



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:46 AM UTC

PDB ID : 7TZO / pdb_00007tzo
EMDB ID : EMD-26213
Title : The apo structure of human mTORC2 complex
Authors : Yu, Z.; Chen, J.; Pearce, D.
Deposited on : 2022-02-16
Resolution : 3.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

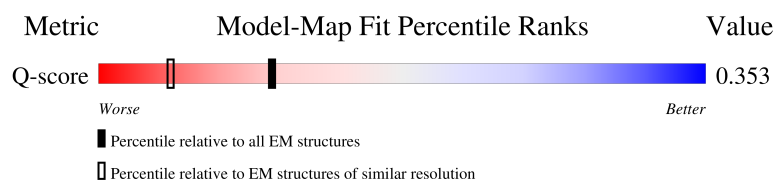
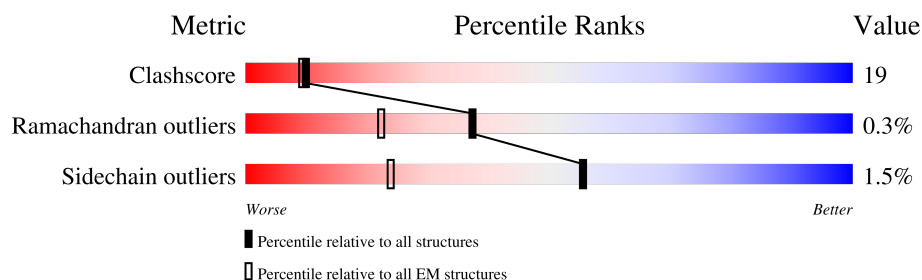
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14492 (2.78 - 3.78)

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	2674	14% 56% 25% 18%
1	B	2674	14% 57% 25% 18%
2	C	347	5% 51% 41% 8%
2	D	347	5% 52% 39% 8%

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Mol	Chain	Length	Quality of chain
3	E	1720	37%27%35%
3	F	1720	37%27%35%
4	G	538	13%5%78%
4	H	538	13%5%78%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 57117 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2184	Total	C	N	O	S	0	0
			16337	10356	2906	2977	98		
1	B	2185	Total	C	N	O	S	0	0
			16304	10330	2904	2972	98		

