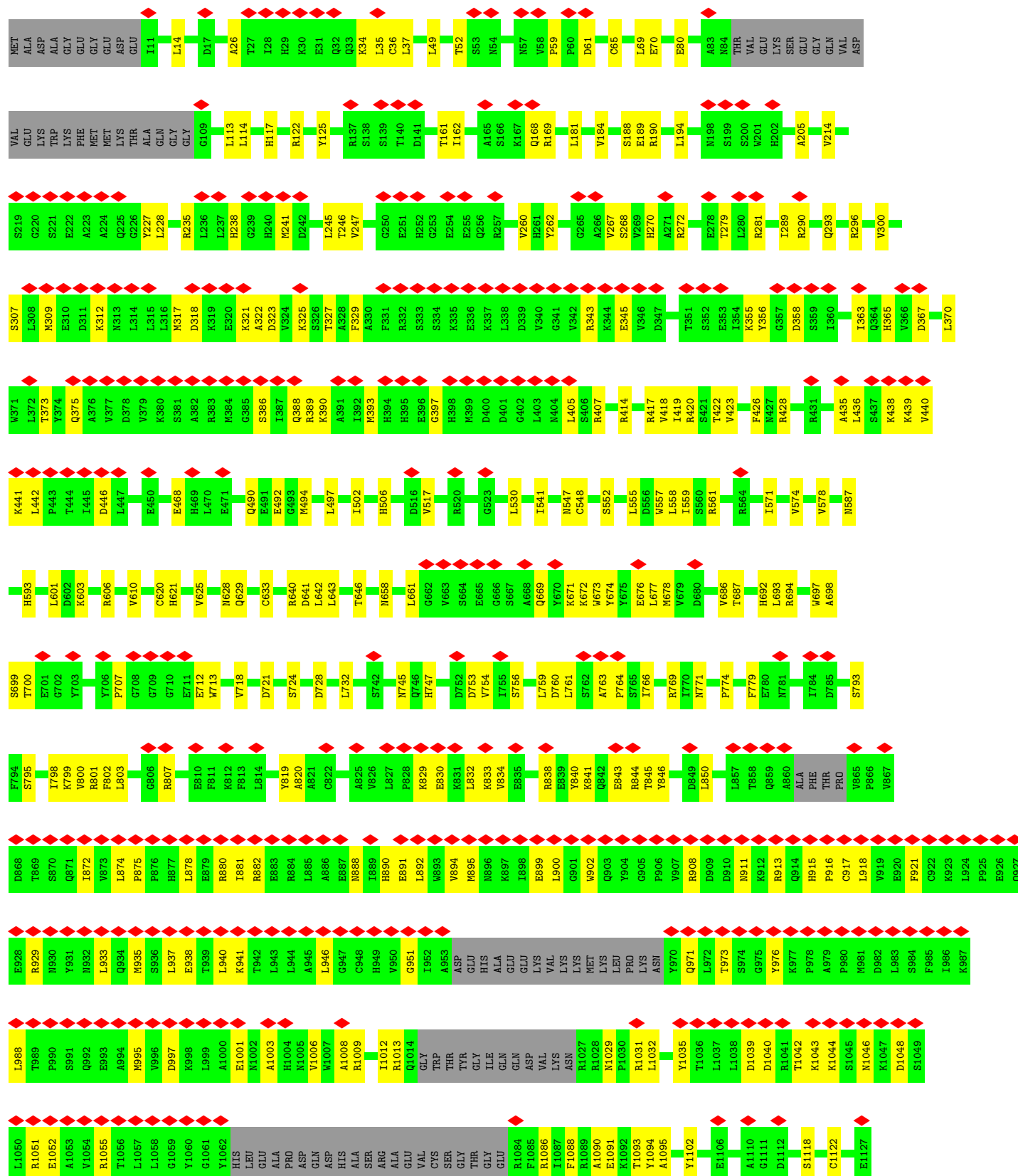
F4040	F3905	L3730	UNK	X3427	X3366	X3306	X3246	X3186	X3126	UNK
V4041	F3909	H3731	UNK	X3428	X3367	X3307	X3247	X3187	X3127	UNK
L4042	I3909	D3732	UNK	X3429	X3368	X3308	X3248	X3188	X3128	UNK
R4044	L3919	R3733	F3611	X3430	X3369	X3309	X3249	X3189	X3129	UNK
R4045	T3920	V3734	V3616	X3431	X3370	X3310	X3250	X3190	UNK	UNK
D4046	E3921	T3737	Q3621	X3432	X3371	X3311	X3251	X3191	UNK	UNK
F4047	Y3922	L3738	Q3621	X3433	X3372	X3312	X3252	X3192	UNK	UNK
H4048	I3923	V3739	E3624	X3434	X3373	X3313	X3253	X3193	UNK	UNK
K4049	L3934	L3742	E3624	UNK	X3374	X3314	X3254	X3194	UNK	UNK
L4050	S3937	G3738	E3631	UNK	X3375	X3315	X3255	X3195	X3136	UNK
M4051	R3938	N3739	E3632	UNK	X3376	X3316	X3256	X3196	X3137	UNK
F4052	L3939	V3740	E3636	UNK	X3377	X3317	X3257	X3197	X3138	UNK
S4053	H4054	V3746	I3640	UNK	X3378	X3318	X3258	X3198	X3139	UNK
K4055	V3940	R3746	I3640	UNK	X3379	X3319	X3259	X3199	X3140	UNK
Q4059	D3941	R3796	I3640	UNK	X3380	X3320	X3260	X3200	X3141	UNK
Q4059	A3942	L3802	A3648	UNK	X3381	X3321	X3261	X3201	X3142	UNK
F4063	Q3954	R3809	GLU	UNK	X3382	X3322	X3262	X3202	X3143	UNK
F4064	M3955	L3816	LEU	UNK	X3383	X3323	X3263	UNK	X3144	UNK
L4065	K3956	G3817	PRO	UNK	X3384	X3324	X3264	UNK	X3145	UNK
E4070	Q3959	X3818	GLU	UNK	X3385	X3325	X3265	UNK	X3146	UNK
T4071	D3960	X3819	GLU	UNK	X3386	X3326	X3266	X3207	X3147	UNK
D4072	S3961	V3820	ASP	UNK	X3387	X3327	X3267	X3208	X3148	UNK
F4073	S3962	E3821	ALA	UNK	X3388	X3328	X3268	X3209	X3149	UNK
N4074	Q3974	X3822	MET	UNK	X3389	X3329	X3269	X3210	X3150	UNK
F4075	L3986	G3823	LYS	UNK	X3390	X3330	X3270	X3211	X3151	UNK
T4076	D4000	S3824	L3669	UNK	X3391	X3331	X3271	X3212	X3152	UNK
D4078	M4001	G3825	L3686	UNK	X3392	X3332	X3272	X3213	X3153	UNK
V4079	L4002	E3826	L3686	UNK	X3393	X3333	X3273	X3214	X3154	UNK
F4082	V4003	K3827	K3696	UNK	X3394	X3334	X3274	X3215	X3155	UNK
V4083	E4004	V3828	K3699	UNK	X3395	X3335	X3275	X3216	X3156	UNK
N4110	V4009	D3831	ASP	UNK	X3396	X3336	X3276	X3217	X3157	X3104
D4111	I4012	D3832	GLU	UNK	X3397	X3337	X3277	X3218	X3158	X3106
T4112	L4012	E3833	GLU	UNK	X3398	X3338	X3278	X3219	X3159	X3107
R4113	L4012	F3834	UNK	UNK	X3399	X3339	X3279	X3220	X3160	X3108
L4114	D4024	Q3843	ASP	UNK	X3400	X3340	X3280	UNK	X3161	X3109
Q4115	L4025	N3864	ASP	UNK	X3401	X3341	X3281	UNK	X3162	X3110
T4116	T4026	T3865	GLY	UNK	X3402	X3342	X3282	UNK	X3163	X3111
E4119	S4027	T3865	GLU	UNK	X3403	X3343	X3283	UNK	X3164	X3112
E4119	S4028	T3865	GLU	UNK	X3404	X3344	X3284	UNK	X3165	X3113
K4142	D4029	L3869	VAL	UNK	X3405	X3345	X3285	UNK	X3166	X3114
E4153	T4030	S3883	LYS	UNK	X3406	X3346	X3286	UNK	X3167	X3115
T4157	F4031	S3883	S3712	UNK	X3407	X3347	X3287	UNK	X3168	X3116
V4164	K4032	D3886	E3719	UNK	X3408	X3348	X3288	X3231	X3169	X3117
S4167	E4033	Y3891	K3722	UNK	X3409	X3349	X3289	X3232	X3170	X3118
S4167	D4035	S3892	K3722	UNK	X3410	X3350	X3290	X3233	X3171	X3119
F4171	P4036	G3893	Q3727	UNK	X3411	X3351	X3291	X3234	X3172	X3120
G4038	D4037	G3893	R3729	UNK	X3412	X3352	X3292	X3235	X3173	X3121
K4039	D4038	L3896	R3729	UNK	X3413	X3353	X3293	X3236	X3174	X3122
V4175	K4039	E3899	R3729	UNK	X3414	X3354	X3294	X3237	X3175	X3123
				UNK	X3417	X3355	X3295	X3238	X3176	X3124
				UNK	X3418	X3356	X3296	X3239	X3177	X3125
				UNK	X3419	X3357	X3297	X3240	X3178	
				UNK	X3420	X3358	X3298	X3241	X3179	
				UNK	X3421	X3359	X3299	X3242	X3180	
				UNK	X3422	X3360	X3300	X3243	X3181	
				UNK	X3423	X3361	X3301	X3244	X3182	
				UNK	X3424	X3362	X3302	X3245	X3183	
				UNK	X3425	X3363	X3303	X3246	X3184	
				UNK	X3426	X3364	X3304	X3247	X3185	
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				UNK			X3364	X3307		
				UNK			X3365	X3308		
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				UNK			X3381	X3324		
				UNK			X3382	X3325		
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				UNK			X3385	X3328		
				UNK			X3386	X3329		
				UNK			X3387	X3330		
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				UNK			X3389	X3332		
				UNK			X3390	X3333		
				UNK			X3391	X3334		
				UNK			X3392	X3335		
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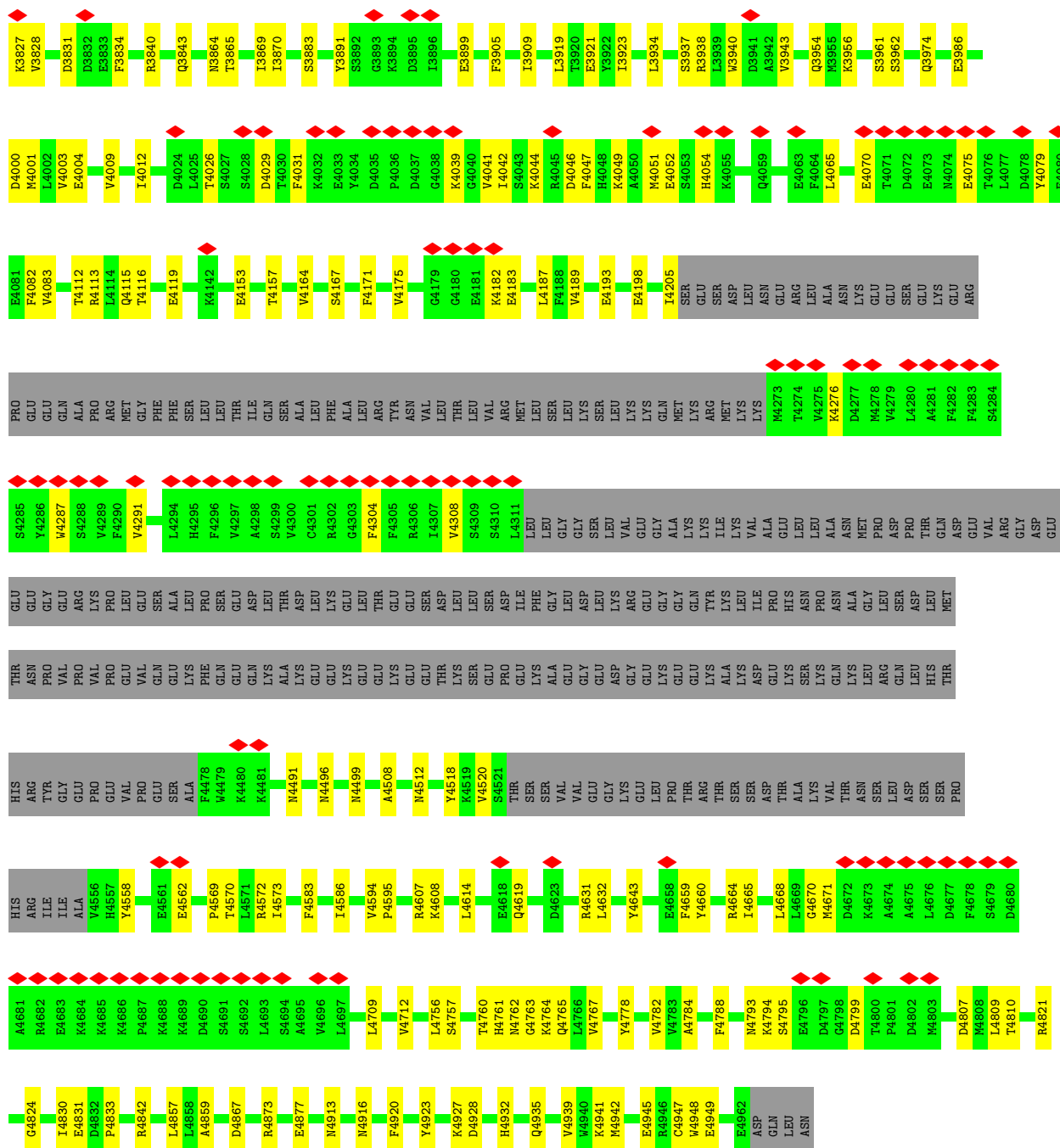




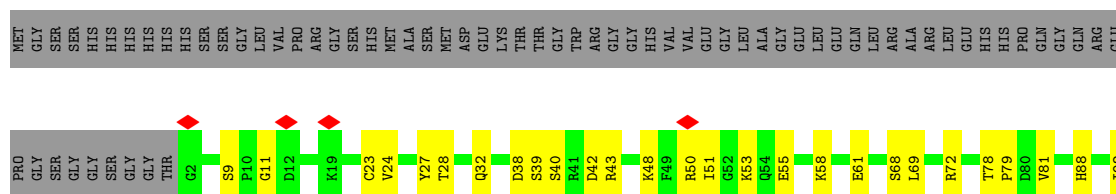


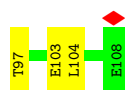






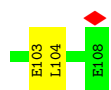
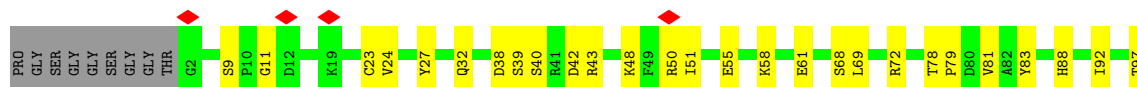
Chain G:





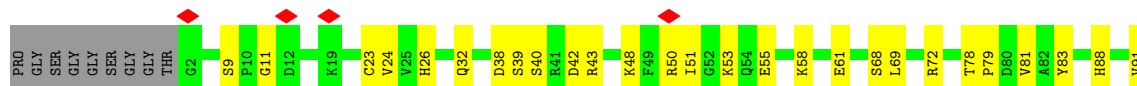
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 44% 16% 39%



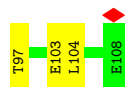
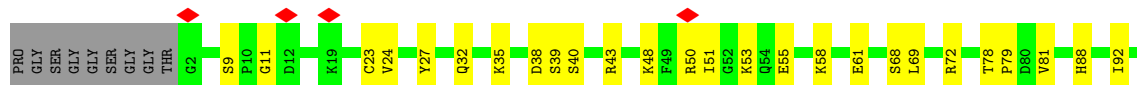
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain I: 43% 18% 39%



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

Chain J: 44% 16% 39%



4 Experimental information

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

5.1 Standard geometry

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	0.13	0/26895	0.33	0/36316
1	B	0.13	0/26895	0.33	0/36316
1	C	0.13	0/26895	0.33	0/36316
1	D	0.13	0/26895	0.33	0/36316
2	G	0.11	0/835	0.33	0/1123
2	H	0.11	0/835	0.33	0/1123
2	I	0.11	0/835	0.33	0/1123
2	J	0.11	0/835	0.33	0/1123
All	All	0.13	0/110920	0.33	0/149756

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	GLU	Peptide

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30071	0	26714	485	0
1	B	30071	0	26714	475	0
1	C	30071	0	26714	484	0
1	D	30071	0	26714	485	0
2	G	819	0	821	19	0
2	H	819	0	821	18	0
2	I	819	0	821	20	0
2	J	819	0	821	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	123564	0	110140	1976	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1976) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2404:GLU:HG3	1:A:2405:MET:H	1.38	0.89
1:B:2404:GLU:HG3	1:B:2405:MET:H	1.38	0.89
1:D:2404:GLU:HG3	1:D:2405:MET:H	1.38	0.88
1:C:2404:GLU:HG3	1:C:2405:MET:H	1.38	0.87
1:A:4821:ARG:NH2	1:D:4824:GLY:O	2.08	0.86
1:D:1190:LEU:HD21	1:D:1193:LYS:HB3	1.58	0.85
1:A:1190:LEU:HD21	1:A:1193:LYS:HB3	1.59	0.85
1:C:1190:LEU:HD21	1:C:1193:LYS:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1190:LEU:HD21	1:B:1193:LYS:HB3	1.59	0.85
1:A:2406:HIS:HA	1:A:2409:HIS:HB3	1.62	0.82
1:B:2406:HIS:HA	1:B:2409:HIS:HB3	1.61	0.82
1:C:2406:HIS:HA	1:C:2409:HIS:HB3	1.62	0.81
1:C:4789:ARG:NH2	1:D:4558:TYR:OH	2.14	0.80
1:A:358:ASP:OD1	1:A:358:ASP:N	2.15	0.80
1:D:2406:HIS:HA	1:D:2409:HIS:HB3	1.62	0.80
1:A:838:ARG:H	1:A:841:LYS:HZ1	1.31	0.79
1:C:358:ASP:OD1	1:C:358:ASP:N	2.15	0.79
1:D:358:ASP:N	1:D:358:ASP:OD1	2.15	0.78
1:B:358:ASP:N	1:B:358:ASP:OD1	2.15	0.77
1:C:4833:PRO:HB3	1:C:4842:ARG:HD3	1.66	0.77
2:J:58:LYS:HA	2:J:61:GLU:HG2	1.66	0.77
2:G:58:LYS:HA	2:G:61:GLU:HG2	1.66	0.77
1:B:4833:PRO:HB3	1:B:4842:ARG:HD3	1.66	0.76
2:H:58:LYS:HA	2:H:61:GLU:HG2	1.66	0.76
1:C:1741:PRO:HB3	1:C:1746:LYS:HE3	1.67	0.76
1:A:4833:PRO:HB3	1:A:4842:ARG:HD3	1.66	0.76
1:D:4833:PRO:HB3	1:D:4842:ARG:HD3	1.66	0.76
2:I:58:LYS:HA	2:I:61:GLU:HG2	1.66	0.76
1:B:1741:PRO:HB3	1:B:1746:LYS:HE3	1.67	0.75
1:D:1741:PRO:HB3	1:D:1746:LYS:HE3	1.67	0.75
1:A:4867:ASP:OD1	1:B:4873:ARG:NH1	2.19	0.74
1:B:838:ARG:H	1:B:841:LYS:HZ1	1.34	0.74
1:A:1741:PRO:HB3	1:A:1746:LYS:HE3	1.67	0.74
1:C:760:ASP:HB3	1:C:764:PRO:HG2	1.70	0.74
1:A:760:ASP:HB3	1:A:764:PRO:HG2	1.70	0.74
1:C:4042:ILE:HG22	1:C:4044:LYS:H	1.53	0.73
1:B:4042:ILE:HG22	1:B:4044:LYS:H	1.53	0.73
1:A:317:MET:HE3	1:A:322:ALA:HA	1.71	0.73
1:D:4042:ILE:HG22	1:D:4044:LYS:H	1.53	0.73
1:A:4042:ILE:HG22	1:A:4044:LYS:H	1.53	0.73
1:C:317:MET:HE3	1:C:322:ALA:HA	1.71	0.73
1:B:317:MET:HE3	1:B:322:ALA:HA	1.71	0.73
1:C:558:LEU:HB3	1:C:571:ILE:HD11	1.71	0.73
1:A:558:LEU:HB3	1:A:571:ILE:HD11	1.71	0.72
1:B:760:ASP:HB3	1:B:764:PRO:HG2	1.70	0.72
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.72	0.72
1:B:694:ARG:HG2	1:B:728:ASP:HB3	1.71	0.72
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.72	0.72
1:B:558:LEU:HB3	1:B:571:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.72	0.72
1:C:838:ARG:H	1:C:841:LYS:HZ1	1.36	0.72
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.72	0.72
1:A:694:ARG:HG2	1:A:728:ASP:HB3	1.72	0.72
1:A:162:ILE:HD11	1:A:181:LEU:HD22	1.72	0.72
1:D:760:ASP:HB3	1:D:764:PRO:HG2	1.70	0.72
1:D:317:MET:HE3	1:D:322:ALA:HA	1.70	0.71
1:D:162:ILE:HD11	1:D:181:LEU:HD22	1.72	0.71
1:D:558:LEU:HB3	1:D:571:ILE:HD11	1.71	0.71
1:C:2853:LYS:HA	1:C:2856:LYS:HE2	1.74	0.70
1:A:4873:ARG:NH1	1:D:4867:ASP:OD1	2.25	0.70
1:C:162:ILE:HD11	1:C:181:LEU:HD22	1.72	0.70
1:B:2853:LYS:HA	1:B:2856:LYS:HE2	1.74	0.70
1:B:162:ILE:HD11	1:B:181:LEU:HD22	1.72	0.70
1:C:694:ARG:HG2	1:C:728:ASP:HB3	1.71	0.70
1:D:694:ARG:HG2	1:D:728:ASP:HB3	1.72	0.70
1:B:1989:GLU:HG2	1:B:1992:ARG:HD3	1.74	0.69
1:D:2853:LYS:HA	1:D:2856:LYS:HE2	1.74	0.69
1:A:2853:LYS:HA	1:A:2856:LYS:HE2	1.74	0.69
1:C:1272:ARG:NH2	1:C:1584:PRO:O	2.26	0.69
1:A:1989:GLU:HG2	1:A:1992:ARG:HD3	1.74	0.69
1:D:1613:SER:O	1:D:1615:ARG:NH2	2.26	0.69
1:A:1613:SER:O	1:A:1615:ARG:NH2	2.26	0.69
1:A:1730:MET:SD	1:A:2106:THR:OG1	2.52	0.68
1:A:1682:ASP:HB2	1:A:1685:GLN:HB3	1.76	0.68
1:C:1682:ASP:HB2	1:C:1685:GLN:HB3	1.76	0.68
1:A:1272:ARG:NH2	1:A:1584:PRO:O	2.26	0.68
1:B:1682:ASP:HB2	1:B:1685:GLN:HB3	1.75	0.68
1:B:1272:ARG:NH2	1:B:1584:PRO:O	2.26	0.68
1:C:671:LYS:HB3	1:C:761:LEU:HB2	1.76	0.68
1:D:1272:ARG:NH2	1:D:1584:PRO:O	2.26	0.68
1:C:1613:SER:O	1:C:1615:ARG:NH2	2.26	0.68
1:C:1989:GLU:HG2	1:C:1992:ARG:HD3	1.74	0.68
1:D:1989:GLU:HG2	1:D:1992:ARG:HD3	1.74	0.67
1:B:1613:SER:O	1:B:1615:ARG:NH2	2.26	0.67
1:A:1262:PRO:HG2	1:A:1265:HIS:HB2	1.77	0.67
1:C:1262:PRO:HG2	1:C:1265:HIS:HB2	1.77	0.67
1:D:900:LEU:HD22	1:D:902:TRP:HE1	1.59	0.67
1:D:1682:ASP:HB2	1:D:1685:GLN:HB3	1.75	0.67
1:C:1730:MET:SD	1:C:2106:THR:OG1	2.52	0.67
1:D:1744:ASN:HD21	1:D:1746:LYS:HE2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LYS:HB3	1:A:761:LEU:HB2	1.76	0.67
1:C:1769:PHE:O	2:I:83:TYR:OH	2.12	0.67
1:B:671:LYS:HB3	1:B:761:LEU:HB2	1.76	0.67
1:D:1262:PRO:HG2	1:D:1265:HIS:HB2	1.77	0.67
1:B:1262:PRO:HG2	1:B:1265:HIS:HB2	1.77	0.66
1:D:1730:MET:SD	1:D:2106:THR:OG1	2.52	0.66
1:D:1775:ASP:OD1	1:D:1776:CYS:N	2.26	0.66
1:A:900:LEU:HD22	1:A:902:TRP:HE1	1.59	0.66
1:C:900:LEU:HD22	1:C:902:TRP:HE1	1.59	0.66
1:C:1775:ASP:OD1	1:C:1776:CYS:N	2.26	0.66
1:D:671:LYS:HB3	1:D:761:LEU:HB2	1.76	0.66
1:D:4619:GLN:HE22	1:D:4631:ARG:HH12	1.44	0.66
1:A:1744:ASN:HD21	1:A:1746:LYS:HE2	1.60	0.66
1:B:900:LEU:HD22	1:B:902:TRP:HE1	1.60	0.66
1:B:1730:MET:SD	1:B:2106:THR:OG1	2.52	0.66
1:C:4115:GLN:O	1:C:4119:GLU:HG2	1.96	0.66
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.29	0.65
1:B:1744:ASN:HD21	1:B:1746:LYS:HE2	1.60	0.65
1:A:759:LEU:HD13	1:A:766:ILE:HG12	1.79	0.65
1:C:4619:GLN:HE22	1:C:4631:ARG:HH12	1.44	0.65
1:B:4115:GLN:O	1:B:4119:GLU:HG2	1.96	0.65
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.29	0.65
1:D:759:LEU:HD13	1:D:766:ILE:HG12	1.79	0.65
1:D:2731:TRP:NE1	1:D:2735:LYS:HZ2	1.95	0.65
1:D:4115:GLN:O	1:D:4119:GLU:HG2	1.96	0.65
1:B:1775:ASP:OD1	1:B:1776:CYS:N	2.26	0.65
1:C:4042:ILE:HG21	1:C:4047:PHE:HB2	1.79	0.65
1:C:759:LEU:HD13	1:C:766:ILE:HG12	1.79	0.65
1:A:1266:GLU:O	1:A:1267:HIS:ND1	2.30	0.65
1:C:1744:ASN:HD21	1:C:1746:LYS:HE2	1.60	0.65
1:C:2731:TRP:NE1	1:C:2735:LYS:HZ2	1.95	0.65
1:A:1267:HIS:O	1:A:1292:SER:OG	2.15	0.65
1:B:1267:HIS:O	1:B:1292:SER:OG	2.15	0.65
1:B:4003:VAL:HG11	1:B:4113:ARG:HG2	1.80	0.64
1:D:2731:TRP:HE1	1:D:2735:LYS:HZ2	1.43	0.64
1:D:4003:VAL:HG11	1:D:4113:ARG:HG2	1.80	0.64
1:C:1266:GLU:O	1:C:1267:HIS:ND1	2.30	0.64
1:A:2731:TRP:HE1	1:A:2735:LYS:HZ2	1.45	0.64
1:A:4115:GLN:O	1:A:4119:GLU:HG2	1.96	0.64
1:A:4619:GLN:HE22	1:A:4631:ARG:HH12	1.44	0.64
1:B:1266:GLU:O	1:B:1267:HIS:ND1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1359:ILE:HG12	1:B:1363:LYS:HD2	1.79	0.64
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.29	0.64
1:D:1266:GLU:O	1:D:1267:HIS:ND1	2.30	0.64
1:D:3818:MET:SD	1:D:3818:MET:N	2.68	0.64
1:C:3818:MET:SD	1:C:3818:MET:N	2.68	0.64
1:D:2836:LEU:HA	1:D:2839:MET:HE3	1.80	0.64
1:C:2836:LEU:HA	1:C:2839:MET:HE3	1.80	0.64
1:B:4619:GLN:HE22	1:B:4631:ARG:HH12	1.44	0.64
1:A:4003:VAL:HG11	1:A:4113:ARG:HG2	1.80	0.64
1:B:426:PHE:HB3	1:B:497:LEU:HD21	1.80	0.64
1:B:759:LEU:HD13	1:B:766:ILE:HG12	1.79	0.64
1:B:3822:GLU:HB3	1:B:3826:GLU:HA	1.80	0.64
1:C:1265:HIS:HD2	1:C:1268:ILE:HB	1.63	0.64
1:C:4003:VAL:HG11	1:C:4113:ARG:HG2	1.80	0.64
1:A:426:PHE:HB3	1:A:497:LEU:HD21	1.80	0.64
1:A:1775:ASP:OD1	1:A:1776:CYS:N	2.26	0.63
1:A:2731:TRP:NE1	1:A:2735:LYS:HZ2	1.94	0.63
1:D:3822:GLU:HB3	1:D:3826:GLU:HA	1.80	0.63
1:A:3822:GLU:HB3	1:A:3826:GLU:HA	1.80	0.63
1:B:2836:LEU:HA	1:B:2839:MET:HE3	1.80	0.63
1:A:4042:ILE:HG21	1:A:4047:PHE:HB2	1.79	0.63
1:B:4042:ILE:HG21	1:B:4047:PHE:HB2	1.79	0.63
1:C:3822:GLU:HB3	1:C:3826:GLU:HA	1.80	0.63
1:A:2836:LEU:HA	1:A:2839:MET:HE3	1.80	0.63
1:B:2731:TRP:NE1	1:B:2735:LYS:HZ2	1.95	0.63
1:D:1267:HIS:O	1:D:1292:SER:OG	2.15	0.63
1:A:1265:HIS:HD2	1:A:1268:ILE:HB	1.63	0.63
1:A:3954:GLN:NE2	1:A:3974:GLN:OE1	2.32	0.63
1:D:1359:ILE:HG12	1:D:1363:LYS:HD2	1.79	0.63
1:C:1267:HIS:O	1:C:1292:SER:OG	2.15	0.63
1:C:3954:GLN:NE2	1:C:3974:GLN:OE1	2.32	0.63
1:C:426:PHE:HB3	1:C:497:LEU:HD21	1.80	0.63
1:B:36:CYS:SG	1:B:37:LEU:N	2.72	0.63
1:B:1847:ILE:HG23	1:B:1892:LEU:HB3	1.81	0.63
1:A:14:LEU:HD11	1:A:214:VAL:HG11	1.81	0.62
1:B:1265:HIS:HD2	1:B:1268:ILE:HB	1.63	0.62
1:B:2731:TRP:HE1	1:B:2735:LYS:HZ2	1.46	0.62
1:B:2735:LYS:HD2	1:B:2740:TRP:CD1	2.34	0.62
1:C:14:LEU:HD11	1:C:214:VAL:HG11	1.81	0.62
1:A:1359:ILE:HG12	1:A:1363:LYS:HD2	1.79	0.62
1:A:4055:LYS:NZ	1:D:4659:PHE:O	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2735:LYS:HD2	1:C:2740:TRP:CD1	2.34	0.62
1:B:3954:GLN:NE2	1:B:3974:GLN:OE1	2.32	0.62
1:C:3822:GLU:OE2	1:C:3824:SER:N	2.32	0.62
1:D:36:CYS:SG	1:D:37:LEU:N	2.72	0.62
1:D:1265:HIS:HD2	1:D:1268:ILE:HB	1.63	0.62
1:D:1847:ILE:HG23	1:D:1892:LEU:HB3	1.81	0.62
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.29	0.62
1:D:4042:ILE:HG21	1:D:4047:PHE:HB2	1.79	0.62
1:C:36:CYS:SG	1:C:37:LEU:N	2.72	0.62
1:D:325:LYS:HG3	1:D:367:ASP:OD1	2.00	0.62
1:D:3954:GLN:NE2	1:D:3974:GLN:OE1	2.32	0.62
1:A:36:CYS:SG	1:A:37:LEU:N	2.72	0.62
1:A:2735:LYS:HD2	1:A:2740:TRP:CD1	2.34	0.62
1:D:426:PHE:HB3	1:D:497:LEU:HD21	1.80	0.62
1:A:325:LYS:HG3	1:A:367:ASP:OD1	2.00	0.62
1:C:325:LYS:HG3	1:C:367:ASP:OD1	2.00	0.62
1:C:1359:ILE:HG12	1:C:1363:LYS:HD2	1.79	0.62
1:C:3754:VAL:HA	1:C:3757:THR:HG22	1.82	0.62
1:A:3822:GLU:OE2	1:A:3824:SER:N	2.32	0.62
1:B:14:LEU:HD11	1:B:214:VAL:HG11	1.81	0.62
1:C:2731:TRP:HE1	1:C:2735:LYS:HZ2	1.46	0.62
1:D:838:ARG:H	1:D:841:LYS:HZ1	1.47	0.62
1:D:2735:LYS:HD2	1:D:2740:TRP:CD1	2.34	0.61
1:D:3754:VAL:HA	1:D:3757:THR:HG22	1.82	0.61
1:A:1847:ILE:HG23	1:A:1892:LEU:HB3	1.81	0.61
1:B:3728:ALA:HA	1:B:3731:HIS:HD1	1.65	0.61
1:A:3754:VAL:HA	1:A:3757:THR:HG22	1.82	0.61
2:H:69:LEU:HA	2:H:104:LEU:HD22	1.82	0.61
1:C:872:ILE:HD11	1:C:941:LYS:HA	1.83	0.61
1:C:1847:ILE:HG23	1:C:1892:LEU:HB3	1.81	0.61
1:A:281:ARG:NH1	1:A:345:GLU:OE2	2.33	0.61
2:I:69:LEU:HA	2:I:104:LEU:HD22	1.83	0.61
1:D:1052:GLU:HA	1:D:1055:ARG:HB2	1.82	0.61
1:B:325:LYS:HG3	1:B:367:ASP:OD1	2.00	0.61
1:B:4079:TYR:O	1:B:4083:VAL:HG13	2.01	0.61
1:D:14:LEU:HD11	1:D:214:VAL:HG11	1.81	0.61
1:B:3754:VAL:HA	1:B:3757:THR:HG22	1.82	0.61
2:H:79:PRO:HD3	2:H:97:THR:HG22	1.83	0.61
1:C:880:ARG:HG3	1:C:881:ILE:HD12	1.82	0.61
1:D:872:ILE:HD11	1:D:941:LYS:HA	1.82	0.61
1:A:4079:TYR:O	1:A:4083:VAL:HG13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1829:LEU:HB3	1:B:1834:ILE:HD11	1.83	0.61
1:A:880:ARG:HG3	1:A:881:ILE:HD12	1.82	0.61
1:D:281:ARG:NH1	1:D:345:GLU:OE2	2.33	0.61
2:J:69:LEU:HA	2:J:104:LEU:HD22	1.83	0.61
1:A:423:VAL:HB	1:A:494:MET:HE3	1.83	0.60
1:A:1829:LEU:HB3	1:A:1834:ILE:HD11	1.83	0.60
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.83	0.60
2:G:79:PRO:HD3	2:G:97:THR:HG22	1.83	0.60
1:B:373:THR:HG22	1:B:397:GLY:HA2	1.82	0.60
1:B:872:ILE:HD11	1:B:941:LYS:HA	1.83	0.60
2:I:24:VAL:HG22	2:I:48:LYS:HG2	1.83	0.60
1:A:3822:GLU:HG3	1:A:3827:LYS:HG3	1.83	0.60
1:C:1829:LEU:HB3	1:C:1834:ILE:HD11	1.83	0.60
1:C:4079:TYR:O	1:C:4083:VAL:HG13	2.01	0.60
2:I:79:PRO:HD3	2:I:97:THR:HG22	1.83	0.60
1:D:4079:TYR:O	1:D:4083:VAL:HG13	2.01	0.60
1:B:3822:GLU:HG3	1:B:3827:LYS:HG3	1.84	0.60
1:B:4044:LYS:HB2	1:B:4075:GLU:HG2	1.83	0.60
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.67	0.60
1:D:1829:LEU:HB3	1:D:1834:ILE:HD11	1.83	0.60
1:D:2275:SER:OG	1:D:2287:ILE:O	2.17	0.60
1:D:3891:TYR:O	1:D:3956:LYS:NZ	2.35	0.60
1:C:281:ARG:NH1	1:C:345:GLU:OE2	2.33	0.60
1:C:373:THR:HG22	1:C:397:GLY:HA2	1.82	0.60
1:C:1052:GLU:HA	1:C:1055:ARG:HB2	1.82	0.60
1:C:2275:SER:OG	1:C:2287:ILE:O	2.17	0.60
1:B:880:ARG:HG3	1:B:881:ILE:HD12	1.82	0.60
1:A:373:THR:HG22	1:A:397:GLY:HA2	1.82	0.60
2:G:69:LEU:HA	2:G:104:LEU:HD22	1.82	0.60
1:B:2855:LYS:HA	1:B:2855:LYS:HE3	1.84	0.60
1:C:1681:VAL:HG23	1:C:1682:ASP:H	1.67	0.60
1:D:4153:GLU:O	1:D:4157:THR:OG1	2.19	0.60
1:A:4044:LYS:HB2	1:A:4075:GLU:HG2	1.83	0.60
1:A:2855:LYS:HE3	1:A:2855:LYS:HA	1.84	0.60
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.84	0.60
2:J:79:PRO:HD3	2:J:97:THR:HG22	1.83	0.60
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.67	0.60
1:B:3822:GLU:OE2	1:B:3824:SER:N	2.32	0.60
1:B:4153:GLU:O	1:B:4157:THR:OG1	2.19	0.60
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.67	0.60
1:C:1684:PRO:HD3	2:I:42:ASP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:ILE:HD11	1:A:941:LYS:HA	1.83	0.60
1:A:4153:GLU:O	1:A:4157:THR:OG1	2.19	0.60
1:B:423:VAL:HB	1:B:494:MET:HE3	1.83	0.60
1:C:69:LEU:HD22	1:C:113:LEU:HD11	1.84	0.60
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.67	0.59
1:B:1052:GLU:HA	1:B:1055:ARG:HB2	1.82	0.59
1:D:69:LEU:HD22	1:D:113:LEU:HD11	1.84	0.59
1:D:279:THR:HG22	1:D:281:ARG:H	1.67	0.59
1:C:279:THR:HG22	1:C:281:ARG:H	1.67	0.59
1:C:4044:LYS:HB2	1:C:4075:GLU:HG2	1.83	0.59
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.67	0.59
1:A:365:HIS:NE2	1:A:367:ASP:OD2	2.35	0.59
1:A:2275:SER:OG	1:A:2287:ILE:O	2.17	0.59
1:B:69:LEU:HD22	1:B:113:LEU:HD11	1.84	0.59
1:B:1681:VAL:HG23	1:B:1682:ASP:H	1.67	0.59
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.84	0.59
1:A:900:LEU:HD22	1:A:902:TRP:NE1	2.18	0.59
1:C:3831:ASP:HB3	1:C:3834:PHE:HB3	1.85	0.59
1:D:373:THR:HG22	1:D:397:GLY:HA2	1.82	0.59
1:D:1681:VAL:HG23	1:D:1682:ASP:H	1.67	0.59
1:B:365:HIS:NE2	1:B:367:ASP:OD2	2.35	0.59
1:B:386:SER:HB3	1:B:388:GLN:HE22	1.67	0.59
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.83	0.59
1:D:4044:LYS:HB2	1:D:4075:GLU:HG2	1.83	0.59
1:A:69:LEU:HD22	1:A:113:LEU:HD11	1.84	0.59
1:A:1052:GLU:HA	1:A:1055:ARG:HB2	1.82	0.59
1:B:279:THR:HG22	1:B:281:ARG:H	1.67	0.59
1:C:4153:GLU:O	1:C:4157:THR:OG1	2.19	0.59
1:C:4778:TYR:O	1:C:4782:VAL:HG12	2.03	0.59
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.67	0.59
1:D:880:ARG:HG3	1:D:881:ILE:HD12	1.82	0.59
1:D:3831:ASP:HB3	1:D:3834:PHE:HB3	1.85	0.59
1:D:4778:TYR:O	1:D:4782:VAL:HG12	2.03	0.59
1:B:2148:ILE:HA	1:B:2151:ASN:HD22	1.68	0.59
1:D:386:SER:HB3	1:D:388:GLN:HE22	1.67	0.59
1:D:423:VAL:HB	1:D:494:MET:HE3	1.83	0.59
1:D:2148:ILE:HA	1:D:2151:ASN:HD22	1.68	0.59
1:D:2855:LYS:HA	1:D:2855:LYS:HE3	1.84	0.59
1:C:386:SER:HB3	1:C:388:GLN:HE22	1.67	0.59
1:C:423:VAL:HB	1:C:494:MET:HE3	1.83	0.59
1:D:3822:GLU:HG3	1:D:3827:LYS:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:24:VAL:HG22	2:J:48:LYS:HG2	1.83	0.59
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.84	0.59
1:C:2148:ILE:HA	1:C:2151:ASN:HD22	1.68	0.59
1:C:3822:GLU:HG3	1:C:3827:LYS:HG3	1.84	0.59
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.67	0.59
1:D:900:LEU:HD22	1:D:902:TRP:NE1	2.18	0.59
1:C:365:HIS:NE2	1:C:367:ASP:OD2	2.35	0.58
1:A:279:THR:HG22	1:A:281:ARG:H	1.67	0.58
1:B:281:ARG:NH1	1:B:345:GLU:OE2	2.33	0.58
1:C:2855:LYS:HA	1:C:2855:LYS:HE3	1.84	0.58
1:A:3831:ASP:HB3	1:A:3834:PHE:HB3	1.85	0.58
1:B:3818:MET:SD	1:B:3818:MET:N	2.68	0.58
1:B:3937:SER:OG	1:B:3938:ARG:N	2.37	0.58
1:B:290:ARG:H	1:B:293:GLN:HE21	1.51	0.58
1:B:900:LEU:HD22	1:B:902:TRP:NE1	2.18	0.58
1:A:2148:ILE:HA	1:A:2151:ASN:HD22	1.68	0.58
1:B:676:GLU:HB2	1:B:803:LEU:HB2	1.84	0.58
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.67	0.58
1:C:2312:VAL:HG23	1:C:2315:ASN:HB2	1.86	0.58
1:D:365:HIS:NE2	1:D:367:ASP:OD2	2.35	0.58
1:D:2312:VAL:HG23	1:D:2315:ASN:HB2	1.86	0.58
1:D:4756:LEU:O	1:D:4760:THR:OG1	2.21	0.58
1:A:4756:LEU:O	1:A:4760:THR:OG1	2.21	0.58
1:C:900:LEU:HD22	1:C:902:TRP:NE1	2.18	0.58
1:B:2275:SER:OG	1:B:2287:ILE:O	2.17	0.58
1:C:3937:SER:OG	1:C:3938:ARG:N	2.37	0.58
1:A:290:ARG:H	1:A:293:GLN:HE21	1.51	0.58
1:A:1814:THR:OG1	1:A:1815:THR:N	2.36	0.58
1:A:1681:VAL:HG23	1:A:1682:ASP:H	1.67	0.58
1:B:3891:TYR:O	1:B:3956:LYS:NZ	2.35	0.58
1:B:4778:TYR:O	1:B:4782:VAL:HG12	2.03	0.58
1:C:1814:THR:OG1	1:C:1815:THR:N	2.36	0.58
1:D:769:ARG:HA	1:D:774:PRO:HA	1.86	0.57
1:D:908:ARG:HG2	1:D:916:PRO:HG3	1.86	0.57
1:A:2325:ARG:NH2	1:D:189:GLU:O	2.36	0.57
1:B:3831:ASP:HB3	1:B:3834:PHE:HB3	1.85	0.57
1:D:3937:SER:OG	1:D:3938:ARG:N	2.37	0.57
1:A:2312:VAL:HG23	1:A:2315:ASN:HB2	1.86	0.57
1:A:4778:TYR:O	1:A:4782:VAL:HG12	2.03	0.57
1:C:769:ARG:HA	1:C:774:PRO:HA	1.87	0.57
1:C:2404:GLU:HG3	1:C:2405:MET:N	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4756:LEU:O	1:C:4760:THR:OG1	2.21	0.57
1:D:933:LEU:O	1:D:937:LEU:HG	2.05	0.57
1:A:908:ARG:HG2	1:A:916:PRO:HG3	1.86	0.57
1:A:1918:ARG:O	1:A:1922:GLU:HG2	2.04	0.57
1:B:2141:MET:SD	1:B:2173:VAL:HG11	2.45	0.57
1:A:386:SER:HB3	1:A:388:GLN:HE22	1.67	0.57
1:D:1918:ARG:O	1:D:1922:GLU:HG2	2.04	0.57
1:A:2276:CYS:SG	1:A:2290:ASN:ND2	2.78	0.57
1:B:1814:THR:OG1	1:B:1815:THR:N	2.36	0.57
1:B:2312:VAL:HG23	1:B:2315:ASN:HB2	1.86	0.57
1:C:908:ARG:HG2	1:C:916:PRO:HG3	1.86	0.57
1:C:3891:TYR:O	1:C:3956:LYS:NZ	2.35	0.57
1:A:933:LEU:O	1:A:937:LEU:HG	2.05	0.57
1:A:2141:MET:SD	1:A:2173:VAL:HG11	2.45	0.57
1:A:3818:MET:SD	1:A:3818:MET:N	2.68	0.57
1:B:1009:ARG:O	1:B:1013:ARG:NH1	2.38	0.57
1:C:933:LEU:O	1:C:937:LEU:HG	2.05	0.57
1:D:2276:CYS:SG	1:D:2290:ASN:ND2	2.78	0.57
1:C:2716:LEU:O	1:C:2720:ILE:HG12	2.05	0.57
1:D:1814:THR:OG1	1:D:1815:THR:N	2.36	0.57
1:A:769:ARG:HA	1:A:774:PRO:HA	1.86	0.57
1:A:2716:LEU:O	1:A:2720:ILE:HG12	2.05	0.57
1:B:1267:HIS:HB2	1:B:1294:ASN:HB2	1.87	0.57
1:B:1918:ARG:O	1:B:1922:GLU:HG2	2.04	0.57
1:B:4756:LEU:O	1:B:4760:THR:OG1	2.21	0.57
1:C:548:CYS:HB3	1:C:578:VAL:HG23	1.86	0.57
1:A:1684:PRO:HD3	2:G:42:ASP:HB3	1.87	0.57
1:A:2228:LEU:HD22	1:A:2296:ARG:HG3	1.87	0.57
1:B:548:CYS:HB3	1:B:578:VAL:HG23	1.86	0.57
1:B:2716:LEU:O	1:B:2720:ILE:HG12	2.05	0.57
1:C:1009:ARG:O	1:C:1013:ARG:NH1	2.38	0.57
1:C:2145:LEU:HD23	1:C:2148:ILE:HD11	1.87	0.57
1:D:290:ARG:H	1:D:293:GLN:HE21	1.51	0.57
1:D:2228:LEU:HD22	1:D:2296:ARG:HG3	1.87	0.57
1:B:769:ARG:HA	1:B:774:PRO:HA	1.86	0.56
1:C:2141:MET:SD	1:C:2173:VAL:HG11	2.45	0.56
1:D:1009:ARG:O	1:D:1013:ARG:NH1	2.38	0.56
1:A:548:CYS:HB3	1:A:578:VAL:HG23	1.86	0.56
1:B:2145:LEU:HD23	1:B:2148:ILE:HD11	1.87	0.56
1:C:290:ARG:H	1:C:293:GLN:HE21	1.51	0.56
1:D:2145:LEU:HD23	1:D:2148:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2145:LEU:HD23	1:A:2148:ILE:HD11	1.87	0.56
1:B:908:ARG:HG2	1:B:916:PRO:HG3	1.86	0.56
1:B:933:LEU:O	1:B:937:LEU:HG	2.05	0.56
1:B:1383:ARG:HE	1:B:1385:LYS:HE2	1.71	0.56
1:B:2070:GLN:O	1:B:3659:ARG:NH1	2.38	0.56
1:B:3796:MET:HE1	1:B:3869:ILE:HG23	1.88	0.56