There are 250 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-124	MET	-	initiating methionine	UNP P42345
A	-123	VAL	-	expression tag	UNP P42345
A	-122	THR	-	expression tag	UNP P42345
A	-121	THR	-	expression tag	UNP P42345
A	-120	LEU	-	expression tag	UNP P42345
A	-119	SER	-	expression tag	UNP P42345
A	-118	GLY	-	expression tag	UNP P42345
A	-117	LEU	-	expression tag	UNP P42345
A	-116	SER	-	expression tag	UNP P42345
A	-115	GLY	-	expression tag	UNP P42345
A	-114	GLU	-	expression tag	UNP P42345
A	-113	GLN	-	expression tag	UNP P42345
A	-112	GLY	-	expression tag	UNP P42345
A	-111	PRO	-	expression tag	UNP P42345
A	-110	SER	-	expression tag	UNP P42345
A	-109	GLY	-	expression tag	UNP P42345
A	-108	ASP	-	expression tag	UNP P42345
A	-107	MET	-	expression tag	UNP P42345
A	-106	THR	-	expression tag	UNP P42345
A	-105	THR	-	expression tag	UNP P42345
A	-104	GLU	-	expression tag	UNP P42345
A	-103	GLU	-	expression tag	UNP P42345
A	-102	ASP	-	expression tag	UNP P42345
A	-101	SER	-	expression tag	UNP P42345
A	-100	ALA	-	expression tag	UNP P42345
A	-99	THR	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-98	HIS	-	expression tag	UNP P42345
A	-97	ILE	-	expression tag	UNP P42345
A	-96	LYS	-	expression tag	UNP P42345
A	-95	PHE	-	expression tag	UNP P42345
A	-94	SER	-	expression tag	UNP P42345
A	-93	LYS	-	expression tag	UNP P42345
A	-92	ARG	-	expression tag	UNP P42345
A	-91	ASP	-	expression tag	UNP P42345
A	-90	GLU	-	expression tag	UNP P42345
A	-89	ASP	-	expression tag	UNP P42345
A	-88	GLY	-	expression tag	UNP P42345
A	-87	ARG	-	expression tag	UNP P42345
A	-86	GLU	-	expression tag	UNP P42345
A	-85	LEU	-	expression tag	UNP P42345
A	-84	ALA	-	expression tag	UNP P42345
A	-83	GLY	-	expression tag	UNP P42345
A	-82	ALA	-	expression tag	UNP P42345
A	-81	THR	-	expression tag	UNP P42345
A	-80	MET	-	expression tag	UNP P42345
A	-79	GLU	-	expression tag	UNP P42345
A	-78	LEU	-	expression tag	UNP P42345
A	-77	ARG	-	expression tag	UNP P42345
A	-76	ASP	-	expression tag	UNP P42345
A	-75	SER	-	expression tag	UNP P42345
A	-74	SER	-	expression tag	UNP P42345
A	-73	GLY	-	expression tag	UNP P42345
A	-72	LYS	-	expression tag	UNP P42345
A	-71	THR	-	expression tag	UNP P42345
A	-70	ILE	-	expression tag	UNP P42345
A	-69	SER	-	expression tag	UNP P42345
A	-68	THR	-	expression tag	UNP P42345
A	-67	TRP	-	expression tag	UNP P42345
A	-66	ILE	-	expression tag	UNP P42345
A	-65	SER	-	expression tag	UNP P42345
A	-64	ASP	-	expression tag	UNP P42345
A	-63	GLY	-	expression tag	UNP P42345
A	-62	HIS	-	expression tag	UNP P42345
A	-61	VAL	-	expression tag	UNP P42345
A	-60	LYS	-	expression tag	UNP P42345
A	-59	ASP	-	expression tag	UNP P42345
A	-58	PHE	-	expression tag	UNP P42345
A	-57	TYR	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-56	LEU	-	expression tag	UNP P42345
A	-55	TYR	-	expression tag	UNP P42345
A	-54	PRO	-	expression tag	UNP P42345
A	-53	GLY	-	expression tag	UNP P42345
A	-52	LYS	-	expression tag	UNP P42345
A	-51	TYR	-	expression tag	UNP P42345
A	-50	THR	-	expression tag	UNP P42345
A	-49	PHE	-	expression tag	UNP P42345
A	-48	VAL	-	expression tag	UNP P42345
A	-47	GLU	-	expression tag	UNP P42345
A	-46	THR	-	expression tag	UNP P42345
A	-45	ALA	-	expression tag	UNP P42345
A	-44	ALA	-	expression tag	UNP P42345
A	-43	PRO	-	expression tag	UNP P42345
A	-42	ASP	-	expression tag	UNP P42345
A	-41	GLY	-	expression tag	UNP P42345
A	-40	TYR	-	expression tag	UNP P42345
A	-39	GLU	-	expression tag	UNP P42345
A	-38	VAL	-	expression tag	UNP P42345
A	-37	ALA	-	expression tag	UNP P42345
A	-36	THR	-	expression tag	UNP P42345
A	-35	PRO	-	expression tag	UNP P42345
A	-34	ILE	-	expression tag	UNP P42345
A	-33	GLU	-	expression tag	UNP P42345
A	-32	PHE	-	expression tag	UNP P42345
A	-31	THR	-	expression tag	UNP P42345
A	-30	VAL	-	expression tag	UNP P42345
A	-29	ASN	-	expression tag	UNP P42345
A	-28	GLU	-	expression tag	UNP P42345
A	-27	ASP	-	expression tag	UNP P42345
A	-26	GLY	-	expression tag	UNP P42345
A	-25	GLN	-	expression tag	UNP P42345
A	-24	VAL	-	expression tag	UNP P42345
A	-23	THR	-	expression tag	UNP P42345
A	-22	VAL	-	expression tag	UNP P42345
A	-21	ASP	-	expression tag	UNP P42345
A	-20	GLY	-	expression tag	UNP P42345
A	-19	GLU	-	expression tag	UNP P42345
A	-18	ALA	-	expression tag	UNP P42345
A	-17	THR	-	expression tag	UNP P42345
A	-16	GLU	-	expression tag	UNP P42345
A	-15	GLY	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ASP	-	expression tag	UNP P42345
A	-13	ALA	-	expression tag	UNP P42345
A	-12	HIS	-	expression tag	UNP P42345
A	-11	THR	-	expression tag	UNP P42345
A	-10	GLY	-	expression tag	UNP P42345
A	-9	SER	-	expression tag	UNP P42345
A	-8	SER	-	expression tag	UNP P42345
A	-7	GLY	-	expression tag	UNP P42345
A	-6	SER	-	expression tag	UNP P42345
A	-5	GLY	-	expression tag	UNP P42345
A	-4	SER	-	expression tag	UNP P42345
A	-3	GLY	-	expression tag	UNP P42345
A	-2	THR	-	expression tag	UNP P42345
A	-1	GLY	-	expression tag	UNP P42345
A	0	SER	-	expression tag	UNP P42345
B	-124	MET	-	initiating methionine	UNP P42345
B	-123	VAL	-	expression tag	UNP P42345
B	-122	THR	-	expression tag	UNP P42345
B	-121	THR	-	expression tag	UNP P42345
B	-120	LEU	-	expression tag	UNP P42345
B	-119	SER	-	expression tag	UNP P42345
B	-118	GLY	-	expression tag	UNP P42345
B	-117	LEU	-	expression tag	UNP P42345
B	-116	SER	-	expression tag	UNP P42345
B	-115	GLY	-	expression tag	UNP P42345
B	-114	GLU	-	expression tag	UNP P42345
B	-113	GLN	-	expression tag	UNP P42345
B	-112	GLY	-	expression tag	UNP P42345
B	-111	PRO	-	expression tag	UNP P42345
B	-110	SER	-	expression tag	UNP P42345
B	-109	GLY	-	expression tag	UNP P42345
B	-108	ASP	-	expression tag	UNP P42345
B	-107	MET	-	expression tag	UNP P42345
B	-106	THR	-	expression tag	UNP P42345
B	-105	THR	-	expression tag	UNP P42345
B	-104	GLU	-	expression tag	UNP P42345
B	-103	GLU	-	expression tag	UNP P42345
B	-102	ASP	-	expression tag	UNP P42345
B	-101	SER	-	expression tag	UNP P42345
B	-100	ALA	-	expression tag	UNP P42345
B	-99	THR	-	expression tag	UNP P42345
B	-98	HIS	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-97	ILE	-	expression tag	UNP P42345
B	-96	LYS	-	expression tag	UNP P42345
B	-95	PHE	-	expression tag	UNP P42345
B	-94	SER	-	expression tag	UNP P42345
B	-93	LYS	-	expression tag	UNP P42345
B	-92	ARG	-	expression tag	UNP P42345
B	-91	ASP	-	expression tag	UNP P42345
B	-90	GLU	-	expression tag	UNP P42345
B	-89	ASP	-	expression tag	UNP P42345
B	-88	GLY	-	expression tag	UNP P42345
B	-87	ARG	-	expression tag	UNP P42345
B	-86	GLU	-	expression tag	UNP P42345
B	-85	LEU	-	expression tag	UNP P42345
B	-84	ALA	-	expression tag	UNP P42345
B	-83	GLY	-	expression tag	UNP P42345
B	-82	ALA	-	expression tag	UNP P42345
B	-81	THR	-	expression tag	UNP P42345
B	-80	MET	-	expression tag	UNP P42345
B	-79	GLU	-	expression tag	UNP P42345
B	-78	LEU	-	expression tag	UNP P42345
B	-77	ARG	-	expression tag	UNP P42345
B	-76	ASP	-	expression tag	UNP P42345
B	-75	SER	-	expression tag	UNP P42345
B	-74	SER	-	expression tag	UNP P42345
B	-73	GLY	-	expression tag	UNP P42345
B	-72	LYS	-	expression tag	UNP P42345
B	-71	THR	-	expression tag	UNP P42345
B	-70	ILE	-	expression tag	UNP P42345
B	-69	SER	-	expression tag	UNP P42345
B	-68	THR	-	expression tag	UNP P42345
B	-67	TRP	-	expression tag	UNP P42345
B	-66	ILE	-	expression tag	UNP P42345
B	-65	SER	-	expression tag	UNP P42345
B	-64	ASP	-	expression tag	UNP P42345
B	-63	GLY	-	expression tag	UNP P42345
B	-62	HIS	-	expression tag	UNP P42345
B	-61	VAL	-	expression tag	UNP P42345
B	-60	LYS	-	expression tag	UNP P42345
B	-59	ASP	-	expression tag	UNP P42345
B	-58	PHE	-	expression tag	UNP P42345
B	-57	TYR	-	expression tag	UNP P42345
B	-56	LEU	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-55	TYR	-	expression tag	UNP P42345
B	-54	PRO	-	expression tag	UNP P42345
B	-53	GLY	-	expression tag	UNP P42345
B	-52	LYS	-	expression tag	UNP P42345
B	-51	TYR	-	expression tag	UNP P42345
B	-50	THR	-	expression tag	UNP P42345
B	-49	PHE	-	expression tag	UNP P42345
B	-48	VAL	-	expression tag	UNP P42345
B	-47	GLU	-	expression tag	UNP P42345
B	-46	THR	-	expression tag	UNP P42345
B	-45	ALA	-	expression tag	UNP P42345
B	-44	ALA	-	expression tag	UNP P42345
B	-43	PRO	-	expression tag	UNP P42345
B	-42	ASP	-	expression tag	UNP P42345
B	-41	GLY	-	expression tag	UNP P42345
B	-40	TYR	-	expression tag	UNP P42345
B	-39	GLU	-	expression tag	UNP P42345
B	-38	VAL	-	expression tag	UNP P42345
B	-37	ALA	-	expression tag	UNP P42345
B	-36	THR	-	expression tag	UNP P42345
B	-35	PRO	-	expression tag	UNP P42345
B	-34	ILE	-	expression tag	UNP P42345
B	-33	GLU	-	expression tag	UNP P42345
B	-32	PHE	-	expression tag	UNP P42345
B	-31	THR	-	expression tag	UNP P42345
B	-30	VAL	-	expression tag	UNP P42345
B	-29	ASN	-	expression tag	UNP P42345
B	-28	GLU	-	expression tag	UNP P42345
B	-27	ASP	-	expression tag	UNP P42345
B	-26	GLY	-	expression tag	UNP P42345
B	-25	GLN	-	expression tag	UNP P42345
B	-24	VAL	-	expression tag	UNP P42345
B	-23	THR	-	expression tag	UNP P42345
B	-22	VAL	-	expression tag	UNP P42345
B	-21	ASP	-	expression tag	UNP P42345
B	-20	GLY	-	expression tag	UNP P42345
B	-19	GLU	-	expression tag	UNP P42345
B	-18	ALA	-	expression tag	UNP P42345
B	-17	THR	-	expression tag	UNP P42345
B	-16	GLU	-	expression tag	UNP P42345
B	-15	GLY	-	expression tag	UNP P42345
B	-14	ASP	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	ALA	-	expression tag	UNP P42345
B	-12	HIS	-	expression tag	UNP P42345
B	-11	THR	-	expression tag	UNP P42345
B	-10	GLY	-	expression tag	UNP P42345
B	-9	SER	-	expression tag	UNP P42345
B	-8	SER	-	expression tag	UNP P42345
B	-7	GLY	-	expression tag	UNP P42345
B	-6	SER	-	expression tag	UNP P42345
B	-5	GLY	-	expression tag	UNP P42345
B	-4	SER	-	expression tag	UNP P42345
B	-3	GLY	-	expression tag	UNP P42345
B	-2	THR	-	expression tag	UNP P42345
B	-1	GLY	-	expression tag	UNP P42345
B	0	SER	-	expression tag	UNP P42345