1:C:1918:ARG:O	1:C:1922:GLU:HG2	2.04	0.56
1:D:3822:GLU:OE2	1:D:3824:SER:N	2.32	0.56
1:A:1267:HIS:HB2	1:A:1294:ASN:HB2	1.87	0.56
1:A:1383:ARG:HE	1:A:1385:LYS:HE2	1.71	0.56
1:A:2404:GLU:HG3	1:A:2405:MET:N	2.16	0.56
2:G:88:HIS:H	2:G:92:ILE:HB	1.71	0.56
1:B:606:ARG:NH2	1:B:1635:GLU:OE1	2.34	0.56
1:C:587:ASN:OD1	1:C:2132:ARG:NH1	2.38	0.56
1:C:1383:ARG:HE	1:C:1385:LYS:HE2	1.71	0.56
1:C:2228:LEU:HD22	1:C:2296:ARG:HG3	1.87	0.56
1:C:2276:CYS:SG	1:C:2290:ASN:ND2	2.78	0.56
1:D:548:CYS:HB3	1:D:578:VAL:HG23	1.86	0.56
1:D:1383:ARG:HE	1:D:1385:LYS:HE2	1.71	0.56
1:D:2716:LEU:O	1:D:2720:ILE:HG12	2.05	0.56
2:J:88:HIS:H	2:J:92:ILE:HB	1.71	0.56
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.88	0.56
1:A:1122:CYS:HA	1:A:1133:ARG:HD3	1.88	0.56
1:B:1684:PRO:HD3	2:H:42:ASP:HB3	1.86	0.56
1:B:2276:CYS:SG	1:B:2290:ASN:ND2	2.78	0.56
1:B:2277:GLN:HA	1:B:2280:VAL:HG22	1.87	0.56
2:H:32:GLN:NE2	2:H:97:THR:OG1	2.34	0.56
1:D:2141:MET:SD	1:D:2173:VAL:HG11	2.45	0.56
1:A:677:LEU:HD12	1:A:802:PHE:HA	1.87	0.56
1:A:1678:CYS:SG	1:A:1679:SER:N	2.78	0.56
1:A:2314:GLU:O	1:A:2318:VAL:HG13	2.06	0.56
1:B:2228:LEU:HD22	1:B:2296:ARG:HG3	1.87	0.56
1:C:4824:GLY:O	1:D:4821:ARG:NH2	2.39	0.56
1:A:587:ASN:OD1	1:A:2132:ARG:NH1	2.38	0.56
1:A:1009:ARG:O	1:A:1013:ARG:NH1	2.38	0.56
1:B:973:THR:OG1	1:B:976:TYR:O	2.18	0.56
1:B:1122:CYS:HA	1:B:1133:ARG:HD3	1.88	0.56
1:C:2314:GLU:O	1:C:2318:VAL:HG13	2.06	0.56
2:I:88:HIS:H	2:I:92:ILE:HB	1.71	0.56
1:D:1678:CYS:SG	1:D:1679:SER:N	2.78	0.56
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLN:HG3	1:B:169:ARG:HG3	1.88	0.56
2:H:88:HIS:H	2:H:92:ILE:HB	1.71	0.56
1:C:606:ARG:NH2	1:C:1635:GLU:OE1	2.34	0.56
1:C:1267:HIS:HB2	1:C:1294:ASN:HB2	1.87	0.56
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.88	0.56
1:D:3796:MET:HE1	1:D:3869:ILE:HG23	1.88	0.56
1:C:2070:GLN:O	1:C:3659:ARG:NH1	2.38	0.56
1:C:3728:ALA:HA	1:C:3731:HIS:ND1	2.21	0.56
1:A:3796:MET:HE1	1:A:3869:ILE:HG23	1.88	0.56
1:D:677:LEU:HD12	1:D:802:PHE:HA	1.87	0.56
1:B:2731:TRP:NE1	1:B:2762:LEU:HD13	2.21	0.55
1:D:3728:ALA:HA	1:D:3731:HIS:ND1	2.21	0.55
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.14	0.55
1:A:3891:TYR:O	1:A:3956:LYS:NZ	2.35	0.55
1:B:1678:CYS:SG	1:B:1679:SER:N	2.78	0.55
1:C:1678:CYS:SG	1:C:1679:SER:N	2.78	0.55
1:C:2064:THR:HG22	1:C:2067:ARG:HH12	1.72	0.55
1:D:1267:HIS:HB2	1:D:1294:ASN:HB2	1.87	0.55
1:B:677:LEU:HD12	1:B:802:PHE:HA	1.87	0.55
1:B:2314:GLU:O	1:B:2318:VAL:HG13	2.06	0.55
1:B:3728:ALA:HA	1:B:3731:HIS:ND1	2.21	0.55
1:C:677:LEU:HD12	1:C:802:PHE:HA	1.87	0.55
1:D:309:MET:HE2	1:D:312:LYS:HZ3	1.72	0.55
1:A:168:GLN:HG3	1:A:169:ARG:HG3	1.87	0.55
1:A:2731:TRP:NE1	1:A:2762:LEU:HD13	2.22	0.55
1:A:3937:SER:OG	1:A:3938:ARG:N	2.37	0.55
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.14	0.55
1:B:235:ARG:NH1	1:B:268:SER:O	2.40	0.55
1:D:2314:GLU:O	1:D:2318:VAL:HG13	2.06	0.55
1:A:732:LEU:HB3	1:A:779:PHE:CZ	2.42	0.55
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.88	0.55
1:C:1122:CYS:HA	1:C:1133:ARG:HD3	1.88	0.55
1:D:2064:THR:HG22	1:D:2067:ARG:HH12	1.72	0.55
1:D:2147:ASP:O	1:D:2151:ASN:ND2	2.40	0.55
1:D:2858:GLU:HG3	1:D:2859:LEU:HD23	1.88	0.55
1:A:2064:THR:HG22	1:A:2067:ARG:HH12	1.72	0.55
1:A:2766:GLU:HA	1:A:2769:ILE:HG23	1.89	0.55
1:B:732:LEU:HB3	1:B:779:PHE:CZ	2.42	0.55
1:B:2220:LEU:HD11	1:B:2242:ALA:HB2	1.89	0.55
1:C:168:GLN:HG3	1:C:169:ARG:HG3	1.87	0.55
1:C:2220:LEU:HD11	1:C:2242:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1122:CYS:HA	1:D:1133:ARG:HD3	1.88	0.55
1:A:2147:ASP:O	1:A:2151:ASN:ND2	2.40	0.55
1:C:2731:TRP:NE1	1:C:2762:LEU:HD13	2.22	0.55
1:C:2851:TRP:HA	1:C:2854:LYS:HE2	1.88	0.55
2:I:32:GLN:NE2	2:I:97:THR:OG1	2.34	0.55
1:D:235:ARG:NH1	1:D:268:SER:O	2.40	0.55
1:D:1042:THR:O	1:D:1046:ASN:ND2	2.40	0.55
1:A:1794:GLN:O	1:A:1798:GLU:HG2	2.06	0.55
1:A:2070:GLN:O	1:A:3659:ARG:NH1	2.38	0.55
1:B:587:ASN:OD1	1:B:2132:ARG:NH1	2.38	0.55
1:C:3796:MET:HE1	1:C:3869:ILE:HG23	1.88	0.55
1:D:2277:GLN:HA	1:D:2280:VAL:HG22	1.88	0.55
1:C:1265:HIS:CD2	1:C:1268:ILE:HB	2.43	0.55
1:D:1794:GLN:O	1:D:1798:GLU:HG2	2.06	0.55
1:D:2731:TRP:NE1	1:D:2762:LEU:HD13	2.22	0.55
1:A:1042:THR:O	1:A:1046:ASN:ND2	2.40	0.54
1:A:2220:LEU:HD11	1:A:2242:ALA:HB2	1.89	0.54
1:A:2851:TRP:HA	1:A:2854:LYS:HE2	1.89	0.54
1:A:3728:ALA:HA	1:A:3731:HIS:ND1	2.21	0.54
1:B:2064:THR:HG22	1:B:2067:ARG:HH12	1.72	0.54
1:B:2766:GLU:HA	1:B:2769:ILE:HG23	1.89	0.54
1:C:732:LEU:HB3	1:C:779:PHE:CZ	2.42	0.54
1:C:1794:GLN:O	1:C:1798:GLU:HG2	2.06	0.54
1:A:235:ARG:NH1	1:A:268:SER:O	2.40	0.54
1:B:1794:GLN:O	1:B:1798:GLU:HG2	2.06	0.54
2:H:39:SER:O	2:H:43:ARG:NH1	2.41	0.54
1:C:235:ARG:NH1	1:C:268:SER:O	2.40	0.54
1:C:2277:GLN:HA	1:C:2280:VAL:HG22	1.88	0.54
2:H:78:THR:O	2:H:81:VAL:HG12	2.08	0.54
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.14	0.54
1:D:168:GLN:HG3	1:D:169:ARG:HG3	1.88	0.54
1:A:2858:GLU:HG3	1:A:2859:LEU:HD23	1.88	0.54
2:I:23:CYS:SG	2:I:51:ILE:HD11	2.48	0.54
1:D:587:ASN:OD1	1:D:2132:ARG:NH1	2.38	0.54
1:D:2404:GLU:HG3	1:D:2405:MET:N	2.16	0.54
1:A:2277:GLN:HA	1:A:2280:VAL:HG22	1.88	0.54
1:B:2147:ASP:O	1:B:2151:ASN:ND2	2.40	0.54
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.14	0.54
2:H:23:CYS:SG	2:H:51:ILE:HD11	2.48	0.54
1:D:1265:HIS:CD2	1:D:1268:ILE:HB	2.42	0.54
1:D:2070:GLN:O	1:D:3659:ARG:NH1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2851:TRP:HA	1:D:2854:LYS:HE2	1.88	0.54
1:A:59:PRO:HB3	1:A:296:ARG:HH12	1.73	0.54
1:B:356:TYR:HA	1:B:405:LEU:HB2	1.90	0.54
1:C:1397:UNK:HA	1:C:1412:UNK:HA	1.90	0.54
1:A:4049:LYS:HA	1:A:4052:GLU:HG2	1.90	0.54
1:B:1610:SER:HB3	1:B:1619:LEU:HB3	1.89	0.54
1:B:2762:LEU:HD23	1:B:2767:LYS:HA	1.90	0.54
1:C:2858:GLU:HG3	1:C:2859:LEU:HD23	1.88	0.54
1:D:2220:LEU:HD11	1:D:2242:ALA:HB2	1.89	0.54
1:B:4049:LYS:HA	1:B:4052:GLU:HG2	1.90	0.54
1:C:2147:ASP:O	1:C:2151:ASN:ND2	2.40	0.54
1:C:4164:VAL:HG22	1:C:4198:GLU:OE2	2.08	0.54
1:D:2766:GLU:HA	1:D:2769:ILE:HG23	1.89	0.54
1:A:2762:LEU:HD23	1:A:2767:LYS:HA	1.90	0.54
1:B:2851:TRP:HA	1:B:2854:LYS:HE2	1.89	0.54
1:C:1042:THR:O	1:C:1046:ASN:ND2	2.40	0.54
1:D:356:TYR:HA	1:D:405:LEU:HB2	1.90	0.54
1:A:902:TRP:HA	1:A:913:ARG:O	2.08	0.54
1:A:1610:SER:HB3	1:A:1619:LEU:HB3	1.89	0.54
1:B:1767:PRO:HG3	1:B:1781:PRO:HB3	1.90	0.54
2:I:78:THR:O	2:I:81:VAL:HG12	2.08	0.54
1:A:1767:PRO:HG3	1:A:1781:PRO:HB3	1.90	0.53
1:A:1845:GLN:NE2	1:A:1848:GLU:OE2	2.41	0.53
2:G:23:CYS:SG	2:G:51:ILE:HD11	2.48	0.53
1:B:59:PRO:HB3	1:B:296:ARG:HH12	1.73	0.53
1:B:228:LEU:HD13	1:B:405:LEU:HD13	1.90	0.53
1:B:902:TRP:HA	1:B:913:ARG:O	2.08	0.53
1:C:59:PRO:HB3	1:C:296:ARG:HH12	1.73	0.53
1:C:902:TRP:HA	1:C:913:ARG:O	2.08	0.53
2:I:39:SER:O	2:I:43:ARG:NH1	2.41	0.53
2:J:78:THR:O	2:J:81:VAL:HG12	2.08	0.53
1:A:973:THR:OG1	1:A:976:TYR:O	2.18	0.53
1:B:1265:HIS:CD2	1:B:1268:ILE:HB	2.42	0.53
1:B:2858:GLU:HG3	1:B:2859:LEU:HD23	1.88	0.53
1:C:1845:GLN:NE2	1:C:1848:GLU:OE2	2.41	0.53
1:D:921:PHE:O	1:D:929:ARG:NH1	2.37	0.53
2:J:23:CYS:SG	2:J:51:ILE:HD11	2.48	0.53
2:G:78:THR:O	2:G:81:VAL:HG12	2.08	0.53
1:B:1042:THR:O	1:B:1046:ASN:ND2	2.40	0.53
2:H:58:LYS:HG3	2:H:81:VAL:HG22	1.91	0.53
1:C:356:TYR:HA	1:C:405:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1397:UNK:HA	1:D:1412:UNK:HA	1.90	0.53
1:C:1199:ASP:OD1	1:C:1199:ASP:N	2.40	0.53
1:D:1767:PRO:HG3	1:D:1781:PRO:HB3	1.91	0.53
1:B:1397:UNK:HA	1:B:1412:UNK:HA	1.90	0.53
2:I:58:LYS:HG3	2:I:81:VAL:HG22	1.91	0.53
1:D:732:LEU:HB3	1:D:779:PHE:CZ	2.42	0.53
1:A:228:LEU:HD13	1:A:405:LEU:HD13	1.90	0.53
1:C:2766:GLU:HA	1:C:2769:ILE:HG23	1.89	0.53
1:B:1845:GLN:NE2	1:B:1848:GLU:OE2	2.41	0.53
1:B:4183:GLU:O	1:B:4187:LEU:HG	2.09	0.53
1:C:61:ASP:OD2	1:C:417:ARG:NH2	2.42	0.53
1:C:1610:SER:HB3	1:C:1619:LEU:HB3	1.89	0.53
1:D:228:LEU:HD13	1:D:405:LEU:HD13	1.90	0.53
1:D:902:TRP:HA	1:D:913:ARG:O	2.08	0.53
1:D:4046:ASP:OD1	1:D:4046:ASP:N	2.42	0.53
1:D:4049:LYS:HA	1:D:4052:GLU:HG2	1.89	0.53
2:J:39:SER:O	2:J:43:ARG:NH1	2.41	0.53
2:G:39:SER:O	2:G:43:ARG:NH1	2.41	0.53
1:B:246:THR:OG1	1:B:247:VAL:N	2.42	0.53
1:C:189:GLU:O	1:D:2325:ARG:NH2	2.41	0.53
1:C:228:LEU:HD13	1:C:405:LEU:HD13	1.90	0.53
1:C:1767:PRO:HG3	1:C:1781:PRO:HB3	1.91	0.53
1:D:61:ASP:OD2	1:D:417:ARG:NH2	2.42	0.53
1:D:1588:HIS:HE1	1:D:1590:GLN:HE21	1.57	0.53
1:D:2728:HIS:O	1:D:2732:SER:OG	2.24	0.53
1:A:1588:HIS:HE1	1:A:1590:GLN:HE21	1.57	0.53
1:B:61:ASP:OD2	1:B:417:ARG:NH2	2.42	0.53
1:B:2404:GLU:HG3	1:B:2405:MET:HG3	1.91	0.53
1:C:2762:LEU:HD23	1:C:2767:LYS:HA	1.90	0.53
1:D:246:THR:OG1	1:D:247:VAL:N	2.42	0.53
1:D:2762:LEU:HD23	1:D:2767:LYS:HA	1.90	0.53
1:A:356:TYR:HA	1:A:405:LEU:HB2	1.90	0.53
1:A:3899:GLU:N	1:A:3899:GLU:OE2	2.42	0.53
1:B:1588:HIS:HE1	1:B:1590:GLN:HE21	1.57	0.53
1:D:1610:SER:HB3	1:D:1619:LEU:HB3	1.89	0.53
1:D:4183:GLU:O	1:D:4187:LEU:HG	2.09	0.53
1:A:629:GLN:HE21	1:A:1670:ASN:HD22	1.57	0.52
1:C:973:THR:OG1	1:C:976:TYR:O	2.18	0.52
1:D:59:PRO:HB3	1:D:296:ARG:HH12	1.73	0.52
1:A:606:ARG:NH2	1:A:1635:GLU:OE1	2.34	0.52
1:A:1397:UNK:HA	1:A:1412:UNK:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:58:LYS:HG3	2:G:81:VAL:HG22	1.91	0.52
1:C:833:LYS:HE3	1:C:834:VAL:H	1.75	0.52
1:C:2125:ILE:HG23	1:C:2141:MET:HE3	1.92	0.52
1:A:707:PRO:O	1:A:838:ARG:NH1	2.43	0.52
1:A:4183:GLU:O	1:A:4187:LEU:HG	2.09	0.52
1:B:707:PRO:O	1:B:838:ARG:NH1	2.43	0.52
1:C:246:THR:OG1	1:C:247:VAL:N	2.42	0.52
1:D:707:PRO:O	1:D:838:ARG:NH1	2.43	0.52
1:B:2125:ILE:HG23	1:B:2141:MET:HE3	1.92	0.52
1:C:707:PRO:O	1:C:838:ARG:NH1	2.43	0.52
1:C:2728:HIS:O	1:C:2732:SER:OG	2.24	0.52
1:C:4183:GLU:O	1:C:4187:LEU:HG	2.09	0.52
1:A:246:THR:OG1	1:A:247:VAL:N	2.42	0.52
1:B:3729:ARG:O	1:B:3733:ARG:NH1	2.43	0.52
1:C:238:HIS:HB2	1:C:241:MET:HB2	1.92	0.52
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.92	0.52
1:C:844:ARG:HE	1:C:845:THR:H	1.57	0.52
1:A:238:HIS:HB2	1:A:241:MET:HB2	1.92	0.52
1:A:4754:THR:OG1	1:D:4765:GLN:OE1	2.28	0.52
1:C:3729:ARG:O	1:C:3733:ARG:NH1	2.43	0.52
1:C:3899:GLU:N	1:C:3899:GLU:OE2	2.42	0.52
1:C:4049:LYS:HA	1:C:4052:GLU:HG2	1.90	0.52
1:D:3729:ARG:O	1:D:3733:ARG:NH1	2.43	0.52
1:D:3961:SER:OG	1:D:3962:SER:N	2.43	0.52
1:A:61:ASP:OD2	1:A:417:ARG:NH2	2.42	0.52
1:A:1265:HIS:CD2	1:A:1268:ILE:HB	2.43	0.52
1:A:1567:LEU:HD22	1:A:1581:PRO:HB3	1.92	0.52
1:A:2404:GLU:HG3	1:A:2405:MET:HG3	1.91	0.52
1:A:3729:ARG:O	1:A:3733:ARG:NH1	2.43	0.52
1:A:4784:ALA:HA	1:A:4788:PHE:HD2	1.75	0.52
1:D:238:HIS:HB2	1:D:241:MET:HB2	1.92	0.52
1:D:2254:LEU:O	1:D:3809:ARG:HD3	2.10	0.52
1:D:2404:GLU:HG3	1:D:2405:MET:HG3	1.91	0.52
2:G:9:SER:HB2	2:G:72:ARG:HB2	1.91	0.52
1:B:629:GLN:HE21	1:B:1670:ASN:HD22	1.57	0.52
1:B:643:LEU:HD13	1:B:1658:THR:HG23	1.92	0.52
1:B:3899:GLU:OE2	1:B:3899:GLU:N	2.42	0.52
1:C:629:GLN:HE21	1:C:1670:ASN:HD22	1.57	0.52
1:C:2254:LEU:O	1:C:3809:ARG:HD3	2.10	0.52
1:D:3899:GLU:N	1:D:3899:GLU:OE2	2.42	0.52
1:A:1048:ASP:HA	1:A:1051:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1567:LEU:HD22	1:B:1581:PRO:HB3	1.92	0.52
1:C:1029:ASN:HB2	1:C:1032:LEU:HD13	1.92	0.52
1:C:1588:HIS:HE1	1:C:1590:GLN:HE21	1.57	0.52
1:D:1845:GLN:NE2	1:D:1848:GLU:OE2	2.41	0.52
1:A:833:LYS:HE3	1:A:834:VAL:H	1.75	0.52
2:H:9:SER:HB2	2:H:72:ARG:HB2	1.91	0.52
1:D:606:ARG:NH2	1:D:1635:GLU:OE1	2.35	0.52
2:J:58:LYS:HG3	2:J:81:VAL:HG22	1.91	0.52
1:A:4164:VAL:HG22	1:A:4198:GLU:OE2	2.10	0.51
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.92	0.51
1:B:2728:HIS:O	1:B:2732:SER:OG	2.24	0.51
1:C:343:ARG:HH21	1:C:345:GLU:H	1.58	0.51
1:C:890:HIS:O	1:C:894:VAL:HG23	2.10	0.51
1:D:1199:ASP:OD1	1:D:1199:ASP:N	2.40	0.51
1:D:2125:ILE:HG23	1:D:2141:MET:HE3	1.92	0.51
2:J:9:SER:HB2	2:J:72:ARG:HB2	1.91	0.51
1:A:844:ARG:HE	1:A:845:THR:H	1.57	0.51
1:A:2254:LEU:O	1:A:3809:ARG:HD3	2.10	0.51
1:B:343:ARG:HH21	1:B:345:GLU:H	1.58	0.51
1:B:833:LYS:HE3	1:B:834:VAL:H	1.75	0.51
1:B:1754:LEU:HG	1:B:1756:THR:HG23	1.93	0.51
1:B:4112:THR:O	1:B:4116:THR:HG23	2.10	0.51
1:D:643:LEU:HD13	1:D:1658:THR:HG23	1.92	0.51
1:D:911:ASN:OD1	1:D:911:ASN:N	2.41	0.51
1:D:4164:VAL:HG22	1:D:4198:GLU:OE2	2.10	0.51
1:A:643:LEU:HD13	1:A:1658:THR:HG23	1.92	0.51
1:B:1048:ASP:HA	1:B:1051:ARG:HD2	1.92	0.51
1:B:4763:GLY:O	1:B:4767:VAL:HG22	2.11	0.51
1:B:4784:ALA:HA	1:B:4788:PHE:HD2	1.75	0.51
1:C:4112:THR:O	1:C:4116:THR:HG23	2.10	0.51
1:C:309:MET:HE2	1:C:312:LYS:HZ3	1.75	0.51
1:C:1257:GLN:HA	1:C:1384:LEU:HD22	1.92	0.51
1:C:2271:CYS:SG	1:C:2294:GLY:N	2.84	0.51
1:C:2404:GLU:HG3	1:C:2405:MET:HG3	1.91	0.51
1:C:4763:GLY:O	1:C:4767:VAL:HG22	2.11	0.51
1:D:343:ARG:HH21	1:D:345:GLU:H	1.58	0.51
1:D:1932:VAL:HG21	1:D:3616:VAL:HA	1.92	0.51
1:D:2271:CYS:SG	1:D:2294:GLY:N	2.84	0.51
1:D:3940:TRP:HA	1:D:3943:VAL:HG22	1.93	0.51
1:B:238:HIS:HB2	1:B:241:MET:HB2	1.92	0.51
1:B:2254:LEU:O	1:B:3809:ARG:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1029:ASN:HB2	1:D:1032:LEU:HD13	1.92	0.51
1:A:2125:ILE:HG23	1:A:2141:MET:HE3	1.92	0.51
1:B:699:SER:OG	1:B:700:THR:N	2.44	0.51
1:B:1932:VAL:HG21	1:B:3616:VAL:HA	1.92	0.51
1:C:1932:VAL:HG21	1:C:3616:VAL:HA	1.92	0.51
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.93	0.51
1:C:921:PHE:O	1:C:929:ARG:NH1	2.37	0.51
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.92	0.51
1:D:4784:ALA:HA	1:D:4788:PHE:HD2	1.75	0.51
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.92	0.51
1:A:721:ASP:N	1:A:721:ASP:OD1	2.43	0.51
1:A:1095:ALA:HB1	1:A:1200:GLY:HA3	1.92	0.51
1:A:4763:GLY:O	1:A:4767:VAL:HG22	2.11	0.51
1:D:633:CYS:SG	1:D:1673:VAL:HG13	2.51	0.51
1:D:844:ARG:HE	1:D:845:THR:H	1.57	0.51
1:D:1095:ALA:HB1	1:D:1200:GLY:HA3	1.92	0.51
1:A:4762:ASN:O	1:A:4764:LYS:N	2.44	0.51
1:B:1095:ALA:HB1	1:B:1200:GLY:HA3	1.92	0.51
1:B:1257:GLN:HA	1:B:1384:LEU:HD22	1.93	0.51
1:C:1321:UNK:HA	1:C:1436:UNK:HA	1.93	0.51
1:C:1567:LEU:HD22	1:C:1581:PRO:HB3	1.92	0.51
1:C:4046:ASP:OD1	1:C:4046:ASP:N	2.42	0.51
1:D:629:GLN:HE21	1:D:1670:ASN:HD22	1.57	0.51
1:D:833:LYS:HE3	1:D:834:VAL:H	1.75	0.51
1:D:890:HIS:O	1:D:894:VAL:HG23	2.10	0.51
1:D:1257:GLN:HA	1:D:1384:LEU:HD22	1.93	0.51
1:D:4762:ASN:O	1:D:4764:LYS:N	2.44	0.51
1:A:633:CYS:SG	1:A:1673:VAL:HG13	2.51	0.51
1:A:2271:CYS:SG	1:A:2294:GLY:N	2.84	0.51
1:B:844:ARG:HE	1:B:845:THR:H	1.57	0.51
1:B:2455:MET:HG3	1:B:2457:ALA:H	1.76	0.51
1:B:3961:SER:OG	1:B:3962:SER:N	2.43	0.51
1:B:3986:GLU:O	1:B:4935:GLN:NE2	2.44	0.51
1:B:4164:VAL:HG22	1:B:4198:GLU:OE2	2.11	0.51
1:B:4665:ILE:O	1:B:4668:LEU:HD23	2.11	0.51
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.93	0.51
1:D:4763:GLY:O	1:D:4767:VAL:HG22	2.11	0.51
2:J:50:ARG:N	2:J:55:GLU:OE2	2.41	0.51
1:A:3986:GLU:O	1:A:4935:GLN:NE2	2.44	0.50
1:B:2080:VAL:HG13	1:B:3669:LEU:HD22	1.93	0.50
1:C:1095:ALA:HB1	1:C:1200:GLY:HA3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2231:PRO:HD3	1:C:2381:ILE:HD11	1.93	0.50
1:C:3940:TRP:HA	1:C:3943:VAL:HG22	1.93	0.50
1:D:1567:LEU:HD22	1:D:1581:PRO:HB3	1.92	0.50
1:D:2206:SER:OG	1:D:2207:ARG:N	2.44	0.50
1:A:1932:VAL:HG21	1:A:3616:VAL:HA	1.92	0.50
1:B:407:ARG:HH21	1:B:3864:ASN:HB3	1.77	0.50
1:B:890:HIS:O	1:B:894:VAL:HG23	2.10	0.50
1:B:2231:PRO:HD3	1:B:2381:ILE:HD11	1.93	0.50
1:B:2271:CYS:SG	1:B:2294:GLY:N	2.84	0.50
1:C:643:LEU:HD13	1:C:1658:THR:HG23	1.92	0.50
1:C:4665:ILE:O	1:C:4668:LEU:HD23	2.11	0.50
2:I:9:SER:HB2	2:I:72:ARG:HB2	1.91	0.50
1:D:4665:ILE:O	1:D:4668:LEU:HD23	2.11	0.50
1:A:4665:ILE:O	1:A:4668:LEU:HD23	2.11	0.50
1:B:1029:ASN:HB2	1:B:1032:LEU:HD13	1.92	0.50
1:B:1321:UNK:HA	1:B:1436:UNK:HA	1.93	0.50
1:C:1754:LEU:HG	1:C:1756:THR:HG23	1.92	0.50
1:C:2080:VAL:HG13	1:C:3669:LEU:HD22	1.93	0.50
1:C:2776:GLU:O	1:C:2780:THR:HG23	2.12	0.50
1:C:4784:ALA:HA	1:C:4788:PHE:HD2	1.75	0.50
1:D:1048:ASP:HA	1:D:1051:ARG:HD2	1.92	0.50
1:A:189:GLU:O	1:B:2325:ARG:NH2	2.44	0.50
1:A:436:LEU:HD21	1:A:517:VAL:HG12	1.94	0.50
1:A:890:HIS:O	1:A:894:VAL:HG23	2.10	0.50
1:A:1029:ASN:HB2	1:A:1032:LEU:HD13	1.92	0.50
1:A:2278:MET:N	1:A:2278:MET:SD	2.85	0.50
1:A:3961:SER:OG	1:A:3962:SER:N	2.43	0.50
1:A:4112:THR:O	1:A:4116:THR:HG23	2.10	0.50
1:B:2776:GLU:O	1:B:2780:THR:HG23	2.12	0.50
1:D:407:ARG:HH21	1:D:3864:ASN:HB3	1.77	0.50
1:D:3986:GLU:O	1:D:4935:GLN:NE2	2.44	0.50
1:D:4112:THR:O	1:D:4116:THR:HG23	2.10	0.50
1:D:4276:LYS:HZ1	1:D:4562:GLU:HG3	1.76	0.50
1:A:699:SER:OG	1:A:700:THR:N	2.44	0.50
1:A:4607:ARG:NE	1:A:4643:TYR:OH	2.45	0.50
1:B:309:MET:HB2	1:B:312:LYS:HZ3	1.76	0.50
1:B:692:HIS:HB3	1:B:795:SER:HB3	1.94	0.50
1:B:4607:ARG:NE	1:B:4643:TYR:OH	2.45	0.50
1:C:2278:MET:N	1:C:2278:MET:SD	2.85	0.50
1:D:1321:UNK:HA	1:D:1436:UNK:HA	1.93	0.50
1:A:407:ARG:HH21	1:A:3864:ASN:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:LYS:HG2	1:B:1573:LYS:HZ1	1.76	0.50
1:B:3940:TRP:HA	1:B:3943:VAL:HG22	1.93	0.50
1:C:1048:ASP:HA	1:C:1051:ARG:HD2	1.92	0.50
1:D:436:LEU:HD21	1:D:517:VAL:HG12	1.94	0.50
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.93	0.50
1:D:1754:LEU:HG	1:D:1756:THR:HG23	1.92	0.50
1:A:343:ARG:HH21	1:A:345:GLU:H	1.58	0.50
1:A:1257:GLN:HA	1:A:1384:LEU:HD22	1.92	0.50
1:A:2776:GLU:O	1:A:2780:THR:HG23	2.12	0.50
1:B:756:SER:OG	1:B:769:ARG:HB2	2.12	0.50
1:B:1001:GLU:HG2	1:B:1035:TYR:CD2	2.47	0.50
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.94	0.50
1:A:2455:MET:HG3	1:A:2457:ALA:H	1.77	0.50
1:B:2206:SER:OG	1:B:2207:ARG:N	2.44	0.50
1:C:633:CYS:SG	1:C:1673:VAL:HG13	2.51	0.50
1:C:2455:MET:HG3	1:C:2457:ALA:H	1.77	0.50
1:D:1677:LEU:HA	1:D:1680:HIS:HB2	1.94	0.50
1:D:2776:GLU:O	1:D:2780:THR:HG23	2.12	0.50
1:A:80:GLU:OE1	1:A:80:GLU:HA	2.12	0.50
1:A:756:SER:OG	1:A:769:ARG:HB2	2.12	0.50
1:A:1199:ASP:OD1	1:A:1199:ASP:N	2.40	0.50
1:C:114:LEU:HB2	1:C:117:HIS:CD2	2.47	0.50
1:A:686:VAL:HG13	1:A:687:THR:HG22	1.93	0.49
1:B:721:ASP:OD1	1:B:721:ASP:N	2.43	0.49
1:B:4070:GLU:OE1	1:B:4070:GLU:N	2.43	0.49
1:A:1001:GLU:HG2	1:A:1035:TYR:CD2	2.47	0.49
1:A:1677:LEU:HA	1:A:1680:HIS:HB2	1.94	0.49
1:A:2080:VAL:HG13	1:A:3669:LEU:HD22	1.93	0.49
1:A:2206:SER:OG	1:A:2207:ARG:N	2.44	0.49
1:A:4029:ASP:OD1	1:A:4029:ASP:N	2.45	0.49
1:B:2278:MET:N	1:B:2278:MET:SD	2.85	0.49
1:C:307:SER:HB3	1:C:317:MET:HE2	1.95	0.49
1:C:3986:GLU:O	1:C:4935:GLN:NE2	2.44	0.49
1:D:80:GLU:OE1	1:D:80:GLU:HA	2.12	0.49
1:D:2080:VAL:HG13	1:D:3669:LEU:HD22	1.93	0.49
1:D:2278:MET:SD	1:D:2278:MET:N	2.85	0.49
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.94	0.49
1:B:763:ALA:HB3	1:B:764:PRO:HD3	1.95	0.49
1:C:692:HIS:HB3	1:C:795:SER:HB3	1.94	0.49
1:C:1986:PRO:HB2	1:C:1988:PRO:HD2	1.95	0.49
1:C:4029:ASP:OD2	1:C:4054:HIS:NE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:TYR:HA	1:D:355:LYS:HA	1.95	0.49
1:D:307:SER:HB3	1:D:317:MET:HE2	1.95	0.49
1:D:4029:ASP:OD2	1:D:4054:HIS:NE2	2.43	0.49
1:A:4029:ASP:OD2	1:A:4054:HIS:NE2	2.43	0.49
2:G:50:ARG:N	2:G:55:GLU:OE2	2.41	0.49
1:B:2141:MET:HE1	1:B:2173:VAL:HG21	1.93	0.49
1:C:878:LEU:HD11	1:C:951:GLY:HA2	1.95	0.49
1:C:1001:GLU:HG2	1:C:1035:TYR:CD2	2.47	0.49
1:C:1677:LEU:HA	1:C:1680:HIS:HB2	1.94	0.49
1:C:4029:ASP:OD1	1:C:4029:ASP:N	2.45	0.49
1:D:756:SER:OG	1:D:769:ARG:HB2	2.12	0.49
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.94	0.49
1:A:1321:UNK:HA	1:A:1436:UNK:HA	1.93	0.49
1:A:2231:PRO:HD3	1:A:2381:ILE:HD11	1.93	0.49
1:A:4508:ALA:O	1:A:4512:ASN:ND2	2.45	0.49
1:B:633:CYS:SG	1:B:1673:VAL:HG13	2.51	0.49
1:B:4046:ASP:N	1:B:4046:ASP:OD1	2.42	0.49
1:C:672:LYS:HB3	1:C:819:TYR:HA	1.94	0.49
1:C:699:SER:OG	1:C:700:THR:N	2.44	0.49
1:C:721:ASP:OD1	1:C:721:ASP:N	2.43	0.49
1:D:4607:ARG:NE	1:D:4643:TYR:OH	2.45	0.49
1:A:428:ARG:HG3	1:A:446:ASP:OD2	2.13	0.49
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.45	0.49
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.93	0.49
1:A:1754:LEU:HG	1:A:1756:THR:HG23	1.92	0.49
1:B:1362:ASP:N	1:B:1362:ASP:OD1	2.45	0.49
1:B:1986:PRO:HB2	1:B:1988:PRO:HD2	1.94	0.49
1:B:3898:ASP:OD1	1:B:3898:ASP:N	2.44	0.49
1:C:435:ALA:HA	1:C:438:LYS:HE3	1.95	0.49
1:C:686:VAL:HG13	1:C:687:THR:HG22	1.93	0.49
1:D:672:LYS:HB3	1:D:819:TYR:HA	1.94	0.49
1:D:699:SER:OG	1:D:700:THR:N	2.44	0.49
1:D:1362:ASP:OD1	1:D:1362:ASP:N	2.45	0.49
1:B:80:GLU:OE1	1:B:80:GLU:HA	2.12	0.49
1:B:686:VAL:HG13	1:B:687:THR:HG22	1.93	0.49
1:C:407:ARG:HH21	1:C:3864:ASN:HB3	1.77	0.49
1:D:692:HIS:HB3	1:D:795:SER:HB3	1.94	0.49
1:D:878:LEU:HD11	1:D:951:GLY:HA2	1.95	0.49
1:D:1001:GLU:HG2	1:D:1035:TYR:CD2	2.47	0.49
1:D:2455:MET:HG3	1:D:2457:ALA:H	1.77	0.49
1:A:307:SER:HB3	1:A:317:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:ALA:O	1:A:1012:ILE:HG23	2.13	0.49
1:A:2101:LEU:O	1:A:2104:THR:HG22	2.13	0.49
1:A:2340:ASN:OD1	1:A:2340:ASN:N	2.46	0.49
1:B:114:LEU:HB2	1:B:117:HIS:CD2	2.47	0.49
1:C:436:LEU:HD21	1:C:517:VAL:HG12	1.94	0.49
1:C:756:SER:OG	1:C:769:ARG:HB2	2.12	0.49
1:C:763:ALA:HB3	1:C:764:PRO:HD3	1.95	0.49
1:C:1359:ILE:HG13	1:C:1360:ASP:H	1.78	0.49
1:C:1362:ASP:N	1:C:1362:ASP:OD1	2.45	0.49
1:C:1985:CYS:SG	1:C:1992:ARG:HD2	2.53	0.49
1:C:2141:MET:HE1	1:C:2173:VAL:HG21	1.93	0.49
1:C:4607:ARG:NE	1:C:4643:TYR:OH	2.45	0.49
1:D:686:VAL:HG13	1:D:687:THR:HG22	1.93	0.49
1:D:2141:MET:HE1	1:D:2173:VAL:HG21	1.93	0.49
1:D:2231:PRO:HD3	1:D:2381:ILE:HD11	1.93	0.49
1:A:227:TYR:HA	1:A:355:LYS:HA	1.94	0.49
1:A:692:HIS:HB3	1:A:795:SER:HB3	1.94	0.49
1:A:878:LEU:HD11	1:A:951:GLY:HA2	1.95	0.49
1:A:1359:ILE:HG13	1:A:1360:ASP:H	1.78	0.49
1:A:1715:TYR:CZ	1:A:1762:MET:HB3	2.48	0.49
1:C:428:ARG:HG3	1:C:446:ASP:OD2	2.13	0.49
1:C:3898:ASP:OD1	1:C:3898:ASP:N	2.44	0.49
1:D:1986:PRO:HB2	1:D:1988:PRO:HD2	1.95	0.49
1:A:114:LEU:HB2	1:A:117:HIS:CD2	2.47	0.49
1:A:2735:LYS:NZ	1:A:2756:MET:HE1	2.28	0.49
1:B:672:LYS:HB3	1:B:819:TYR:HA	1.94	0.49
1:B:1677:LEU:HA	1:B:1680:HIS:HB2	1.94	0.49
1:B:4762:ASN:O	1:B:4764:LYS:N	2.44	0.49
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.94	0.49
1:D:603:LYS:HG2	1:D:1573:LYS:HZ1	1.78	0.49
1:D:2735:LYS:NZ	1:D:2756:MET:HE1	2.28	0.49
1:A:309:MET:HE2	1:A:312:LYS:HZ3	1.78	0.48
1:A:3940:TRP:HA	1:A:3943:VAL:HG22	1.93	0.48
1:A:4928:ASP:O	1:A:4932:HIS:NE2	2.46	0.48
1:B:307:SER:HB3	1:B:317:MET:HE2	1.94	0.48
1:C:3961:SER:OG	1:C:3962:SER:N	2.43	0.48
1:C:4709:LEU:HA	1:C:4712:VAL:HG22	1.95	0.48
1:D:370:LEU:HB2	1:D:393:MET:HB2	1.95	0.48
1:D:2484:LEU:O	1:D:2488:GLU:HG2	2.13	0.48
1:A:300:VAL:O	1:A:420:ARG:NH1	2.40	0.48
1:A:921:PHE:O	1:A:929:ARG:NH1	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ARG:HG3	1:B:446:ASP:OD2	2.13	0.48
1:B:435:ALA:HA	1:B:438:LYS:HE3	1.95	0.48
1:B:436:LEU:HD21	1:B:517:VAL:HG12	1.94	0.48
1:B:878:LEU:HD11	1:B:951:GLY:HA2	1.95	0.48
1:C:80:GLU:OE1	1:C:80:GLU:HA	2.12	0.48
1:C:1715:TYR:CZ	1:C:1762:MET:HB3	2.48	0.48
1:C:2484:LEU:O	1:C:2488:GLU:HG2	2.13	0.48
1:D:114:LEU:HB2	1:D:117:HIS:CD2	2.47	0.48
1:D:1008:ALA:O	1:D:1012:ILE:HG23	2.13	0.48
1:D:1985:CYS:SG	1:D:1992:ARG:HD2	2.53	0.48
1:A:672:LYS:HB3	1:A:819:TYR:HA	1.94	0.48
1:B:4029:ASP:OD1	1:B:4029:ASP:N	2.45	0.48
1:C:370:LEU:HB2	1:C:393:MET:HB2	1.95	0.48
1:C:1008:ALA:O	1:C:1012:ILE:HG23	2.13	0.48
1:A:1985:CYS:SG	1:A:1992:ARG:HD2	2.53	0.48
1:A:1986:PRO:HB2	1:A:1988:PRO:HD2	1.94	0.48
1:B:370:LEU:HB2	1:B:393:MET:HB2	1.95	0.48
1:B:1008:ALA:O	1:B:1012:ILE:HG23	2.13	0.48
1:C:227:TYR:HA	1:C:355:LYS:HA	1.94	0.48
1:C:2206:SER:OG	1:C:2207:ARG:N	2.44	0.48
1:D:1359:ILE:HG13	1:D:1360:ASP:H	1.78	0.48
1:A:490:GLN:O	1:A:490:GLN:NE2	2.45	0.48
1:A:658:ASN:HD22	1:A:833:LYS:H	1.61	0.48
1:A:2141:MET:HE1	1:A:2173:VAL:HG21	1.94	0.48
1:C:2331:GLY:HA3	1:C:2391:TYR:HE1	1.79	0.48
1:C:4570:THR:HA	1:C:4573:ILE:HG12	1.96	0.48
1:C:4757:SER:O	1:C:4761:HIS:HB2	2.14	0.48
1:C:4928:ASP:O	1:C:4932:HIS:NE2	2.46	0.48
1:C:4947:CYS:SG	1:C:4948:TRP:N	2.87	0.48
1:D:763:ALA:HB3	1:D:764:PRO:HD3	1.95	0.48
1:A:2484:LEU:O	1:A:2488:GLU:HG2	2.13	0.48
1:A:4709:LEU:HA	1:A:4712:VAL:HG22	1.95	0.48
1:B:1359:ILE:HG13	1:B:1360:ASP:H	1.78	0.48
1:B:1769:PHE:O	2:H:83:TYR:OH	2.28	0.48
1:B:1985:CYS:SG	1:B:1992:ARG:HD2	2.53	0.48
1:B:2101:LEU:O	1:B:2104:THR:HG22	2.13	0.48
1:C:4808:MET:HB2	1:D:4518:TYR:H	1.79	0.48
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.94	0.48
1:B:2331:GLY:HA3	1:B:2391:TYR:HE1	1.79	0.48
1:D:2101:LEU:O	1:D:2104:THR:HG22	2.13	0.48
1:B:2404:GLU:HG3	1:B:2405:MET:N	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4709:LEU:HA	1:B:4712:VAL:HG22	1.95	0.48
1:C:2836:LEU:HD22	1:C:2839:MET:HE3	1.95	0.48
1:D:70:GLU:OE1	1:D:122:ARG:NE	2.44	0.48
1:D:721:ASP:N	1:D:721:ASP:OD1	2.43	0.48
1:A:718:VAL:HG23	1:A:724:SER:HB3	1.96	0.48
1:B:2735:LYS:NZ	1:B:2756:MET:HE1	2.28	0.48
1:B:4757:SER:O	1:B:4761:HIS:HB2	2.14	0.48
1:C:2722:LYS:HD2	1:C:2722:LYS:HA	1.63	0.48
1:D:428:ARG:HG3	1:D:446:ASP:OD2	2.13	0.48
1:D:435:ALA:HA	1:D:438:LYS:HE3	1.95	0.48
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.47	0.48
1:A:2296:ARG:NH1	1:A:2299:ASP:OD2	2.47	0.48
1:B:552:SER:HA	1:B:555:LEU:HD13	1.96	0.48
1:B:712:GLU:HB3	1:B:713:TRP:CD2	2.49	0.48
1:B:718:VAL:HG23	1:B:724:SER:HB3	1.96	0.48
1:B:1715:TYR:CZ	1:B:1762:MET:HB3	2.48	0.48
1:B:3923:ILE:HD13	1:B:3934:LEU:HD12	1.96	0.48
1:B:4029:ASP:OD2	1:B:4054:HIS:NE2	2.43	0.48
1:B:4928:ASP:O	1:B:4932:HIS:NE2	2.46	0.48
1:B:4947:CYS:SG	1:B:4948:TRP:N	2.87	0.48
1:C:552:SER:HA	1:C:555:LEU:HD13	1.96	0.48
1:C:658:ASN:HD22	1:C:833:LYS:H	1.61	0.48
1:D:4709:LEU:HA	1:D:4712:VAL:HG22	1.95	0.48
1:D:4757:SER:O	1:D:4761:HIS:HB2	2.14	0.48
1:D:4928:ASP:O	1:D:4932:HIS:NE2	2.46	0.48
1:A:435:ALA:HA	1:A:438:LYS:HE3	1.95	0.47
1:B:227:TYR:HA	1:B:355:LYS:HA	1.94	0.47
1:B:620:CYS:SG	1:B:621:HIS:N	2.87	0.47
1:B:658:ASN:HD22	1:B:833:LYS:H	1.61	0.47
1:B:1709:ASP:HA	1:B:1713:SER:HB3	1.96	0.47
1:C:712:GLU:HB3	1:C:713:TRP:CD2	2.49	0.47
1:A:641:ASP:OD1	1:A:642:LEU:N	2.47	0.47
1:A:4046:ASP:OD1	1:A:4046:ASP:N	2.42	0.47
1:B:441:LYS:HG2	1:B:442:LEU:HD23	1.95	0.47
1:B:875:PRO:O	1:B:882:ARG:NH2	2.46	0.47
1:B:2484:LEU:O	1:B:2488:GLU:HG2	2.13	0.47
1:B:2836:LEU:HD22	1:B:2839:MET:HE3	1.95	0.47
1:B:2892:PHE:O	1:B:2896:GLN:HG2	2.14	0.47
1:C:620:CYS:SG	1:C:621:HIS:N	2.87	0.47
1:C:1090:ALA:HB3	1:C:1202:ILE:HD11	1.96	0.47
1:C:1700:ARG:NH1	1:C:1817:PHE:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2735:LYS:NZ	1:C:2756:MET:HE1	2.28	0.47
1:C:2892:PHE:O	1:C:2896:GLN:HG2	2.14	0.47
1:D:1715:TYR:CZ	1:D:1762:MET:HB3	2.48	0.47
1:D:2296:ARG:NH1	1:D:2299:ASP:OD2	2.47	0.47
1:A:603:LYS:HG2	1:A:1573:LYS:HZ1	1.79	0.47
1:A:1343:PHE:HB2	1:A:1376:TYR:HD2	1.80	0.47
2:G:32:GLN:NE2	2:G:97:THR:OG1	2.34	0.47
1:B:672:LYS:NZ	1:B:760:ASP:OD2	2.35	0.47
1:B:4570:THR:HA	1:B:4573:ILE:HG12	1.96	0.47
1:C:3923:ILE:HD13	1:C:3934:LEU:HD12	1.96	0.47
1:A:620:CYS:SG	1:A:621:HIS:N	2.87	0.47
1:A:2331:GLY:HA3	1:A:2391:TYR:HE1	1.79	0.47
1:A:2903:SER:OG	1:A:2904:ARG:N	2.48	0.47
1:A:4570:THR:HA	1:A:4573:ILE:HG12	1.96	0.47
1:B:641:ASP:OD1	1:B:642:LEU:N	2.47	0.47
1:B:1343:PHE:HB2	1:B:1376:TYR:HD2	1.80	0.47
1:B:1700:ARG:NH1	1:B:1817:PHE:O	2.47	0.47
1:B:4942:MET:HE1	1:B:4949:GLU:HB2	1.96	0.47
2:H:50:ARG:N	2:H:55:GLU:OE2	2.41	0.47
1:C:718:VAL:HG23	1:C:724:SER:HB3	1.96	0.47
2:I:50:ARG:N	2:I:55:GLU:OE2	2.41	0.47
1:D:718:VAL:HG23	1:D:724:SER:HB3	1.96	0.47
1:A:712:GLU:HB3	1:A:713:TRP:CD2	2.49	0.47
1:A:844:ARG:HE	1:A:845:THR:HG22	1.80	0.47
1:A:3923:ILE:HD13	1:A:3934:LEU:HD12	1.96	0.47
1:A:4757:SER:O	1:A:4761:HIS:HB2	2.14	0.47
1:A:4947:CYS:SG	1:A:4948:TRP:N	2.87	0.47
1:B:1743:GLU:CD	1:B:1744:ASN:HD22	2.22	0.47
1:B:4608:LYS:HG3	1:B:4614:LEU:HB2	1.97	0.47
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.47	0.47
1:C:1343:PHE:HB2	1:C:1376:TYR:HD2	1.80	0.47
1:D:267:VAL:HA	1:D:270:HIS:ND1	2.29	0.47
1:D:844:ARG:HE	1:D:845:THR:HG22	1.80	0.47
1:D:2331:GLY:HA3	1:D:2391:TYR:HE1	1.79	0.47
1:D:2340:ASN:OD1	1:D:2340:ASN:N	2.46	0.47
1:D:2836:LEU:HD22	1:D:2839:MET:HE3	1.95	0.47
1:D:4947:CYS:SG	1:D:4948:TRP:N	2.87	0.47
1:A:370:LEU:HB2	1:A:393:MET:HB2	1.95	0.47
1:A:4905:GLU:OE2	1:D:4182:LYS:HD3	2.15	0.47
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.47	0.47
1:C:267:VAL:HA	1:C:270:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LYS:HG2	1:C:442:LEU:HD23	1.96	0.47
1:C:911:ASN:OD1	1:C:911:ASN:N	2.41	0.47
1:C:1709:ASP:HA	1:C:1713:SER:HB3	1.96	0.47
1:D:441:LYS:HG2	1:D:442:LEU:HD23	1.96	0.47
1:D:712:GLU:HB3	1:D:713:TRP:CD2	2.49	0.47
1:A:915:HIS:CE1	1:A:917:CYS:HB2	2.50	0.47
1:A:1700:ARG:NH1	1:A:1817:PHE:O	2.47	0.47
1:A:1743:GLU:CD	1:A:1744:ASN:HD22	2.22	0.47
1:A:1981:ASP:OD1	1:A:1982:LYS:N	2.48	0.47
1:A:2728:HIS:O	1:A:2732:SER:OG	2.24	0.47
1:A:2765:LYS:O	1:A:2769:ILE:HG23	2.15	0.47
1:A:2836:LEU:HD22	1:A:2839:MET:HE3	1.95	0.47
1:A:4942:MET:HE1	1:A:4949:GLU:HB2	1.96	0.47
1:B:228:LEU:HD23	1:B:289:ILE:HB	1.96	0.47
1:B:2092:ASP:OD1	1:B:2093:GLY:N	2.48	0.47
1:B:2271:CYS:SG	1:B:2293:GLU:HB2	2.55	0.47
1:B:2296:ARG:NH1	1:B:2299:ASP:OD2	2.47	0.47
1:B:2903:SER:OG	1:B:2904:ARG:N	2.48	0.47
1:B:3640:ILE:HG22	1:B:3729:ARG:HH11	1.80	0.47
1:C:70:GLU:OE1	1:C:122:ARG:NE	2.44	0.47
1:C:671:LYS:HA	1:C:761:LEU:HD12	1.97	0.47
1:C:844:ARG:HE	1:C:845:THR:HG22	1.80	0.47
1:C:875:PRO:O	1:C:882:ARG:NH2	2.46	0.47
1:C:1704:TYR:O	1:C:1708:ILE:HG12	2.15	0.47
1:C:1743:GLU:CD	1:C:1744:ASN:HD22	2.22	0.47
1:C:1981:ASP:OD1	1:C:1982:LYS:N	2.48	0.47
1:C:2296:ARG:NH1	1:C:2299:ASP:OD2	2.47	0.47
1:C:4608:LYS:HG3	1:C:4614:LEU:HB2	1.97	0.47
1:C:4762:ASN:O	1:C:4764:LYS:N	2.44	0.47
2:I:11:GLY:O	2:I:68:SER:OG	2.32	0.47
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.47	0.47
1:D:1700:ARG:NH1	1:D:1817:PHE:O	2.47	0.47
1:D:1981:ASP:OD1	1:D:1982:LYS:N	2.48	0.47
1:D:2092:ASP:OD1	1:D:2093:GLY:N	2.48	0.47
1:A:441:LYS:HG2	1:A:442:LEU:HD23	1.95	0.47
1:A:2081:ARG:HG3	1:A:3686:LEU:HD22	1.97	0.47
1:A:3640:ILE:HG22	1:A:3729:ARG:HH11	1.80	0.47
1:A:4070:GLU:OE1	1:A:4070:GLU:N	2.43	0.47
1:B:439:LYS:HD2	1:B:440:VAL:O	2.15	0.47
1:C:2716:LEU:HD22	1:C:2778:LEU:HD21	1.97	0.47
1:D:228:LEU:HD23	1:D:289:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:THR:OG1	1:D:494:MET:HE1	2.15	0.47
1:D:2892:PHE:O	1:D:2896:GLN:HG2	2.14	0.47
1:D:2903:SER:OG	1:D:2904:ARG:N	2.48	0.47
2:J:32:GLN:NE2	2:J:97:THR:OG1	2.34	0.47
1:A:267:VAL:HA	1:A:270:HIS:ND1	2.30	0.47
1:A:2068:TRP:HE3	1:A:2083:MET:HE2	1.80	0.47
1:A:2716:LEU:HD22	1:A:2778:LEU:HD21	1.97	0.47
1:B:1981:ASP:OD1	1:B:1982:LYS:N	2.48	0.47
1:C:2101:LEU:O	1:C:2104:THR:HG22	2.13	0.47
1:C:2765:LYS:O	1:C:2769:ILE:HG23	2.15	0.47
1:C:4830:ILE:HB	1:C:4842:ARG:HH21	1.80	0.47
1:D:552:SER:HA	1:D:555:LEU:HD13	1.96	0.47
1:D:658:ASN:HD22	1:D:833:LYS:H	1.61	0.47
1:D:1793:ILE:HG12	1:D:1843:ILE:HD11	1.97	0.47
1:D:4070:GLU:OE1	1:D:4070:GLU:N	2.43	0.47
1:A:228:LEU:HD23	1:A:289:ILE:HB	1.96	0.47
1:A:309:MET:HB2	1:A:312:LYS:HZ3	1.78	0.47
1:A:552:SER:HA	1:A:555:LEU:HD13	1.96	0.47
1:A:646:THR:HG21	1:A:1685:GLN:HE22	1.80	0.47
1:A:1090:ALA:HB3	1:A:1202:ILE:HD11	1.96	0.47
1:A:1704:TYR:O	1:A:1708:ILE:HG12	2.15	0.47
1:B:1902:LYS:HG3	1:B:2079:LEU:HD11	1.97	0.47
1:B:2716:LEU:HD22	1:B:2778:LEU:HD21	1.97	0.47
1:B:2765:LYS:O	1:B:2769:ILE:HG23	2.15	0.47
1:B:4830:ILE:HB	1:B:4842:ARG:HH21	1.80	0.47
2:H:11:GLY:O	2:H:68:SER:OG	2.32	0.47
1:C:1902:LYS:HG3	1:C:2079:LEU:HD11	1.97	0.47
1:C:4070:GLU:OE1	1:C:4070:GLU:N	2.43	0.47
1:D:620:CYS:SG	1:D:621:HIS:N	2.87	0.47
1:D:646:THR:HG21	1:D:1685:GLN:HE22	1.80	0.47
1:D:671:LYS:HA	1:D:761:LEU:HD12	1.96	0.47
1:D:1743:GLU:CD	1:D:1744:ASN:HD22	2.22	0.47
1:D:2081:ARG:HG3	1:D:3686:LEU:HD22	1.97	0.47
1:D:2765:LYS:O	1:D:2769:ILE:HG23	2.15	0.47
1:A:439:LYS:HD2	1:A:440:VAL:O	2.15	0.46
1:A:923:LYS:HB2	1:A:923:LYS:HE3	1.71	0.46
1:A:2271:CYS:SG	1:A:2293:GLU:HB2	2.55	0.46
1:B:915:HIS:CE1	1:B:917:CYS:HB2	2.50	0.46
1:B:1090:ALA:HB3	1:B:1202:ILE:HD11	1.96	0.46
1:B:1793:ILE:HG12	1:B:1843:ILE:HD11	1.97	0.46
1:B:3822:GLU:OE2	1:B:3823:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:874:LEU:HD11	1:C:941:LYS:HD3	1.97	0.46
1:C:915:HIS:CE1	1:C:917:CYS:HB2	2.50	0.46
1:C:2903:SER:OG	1:C:2904:ARG:N	2.48	0.46
1:C:3640:ILE:HG22	1:C:3729:ARG:HH11	1.80	0.46
1:C:4942:MET:HE1	1:C:4949:GLU:HB2	1.96	0.46
1:D:754:VAL:HG23	1:D:771:ASN:HA	1.97	0.46
1:D:997:ASP:O	1:D:1001:GLU:HG3	2.16	0.46
1:D:4570:THR:HA	1:D:4573:ILE:HG12	1.96	0.46
1:A:671:LYS:HA	1:A:761:LEU:HD12	1.96	0.46
1:A:997:ASP:O	1:A:1001:GLU:HG3	2.16	0.46
1:A:2892:PHE:O	1:A:2896:GLN:HG2	2.14	0.46
1:A:3786:VAL:HG11	1:A:3865:THR:HG23	1.98	0.46
1:A:4830:ILE:HB	1:A:4842:ARG:HH21	1.80	0.46
1:B:267:VAL:HA	1:B:270:HIS:ND1	2.30	0.46
1:B:309:MET:HE2	1:B:312:LYS:HZ3	1.80	0.46
1:C:1793:ILE:HG12	1:C:1843:ILE:HD11	1.97	0.46
1:D:1343:PHE:HB2	1:D:1376:TYR:HD2	1.80	0.46
1:D:2716:LEU:HD22	1:D:2778:LEU:HD21	1.97	0.46
1:D:2848:HIS:HE1	1:D:2869:LEU:HD13	1.80	0.46
1:D:4830:ILE:HG22	1:D:4831:GLU:H	1.80	0.46
1:A:874:LEU:HD11	1:A:941:LYS:HD3	1.97	0.46
1:B:1102:TYR:HB2	1:B:1165:MET:HG3	1.97	0.46
1:B:3786:VAL:HG11	1:B:3865:THR:HG23	1.98	0.46
1:C:300:VAL:O	1:C:420:ARG:NH1	2.40	0.46
1:C:641:ASP:OD1	1:C:642:LEU:N	2.47	0.46
1:C:2271:CYS:SG	1:C:2293:GLU:HB2	2.55	0.46
1:D:641:ASP:OD1	1:D:642:LEU:N	2.48	0.46
1:D:1709:ASP:HA	1:D:1713:SER:HB3	1.96	0.46
1:D:4508:ALA:O	1:D:4512:ASN:ND2	2.45	0.46
1:D:4942:MET:HE1	1:D:4949:GLU:HB2	1.96	0.46
1:A:1709:ASP:HA	1:A:1713:SER:HB3	1.96	0.46
1:A:1793:ILE:HG12	1:A:1843:ILE:HD11	1.97	0.46
1:B:844:ARG:HE	1:B:845:THR:HG22	1.80	0.46
1:B:921:PHE:O	1:B:929:ARG:NH1	2.37	0.46
1:C:309:MET:HB2	1:C:312:LYS:HZ3	1.81	0.46
1:C:1677:LEU:O	1:C:1681:VAL:HG22	2.16	0.46
1:D:1102:TYR:HB2	1:D:1165:MET:HG3	1.97	0.46
1:D:1305:SER:OG	1:D:1588:HIS:O	2.34	0.46
1:D:2068:TRP:HE3	1:D:2083:MET:HE2	1.80	0.46
1:A:284:TRP:O	1:A:287:SER:OG	2.29	0.46
1:A:892:LEU:HA	1:A:895:MET:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4608:LYS:HG3	1:A:4614:LEU:HB2	1.97	0.46
1:B:671:LYS:HA	1:B:761:LEU:HD12	1.96	0.46
1:B:2081:ARG:HG3	1:B:3686:LEU:HD22	1.97	0.46
1:C:422:THR:OG1	1:C:494:MET:HE1	2.15	0.46
1:C:892:LEU:HA	1:C:895:MET:HB2	1.98	0.46
1:C:2735:LYS:HZ3	1:C:2756:MET:HE1	1.81	0.46
1:C:4276:LYS:HZ1	1:C:4562:GLU:HG3	1.80	0.46
1:D:915:HIS:CE1	1:D:917:CYS:HB2	2.50	0.46
1:D:1090:ALA:HB3	1:D:1202:ILE:HD11	1.96	0.46
1:D:3923:ILE:HD13	1:D:3934:LEU:HD12	1.96	0.46
1:A:422:THR:OG1	1:A:494:MET:HE1	2.15	0.46
1:B:2848:HIS:HE1	1:B:2869:LEU:HD13	1.80	0.46
1:C:228:LEU:HD23	1:C:289:ILE:HB	1.96	0.46
1:C:417:ARG:NH1	1:C:420:ARG:HH22	2.14	0.46
1:C:2340:ASN:OD1	1:C:2340:ASN:N	2.46	0.46
1:D:442:LEU:HD23	1:D:442:LEU:H	1.81	0.46
1:D:1902:LYS:HG3	1:D:2079:LEU:HD11	1.97	0.46
1:D:2271:CYS:SG	1:D:2293:GLU:HB2	2.55	0.46
1:A:1305:SER:OG	1:A:1588:HIS:O	2.34	0.46
1:A:2092:ASP:OD1	1:A:2093:GLY:N	2.48	0.46
1:A:4830:ILE:HG22	1:A:4831:GLU:H	1.80	0.46
1:B:799:LYS:HG2	1:B:1621:GLN:NE2	2.31	0.46
1:B:800:VAL:HB	1:B:1620:VAL:HG23	1.98	0.46
1:B:892:LEU:HA	1:B:895:MET:HB2	1.98	0.46
1:B:1677:LEU:O	1:B:1681:VAL:HG22	2.16	0.46
1:B:3621:GLN:O	1:B:3624:GLU:HG3	2.16	0.46
1:C:603:LYS:HG2	1:C:1573:LYS:HZ1	1.81	0.46
1:C:2092:ASP:OD1	1:C:2093:GLY:N	2.48	0.46
1:D:1139:GLY:O	1:D:1155:SER:OG	2.30	0.46
1:D:1704:TYR:O	1:D:1708:ILE:HG12	2.15	0.46
1:D:2201:TYR:O	1:D:2205:ILE:HG22	2.16	0.46
1:D:4608:LYS:HG3	1:D:4614:LEU:HB2	1.97	0.46
1:A:442:LEU:HD23	1:A:442:LEU:H	1.81	0.46
1:A:1902:LYS:HG3	1:A:2079:LEU:HD11	1.97	0.46
1:B:247:VAL:O	1:B:272:ARG:NH1	2.44	0.46
1:B:2735:LYS:HZ3	1:B:2756:MET:HE1	1.81	0.46
1:C:3822:GLU:OE2	1:C:3823:GLY:N	2.49	0.46
1:D:629:GLN:NE2	1:D:1670:ASN:HD22	2.13	0.46
1:D:3640:ILE:HG22	1:D:3729:ARG:HH11	1.80	0.46
1:D:3822:GLU:OE2	1:D:3823:GLY:N	2.49	0.46
1:A:1747:HIS:O	1:A:1747:HIS:ND1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2201:TYR:O	1:A:2205:ILE:HG22	2.16	0.46
1:B:422:THR:OG1	1:B:494:MET:HE1	2.15	0.46
1:B:801:ARG:HA	1:B:1618:TRP:O	2.16	0.46
1:B:2107:ILE:HG13	1:B:2108:ASN:H	1.81	0.46
2:H:72:ARG:HG2	2:H:103:GLU:HB2	1.98	0.46
1:C:2081:ARG:HG3	1:C:3686:LEU:HD22	1.97	0.46
1:C:2771:ARG:HH22	1:C:2775:LYS:HD3	1.81	0.46
1:C:2848:HIS:HE1	1:C:2869:LEU:HD13	1.80	0.46
1:C:4830:ILE:HG22	1:C:4831:GLU:H	1.80	0.46
1:D:380:LYS:HD3	1:D:380:LYS:HA	1.71	0.46
1:D:417:ARG:NH1	1:D:420:ARG:HH22	2.14	0.46
1:A:629:GLN:NE2	1:A:1670:ASN:HD22	2.13	0.46
1:A:754:VAL:HG23	1:A:771:ASN:HA	1.97	0.46
1:A:800:VAL:HB	1:A:1620:VAL:HG23	1.98	0.46
1:A:2848:HIS:HE1	1:A:2869:LEU:HD13	1.80	0.46
1:A:3822:GLU:OE2	1:A:3823:GLY:N	2.48	0.46
1:B:442:LEU:HD23	1:B:442:LEU:H	1.81	0.46
1:B:646:THR:HG21	1:B:1685:GLN:HE22	1.80	0.46
1:C:629:GLN:NE2	1:C:1670:ASN:HD22	2.13	0.46
1:C:799:LYS:HG2	1:C:1621:GLN:NE2	2.31	0.46
1:C:801:ARG:HA	1:C:1618:TRP:O	2.16	0.46
1:C:997:ASP:O	1:C:1001:GLU:HG3	2.16	0.46
1:C:1747:HIS:O	1:C:1747:HIS:ND1	2.47	0.46
1:D:373:THR:O	1:D:375:GLN:NE2	2.43	0.46
1:D:439:LYS:HD2	1:D:440:VAL:O	2.15	0.46
1:A:799:LYS:HG2	1:A:1621:GLN:NE2	2.31	0.45
1:B:2238:PRO:O	1:B:2241:VAL:HG12	2.17	0.45