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	319	Total	C	N	O	S	0	0
			2465	1533	437	477	18		
2	D	319	Total	C	N	O	S	0	0
			2465	1533	437	477	18		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	initiating methionine	UNP Q9BVC4
C	-19	GLY	-	expression tag	UNP Q9BVC4
C	-18	TYR	-	expression tag	UNP Q9BVC4
C	-17	PRO	-	expression tag	UNP Q9BVC4
C	-16	TYR	-	expression tag	UNP Q9BVC4
C	-15	ASP	-	expression tag	UNP Q9BVC4
C	-14	VAL	-	expression tag	UNP Q9BVC4
C	-13	PRO	-	expression tag	UNP Q9BVC4
C	-12	ASP	-	expression tag	UNP Q9BVC4
C	-11	TYR	-	expression tag	UNP Q9BVC4
C	-10	ALA	-	expression tag	UNP Q9BVC4
C	-9	ASP	-	expression tag	UNP Q9BVC4
C	-8	LEU	-	expression tag	UNP Q9BVC4
C	-7	ASN	-	expression tag	UNP Q9BVC4
C	-6	GLY	-	expression tag	UNP Q9BVC4
C	-5	GLY	-	expression tag	UNP Q9BVC4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q9BVC4
C	-3	GLY	-	expression tag	UNP Q9BVC4
C	-2	GLY	-	expression tag	UNP Q9BVC4
C	-1	SER	-	expression tag	UNP Q9BVC4
C	0	THR	-	expression tag	UNP Q9BVC4
D	-20	MET	-	initiating methionine	UNP Q9BVC4
D	-19	GLY	-	expression tag	UNP Q9BVC4
D	-18	TYR	-	expression tag	UNP Q9BVC4
D	-17	PRO	-	expression tag	UNP Q9BVC4
D	-16	TYR	-	expression tag	UNP Q9BVC4
D	-15	ASP	-	expression tag	UNP Q9BVC4
D	-14	VAL	-	expression tag	UNP Q9BVC4
D	-13	PRO	-	expression tag	UNP Q9BVC4
D	-12	ASP	-	expression tag	UNP Q9BVC4
D	-11	TYR	-	expression tag	UNP Q9BVC4
D	-10	ALA	-	expression tag	UNP Q9BVC4
D	-9	ASP	-	expression tag	UNP Q9BVC4
D	-8	LEU	-	expression tag	UNP Q9BVC4
D	-7	ASN	-	expression tag	UNP Q9BVC4
D	-6	GLY	-	expression tag	UNP Q9BVC4
D	-5	GLY	-	expression tag	UNP Q9BVC4
D	-4	GLY	-	expression tag	UNP Q9BVC4
D	-3	GLY	-	expression tag	UNP Q9BVC4
D	-2	GLY	-	expression tag	UNP Q9BVC4
D	-1	SER	-	expression tag	UNP Q9BVC4
D	0	THR	-	expression tag	UNP Q9BVC4

- Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1117	Total	C	N	O	S	0	0
			8931	5689	1584	1611	47		
3	F	1117	Total	C	N	O	S	0	0
			8931	5689	1584	1611	47		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	MET	-	initiating methionine	UNP Q6R327
E	-10	ASP	-	expression tag	UNP Q6R327
E	-9	TYR	-	expression tag	UNP Q6R327
E	-8	LYS	-	expression tag	UNP Q6R327

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	ASP	-	expression tag	UNP Q6R327
E	-6	ASP	-	expression tag	UNP Q6R327
E	-5	ASP	-	expression tag	UNP Q6R327
E	-4	ASP	-	expression tag	UNP Q6R327
E	-3	LYS	-	expression tag	UNP Q6R327
E	-2	GLY	-	expression tag	UNP Q6R327
E	-1	SER	-	expression tag	UNP Q6R327
E	0	THR	-	expression tag	UNP Q6R327
F	-11	MET	-	initiating methionine	UNP Q6R327
F	-10	ASP	-	expression tag	UNP Q6R327
F	-9	TYR	-	expression tag	UNP Q6R327
F	-8	LYS	-	expression tag	UNP Q6R327
F	-7	ASP	-	expression tag	UNP Q6R327
F	-6	ASP	-	expression tag	UNP Q6R327
F	-5	ASP	-	expression tag	UNP Q6R327
F	-4	ASP	-	expression tag	UNP Q6R327
F	-3	LYS	-	expression tag	UNP Q6R327
F	-2	GLY	-	expression tag	UNP Q6R327
F	-1	SER	-	expression tag	UNP Q6R327
F	0	THR	-	expression tag	UNP Q6R327

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	120	Total	C	N	O	S	0	0
			842	518	158	162	4		
4	H	120	Total	C	N	O	S	0	0
			842	518	158	162	4		

There are 32 discrepancies between the modelled and reference sequences:

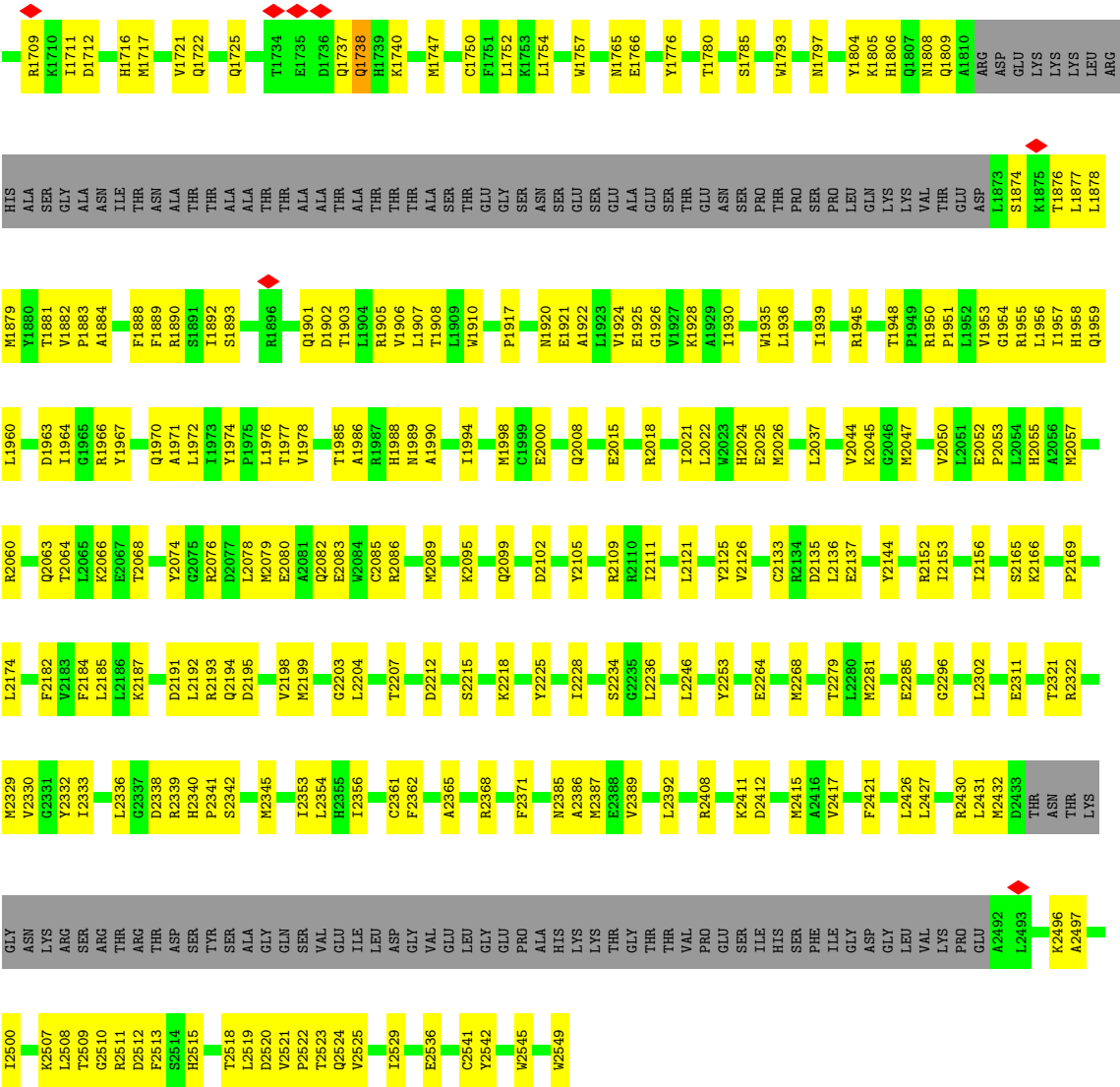
Chain	Residue	Modelled	Actual	Comment	Reference
G	523	ALA	-	expression tag	UNP Q9BPZ7
G	524	ALA	-	expression tag	UNP Q9BPZ7
G	525	ALA	-	expression tag	UNP Q9BPZ7
G	526	GLY	-	expression tag	UNP Q9BPZ7
G	527	GLY	-	expression tag	UNP Q9BPZ7
G	528	GLY	-	expression tag	UNP Q9BPZ7
G	529	GLY	-	expression tag	UNP Q9BPZ7
G	530	TYR	-	expression tag	UNP Q9BPZ7
G	531	PRO	-	expression tag	UNP Q9BPZ7
G	532	TYR	-	expression tag	UNP Q9BPZ7

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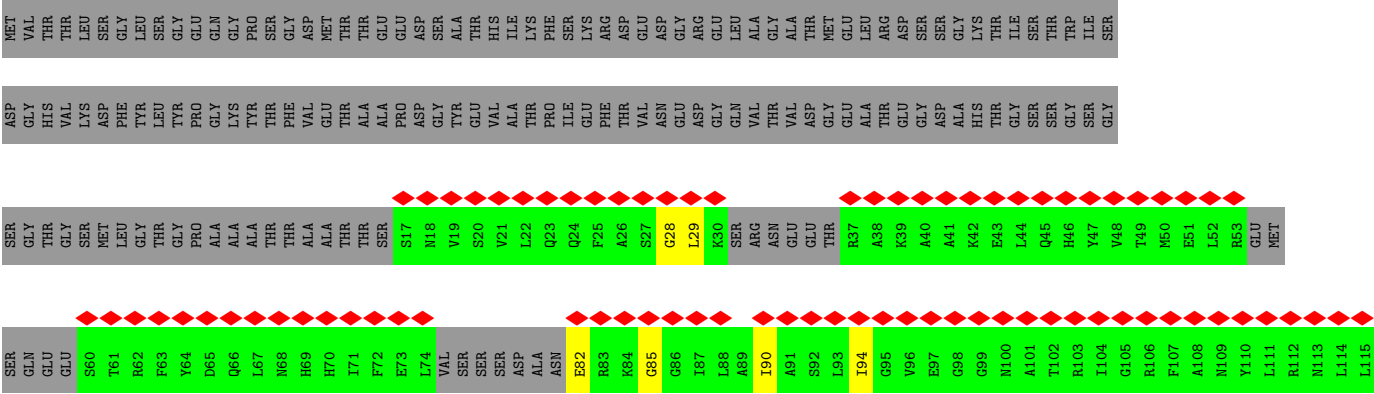
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Chain	Residue	Modelled	Actual	Comment	Reference
G	533	ASP	-	expression tag	UNP Q9BPZ7
G	534	VAL	-	expression tag	UNP Q9BPZ7
G	535	PRO	-	expression tag	UNP Q9BPZ7
G	536	ASP	-	expression tag	UNP Q9BPZ7
G	537	TYR	-	expression tag	UNP Q9BPZ7
G	538	ALA	-	expression tag	UNP Q9BPZ7
H	523	ALA	-	expression tag	UNP Q9BPZ7
H	524	ALA	-	expression tag	UNP Q9BPZ7
H	525	ALA	-	expression tag	UNP Q9BPZ7
H	526	GLY	-	expression tag	UNP Q9BPZ7
H	527	GLY	-	expression tag	UNP Q9BPZ7
H	528	GLY	-	expression tag	UNP Q9BPZ7
H	529	GLY	-	expression tag	UNP Q9BPZ7
H	530	TYR	-	expression tag	UNP Q9BPZ7
H	531	PRO	-	expression tag	UNP Q9BPZ7
H	532	TYR	-	expression tag	UNP Q9BPZ7
H	533	ASP	-	expression tag	UNP Q9BPZ7
H	534	VAL	-	expression tag	UNP Q9BPZ7
H	535	PRO	-	expression tag	UNP Q9BPZ7
H	536	ASP	-	expression tag	UNP Q9BPZ7
H	537	TYR	-	expression tag	UNP Q9BPZ7
H	538	ALA	-	expression tag	UNP Q9BPZ7