1:C:754:VAL:HG23	1:C:771:ASN:HA	1.97	0.45
1:C:2201:TYR:O	1:C:2205:ILE:HG22	2.16	0.45
1:C:2238:PRO:O	1:C:2241:VAL:HG12	2.17	0.45
1:C:4508:ALA:O	1:C:4512:ASN:ND2	2.45	0.45
2:I:72:ARG:HG2	2:I:103:GLU:HB2	1.98	0.45
1:D:799:LYS:HG2	1:D:1621:GLN:NE2	2.31	0.45
1:D:946:LEU:HD13	1:D:995:MET:SD	2.56	0.45
1:D:2771:ARG:HH22	1:D:2775:LYS:HD3	1.81	0.45
1:A:875:PRO:O	1:A:882:ARG:NH2	2.46	0.45
1:A:1102:TYR:HB2	1:A:1165:MET:HG3	1.97	0.45
1:A:1677:LEU:O	1:A:1681:VAL:HG22	2.16	0.45
1:A:2771:ARG:HH22	1:A:2775:LYS:HD3	1.81	0.45
1:B:417:ARG:NH1	1:B:420:ARG:HH22	2.14	0.45
1:B:629:GLN:NE2	1:B:1670:ASN:HD22	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4276:LYS:HZ1	1:B:4562:GLU:HG3	1.81	0.45
1:B:4793:ASN:O	1:B:4795:SER:N	2.49	0.45
1:C:439:LYS:HD2	1:C:440:VAL:O	2.15	0.45
1:C:646:THR:HG21	1:C:1685:GLN:HE22	1.80	0.45
1:C:2068:TRP:HE3	1:C:2083:MET:HE2	1.80	0.45
1:D:1677:LEU:O	1:D:1681:VAL:HG22	2.16	0.45
1:A:946:LEU:HD13	1:A:995:MET:SD	2.56	0.45
2:G:72:ARG:HG2	2:G:103:GLU:HB2	1.98	0.45
1:B:874:LEU:HD11	1:B:941:LYS:HD3	1.97	0.45
1:B:997:ASP:O	1:B:1001:GLU:HG3	2.16	0.45
1:B:2201:TYR:O	1:B:2205:ILE:HG22	2.16	0.45
1:D:490:GLN:O	1:D:490:GLN:NE2	2.44	0.45
1:D:2057:LEU:O	1:D:2060:LEU:HD23	2.17	0.45
1:D:3621:GLN:O	1:D:3624:GLU:HG3	2.16	0.45
2:J:72:ARG:HG2	2:J:103:GLU:HB2	1.98	0.45
1:B:1747:HIS:O	1:B:1747:HIS:ND1	2.47	0.45
1:C:1591:PHE:CZ	1:C:1593:SER:HB2	2.52	0.45
1:C:3621:GLN:O	1:C:3624:GLU:HG3	2.16	0.45
1:D:874:LEU:HD11	1:D:941:LYS:HD3	1.97	0.45
1:A:4044:LYS:HE2	1:A:4044:LYS:HB3	1.82	0.45
1:A:4873:ARG:O	1:A:4877:GLU:HG2	2.17	0.45
1:B:207:PHE:CE1	1:C:2324:ILE:HB	2.52	0.45
1:B:373:THR:O	1:B:375:GLN:NE2	2.43	0.45
1:B:490:GLN:O	1:B:490:GLN:NE2	2.44	0.45
1:B:4830:ILE:HG22	1:B:4831:GLU:H	1.80	0.45
1:D:973:THR:OG1	1:D:976:TYR:O	2.18	0.45
1:D:2238:PRO:O	1:D:2241:VAL:HG12	2.16	0.45
1:D:4830:ILE:HB	1:D:4842:ARG:HH21	1.80	0.45
1:A:2057:LEU:O	1:A:2060:LEU:HD23	2.17	0.45
1:A:4793:ASN:O	1:A:4795:SER:N	2.49	0.45
1:B:1704:TYR:O	1:B:1708:ILE:HG12	2.15	0.45
1:B:2068:TRP:HE3	1:B:2083:MET:HE2	1.80	0.45
1:C:442:LEU:HD23	1:C:442:LEU:H	1.81	0.45
1:C:800:VAL:HB	1:C:1620:VAL:HG23	1.98	0.45
1:C:2107:ILE:HG13	1:C:2108:ASN:H	1.81	0.45
1:C:3786:VAL:HG11	1:C:3865:THR:HG23	1.98	0.45
1:D:1591:PHE:CZ	1:D:1593:SER:HB2	2.52	0.45
1:A:2107:ILE:HG22	1:A:2157:HIS:CD2	2.52	0.45
1:A:2107:ILE:HG13	1:A:2108:ASN:H	1.81	0.45
1:A:3621:GLN:O	1:A:3624:GLU:HG3	2.16	0.45
1:B:754:VAL:HG23	1:B:771:ASN:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1367:LYS:NZ	1:B:1369:GLU:OE2	2.35	0.45
1:B:2107:ILE:HG22	1:B:2157:HIS:CD2	2.52	0.45
1:C:1102:TYR:HB2	1:C:1165:MET:HG3	1.97	0.45
1:D:2385:ASN:HA	1:D:2388:MET:HE3	1.99	0.45
1:D:3786:VAL:HG11	1:D:3865:THR:HG23	1.98	0.45
1:A:625:VAL:HG23	1:A:628:ASN:HB2	1.99	0.45
1:A:4187:LEU:HG	1:A:4187:LEU:H	1.68	0.45
2:G:38:ASP:OD1	2:G:39:SER:N	2.50	0.45
1:B:692:HIS:NE2	1:B:793:SER:OG	2.47	0.45
1:B:946:LEU:HD13	1:B:995:MET:SD	2.56	0.45
1:B:1305:SER:OG	1:B:1588:HIS:O	2.34	0.45
1:C:2057:LEU:O	1:C:2060:LEU:HD23	2.17	0.45
1:C:2498:ALA:O	1:C:2501:LEU:HD23	2.16	0.45
1:D:892:LEU:HA	1:D:895:MET:HB2	1.98	0.45
1:D:2848:HIS:CE1	1:D:2869:LEU:HD13	2.52	0.45
1:D:4873:ARG:O	1:D:4877:GLU:HG2	2.17	0.45
1:A:417:ARG:NH1	1:A:420:ARG:HH22	2.14	0.45
1:C:2107:ILE:HG22	1:C:2157:HIS:CD2	2.52	0.45
1:D:290:ARG:H	1:D:293:GLN:NE2	2.15	0.45
1:D:2107:ILE:HG13	1:D:2108:ASN:H	1.81	0.45
1:D:4583:PHE:O	1:D:4586:ILE:HG22	2.17	0.45
1:A:70:GLU:OE1	1:A:122:ARG:NE	2.45	0.45
1:A:801:ARG:HA	1:A:1618:TRP:O	2.16	0.45
1:A:2238:PRO:O	1:A:2241:VAL:HG12	2.17	0.45
1:A:3943:VAL:HG23	1:A:4001:MET:HE3	1.99	0.45
1:B:2771:ARG:HH22	1:B:2775:LYS:HD3	1.81	0.45
1:B:4508:ALA:O	1:B:4512:ASN:ND2	2.45	0.45
1:C:2848:HIS:CE1	1:C:2869:LEU:HD13	2.52	0.45
1:C:4026:THR:O	1:C:4031:PHE:HB3	2.17	0.45
1:D:419:ILE:HD13	1:D:492:GLU:HG3	1.99	0.45
2:J:38:ASP:OD1	2:J:39:SER:N	2.50	0.45
1:A:419:ILE:HD13	1:A:492:GLU:HG3	1.99	0.44
1:A:2720:ILE:HD11	1:A:2778:LEU:HD22	1.99	0.44
1:A:4583:PHE:O	1:A:4586:ILE:HG22	2.17	0.44
1:B:14:LEU:HB3	1:B:113:LEU:HD12	2.00	0.44
1:B:1591:PHE:CZ	1:B:1593:SER:HB2	2.52	0.44
1:B:1970:GLU:HA	1:B:1973:ASN:HB2	1.99	0.44
1:C:1968:PRO:HA	1:C:1971:GLN:HB3	1.99	0.44
1:C:1970:GLU:HA	1:C:1973:ASN:HB2	1.99	0.44
1:C:2058:GLN:HG3	1:C:2090:GLN:NE2	2.32	0.44
1:D:625:VAL:HG23	1:D:628:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2058:GLN:HG3	1:D:2090:GLN:NE2	2.32	0.44
1:B:300:VAL:O	1:B:420:ARG:NH1	2.40	0.44
1:B:923:LYS:HB2	1:B:923:LYS:HE3	1.71	0.44
1:B:3943:VAL:HG23	1:B:4001:MET:HE3	1.99	0.44
1:C:1305:SER:OG	1:C:1588:HIS:O	2.34	0.44
1:C:2763:SER:H	1:C:2766:GLU:HB2	1.82	0.44
1:D:923:LYS:HB2	1:D:923:LYS:HE3	1.71	0.44
1:D:2498:ALA:O	1:D:2501:LEU:HD23	2.16	0.44
1:D:3919:LEU:O	1:D:3923:ILE:HG12	2.18	0.44
1:D:3943:VAL:HG23	1:D:4001:MET:HE3	1.99	0.44
1:D:4026:THR:O	1:D:4031:PHE:HB3	2.18	0.44
1:A:833:LYS:HE3	1:A:834:VAL:N	2.33	0.44
1:B:414:ARG:O	1:B:418:VAL:HG12	2.18	0.44
1:B:2058:GLN:HG3	1:B:2090:GLN:NE2	2.32	0.44
1:B:4873:ARG:O	1:B:4877:GLU:HG2	2.17	0.44
1:C:14:LEU:HB3	1:C:113:LEU:HD12	2.00	0.44
1:C:946:LEU:HD13	1:C:995:MET:SD	2.56	0.44
1:C:4793:ASN:O	1:C:4795:SER:N	2.49	0.44
1:D:801:ARG:HA	1:D:1618:TRP:O	2.16	0.44
1:D:1798:GLU:O	1:D:1802:GLU:HG2	2.18	0.44
1:D:2107:ILE:HG22	1:D:2157:HIS:CD2	2.52	0.44
1:A:2385:ASN:HA	1:A:2388:MET:HE3	1.99	0.44
1:B:189:GLU:O	1:C:2325:ARG:NH2	2.49	0.44
1:B:3919:LEU:O	1:B:3923:ILE:HG12	2.18	0.44
1:C:36:CYS:SG	1:C:65:CYS:HB3	2.58	0.44
1:C:1320:UNK:HA	1:C:1325:UNK:HA	2.00	0.44
1:C:3919:LEU:O	1:C:3923:ILE:HG12	2.18	0.44
1:C:4039:LYS:O	1:C:4041:VAL:HG23	2.17	0.44
1:D:317:MET:HB2	1:D:321:LYS:HE3	2.00	0.44
1:D:800:VAL:HB	1:D:1620:VAL:HG23	1.98	0.44
1:D:4799:ASP:N	1:D:4799:ASP:OD1	2.51	0.44
1:A:2058:GLN:HG3	1:A:2090:GLN:NE2	2.32	0.44
1:A:2763:SER:H	1:A:2766:GLU:HB2	1.83	0.44
1:A:4039:LYS:O	1:A:4041:VAL:HG23	2.18	0.44
1:B:1972:ILE:HA	1:B:1975:LEU:HG	1.99	0.44
1:B:2498:ALA:O	1:B:2501:LEU:HD23	2.16	0.44
1:C:317:MET:HB2	1:C:321:LYS:HE3	2.00	0.44
1:C:2720:ILE:HD11	1:C:2778:LEU:HD22	1.99	0.44
1:C:2858:GLU:O	1:C:2862:LYS:HG2	2.17	0.44
1:C:4583:PHE:O	1:C:4586:ILE:HG22	2.17	0.44
1:D:36:CYS:SG	1:D:65:CYS:HB3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1970:GLU:HA	1:D:1973:ASN:HB2	1.99	0.44
1:A:2498:ALA:O	1:A:2501:LEU:HD23	2.16	0.44
1:B:833:LYS:HE3	1:B:834:VAL:N	2.33	0.44
1:B:2385:ASN:HA	1:B:2388:MET:HE3	1.99	0.44
1:B:4039:LYS:O	1:B:4041:VAL:HG23	2.18	0.44
1:C:414:ARG:O	1:C:418:VAL:HG12	2.18	0.44
1:C:2342:LEU:N	1:C:2430:ASP:OD2	2.47	0.44
1:C:4873:ARG:O	1:C:4877:GLU:HG2	2.17	0.44
1:D:2346:MET:HE3	1:D:2346:MET:HB3	1.93	0.44
1:D:2471:LEU:HD23	1:D:2471:LEU:HA	1.80	0.44
1:D:2858:GLU:O	1:D:2862:LYS:HG2	2.17	0.44
1:A:14:LEU:HB3	1:A:113:LEU:HD12	2.00	0.44
1:A:36:CYS:SG	1:A:65:CYS:HB3	2.58	0.44
1:A:935:MET:O	1:A:938:GLU:HG3	2.18	0.44
1:A:1591:PHE:CZ	1:A:1593:SER:HB2	2.52	0.44
1:A:1972:ILE:HA	1:A:1975:LEU:HG	2.00	0.44
1:A:2346:MET:HE3	1:A:2346:MET:HB3	1.93	0.44
1:A:3919:LEU:O	1:A:3923:ILE:HG12	2.18	0.44
1:B:419:ILE:HD13	1:B:492:GLU:HG3	1.99	0.44
1:B:625:VAL:HG23	1:B:628:ASN:HB2	1.99	0.44
1:C:799:LYS:HG2	1:C:1621:GLN:HE22	1.83	0.44
1:C:1347:MET:HG2	1:C:1371:ASN:HD22	1.83	0.44
1:C:2282:LYS:HA	1:C:2282:LYS:HD2	1.90	0.44
1:D:4009:VAL:HA	1:D:4012:ILE:HG12	2.00	0.44
1:A:2867:HIS:HB2	1:A:2870:LEU:HG	2.00	0.44
1:B:36:CYS:SG	1:B:65:CYS:HB3	2.58	0.44
1:B:674:TYR:N	1:B:820:ALA:O	2.51	0.44
1:B:1811:VAL:HB	1:B:1818:LEU:HD13	2.00	0.44
1:B:2057:LEU:O	1:B:2060:LEU:HD23	2.17	0.44
1:B:4496:ASN:HD22	1:B:4499:ASN:HD22	1.66	0.44
1:C:329:PHE:HB3	1:C:363:ILE:HD11	2.00	0.44
1:C:674:TYR:N	1:C:820:ALA:O	2.51	0.44
1:C:882:ARG:HG2	1:C:940:LEU:HD12	2.00	0.44
1:C:935:MET:O	1:C:938:GLU:HG3	2.18	0.44
1:D:14:LEU:HB3	1:D:113:LEU:HD12	2.00	0.44
1:D:329:PHE:HB3	1:D:363:ILE:HD11	2.00	0.44
1:D:1347:MET:HG2	1:D:1371:ASN:HD22	1.83	0.44
1:D:2894:PHE:HA	1:D:2897:ILE:HG12	2.00	0.44
1:A:26:ALA:HB2	1:A:194:LEU:HD21	2.00	0.44
1:A:799:LYS:HG2	1:A:1621:GLN:HE22	1.83	0.44
1:A:2160:LEU:HB3	1:A:2161:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2258:GLU:HG3	1:A:2261:LEU:HB2	2.00	0.44
1:B:438:LYS:HZ1	1:B:441:LYS:HD2	1.83	0.44
1:B:1347:MET:HG2	1:B:1371:ASN:HD22	1.83	0.44
1:B:1968:PRO:HA	1:B:1971:GLN:HB3	1.99	0.44
1:B:2720:ILE:HD11	1:B:2778:LEU:HD22	1.99	0.44
1:C:625:VAL:HG23	1:C:628:ASN:HB2	1.99	0.44
1:C:1798:GLU:O	1:C:1802:GLU:HG2	2.18	0.44
1:C:2867:HIS:HB2	1:C:2870:LEU:HG	2.00	0.44
1:D:833:LYS:HE3	1:D:834:VAL:N	2.33	0.44
1:D:2342:LEU:N	1:D:2430:ASP:OD2	2.47	0.44
1:A:1798:GLU:O	1:A:1802:GLU:HG2	2.18	0.43
1:A:1970:GLU:HA	1:A:1973:ASN:HB2	1.99	0.43
1:A:4659:PHE:O	1:B:4055:LYS:NZ	2.41	0.43
1:B:70:GLU:OE1	1:B:122:ARG:NE	2.45	0.43
1:B:2258:GLU:HG3	1:B:2261:LEU:HB2	2.00	0.43
1:B:2763:SER:H	1:B:2766:GLU:HB2	1.83	0.43
1:C:2385:ASN:HA	1:C:2388:MET:HE3	1.99	0.43
1:D:414:ARG:O	1:D:418:VAL:HG12	2.18	0.43
1:D:1320:UNK:HA	1:D:1325:UNK:HA	2.00	0.43
1:D:4039:LYS:O	1:D:4041:VAL:HG23	2.17	0.43
1:A:1165:MET:HB3	1:A:1236:TYR:CE2	2.53	0.43
1:A:1347:MET:HG2	1:A:1371:ASN:HD22	1.83	0.43
1:A:4496:ASN:HD22	1:A:4499:ASN:HD22	1.66	0.43
1:B:329:PHE:HB3	1:B:363:ILE:HD11	2.00	0.43
1:B:1040:ASP:HA	1:B:1043:LYS:HG3	2.01	0.43
1:B:1798:GLU:O	1:B:1802:GLU:HG2	2.18	0.43
1:C:490:GLN:O	1:C:490:GLN:NE2	2.45	0.43
2:I:38:ASP:OD1	2:I:39:SER:N	2.50	0.43
1:D:300:VAL:O	1:D:420:ARG:NH1	2.40	0.43
1:D:1811:VAL:HB	1:D:1818:LEU:HD13	2.00	0.43
1:A:317:MET:HB2	1:A:321:LYS:HE3	2.00	0.43
1:A:595:LYS:HE2	1:A:595:LYS:HB3	1.89	0.43
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.99	0.43
1:B:3712:SER:OG	1:B:3715:GLU:OE2	2.33	0.43
1:C:1165:MET:HB3	1:C:1236:TYR:CE2	2.53	0.43
1:C:1972:ILE:HA	1:C:1975:LEU:HG	2.00	0.43
1:D:674:TYR:N	1:D:820:ALA:O	2.51	0.43
1:D:935:MET:O	1:D:938:GLU:HG3	2.18	0.43
1:D:1747:HIS:O	1:D:1747:HIS:ND1	2.47	0.43
1:D:2720:ILE:HD11	1:D:2778:LEU:HD22	1.99	0.43
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:TYR:N	1:A:820:ALA:O	2.51	0.43
1:A:1786:ASP:O	1:A:1789:LYS:HG2	2.18	0.43
1:A:2722:LYS:HD2	1:A:2722:LYS:HA	1.63	0.43
1:B:850:LEU:H	1:B:850:LEU:HG	1.57	0.43
1:B:1031:ARG:NH1	1:B:1039:ASP:OD2	2.52	0.43
1:B:4026:THR:O	1:B:4031:PHE:HB3	2.18	0.43
1:C:419:ILE:HD13	1:C:492:GLU:HG3	1.99	0.43
1:C:1786:ASP:O	1:C:1789:LYS:HG2	2.18	0.43
1:C:4799:ASP:N	1:C:4799:ASP:OD1	2.51	0.43
1:D:640:ARG:HD3	2:J:35:LYS:HD3	2.00	0.43
1:D:799:LYS:HG2	1:D:1621:GLN:HE22	1.83	0.43
1:D:1972:ILE:HA	1:D:1975:LEU:HG	2.00	0.43
1:D:2278:MET:O	1:D:2282:LYS:HG2	2.19	0.43
1:D:2867:HIS:HB2	1:D:2870:LEU:HG	2.00	0.43
1:A:1968:PRO:HA	1:A:1971:GLN:HB3	1.99	0.43
1:A:2848:HIS:CE1	1:A:2869:LEU:HD13	2.52	0.43
1:A:2894:PHE:HA	1:A:2897:ILE:HG12	2.00	0.43
1:A:4009:VAL:HA	1:A:4012:ILE:HG12	2.00	0.43
1:B:317:MET:HB2	1:B:321:LYS:HE3	2.00	0.43
1:B:911:ASN:OD1	1:B:911:ASN:N	2.41	0.43
1:B:2848:HIS:CE1	1:B:2869:LEU:HD13	2.52	0.43
1:B:4009:VAL:HA	1:B:4012:ILE:HG12	2.00	0.43
1:C:807:ARG:O	1:C:1615:ARG:NE	2.48	0.43
1:C:1776:CYS:SG	1:C:1778:GLN:HB2	2.59	0.43
1:C:1811:VAL:HB	1:C:1818:LEU:HD13	2.00	0.43
1:C:3943:VAL:HG23	1:C:4001:MET:HE3	1.99	0.43
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.99	0.43
1:D:882:ARG:HG2	1:D:940:LEU:HD12	2.00	0.43
1:D:1165:MET:HB3	1:D:1236:TYR:CE2	2.53	0.43
1:D:1776:CYS:SG	1:D:1778:GLN:HB2	2.59	0.43
1:D:2763:SER:H	1:D:2766:GLU:HB2	1.83	0.43
1:D:4205:ILE:HG23	1:D:4491:ASN:HB3	2.01	0.43
1:D:4807:ASP:HB3	1:D:4810:THR:HB	2.00	0.43
1:A:414:ARG:O	1:A:418:VAL:HG12	2.18	0.43
1:A:2278:MET:O	1:A:2282:LYS:HG2	2.19	0.43
1:B:1320:UNK:HA	1:B:1325:UNK:HA	1.99	0.43
1:B:4670:GLY:O	1:B:4671:MET:HG2	2.19	0.43
1:B:4799:ASP:OD1	1:B:4799:ASP:N	2.51	0.43
2:H:38:ASP:OD1	2:H:39:SER:N	2.50	0.43
1:C:894:VAL:HG13	1:C:918:LEU:HB3	2.01	0.43
1:D:190:ARG:HD3	1:D:205:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1091:GLU:HB3	1:D:1094:TYR:CD2	2.52	0.43
1:D:1118:SER:HA	1:D:1134:ALA:HA	2.01	0.43
1:D:1786:ASP:O	1:D:1789:LYS:HG2	2.18	0.43
1:D:1945:GLU:O	1:D:1948:GLN:HG3	2.19	0.43
1:D:4000:ASP:O	1:D:4004:GLU:HG3	2.19	0.43
1:D:4496:ASN:HD22	1:D:4499:ASN:HD22	1.66	0.43
1:A:290:ARG:H	1:A:293:GLN:NE2	2.15	0.43
1:A:329:PHE:HB3	1:A:363:ILE:HD11	2.00	0.43
1:A:1091:GLU:HB3	1:A:1094:TYR:CD2	2.52	0.43
1:A:2735:LYS:HZ3	1:A:2756:MET:HE1	1.83	0.43
1:A:2858:GLU:O	1:A:2862:LYS:HG2	2.17	0.43
1:A:4287:TRP:O	1:A:4291:VAL:HG13	2.19	0.43
1:A:4799:ASP:N	1:A:4799:ASP:OD1	2.51	0.43
1:B:140:THR:OG1	1:C:2337:GLU:HG3	2.19	0.43
1:B:799:LYS:HG2	1:B:1621:GLN:HE22	1.83	0.43
1:B:2858:GLU:O	1:B:2862:LYS:HG2	2.17	0.43
1:C:4009:VAL:HA	1:C:4012:ILE:HG12	2.00	0.43
1:C:4205:ILE:HG23	1:C:4491:ASN:HB3	2.01	0.43
1:D:1968:PRO:HA	1:D:1971:GLN:HB3	1.99	0.43
1:D:2160:LEU:HB3	1:D:2161:MET:HE2	2.00	0.43
1:A:1945:GLU:O	1:A:1948:GLN:HG3	2.19	0.43
1:A:4026:THR:O	1:A:4031:PHE:HB3	2.17	0.43
1:A:4670:GLY:O	1:A:4671:MET:HG2	2.19	0.43
1:B:882:ARG:HG2	1:B:940:LEU:HD12	2.00	0.43
1:B:935:MET:O	1:B:938:GLU:HG3	2.18	0.43
1:B:2160:LEU:HB3	1:B:2161:MET:HE2	2.00	0.43
1:B:4583:PHE:O	1:B:4586:ILE:HG22	2.18	0.43
1:C:161:THR:HG23	1:C:184:VAL:HB	2.01	0.43
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.99	0.43
1:C:829:LYS:O	1:C:830:GLU:HG3	2.19	0.43
1:C:988:LEU:HD11	1:C:1055:ARG:HG2	2.00	0.43
1:C:1271:THR:OG1	1:C:1272:ARG:N	2.52	0.43
1:C:2258:GLU:HG3	1:C:2261:LEU:HB2	2.00	0.43
1:C:2894:PHE:HA	1:C:2897:ILE:HG12	2.00	0.43
1:D:26:ALA:HB2	1:D:194:LEU:HD21	2.00	0.43
1:D:829:LYS:O	1:D:830:GLU:HG3	2.19	0.43
1:D:4029:ASP:OD1	1:D:4029:ASP:N	2.45	0.43
1:A:672:LYS:NZ	1:A:760:ASP:OD2	2.35	0.43
1:A:882:ARG:HG2	1:A:940:LEU:HD12	2.00	0.43
1:A:899:GLU:HG2	1:A:971:GLN:HE22	1.84	0.43
1:A:988:LEU:HD11	1:A:1055:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1811:VAL:HB	1:A:1818:LEU:HD13	2.00	0.43
1:A:2342:LEU:N	1:A:2430:ASP:OD2	2.47	0.43
1:A:4193:GLU:OE2	1:A:4943:TYR:OH	2.30	0.43
1:A:4807:ASP:HB3	1:A:4810:THR:HB	2.00	0.43
1:B:698:ALA:HA	1:B:724:SER:HA	2.00	0.43
1:B:1786:ASP:O	1:B:1789:LYS:HG2	2.18	0.43
1:B:2278:MET:O	1:B:2282:LYS:HG2	2.19	0.43
1:B:4205:ILE:HG23	1:B:4491:ASN:HB3	2.01	0.43
1:C:373:THR:O	1:C:375:GLN:NE2	2.43	0.43
1:C:698:ALA:HA	1:C:724:SER:HA	2.00	0.43
1:C:1040:ASP:HA	1:C:1043:LYS:HG3	2.01	0.43
1:C:3758:LEU:O	1:C:3762:ILE:HG12	2.19	0.43
1:D:899:GLU:HG2	1:D:971:GLN:HE22	1.84	0.43
1:D:2837:HIS:ND1	1:D:2838:ALA:N	2.67	0.43
1:D:4287:TRP:O	1:D:4291:VAL:HG13	2.19	0.43
1:D:4793:ASN:O	1:D:4795:SER:N	2.49	0.43
1:A:829:LYS:O	1:A:830:GLU:HG3	2.19	0.43
1:A:911:ASN:OD1	1:A:911:ASN:N	2.41	0.43
1:A:1031:ARG:HA	1:A:1031:ARG:HD3	1.84	0.43
1:A:1217:PHE:O	1:A:1240:ALA:N	2.52	0.43
1:B:1165:MET:HB3	1:B:1236:TYR:CE2	2.53	0.43
1:B:1945:GLU:O	1:B:1948:GLN:HG3	2.19	0.43
1:B:2867:HIS:HB2	1:B:2870:LEU:HG	2.00	0.43
1:B:4287:TRP:O	1:B:4291:VAL:HG13	2.19	0.43
1:C:26:ALA:HB2	1:C:194:LEU:HD21	2.00	0.43
1:C:697:TRP:HB2	1:C:766:ILE:HD13	2.01	0.43
1:C:845:THR:OG1	1:C:846:TYR:N	2.51	0.43
1:C:1031:ARG:NH1	1:C:1039:ASP:OD2	2.52	0.43
1:C:1945:GLU:O	1:C:1948:GLN:HG3	2.19	0.43
1:C:4806:ASP:HA	1:D:4520:VAL:HG12	2.01	0.43
2:I:53:LYS:HD3	2:I:53:LYS:HA	1.92	0.43
1:D:3758:LEU:O	1:D:3762:ILE:HG12	2.19	0.43
1:A:661:LEU:HD13	1:A:673:TRP:CD1	2.54	0.42
1:A:838:ARG:N	1:A:841:LYS:HZ1	2.09	0.42
1:A:843:GLU:HB3	1:A:1606:LYS:HD3	2.01	0.42
1:A:1031:ARG:NH1	1:A:1039:ASP:OD2	2.52	0.42
1:A:1608:ASP:OD1	1:A:1608:ASP:N	2.52	0.42
1:A:4516:LEU:HD23	1:D:4809:LEU:HD13	2.01	0.42
1:B:26:ALA:HB2	1:B:194:LEU:HD21	2.00	0.42
1:B:894:VAL:HG13	1:B:918:LEU:HB3	2.01	0.42
1:B:1776:CYS:SG	1:B:1778:GLN:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ASN:HB2	1:C:832:LEU:HD12	2.01	0.42
1:C:1987:CYS:N	1:C:1988:PRO:HD2	2.34	0.42
1:C:2876:LEU:O	1:C:2881:LYS:NZ	2.43	0.42
1:D:798:ILE:HD12	1:D:798:ILE:HA	1.91	0.42
1:D:807:ARG:O	1:D:1615:ARG:NE	2.48	0.42
2:J:27:TYR:N	2:J:40:SER:OG	2.51	0.42
1:A:4205:ILE:HG23	1:A:4491:ASN:HB3	2.01	0.42
1:B:190:ARG:HD3	1:B:205:ALA:O	2.19	0.42
1:B:674:TYR:CE2	1:B:756:SER:HB2	2.54	0.42
1:B:843:GLU:HB3	1:B:1606:LYS:HD3	2.01	0.42
1:B:988:LEU:HD11	1:B:1055:ARG:HG2	2.00	0.42
1:B:1987:CYS:N	1:B:1988:PRO:HD2	2.34	0.42
1:C:850:LEU:H	1:C:850:LEU:HG	1.57	0.42
1:C:2160:LEU:HB3	1:C:2161:MET:HE2	2.00	0.42
1:D:247:VAL:O	1:D:272:ARG:NH1	2.44	0.42
1:D:438:LYS:HZ1	1:D:441:LYS:HD2	1.83	0.42
1:D:661:LEU:HD13	1:D:673:TRP:CD1	2.54	0.42
1:D:674:TYR:CE2	1:D:756:SER:HB2	2.54	0.42
1:D:1031:ARG:NH1	1:D:1039:ASP:OD2	2.52	0.42
1:D:2258:GLU:HG3	1:D:2261:LEU:HB2	2.00	0.42
1:A:161:THR:HG23	1:A:184:VAL:HB	2.01	0.42
1:A:692:HIS:NE2	1:A:793:SER:OG	2.47	0.42
1:A:1320:UNK:HA	1:A:1325:UNK:HA	2.00	0.42
1:A:1776:CYS:SG	1:A:1778:GLN:HB2	2.59	0.42
1:B:845:THR:OG1	1:B:846:TYR:N	2.51	0.42
1:B:1827:TYR:CZ	1:B:1831:ILE:HD11	2.54	0.42
1:B:3758:LEU:O	1:B:3762:ILE:HG12	2.19	0.42
1:C:1118:SER:HA	1:C:1134:ALA:HA	2.01	0.42
1:C:1641:ASP:HB2	1:C:1644:GLU:HG3	2.00	0.42
1:C:2278:MET:O	1:C:2282:LYS:HG2	2.19	0.42
1:C:4670:GLY:O	1:C:4671:MET:HG2	2.19	0.42
1:C:4923:TYR:CZ	1:C:4927:LYS:HD2	2.55	0.42
1:D:245:LEU:HD11	1:D:260:VAL:HG12	2.01	0.42
1:D:658:ASN:HB2	1:D:832:LEU:HD12	2.01	0.42
1:D:875:PRO:O	1:D:882:ARG:NH2	2.46	0.42
1:D:894:VAL:HG13	1:D:918:LEU:HB3	2.01	0.42
1:D:988:LEU:HD11	1:D:1055:ARG:HG2	2.00	0.42
1:D:1271:THR:OG1	1:D:1272:ARG:N	2.52	0.42
1:D:1641:ASP:HB2	1:D:1644:GLU:HG3	2.01	0.42
1:D:3905:PHE:O	1:D:3909:ILE:HG12	2.20	0.42
1:D:4189:VAL:HG21	1:D:4948:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1827:TYR:CZ	1:A:1831:ILE:HD11	2.54	0.42
1:A:3719:GLU:HA	1:A:3722:LYS:HG2	2.01	0.42
1:B:661:LEU:HD13	1:B:673:TRP:CD1	2.54	0.42
1:B:802:PHE:HB2	1:B:1618:TRP:HB2	2.01	0.42
1:B:2282:LYS:HA	1:B:2282:LYS:HD2	1.90	0.42
1:B:2894:PHE:HA	1:B:2897:ILE:HG12	2.00	0.42
1:C:4509:PHE:HD1	1:C:4509:PHE:HA	1.78	0.42
1:D:3719:GLU:HA	1:D:3722:LYS:HG2	2.01	0.42
1:D:4857:LEU:HD23	1:D:4857:LEU:HA	1.91	0.42
1:A:190:ARG:HD3	1:A:205:ALA:O	2.19	0.42
1:A:1088:PHE:HB2	1:A:1205:CYS:SG	2.60	0.42
1:A:1271:THR:OG1	1:A:1272:ARG:N	2.52	0.42
1:A:4000:ASP:O	1:A:4004:GLU:HG3	2.19	0.42
1:B:697:TRP:HB2	1:B:766:ILE:HD13	2.01	0.42
1:B:829:LYS:O	1:B:830:GLU:HG3	2.19	0.42
1:B:1706:LEU:O	1:B:1710:ILE:HG13	2.20	0.42
1:B:1789:LYS:HB2	1:B:1835:PHE:CE1	2.55	0.42
1:B:2722:LYS:HD2	1:B:2722:LYS:HA	1.63	0.42
1:B:4000:ASP:O	1:B:4004:GLU:HG3	2.19	0.42
1:C:2305:VAL:O	1:C:2312:VAL:HG22	2.20	0.42
1:C:4182:LYS:HA	1:C:4182:LYS:HD2	1.89	0.42
1:D:697:TRP:HB2	1:D:766:ILE:HD13	2.01	0.42
1:D:1827:TYR:CZ	1:D:1831:ILE:HD11	2.54	0.42
1:A:698:ALA:HA	1:A:724:SER:HA	2.00	0.42
1:A:1118:SER:HA	1:A:1134:ALA:HA	2.01	0.42
1:A:1233:GLN:HG3	1:B:3493:UNK:CB	2.49	0.42
1:A:1595:VAL:O	1:A:1595:VAL:HG23	2.20	0.42
1:A:2487:LEU:O	1:A:2492:LEU:HG	2.20	0.42
1:A:2876:LEU:O	1:A:2881:LYS:NZ	2.43	0.42
1:B:557:TRP:CE3	1:B:558:LEU:HD23	2.55	0.42
1:B:1608:ASP:OD1	1:B:1608:ASP:N	2.52	0.42
1:B:4913:ASN:HB3	1:B:4916:ASN:HB2	2.02	0.42
1:C:1706:LEU:O	1:C:1710:ILE:HG13	2.20	0.42
1:C:1789:LYS:HB2	1:C:1835:PHE:CE1	2.55	0.42
1:C:2471:LEU:HD23	1:C:2471:LEU:HA	1.80	0.42
1:C:4000:ASP:O	1:C:4004:GLU:HG3	2.19	0.42
1:C:4496:ASN:HD22	1:C:4499:ASN:HD22	1.66	0.42
1:D:843:GLU:HB3	1:D:1606:LYS:HD3	2.01	0.42
1:D:1744:ASN:ND2	1:D:1746:LYS:HE2	2.31	0.42
1:D:1789:LYS:HB2	1:D:1835:PHE:CE1	2.55	0.42
1:D:1959:ARG:HH21	1:D:1962:ARG:HH12	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4923:TYR:CZ	1:D:4927:LYS:HD2	2.55	0.42
2:J:53:LYS:HD3	2:J:53:LYS:HA	1.92	0.42
1:A:674:TYR:CE2	1:A:756:SER:HB2	2.54	0.42
1:A:1643:LEU:HD22	1:A:1694:TYR:O	2.20	0.42
1:A:4923:TYR:CZ	1:A:4927:LYS:HD2	2.54	0.42
1:B:1044:LYS:HD2	1:B:1044:LYS:HA	1.78	0.42
1:B:2837:HIS:ND1	1:B:2838:ALA:N	2.67	0.42
1:B:3905:PHE:O	1:B:3909:ILE:HG12	2.20	0.42
1:B:4189:VAL:HG21	1:B:4948:TRP:CZ2	2.55	0.42
2:H:27:TYR:N	2:H:40:SER:OG	2.51	0.42
1:C:438:LYS:HZ1	1:C:441:LYS:HD2	1.84	0.42
1:C:557:TRP:CE3	1:C:558:LEU:HD23	2.55	0.42
1:C:2837:HIS:ND1	1:C:2838:ALA:N	2.67	0.42
1:C:4287:TRP:O	1:C:4291:VAL:HG13	2.19	0.42
1:D:698:ALA:HA	1:D:724:SER:HA	2.00	0.42
1:D:1643:LEU:HD22	1:D:1694:TYR:O	2.20	0.42
1:A:697:TRP:HB2	1:A:766:ILE:HD13	2.01	0.42
1:A:1835:PHE:O	1:A:1840:LEU:HD12	2.20	0.42
1:A:3905:PHE:O	1:A:3909:ILE:HG12	2.20	0.42
1:B:245:LEU:HD11	1:B:260:VAL:HG12	2.01	0.42
1:B:987:LYS:HE2	1:B:987:LYS:HB3	1.92	0.42
1:B:1303:ARG:NH2	1:B:1590:GLN:OE1	2.53	0.42
1:B:1595:VAL:HG23	1:B:1595:VAL:O	2.20	0.42
1:B:1835:PHE:O	1:B:1840:LEU:HD12	2.20	0.42
1:B:4660:TYR:HB3	1:B:4664:ARG:HH21	1.85	0.42
1:B:4807:ASP:HB3	1:B:4810:THR:HB	2.00	0.42
1:C:247:VAL:O	1:C:272:ARG:NH1	2.44	0.42
1:C:661:LEU:HD13	1:C:673:TRP:CD1	2.54	0.42
1:C:693:LEU:HD13	1:C:798:ILE:HG12	2.02	0.42
1:C:899:GLU:HG2	1:C:971:GLN:HE22	1.84	0.42
1:C:1088:PHE:HB2	1:C:1205:CYS:SG	2.60	0.42
1:C:1668:LEU:HD23	1:C:2131:VAL:HG22	2.02	0.42
1:C:4807:ASP:HB3	1:C:4810:THR:HB	2.00	0.42
1:D:34:LYS:O	1:D:52:THR:OG1	2.37	0.42
1:D:1367:LYS:NZ	1:D:1369:GLU:OE2	2.35	0.42
1:D:1608:ASP:OD1	1:D:1608:ASP:N	2.52	0.42
1:D:1682:ASP:HB3	1:D:1684:PRO:HD2	2.01	0.42
1:D:2305:VAL:O	1:D:2312:VAL:HG22	2.20	0.42
1:D:4569:PRO:HB3	1:D:4572:ARG:HH21	1.85	0.42
1:D:4670:GLY:O	1:D:4671:MET:HG2	2.19	0.42
1:A:547:ASN:OD1	1:A:547:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1641:ASP:HB2	1:A:1644:GLU:HG3	2.00	0.42
1:A:1668:LEU:HD23	1:A:2131:VAL:HG22	2.02	0.42
1:A:1789:LYS:HB2	1:A:1835:PHE:CE1	2.55	0.42
2:G:27:TYR:N	2:G:40:SER:OG	2.51	0.42
1:B:161:THR:HG23	1:B:184:VAL:HB	2.01	0.42
1:B:1217:PHE:O	1:B:1240:ALA:N	2.52	0.42
1:B:1271:THR:OG1	1:B:1272:ARG:N	2.52	0.42
1:B:2755:LEU:HD12	1:B:2767:LYS:CD	2.50	0.42
1:B:3636:GLU:HG2	1:B:3696:LYS:HE3	2.01	0.42
1:B:4923:TYR:CZ	1:B:4927:LYS:HD2	2.54	0.42
1:C:833:LYS:HE3	1:C:834:VAL:N	2.33	0.42
1:C:840:TYR:CE2	1:C:850:LEU:HA	2.55	0.42
1:C:1608:ASP:OD1	1:C:1608:ASP:N	2.52	0.42
1:C:4913:ASN:HB3	1:C:4916:ASN:HB2	2.02	0.42
1:D:161:THR:HG23	1:D:184:VAL:HB	2.01	0.42
1:D:674:TYR:HB2	1:D:819:TYR:HB3	2.02	0.42
1:D:1088:PHE:HB2	1:D:1205:CYS:SG	2.60	0.42
1:D:1273:ILE:HG13	1:D:1274:ASP:N	2.32	0.42
1:D:3636:GLU:HG2	1:D:3696:LYS:HE3	2.01	0.42
1:D:4913:ASN:HB3	1:D:4916:ASN:HB2	2.02	0.42
1:A:28:ILE:HG21	1:A:201:TRP:HH2	1.85	0.42
1:A:658:ASN:HB2	1:A:832:LEU:HD12	2.01	0.42
1:A:4632:LEU:H	1:A:4632:LEU:HD23	1.85	0.42
1:B:2487:LEU:O	1:B:2492:LEU:HG	2.20	0.42
1:B:4079:TYR:HA	1:B:4082:PHE:HB3	2.02	0.42
1:C:245:LEU:HD11	1:C:260:VAL:HG12	2.01	0.42
1:C:674:TYR:CE2	1:C:756:SER:HB2	2.54	0.42
1:C:692:HIS:NE2	1:C:793:SER:OG	2.47	0.42
1:C:745:ASN:O	1:C:747:HIS:ND1	2.49	0.42
1:C:802:PHE:HB2	1:C:1618:TRP:HB2	2.01	0.42
1:C:1044:LYS:HD2	1:C:1044:LYS:HA	1.78	0.42
1:C:3905:PHE:O	1:C:3909:ILE:HG12	2.20	0.42
1:C:4189:VAL:HG21	1:C:4948:TRP:CZ2	2.55	0.42
1:D:557:TRP:CZ2	1:D:561:ARG:HG3	2.55	0.42
1:D:840:TYR:CE2	1:D:850:LEU:HA	2.55	0.42
1:D:1040:ASP:HA	1:D:1043:LYS:HG3	2.01	0.42
1:D:1217:PHE:O	1:D:1240:ALA:N	2.52	0.42
1:D:1303:ARG:NH2	1:D:1590:GLN:OE1	2.53	0.42
1:D:1595:VAL:O	1:D:1595:VAL:HG23	2.20	0.42
1:D:1987:CYS:N	1:D:1988:PRO:HD2	2.34	0.42
1:D:4047:PHE:O	1:D:4051:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:TRP:CZ2	1:A:561:ARG:HG3	2.55	0.41
1:A:894:VAL:HG13	1:A:918:LEU:HB3	2.01	0.41
1:A:1303:ARG:NH2	1:A:1590:GLN:OE1	2.53	0.41
1:A:1977:ASN:OD1	1:A:1977:ASN:N	2.53	0.41
1:A:4569:PRO:HB3	1:A:4572:ARG:HH21	1.85	0.41
1:B:290:ARG:H	1:B:293:GLN:NE2	2.15	0.41
1:B:899:GLU:HG2	1:B:971:GLN:HE22	1.84	0.41
1:B:1643:LEU:HD22	1:B:1694:TYR:O	2.20	0.41
1:B:1744:ASN:ND2	1:B:1746:LYS:HE2	2.30	0.41
1:B:3802:LEU:HB2	1:B:3883:SER:OG	2.20	0.41
1:C:190:ARG:HD3	1:C:205:ALA:O	2.19	0.41
1:C:375:GLN:NE2	1:C:390:LYS:O	2.53	0.41
1:C:557:TRP:CZ2	1:C:561:ARG:HG3	2.55	0.41
1:C:2487:LEU:O	1:C:2492:LEU:HG	2.20	0.41
1:C:3636:GLU:HG2	1:C:3696:LYS:HE3	2.01	0.41
1:C:3825:GLY:O	1:C:3828:VAL:HG12	2.20	0.41
1:D:669:GLN:HB3	1:D:673:TRP:HZ2	1.85	0.41
1:D:845:THR:OG1	1:D:846:TYR:N	2.51	0.41
1:D:2486:LEU:HD13	1:D:2486:LEU:HA	1.87	0.41
1:D:4079:TYR:HA	1:D:4082:PHE:HB3	2.02	0.41
1:A:125:TYR:CE1	1:A:417:ARG:HD3	2.55	0.41
1:A:2837:HIS:ND1	1:A:2838:ALA:N	2.67	0.41
1:A:4913:ASN:HB3	1:A:4916:ASN:HB2	2.02	0.41
1:B:557:TRP:CZ2	1:B:561:ARG:HG3	2.55	0.41
1:B:3825:GLY:O	1:B:3828:VAL:HG12	2.20	0.41
1:C:323:ASP:O	1:C:327:THR:OG1	2.27	0.41
1:C:843:GLU:HB3	1:C:1606:LYS:HD3	2.01	0.41
1:C:1744:ASN:ND2	1:C:1746:LYS:HE2	2.30	0.41
1:C:1977:ASN:OD1	1:C:1977:ASN:N	2.53	0.41
1:C:4175:VAL:HG22	1:C:4187:LEU:HD13	2.02	0.41
1:D:125:TYR:CE1	1:D:417:ARG:HD3	2.56	0.41
1:D:1706:LEU:O	1:D:1710:ILE:HG13	2.20	0.41
1:D:2487:LEU:O	1:D:2492:LEU:HG	2.20	0.41
1:D:2755:LEU:HD12	1:D:2767:LYS:CD	2.50	0.41
1:A:557:TRP:CE3	1:A:558:LEU:HD23	2.55	0.41
1:A:745:ASN:O	1:A:747:HIS:ND1	2.49	0.41
1:A:1040:ASP:HA	1:A:1043:LYS:HG3	2.01	0.41
1:A:1706:LEU:O	1:A:1710:ILE:HG13	2.20	0.41
1:A:1744:ASN:ND2	1:A:1746:LYS:HE2	2.30	0.41
1:A:1931:PHE:CE1	1:A:1995:LEU:HB2	2.55	0.41
1:A:4051:MET:HE1	1:A:4065:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4928:ASP:OD1	1:A:4929:GLU:N	2.46	0.41
2:G:53:LYS:HD3	2:G:53:LYS:HA	1.92	0.41
1:B:541:ILE:HD11	1:B:574:VAL:HG13	2.02	0.41
1:B:547:ASN:OD1	1:B:547:ASN:N	2.53	0.41
1:B:658:ASN:HB2	1:B:832:LEU:HD12	2.01	0.41
1:B:1682:ASP:HB3	1:B:1684:PRO:HD2	2.01	0.41
1:B:4574:LEU:HD12	1:B:4574:LEU:HA	1.90	0.41
1:C:34:LYS:O	1:C:52:THR:OG1	2.37	0.41
1:C:125:TYR:CE1	1:C:417:ARG:HD3	2.56	0.41
1:C:1303:ARG:NH2	1:C:1590:GLN:OE1	2.53	0.41
1:D:28:ILE:HG21	1:D:201:TRP:HH2	1.85	0.41
1:D:557:TRP:CE3	1:D:558:LEU:HD23	2.55	0.41
1:D:1682:ASP:CB	1:D:1685:GLN:HB3	2.48	0.41
1:D:4051:MET:HE1	1:D:4065:LEU:HB2	2.02	0.41
1:D:4608:LYS:HG2	1:D:4614:LEU:HD22	2.03	0.41
1:D:4941:LYS:O	1:D:4945:GLU:HG3	2.21	0.41
1:A:669:GLN:HB3	1:A:673:TRP:HZ2	1.86	0.41
1:A:802:PHE:HB2	1:A:1618:TRP:HB2	2.01	0.41
1:A:1682:ASP:HB3	1:A:1684:PRO:HD2	2.01	0.41
1:A:3758:LEU:O	1:A:3762:ILE:HG12	2.19	0.41
1:A:4189:VAL:HG21	1:A:4948:TRP:CZ2	2.55	0.41
1:B:1118:SER:HA	1:B:1134:ALA:HA	2.01	0.41
1:B:3719:GLU:HA	1:B:3722:LYS:HG2	2.02	0.41
1:B:3870:ILE:H	1:B:3870:ILE:HG12	1.67	0.41
1:B:4175:VAL:HG22	1:B:4187:LEU:HD13	2.02	0.41
1:B:4569:PRO:HB3	1:B:4572:ARG:HH21	1.85	0.41
1:C:318:ASP:OD1	1:C:318:ASP:N	2.54	0.41
1:C:3719:GLU:HA	1:C:3722:LYS:HG2	2.02	0.41
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.85	0.41
1:D:2282:LYS:HA	1:D:2282:LYS:HD2	1.90	0.41
1:D:4171:PHE:CE1	1:D:4175:VAL:HG21	2.56	0.41
1:D:4660:TYR:HB3	1:D:4664:ARG:HH21	1.85	0.41
1:A:1091:GLU:HG2	1:A:1093:THR:H	1.85	0.41
1:A:1987:CYS:N	1:A:1988:PRO:HD2	2.34	0.41
1:A:4941:LYS:O	1:A:4945:GLU:HG3	2.21	0.41
1:C:1091:GLU:HG2	1:C:1093:THR:H	1.85	0.41
1:C:1740:PHE:CD1	1:C:1923:ALA:HB1	2.56	0.41
1:C:2755:LEU:HD12	1:C:2767:LYS:CD	2.50	0.41
1:D:1809:ASP:N	1:D:1809:ASP:OD1	2.54	0.41
1:D:2722:LYS:HD2	1:D:2722:LYS:HA	1.63	0.41
1:A:16:THR:OG1	1:A:109:GLY:O	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:HIS:C	1:A:399:MET:HE2	2.46	0.41
1:A:693:LEU:HD13	1:A:798:ILE:HG12	2.01	0.41
1:A:840:TYR:CE2	1:A:850:LEU:HA	2.55	0.41
1:A:1086:ARG:HH21	1:A:1251:LEU:HD13	1.86	0.41
1:A:1829:LEU:O	1:A:1834:ILE:HG12	2.21	0.41
1:A:2733:MET:O	1:A:2736:LEU:HG	2.21	0.41
1:A:2755:LEU:HD12	1:A:2767:LYS:CD	2.50	0.41
1:A:4171:PHE:CE1	1:A:4175:VAL:HG21	2.56	0.41
1:B:888:ASN:O	1:B:891:GLU:HG2	2.21	0.41
1:B:1641:ASP:HB2	1:B:1644:GLU:HG3	2.00	0.41
1:B:1931:PHE:CE1	1:B:1995:LEU:HB2	2.55	0.41
1:B:4171:PHE:CE1	1:B:4175:VAL:HG21	2.56	0.41
1:C:1643:LEU:HD22	1:C:1694:TYR:O	2.20	0.41
1:C:1809:ASP:OD1	1:C:1809:ASP:N	2.54	0.41
1:C:1827:TYR:CZ	1:C:1831:ILE:HD11	2.54	0.41
1:C:1829:LEU:O	1:C:1834:ILE:HG12	2.21	0.41
1:C:1835:PHE:O	1:C:1840:LEU:HD12	2.20	0.41
1:C:1959:ARG:HH21	1:C:1962:ARG:HH12	1.68	0.41
1:C:3802:LEU:HB2	1:C:3883:SER:OG	2.20	0.41
1:C:4047:PHE:O	1:C:4051:MET:HG2	2.20	0.41
1:C:4569:PRO:HB3	1:C:4572:ARG:HH21	1.85	0.41
1:C:4632:LEU:HD23	1:C:4632:LEU:H	1.85	0.41
1:D:323:ASP:O	1:D:327:THR:OG1	2.27	0.41
1:D:748:LEU:HD23	1:D:748:LEU:HA	1.91	0.41
1:D:1740:PHE:CD1	1:D:1923:ALA:HB1	2.56	0.41
1:D:1931:PHE:CE1	1:D:1995:LEU:HB2	2.56	0.41
1:D:4044:LYS:HE2	1:D:4044:LYS:HB3	1.82	0.41
1:A:245:LEU:HD11	1:A:260:VAL:HG12	2.01	0.41
1:A:674:TYR:HB2	1:A:819:TYR:HB3	2.02	0.41
1:A:773:GLN:H	1:A:773:GLN:HG2	1.70	0.41
1:A:3636:GLU:HG2	1:A:3696:LYS:HE3	2.02	0.41
1:A:3802:LEU:HB2	1:A:3883:SER:OG	2.21	0.41
1:B:318:ASP:OD1	1:B:318:ASP:N	2.54	0.41
1:B:398:HIS:C	1:B:399:MET:HE2	2.46	0.41
1:B:1088:PHE:HB2	1:B:1205:CYS:SG	2.60	0.41
1:B:2340:ASN:OD1	1:B:2340:ASN:N	2.46	0.41
1:C:669:GLN:HB3	1:C:673:TRP:HZ2	1.85	0.41
1:C:888:ASN:O	1:C:891:GLU:HG2	2.21	0.41
1:C:1567:LEU:HD11	1:C:1579:PRO:C	2.45	0.41
1:C:1609:VAL:HG12	1:C:1611:ARG:H	1.86	0.41
1:C:1931:PHE:CE1	1:C:1995:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4928:ASP:OD1	1:C:4929:GLU:N	2.46	0.41
1:D:557:TRP:CE2	1:D:561:ARG:HG3	2.56	0.41
1:D:1829:LEU:O	1:D:1834:ILE:HG12	2.21	0.41
1:D:1835:PHE:O	1:D:1840:LEU:HD12	2.20	0.41
1:D:2188:PHE:HB3	1:D:2191:MET:HB3	2.03	0.41
1:D:2733:MET:O	1:D:2736:LEU:HG	2.21	0.41
1:A:987:LYS:HE2	1:A:987:LYS:HB3	1.92	0.41
1:A:1682:ASP:CB	1:A:1685:GLN:HB3	2.48	0.41
1:A:4079:TYR:HA	1:A:4082:PHE:HB3	2.02	0.41
1:B:125:TYR:CE1	1:B:417:ARG:HD3	2.56	0.41
1:B:557:TRP:CE2	1:B:561:ARG:HG3	2.56	0.41
1:B:1809:ASP:N	1:B:1809:ASP:OD1	2.54	0.41
1:B:2733:MET:O	1:B:2736:LEU:HG	2.21	0.41
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.85	0.41
1:C:290:ARG:H	1:C:293:GLN:NE2	2.15	0.41
1:C:557:TRP:CE2	1:C:561:ARG:HG3	2.56	0.41
1:C:674:TYR:HB2	1:C:819:TYR:HB3	2.02	0.41
1:C:1031:ARG:HA	1:C:1031:ARG:HD3	1.84	0.41
1:C:1682:ASP:HB3	1:C:1684:PRO:HD2	2.01	0.41
1:C:4660:TYR:HB3	1:C:4664:ARG:HH21	1.85	0.41
1:D:541:ILE:HD11	1:D:574:VAL:HG13	2.02	0.41
1:D:802:PHE:HB2	1:D:1618:TRP:HB2	2.01	0.41
1:D:1086:ARG:HH21	1:D:1251:LEU:HD13	1.86	0.41
2:J:11:GLY:O	2:J:68:SER:OG	2.32	0.41
1:A:34:LYS:O	1:A:52:THR:OG1	2.37	0.41
1:A:527:LYS:NZ	1:A:531:ASN:OD1	2.38	0.41
1:A:1567:LEU:HD11	1:A:1579:PRO:C	2.45	0.41
1:A:1959:ARG:HH21	1:A:1962:ARG:HH12	1.68	0.41
1:A:2305:VAL:O	1:A:2312:VAL:HG22	2.20	0.41
1:A:4608:LYS:HG2	1:A:4614:LEU:HD22	2.03	0.41
1:A:4660:TYR:HB3	1:A:4664:ARG:HH21	1.85	0.41
1:A:4794:LYS:HE3	1:A:4794:LYS:HB3	1.95	0.41
2:G:11:GLY:O	2:G:68:SER:OG	2.32	0.41
2:G:28:THR:O	2:G:28:THR:OG1	2.36	0.41
1:B:16:THR:OG1	1:B:109:GLY:O	2.35	0.41
1:B:530:LEU:HD23	1:B:530:LEU:HA	1.87	0.41
1:B:840:TYR:CE2	1:B:850:LEU:HA	2.55	0.41
1:B:1086:ARG:HH21	1:B:1251:LEU:HD13	1.86	0.41
1:B:1091:GLU:HG2	1:B:1093:THR:H	1.85	0.41
1:B:1829:LEU:O	1:B:1834:ILE:HG12	2.21	0.41
1:B:2234:ARG:HD2	1:B:2234:ARG:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2260:ASP:N	1:B:2260:ASP:OD1	2.54	0.41
1:B:2305:VAL:O	1:B:2312:VAL:HG22	2.20	0.41
1:B:2887:LYS:O	1:B:2891:ILE:HG23	2.21	0.41
1:B:4047:PHE:O	1:B:4051:MET:HG2	2.20	0.41
1:B:4608:LYS:HG2	1:B:4614:LEU:HD22	2.03	0.41
1:B:4632:LEU:HD23	1:B:4632:LEU:H	1.85	0.41
1:B:4867:ASP:OD1	1:C:4873:ARG:NH1	2.54	0.41
1:C:640:ARG:HH22	2:I:91:VAL:HG13	1.86	0.41
1:C:1086:ARG:HH21	1:C:1251:LEU:HD13	1.86	0.41
1:C:1091:GLU:HB3	1:C:1094:TYR:CD2	2.52	0.41
1:C:1595:VAL:HG23	1:C:1595:VAL:O	2.20	0.41
1:C:4171:PHE:CE1	1:C:4175:VAL:HG21	2.56	0.41
1:C:4636:THR:OG1	1:C:4637:GLN:N	2.54	0.41
1:C:4941:LYS:O	1:C:4945:GLU:HG3	2.21	0.41
1:D:309:MET:HB2	1:D:312:LYS:HZ3	1.85	0.41
1:D:987:LYS:HE2	1:D:987:LYS:HB3	1.92	0.41
1:D:1091:GLU:HG2	1:D:1093:THR:H	1.85	0.41
1:D:3802:LEU:HB2	1:D:3883:SER:OG	2.21	0.41
1:D:4304:PHE:O	1:D:4308:VAL:HG22	2.21	0.41
1:D:4594:VAL:N	1:D:4595:PRO:HD2	2.36	0.41
1:D:4794:LYS:HE3	1:D:4794:LYS:HB3	1.96	0.41
1:A:850:LEU:H	1:A:850:LEU:HG	1.57	0.41
1:A:1740:PHE:CD1	1:A:1923:ALA:HB1	2.56	0.41
1:A:3825:GLY:O	1:A:3828:VAL:HG12	2.20	0.41
1:B:28:ILE:HG21	1:B:201:TRP:HH2	1.85	0.41
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.93	0.41
1:B:693:LEU:HD13	1:B:798:ILE:HG12	2.02	0.41
1:B:1363:LYS:HE2	1:B:1365:THR:HG22	2.03	0.41
1:B:1567:LEU:HD11	1:B:1579:PRO:C	2.45	0.41
1:B:3612:ARG:O	1:B:3612:ARG:NH1	2.54	0.41
1:C:541:ILE:HD11	1:C:574:VAL:HG13	2.02	0.41
1:C:4079:TYR:HA	1:C:4082:PHE:HB3	2.02	0.41
1:C:4594:VAL:N	1:C:4595:PRO:HD2	2.36	0.41
1:D:1567:LEU:HD11	1:D:1579:PRO:C	2.45	0.41
1:D:1668:LEU:HD23	1:D:2131:VAL:HG22	2.02	0.41
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.85	0.41
1:A:318:ASP:OD1	1:A:318:ASP:N	2.54	0.40
1:A:380:LYS:HA	1:A:380:LYS:HD3	1.71	0.40
1:A:4304:PHE:O	1:A:4308:VAL:HG22	2.21	0.40
1:B:1740:PHE:CD1	1:B:1923:ALA:HB1	2.56	0.40
1:C:2260:ASP:OD1	1:C:2260:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2331:GLY:HA3	1:C:2391:TYR:CE1	2.56	0.40
1:C:4924:LEU:HD23	1:C:4924:LEU:HA	1.92	0.40
1:D:644:LEU:HD11	1:D:1651:LEU:HD22	2.03	0.40
1:D:3870:ILE:H	1:D:3870:ILE:HG12	1.67	0.40
1:D:4164:VAL:HA	1:D:4167:SER:OG	2.21	0.40
1:A:888:ASN:O	1:A:891:GLU:HG2	2.21	0.40
1:A:1003:ALA:O	1:A:1006:VAL:HG22	2.22	0.40
1:A:1363:LYS:HE2	1:A:1365:THR:HG22	2.03	0.40
1:A:4047:PHE:O	1:A:4051:MET:HG2	2.20	0.40
1:A:4276:LYS:NZ	1:A:4562:GLU:HG3	2.36	0.40
1:A:4862:GLN:HG2	1:D:4859:ALA:HB2	2.03	0.40
1:B:674:TYR:HB2	1:B:819:TYR:HB3	2.02	0.40
1:B:2747:SER:O	1:B:2753:GLN:NE2	2.49	0.40
1:C:4276:LYS:NZ	1:C:4562:GLU:HG3	2.36	0.40
1:D:527:LYS:NZ	1:D:531:ASN:OD1	2.38	0.40
1:D:693:LEU:HD13	1:D:798:ILE:HG12	2.02	0.40
1:D:3825:GLY:O	1:D:3828:VAL:HG12	2.20	0.40
1:D:4830:ILE:HB	1:D:4842:ARG:NH2	2.36	0.40
1:A:313:ASN:HD21	1:A:392:ILE:HA	1.87	0.40
1:A:373:THR:O	1:A:375:GLN:NE2	2.43	0.40
1:A:541:ILE:HD11	1:A:574:VAL:HG13	2.02	0.40
1:A:557:TRP:CE2	1:A:561:ARG:HG3	2.56	0.40
1:A:1131:ASP:HB3	1:A:1133:ARG:HG2	2.04	0.40
1:A:1809:ASP:N	1:A:1809:ASP:OD1	2.54	0.40
1:A:2260:ASP:N	1:A:2260:ASP:OD1	2.54	0.40
1:A:2331:GLY:HA3	1:A:2391:TYR:CE1	2.56	0.40
1:A:2887:LYS:O	1:A:2891:ILE:HG23	2.21	0.40
1:A:4164:VAL:HA	1:A:4167:SER:OG	2.22	0.40
1:A:4276:LYS:HZ1	1:A:4562:GLU:HG3	1.86	0.40
1:A:4594:VAL:N	1:A:4595:PRO:HD2	2.36	0.40
1:A:4857:LEU:HD23	1:A:4857:LEU:HA	1.91	0.40
1:B:669:GLN:HB3	1:B:673:TRP:HZ2	1.85	0.40
1:B:1131:ASP:HB3	1:B:1133:ARG:HG2	2.04	0.40
1:B:2065:MET:SD	1:B:2083:MET:HG3	2.62	0.40
1:B:4001:MET:HE2	1:B:4001:MET:HB2	1.95	0.40
1:C:502:ILE:HG22	1:C:506:HIS:CD2	2.56	0.40
1:C:530:LEU:HD23	1:C:530:LEU:HA	1.87	0.40
1:C:1682:ASP:CB	1:C:1685:GLN:HB3	2.48	0.40
1:C:2733:MET:O	1:C:2736:LEU:HG	2.21	0.40
1:C:3954:GLN:NE2	1:C:3971:MET:SD	2.95	0.40
1:D:313:ASN:HD21	1:D:392:ILE:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:HIS:C	1:D:399:MET:HE2	2.46	0.40
1:D:1609:VAL:HG12	1:D:1611:ARG:H	1.86	0.40
1:D:4632:LEU:HD23	1:D:4632:LEU:H	1.85	0.40
1:A:1609:VAL:HG12	1:A:1611:ARG:H	1.86	0.40
1:A:1731:THR:O	1:A:1735:LYS:HG3	2.21	0.40
1:A:2166:MET:HE3	1:A:2166:MET:HB2	1.92	0.40
1:B:773:GLN:H	1:B:773:GLN:HG2	1.70	0.40
1:B:1003:ALA:O	1:B:1006:VAL:HG22	2.22	0.40
1:B:4010:GLU:HG2	1:B:4120:LEU:HD13	2.03	0.40
1:C:547:ASN:OD1	1:C:547:ASN:N	2.53	0.40
1:C:678:MET:HA	1:C:753:ASP:O	2.22	0.40
1:C:1982:LYS:HD2	1:C:1983:SER:H	1.86	0.40
1:C:2085:VAL:HG12	1:C:3686:LEU:HD13	2.03	0.40
1:C:2134:GLY:H	1:C:2137:GLU:HB2	1.87	0.40
1:C:2188:PHE:HB3	1:C:2191:MET:HB3	2.03	0.40
1:C:2859:LEU:HD22	1:C:2859:LEU:HA	1.93	0.40
1:C:3874:VAL:HG11	1:C:3937:SER:OG	2.22	0.40
1:C:4083:VAL:O	1:C:4087:HIS:HB3	2.22	0.40
1:C:4093:ILE:O	1:C:4097:VAL:HG23	2.22	0.40
1:C:4164:VAL:HA	1:C:4167:SER:OG	2.21	0.40
1:C:4185:MET:HE1	1:C:4889:ILE:HA	2.04	0.40
1:D:418:VAL:O	1:D:422:THR:HG23	2.22	0.40
1:D:888:ASN:O	1:D:891:GLU:HG2	2.21	0.40
1:D:1733:GLU:O	1:D:1736:SER:OG	2.32	0.40
1:D:2085:VAL:HG12	1:D:3686:LEU:HD13	2.03	0.40
1:D:2260:ASP:OD1	1:D:2260:ASP:N	2.54	0.40
1:D:3762:ILE:HD12	1:D:3840:ARG:HG3	2.03	0.40
1:A:1289:SER:HA	1:A:1353:HIS:HB3	2.04	0.40
1:B:502:ILE:HG22	1:B:506:HIS:CD2	2.56	0.40
1:B:1127:GLU:HG3	1:B:1128:LEU:N	2.37	0.40
1:B:1982:LYS:HD2	1:B:1983:SER:H	1.86	0.40
1:B:4185:MET:HE1	1:B:4889:ILE:HA	2.04	0.40
1:B:4589:TYR:OH	1:B:4715:ASP:OD2	2.38	0.40
1:B:4594:VAL:N	1:B:4595:PRO:HD2	2.36	0.40
1:B:4603:LYS:HD2	1:B:4607:ARG:NH1	2.37	0.40
1:C:1003:ALA:O	1:C:1006:VAL:HG22	2.22	0.40
2:I:26:HIS:HD2	2:I:40:SER:OG	2.05	0.40
1:D:37:LEU:HD13	1:D:203:VAL:HG21	2.04	0.40
1:D:479:LEU:HD23	1:D:482:LEU:HD21	2.04	0.40
1:D:678:MET:HA	1:D:753:ASP:O	2.22	0.40
1:D:745:ASN:O	1:D:747:HIS:ND1	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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%)	3051 (94%)	204 (6%)	0	100	100
1	B	3255/4966 (66%)	3050 (94%)	205 (6%)	0	100	100
1	C	3255/4966 (66%)	3050 (94%)	205 (6%)	0	100	100
1	D	3255/4966 (66%)	3049 (94%)	206 (6%)	0	100	100
2	G	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	H	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	I	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
2	J	105/176 (60%)	102 (97%)	3 (3%)	0	100	100
All	All	13440/20568 (65%)	12608 (94%)	832 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