● Molecule 1: Serine/threonine-protein kinase mTOR

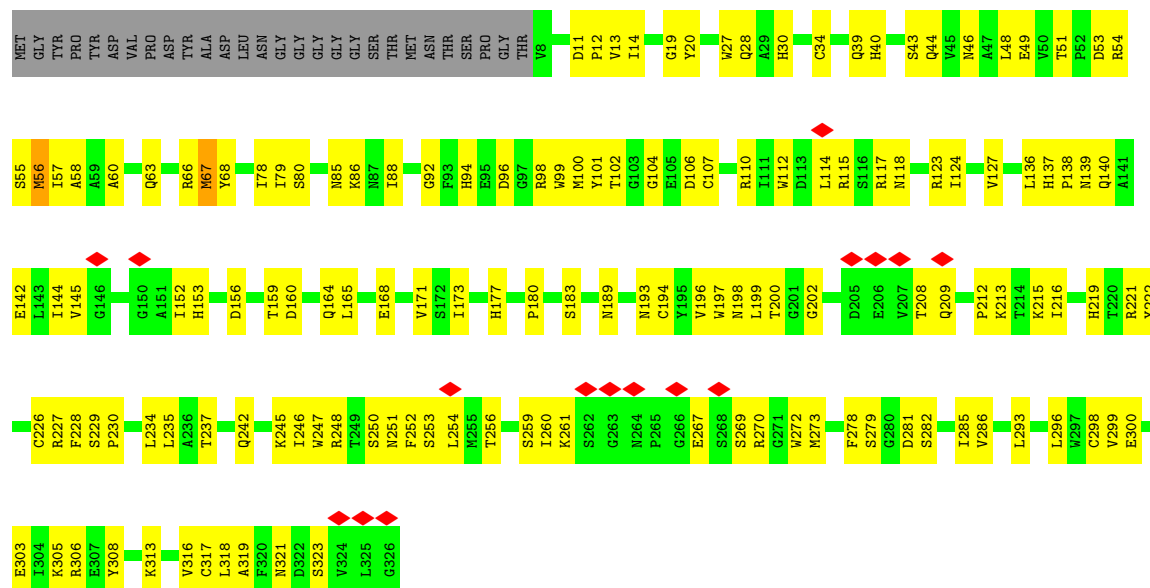




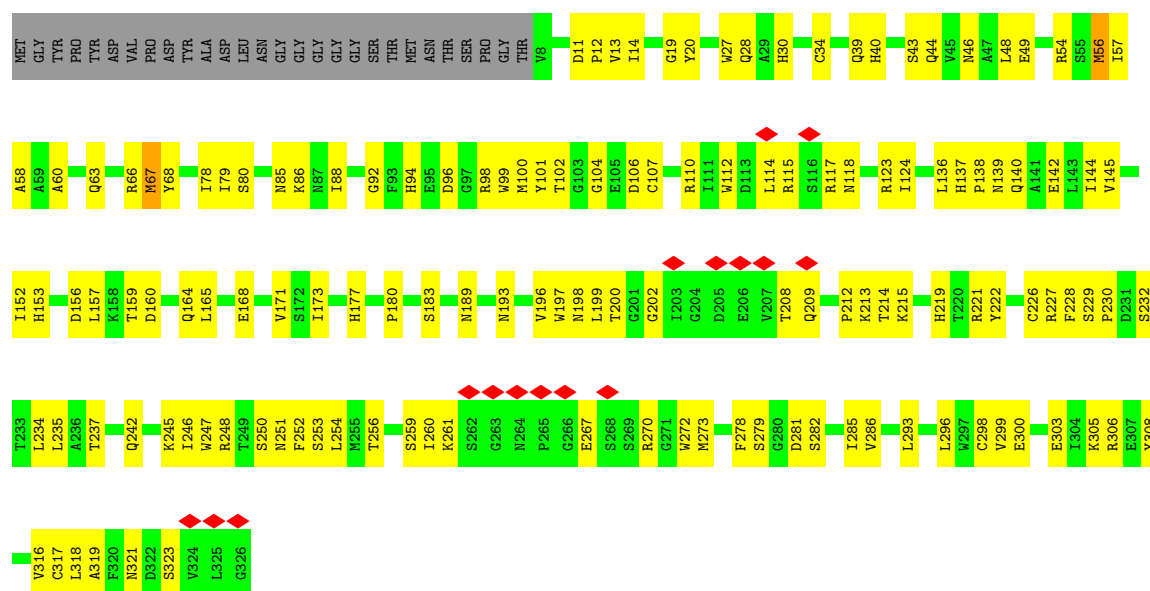




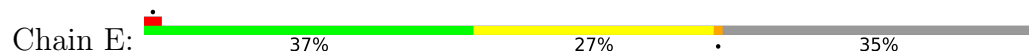
• Molecule 2: Target of rapamycin complex subunit LST8