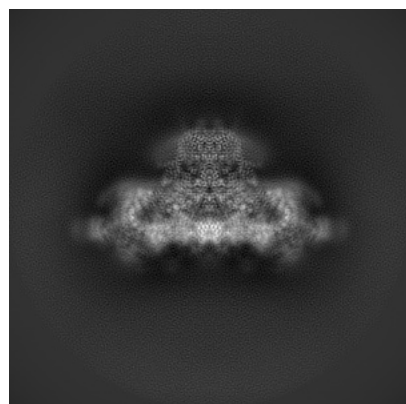
6 Map visualisation [i](#)

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

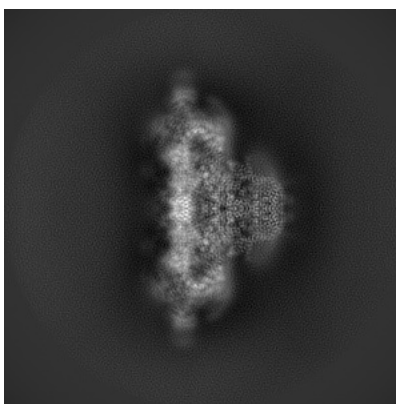
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

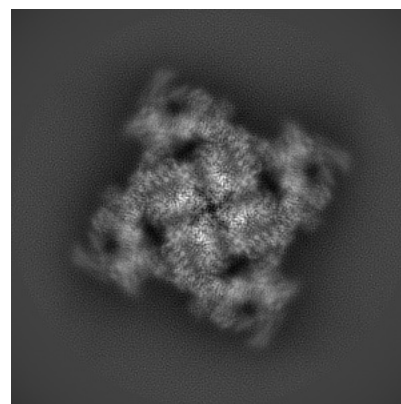
6.1.1 Primary map



X

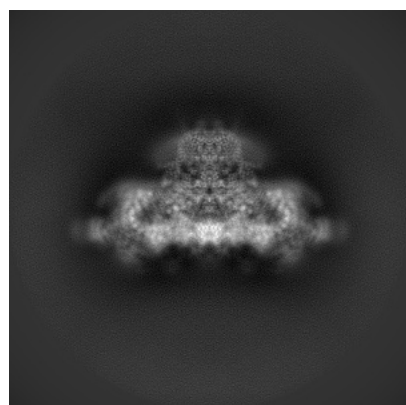


Y

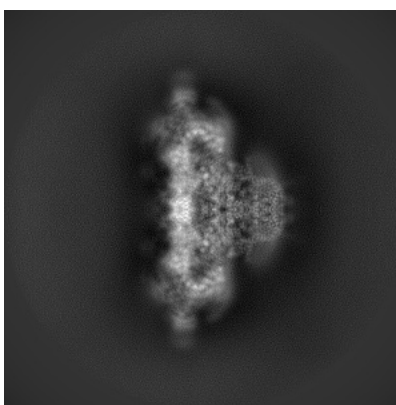


Z

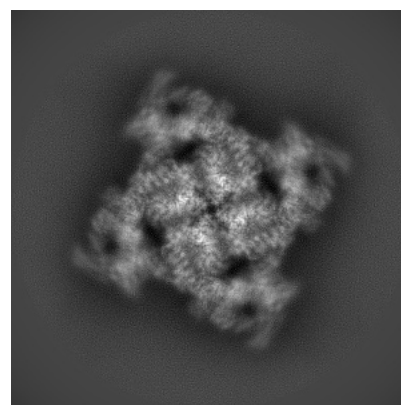
6.1.2 Raw map



X



Y

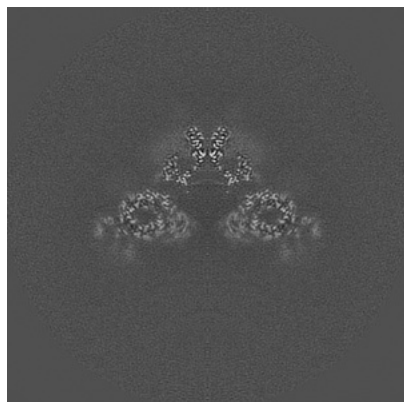


Z

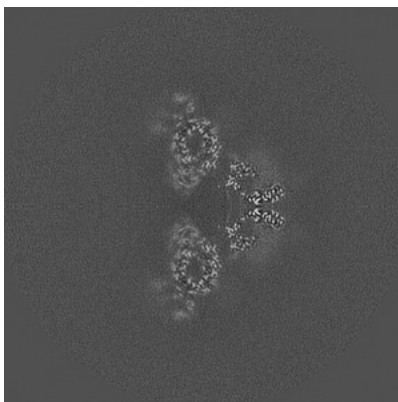
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

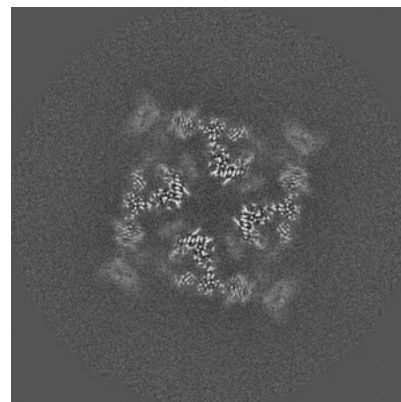
6.2.1 Primary map



X Index: 200

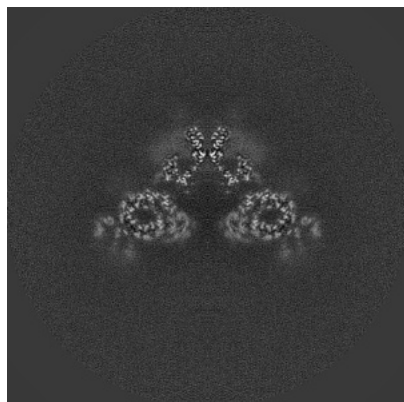


Y Index: 200

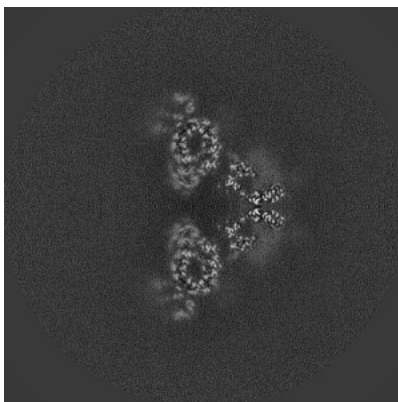


Z Index: 200

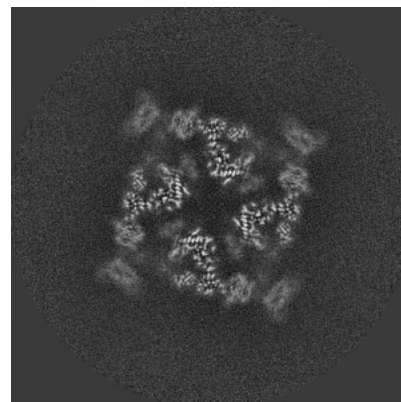
6.2.2 Raw map



X Index: 200



Y Index: 200

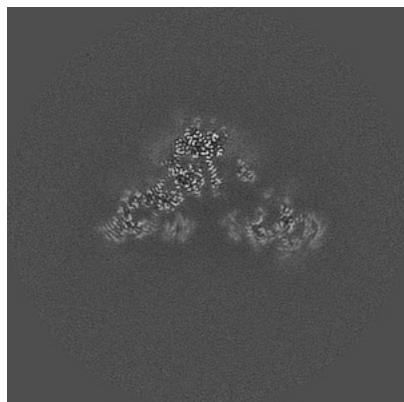


Z Index: 200

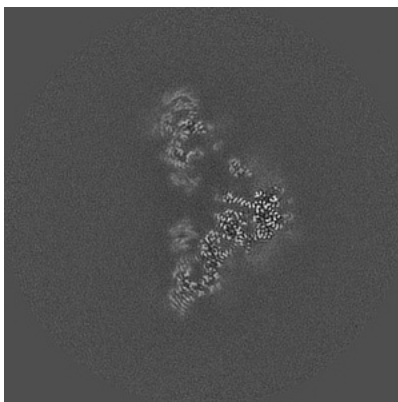
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

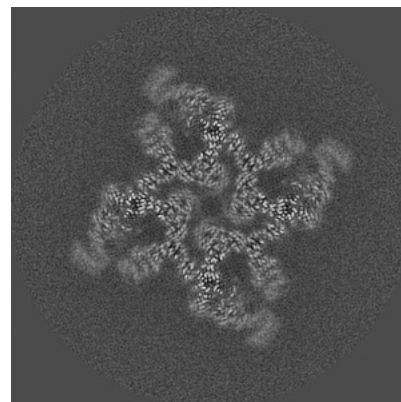
6.3.1 Primary map



X Index: 193

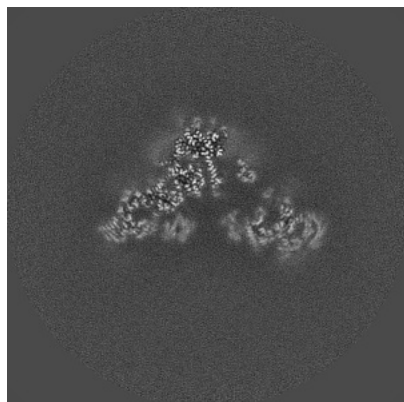


Y Index: 207

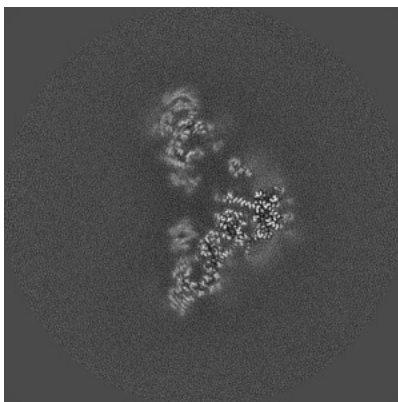


Z Index: 180

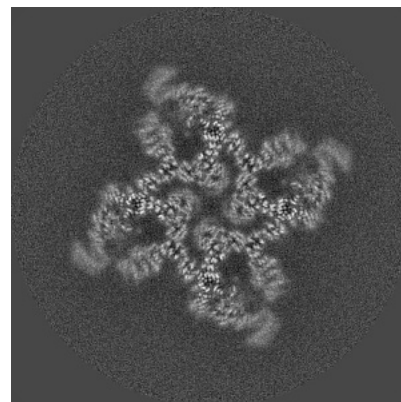
6.3.2 Raw map



X Index: 193



Y Index: 207

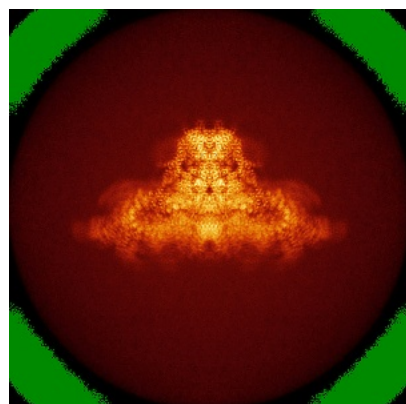


Z Index: 180

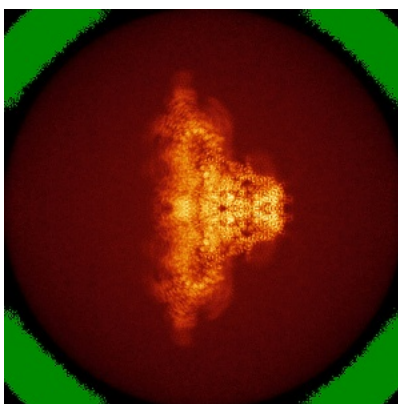
The images above show the largest variance slices of the map in three orthogonal directions.

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

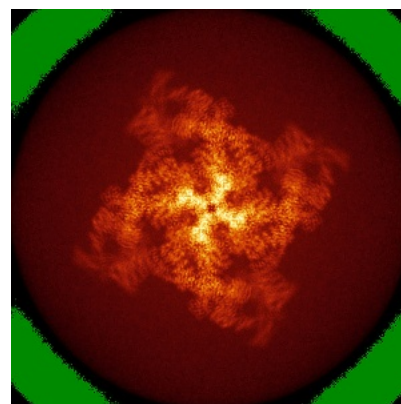
6.4.1 Primary map



X

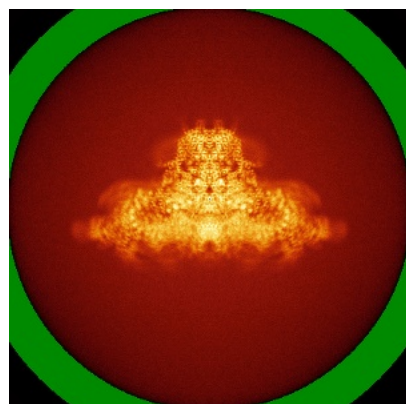


Y

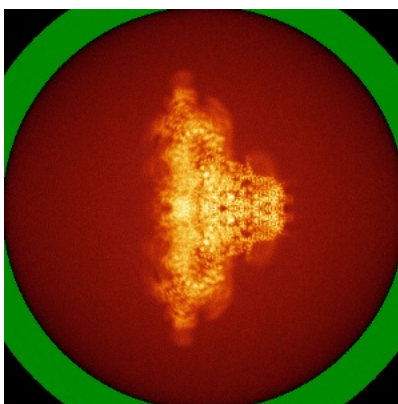


Z

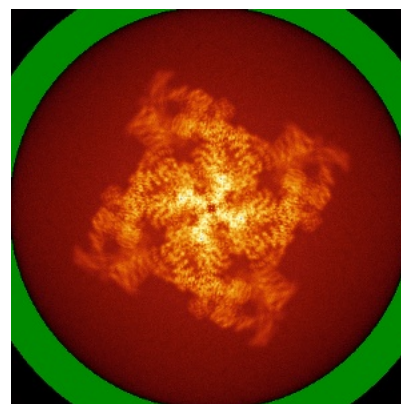
6.4.2 Raw map



X



Y

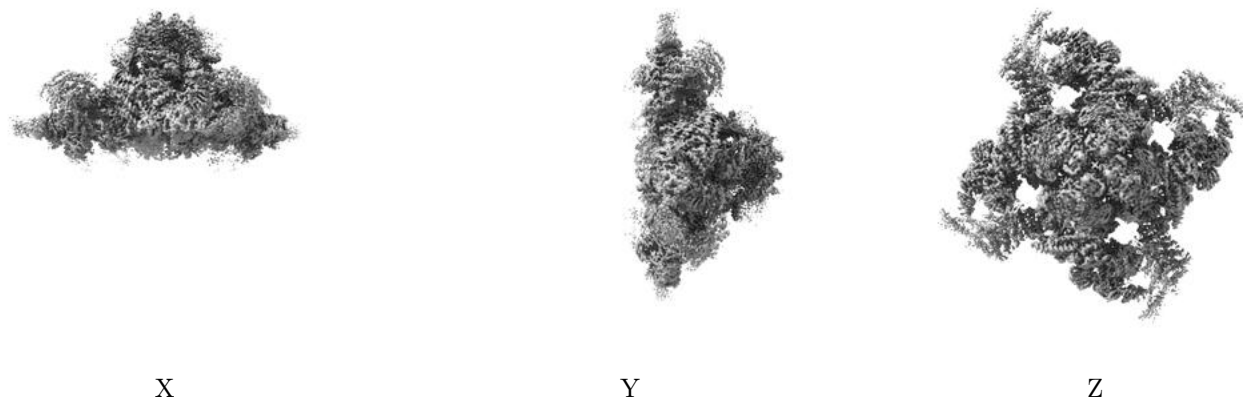


Z

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 0.019. 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.

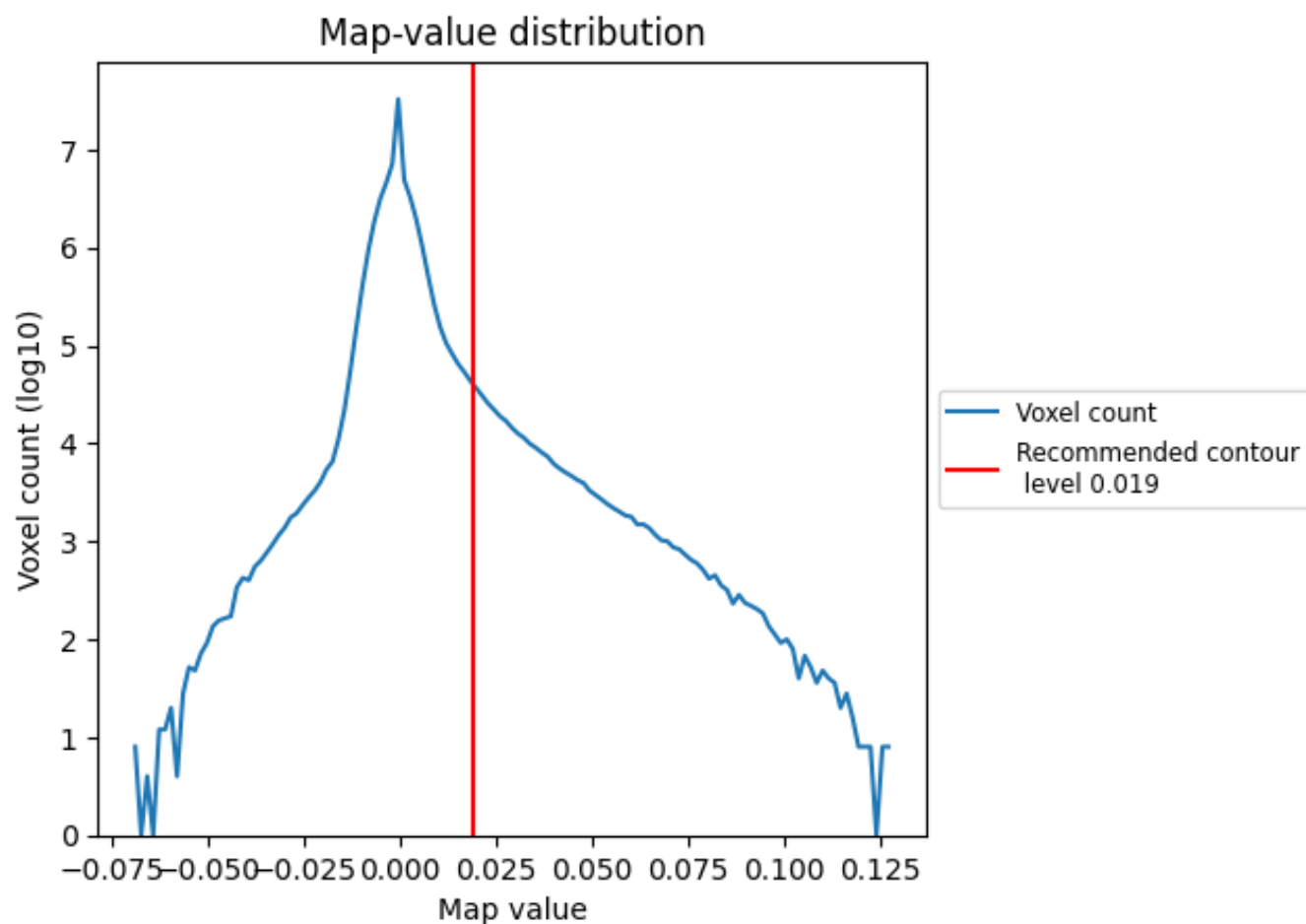
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

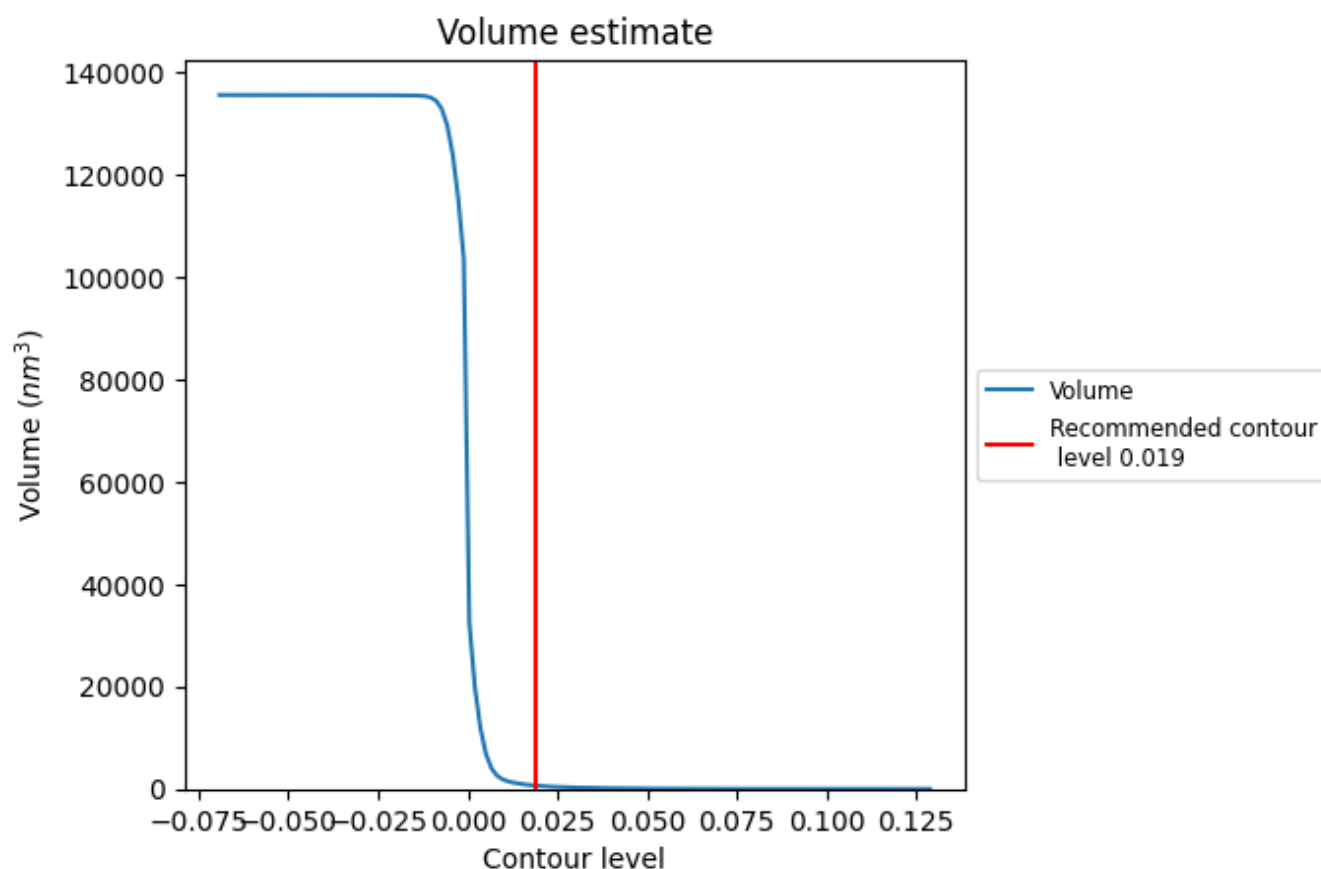
This section contains the results of statistical analysis of the map.

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.

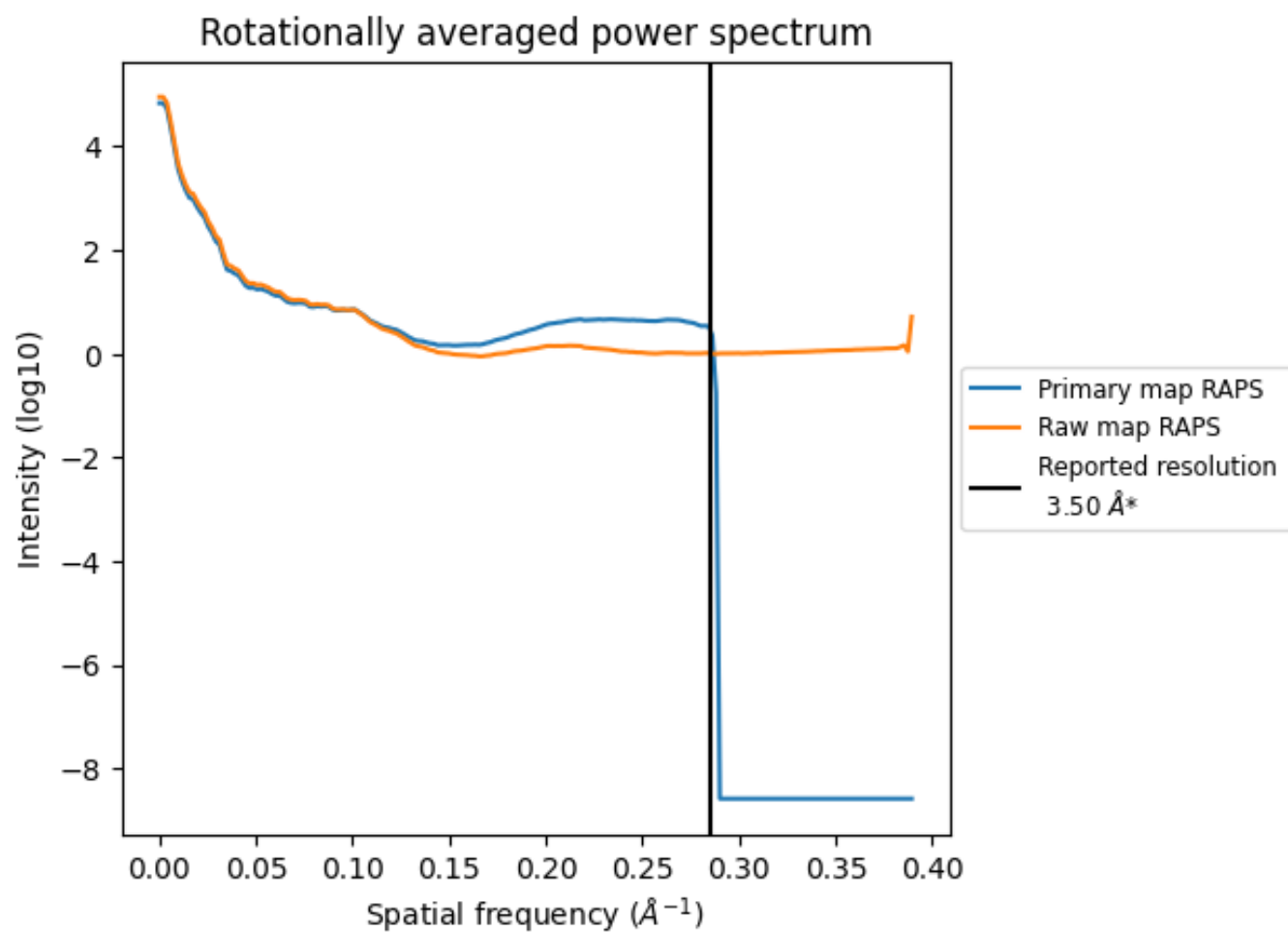
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 653 nm³; this corresponds to an approximate mass of 590 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

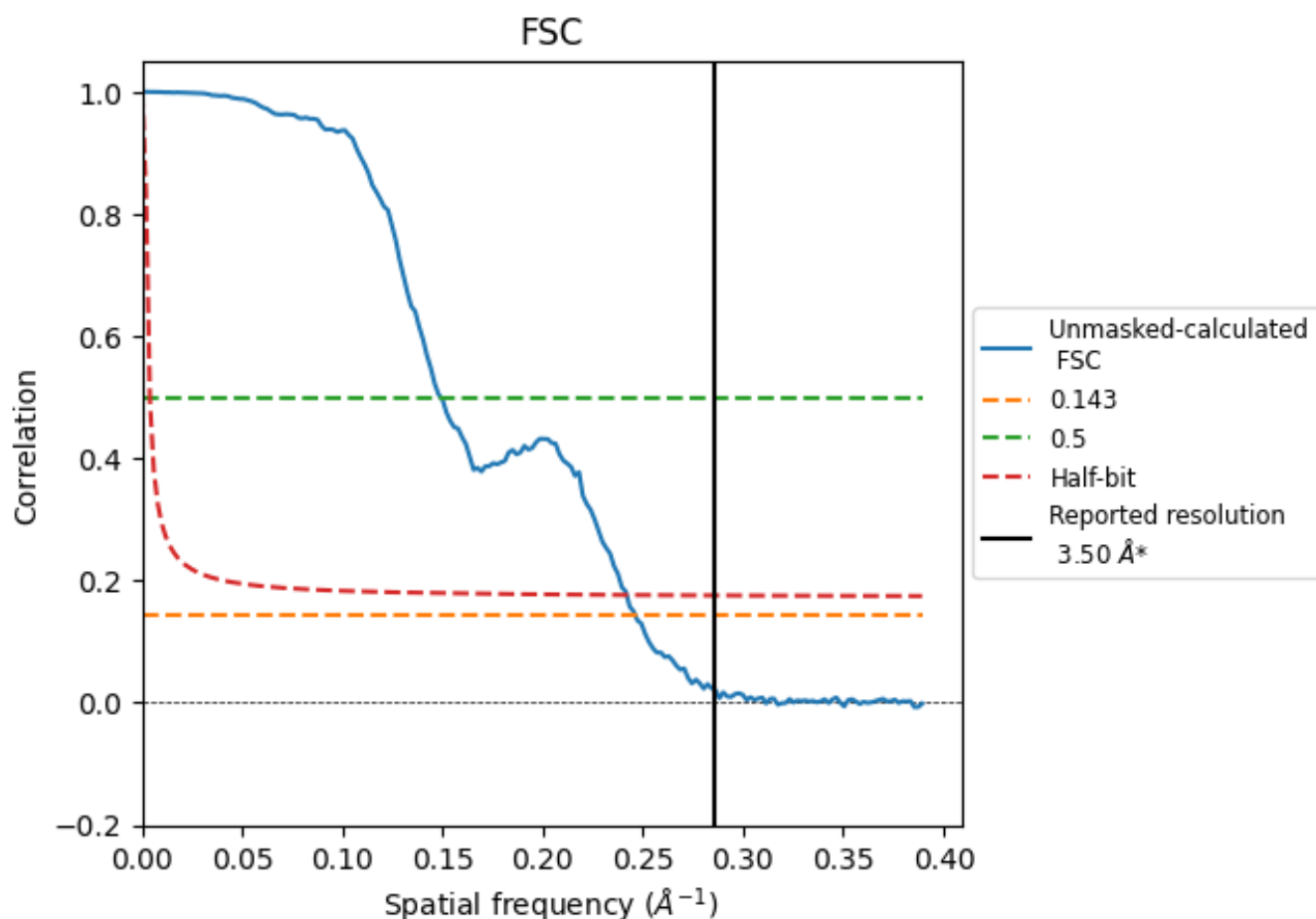


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

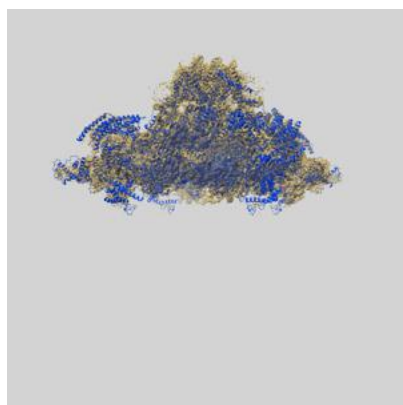
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	6.71	4.13

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

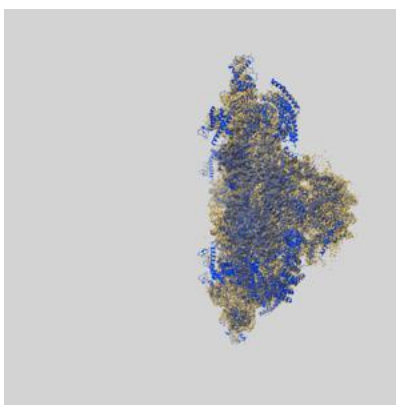
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33936 and PDB model 7VMM. Per-residue inclusion information can be found in section 3 on page 12.

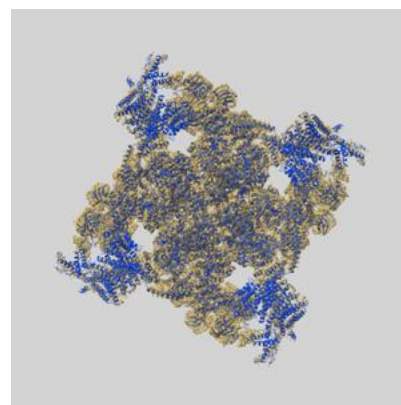
9.1 Map-model overlay [i](#)



X



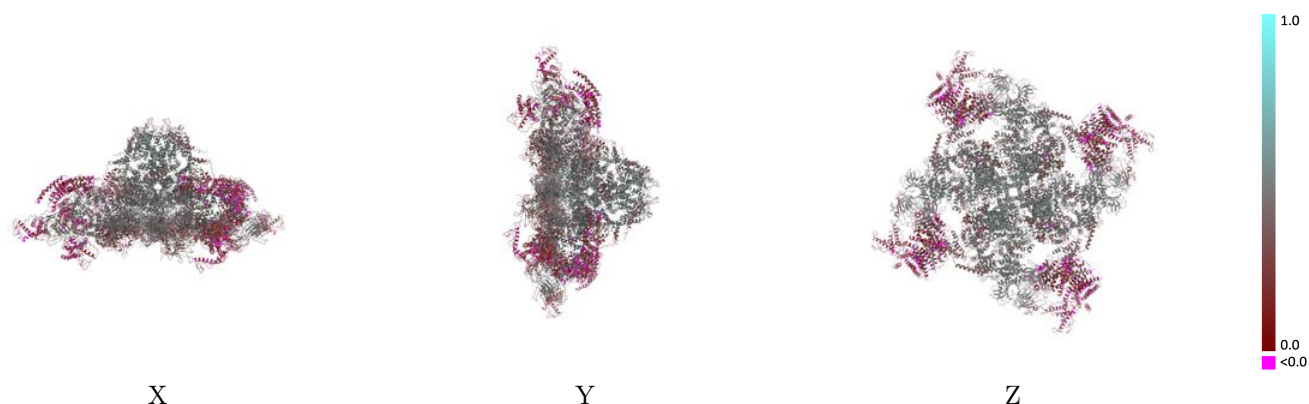
Y



Z

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

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

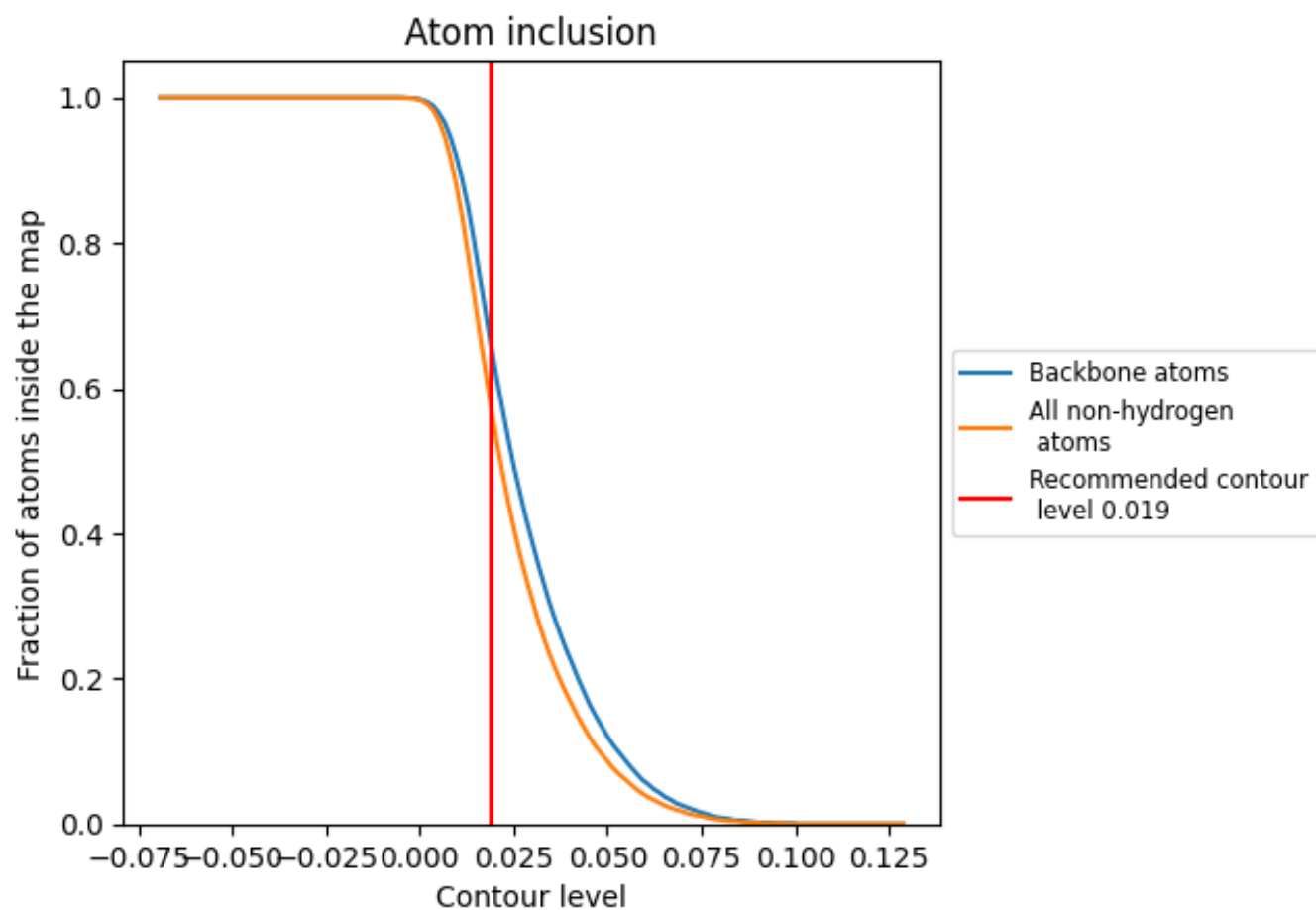


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5730	0.3810
A	0.5700	0.3790
B	0.5720	0.3820
C	0.5710	0.3780
D	0.5690	0.3760
G	0.6850	0.4520
H	0.6910	0.4520
I	0.6810	0.4520
J	0.6880	0.4520