• Molecule 2: Target of rapamycin complex subunit LST8

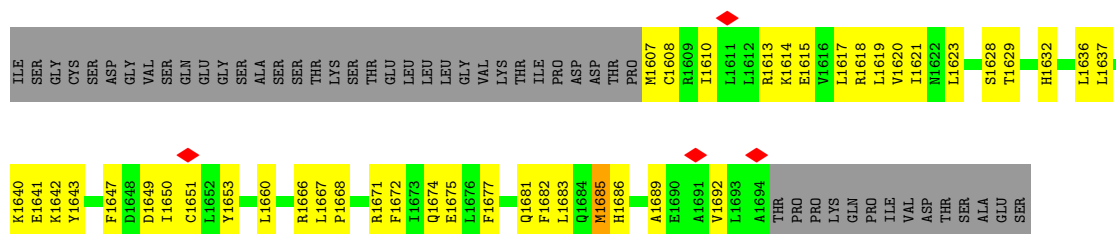


• Molecule 3: Rapamycin-insensitive companion of mTOR

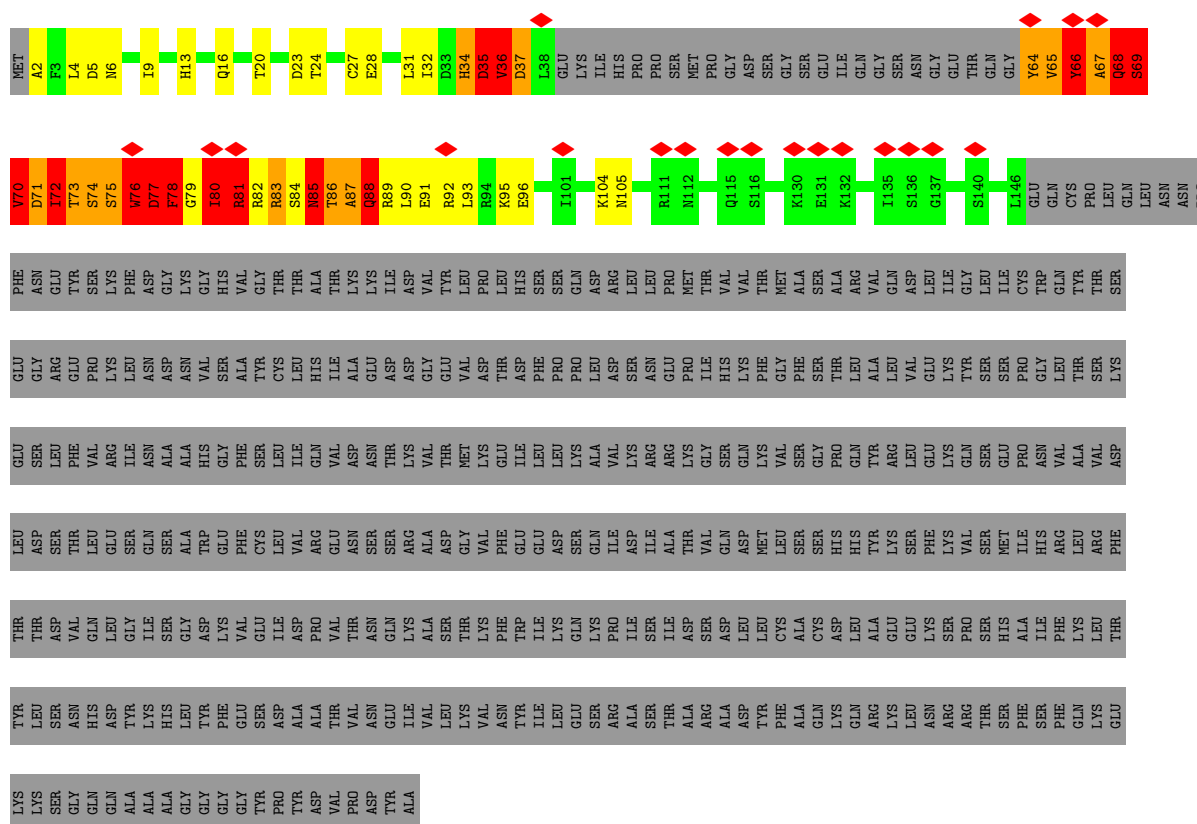




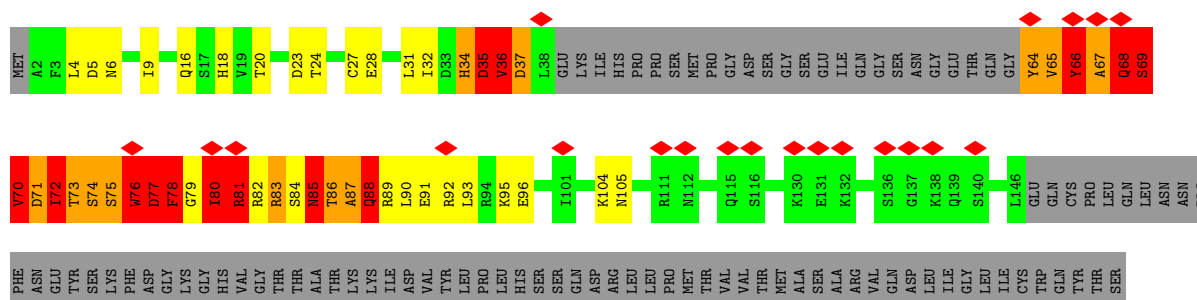




• Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1



• Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288538	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	22.607	Depositor
Minimum map value	-11.647	Depositor
Average map value	0.026	Depositor
Map value standard deviation	1.029	Depositor
Recommended contour level	2.64	Depositor
Map size ($\text{\AA}$)	356.4, 356.4, 356.4	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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	0.24	0/16632	0.52	2/22593 (0.0%)
1	B	0.24	0/16598	0.52	1/22552 (0.0%)
2	C	0.20	0/2523	0.52	0/3438
2	D	0.19	0/2523	0.52	0/3438
3	E	0.25	0/9092	0.56	5/12300 (0.0%)
3	F	0.25	0/9092	0.56	5/12300 (0.0%)
4	G	2.60	60/852 (7.0%)	2.44	63/1161 (5.4%)
4	H	2.60	61/852 (7.2%)	2.44	63/1161 (5.4%)
All	All	0.50	121/58164 (0.2%)	0.67	139/78943 (0.2%)

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
3	E	0	1
3	F	0	1
4	G	2	6
4	H	2	6
All	All	4	14

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	85	ASN	CA-C	-18.24	1.28	1.52
4	G	85	ASN	CA-C	-18.17	1.28	1.52
4	H	87	ALA	N-CA	-17.66	1.25	1.46
4	G	87	ALA	N-CA	-17.62	1.25	1.46
4	G	86	THR	C-O	16.33	1.44	1.24
4	H	86	THR	C-O	16.28	1.44	1.24
4	H	83	ARG	C-O	-15.69	1.07	1.24
4	G	83	ARG	C-O	-15.69	1.07	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	85	ASN	C-O	-15.65	1.04	1.24
4	H	85	ASN	C-O	-15.56	1.04	1.24
4	H	83	ARG	CA-C	-14.94	1.38	1.53
4	G	83	ARG	CA-C	-14.84	1.38	1.53
4	H	87	ALA	CA-C	-11.94	1.37	1.52
4	G	87	ALA	CA-C	-11.91	1.37	1.52
4	H	81	ARG	C-O	-11.37	1.11	1.24
4	G	81	ARG	C-O	-11.37	1.11	1.24
4	H	77	ASP	CG-OD2	-11.19	1.04	1.25
4	G	77	ASP	CG-OD2	-11.18	1.04	1.25
4	G	85	ASN	N-CA	-10.90	1.32	1.46
4	G	83	ARG	CZ-NH2	-10.88	1.19	1.33
4	H	83	ARG	CZ-NH2	-10.82	1.19	1.33
4	H	85	ASN	N-CA	-10.71	1.32	1.46
4	H	88	GLN	CG-CD	-10.43	1.25	1.52
4	G	88	GLN	CG-CD	-10.42	1.26	1.52
4	G	80	ILE	C-O	-10.23	1.11	1.24
4	H	80	ILE	C-O	-10.20	1.11	1.24
4	G	85	ASN	CA-CB	-9.86	1.36	1.53
4	G	77	ASP	CB-CG	-9.84	1.27	1.52
4	H	85	ASN	CA-CB	-9.82	1.36	1.53
4	H	77	ASP	CB-CG	-9.82	1.27	1.52
4	H	85	ASN	C-N	-9.59	1.20	1.33
4	G	85	ASN	C-N	-9.58	1.20	1.33
4	H	84	SER	C-N	-9.41	1.20	1.33
4	G	83	ARG	N-CA	-9.39	1.35	1.46
4	G	84	SER	C-N	-9.32	1.20	1.33
4	H	83	ARG	N-CA	-9.25	1.35	1.46
4	G	85	ASN	CG-ND2	-8.99	1.14	1.33
4	H	85	ASN	CG-ND2	-8.99	1.14	1.33
4	G	88	GLN	CD-NE2	-8.77	1.14	1.33
4	H	88	GLN	CD-NE2	-8.75	1.14	1.33
4	G	83	ARG	CA-CB	-8.68	1.41	1.53
4	H	83	ARG	CA-CB	-8.64	1.41	1.53
4	G	79	GLY	C-O	-8.34	1.12	1.23
4	H	79	GLY	C-O	-8.32	1.12	1.23
4	H	84	SER	CA-CB	-8.19	1.39	1.53
4	G	84	SER	CA-CB	-8.17	1.39	1.53
4	G	88	GLN	CA-C	-7.89	1.42	1.52
4	H	88	GLN	CA-C	-7.89	1.42	1.52
4	H	83	ARG	CD-NE	-7.63	1.35	1.46
4	G	83	ARG	CD-NE	-7.57	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	82	ARG	C-O	-7.53	1.14	1.24
4	G	82	ARG	C-O	-7.49	1.14	1.24
4	H	77	ASP	CG-OD1	-7.48	1.11	1.25
4	G	77	ASP	CG-OD1	-7.47	1.11	1.25
4	H	77	ASP	CA-CB	-7.41	1.41	1.53
4	G	77	ASP	CA-CB	-7.41	1.41	1.53
4	H	87	ALA	CA-CB	-7.21	1.42	1.53
4	G	87	ALA	CA-CB	-7.17	1.42	1.53
4	G	72	ILE	CA-C	7.04	1.61	1.52
4	H	72	ILE	CA-C	7.03	1.61	1.52
4	H	81	ARG	CZ-NH1	-7.00	1.23	1.32
4	G	81	ARG	CZ-NH1	-6.98	1.23	1.32
4	G	82	ARG	N-CA	6.97	1.55	1.46
4	H	68	GLN	CA-C	-6.90	1.43	1.52
4	G	86	THR	CB-CG2	-6.88	1.29	1.52
4	G	68	GLN	CA-C	-6.84	1.43	1.52
4	G	78	PHE	C-O	-6.83	1.15	1.24
4	H	86	THR	CB-CG2	-6.83	1.29	1.52
4	H	86	THR	CB-OG1	-6.83	1.32	1.43
4	H	78	PHE	C-O	-6.83	1.15	1.24
4	G	86	THR	CB-OG1	-6.82	1.32	1.43
4	H	84	SER	CB-OG	-6.82	1.28	1.42
4	H	82	ARG	N-CA	6.81	1.54	1.46
4	G	84	SER	CB-OG	-6.80	1.28	1.42
4	H	69	SER	CA-C	-6.69	1.44	1.53
4	G	69	SER	CA-C	-6.65	1.44	1.53
4	H	68	GLN	N-CA	-6.43	1.37	1.46
4	G	68	GLN	N-CA	-6.41	1.38	1.46
4	G	81	ARG	CA-CB	-6.39	1.43	1.53
4	H	81	ARG	CA-CB	-6.35	1.43	1.53
4	G	86	THR	CA-C	6.13	1.60	1.52
4	H	86	THR	CA-C	6.11	1.60	1.52
4	G	86	THR	N-CA	-6.07	1.38	1.46
4	H	86	THR	N-CA	-6.05	1.38	1.46
4	H	66	TYR	N-CA	-6.03	1.38	1.46
4	H	74	SER	N-CA	6.02	1.53	1.46
4	G	81	ARG	CZ-NH2	-6.01	1.25	1.33
4	H	81	ARG	CZ-NH2	-6.00	1.25	1.33
4	G	66	TYR	N-CA	-5.92	1.38	1.46
4	G	74	SER	N-CA	5.89	1.53	1.46
4	H	66	TYR	CA-C	-5.88	1.45	1.52
4	G	80	ILE	CB-CG2	5.86	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	66	TYR	CA-C	-5.86	1.45	1.52
4	H	80	ILE	CB-CG2	5.85	1.71	1.52
4	G	84	SER	CA-C	-5.76	1.45	1.52
4	H	84	SER	CA-C	-5.71	1.45	1.52
4	H	81	ARG	CA-C	-5.67	1.45	1.52
4	G	81	ARG	CA-C	-5.67	1.45	1.52
4	H	84	SER	C-O	5.63	1.30	1.23
4	G	84	SER	C-O	5.62	1.30	1.23
4	H	36	VAL	CA-CB	5.58	1.62	1.54
4	G	36	VAL	CA-CB	5.55	1.62	1.54
4	H	65	VAL	C-O	-5.50	1.17	1.24
4	G	88	GLN	CA-CB	5.48	1.62	1.53
4	G	75	SER	CA-C	-5.46	1.45	1.52
4	G	75	SER	C-O	-5.46	1.17	1.24
4	H	75	SER	C-O	-5.46	1.17	1.24
4	H	75	SER	CA-C	-5.43	1.45	1.52
4	H	88	GLN	CA-CB	5.42	1.61	1.53
4	G	65	VAL	C-O	-5.40	1.17	1.24
4	H	82	ARG	CZ-NH1	-5.39	1.25	1.32
4	H	76	TRP	CB-CG	-5.36	1.33	1.50
4	G	76	TRP	CB-CG	-5.35	1.33	1.50
4	G	82	ARG	CZ-NH1	-5.34	1.25	1.32
4	H	70	VAL	C-O	-5.26	1.17	1.24
4	G	66	TYR	C-O	-5.17	1.17	1.24
4	G	70	VAL	C-O	-5.17	1.18	1.24
4	H	75	SER	CA-CB	-5.14	1.44	1.53
4	G	75	SER	CA-CB	-5.14	1.44	1.53
4	H	66	TYR	C-O	-5.14	1.17	1.24
4	H	70	VAL	N-CA	5.04	1.52	1.46

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	88	GLN	CA-C-N	-21.41	92.61	120.44
4	H	88	GLN	C-N-CA	-21.41	92.61	120.44
4	G	88	GLN	CA-C-N	-21.39	92.63	120.44
4	G	88	GLN	C-N-CA	-21.39	92.63	120.44
4	H	77	ASP	N-CA-C	21.28	156.12	110.80
4	G	77	ASP	N-CA-C	21.26	156.08	110.80
4	G	77	ASP	CB-CA-C	-16.27	78.05	110.42
4	H	77	ASP	CB-CA-C	-16.23	78.12	110.42
4	H	88	GLN	N-CA-C	-15.22	92.91	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	88	GLN	N-CA-C	-15.21	92.92	111.33
4	G	84	SER	CA-C-O	15.10	137.90	120.99
4	H	84	SER	CA-C-O	15.04	137.83	120.99
4	H	71	ASP	N-CA-C	-12.25	96.39	112.68
4	G	71	ASP	N-CA-C	-12.25	96.39	112.68
4	H	72	ILE	N-CA-C	11.92	134.14	109.34
4	G	72	ILE	N-CA-C	11.92	134.13	109.34
4	H	84	SER	N-CA-C	11.56	127.14	108.99
4	G	84	SER	N-CA-C	11.56	127.13	108.99
4	G	86	THR	CA-C-O	10.15	135.02	120.51
4	H	86	THR	CA-C-O	10.14	135.02	120.51
4	H	81	ARG	N-CA-C	9.99	124.73	108.34
4	G	81	ARG	N-CA-C	9.99	124.72	108.34
4	H	88	GLN	CA-C-O	9.84	131.25	120.63
4	H	79	GLY	CA-C-N	9.81	139.64	121.97
4	H	79	GLY	C-N-CA	9.81	139.64	121.97
4	G	88	GLN	CA-C-O	9.79	131.21	120.63
4	G	79	GLY	CA-C-N	9.79	139.60	121.97
4	G	79	GLY	C-N-CA	9.79	139.60	121.97
4	G	72	ILE	CB-CA-C	-9.76	95.28	111.29
4	H	87	ALA	O-C-N	9.75	132.12	122.07
4	G	87	ALA	O-C-N	9.73	132.09	122.07
4	H	72	ILE	CB-CA-C	-9.72	95.34	111.29
4	H	79	GLY	N-CA-C	8.89	134.25	113.18
4	G	79	GLY	N-CA-C	8.89	134.24	113.18
4	H	80	ILE	CA-C-O	-8.82	109.75	120.78
4	H	77	ASP	N-CA-CB	-8.81	95.60	110.49
4	G	80	ILE	CA-C-O	-8.80	109.78	120.78
4	G	77	ASP	N-CA-CB	-8.77	95.67	110.49
4	G	67	ALA	CA-C-N	-8.65	105.03	121.54
4	G	67	ALA	C-N-CA	-8.65	105.03	121.54
4	H	67	ALA	CA-C-N	-8.62	105.07	121.54
4	H	67	ALA	C-N-CA	-8.62	105.07	121.54
4	H	70	VAL	CB-CA-C	8.58	125.37	111.29
4	G	70	VAL	CB-CA-C	8.58	125.36	111.29
4	G	73	THR	CA-C-N	7.98	136.78	121.54
4	G	73	THR	C-N-CA	7.98	136.78	121.54
4	H	67	ALA	CA-C-O	7.97	131.91	120.51
4	G	67	ALA	CA-C-O	7.96	131.89	120.51
4	H	73	THR	CA-C-N	7.95	136.73	121.54
4	H	73	THR	C-N-CA	7.95	136.73	121.54
4	G	36	VAL	N-CA-C	7.91	125.79	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	36	VAL	N-CA-C	7.91	125.79	109.34
4	H	84	SER	CA-C-N	-7.81	106.62	121.54
4	H	84	SER	C-N-CA	-7.81	106.62	121.54
4	G	84	SER	CA-C-N	-7.76	106.72	121.54
4	G	84	SER	C-N-CA	-7.76	106.72	121.54
4	G	35	ASP	CB-CG-OD1	7.49	135.62	118.40
4	H	84	SER	CB-CA-C	-7.47	94.04	109.94
4	G	84	SER	CB-CA-C	-7.45	94.06	109.94
4	H	35	ASP	CB-CG-OD1	7.45	135.54	118.40
4	H	86	THR	N-CA-C	7.20	126.13	110.80
4	G	86	THR	N-CA-C	7.17	126.07	110.80
4	G	81	ARG	CA-C-N	7.15	135.19	121.54
4	G	81	ARG	C-N-CA	7.15	135.19	121.54
4	H	81	ARG	CA-C-N	7.15	135.19	121.54
4	H	81	ARG	C-N-CA	7.15	135.19	121.54
3	E	729	ARG	CA-CB-CG	6.96	128.03	114.10
4	G	87	ALA	CA-C-O	-6.96	113.52	120.82
3	F	729	ARG	CA-CB-CG	6.92	127.94	114.10
4	H	87	ALA	CA-C-O	-6.91	113.56	120.82
4	H	80	ILE	CB-CA-C	6.80	122.44	111.29
4	G	80	ILE	CB-CA-C	6.77	122.39	111.29
4	G	85	ASN	CA-C-N	-6.37	109.38	121.54
4	G	85	ASN	C-N-CA	-6.37	109.38	121.54
4	H	86	THR	O-C-N	6.35	131.04	122.59
4	H	85	ASN	CA-C-N	-6.35	109.41	121.54
4	H	85	ASN	C-N-CA	-6.35	109.41	121.54
4	G	86	THR	O-C-N	6.33	131.01	122.59
4	H	82	ARG	CA-CB-CG	-6.30	101.51	114.10
4	G	82	ARG	CA-CB-CG	-6.28	101.54	114.10
4	G	36	VAL	CA-CB-CG1	6.26	121.03	110.40
4	H	36	VAL	CA-CB-CG1	6.25	121.03	110.40
4	H	86	THR	N-CA-CB	-6.19	100.03	110.49
3	E	270	GLU	CA-CB-CG	6.16	126.41	114.10
3	F	322	GLU	CA-CB-CG	6.14	126.39	114.10
3	E	322	GLU	CA-CB-CG	6.14	126.38	114.10
3	F	270	GLU	CA-CB-CG	6.14	126.37	114.10
4	H	78	PHE	N-CA-C	6.13	123.86	110.80
4	G	78	PHE	N-CA-C	6.13	123.85	110.80
4	G	86	THR	N-CA-CB	-6.13	100.13	110.49
4	G	85	ASN	CA-C-O	6.05	129.16	120.51
4	G	80	ILE	CG1-CB-CG2	6.03	128.79	110.70
4	G	74	SER	CA-C-N	6.02	133.04	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	74	SER	C-N-CA	6.02	133.04	121.54
4	H	80	ILE	CG1-CB-CG2	6.02	128.76	110.70
4	H	74	SER	CA-C-N	6.01	133.03	121.54
4	H	74	SER	C-N-CA	6.01	133.03	121.54
4	H	85	ASN	CA-C-O	5.99	129.08	120.51
4	H	77	ASP	CB-CG-OD1	-5.98	104.64	118.40
4	G	77	ASP	CB-CG-OD1	-5.97	104.66	118.40
4	G	83	ARG	NE-CZ-NH1	5.92	127.42	121.50
4	G	87	ALA	N-CA-CB	-5.91	101.44	110.01
4	H	83	ARG	NE-CZ-NH1	5.88	127.38	121.50
4	H	88	GLN	CA-CB-CG	5.87	125.84	114.10
4	G	88	GLN	CA-CB-CG	5.87	125.83	114.10
4	H	87	ALA	N-CA-CB	-5.87	101.50	110.01
4	G	85	ASN	N-CA-C	5.82	123.20	110.80
4	H	85	ASN	N-CA-C	5.79	123.14	110.80
4	H	65	VAL	CA-C-O	5.74	127.96	120.78
4	G	65	VAL	CA-C-O	5.72	127.93	120.78
4	H	76	TRP	CB-CA-C	-5.60	99.28	110.42
4	G	76	TRP	CB-CA-C	-5.59	99.29	110.42
4	H	80	ILE	CA-CB-CG2	5.56	119.94	110.50
4	G	80	ILE	CA-CB-CG2	5.50	119.86	110.50
4	H	85	ASN	CA-CB-CG	-5.45	107.15	112.60
1	B	854	VAL	N-CA-C	5.44	115.92	111.62
4	H	69	SER	N-CA-C	-5.44	103.50	111.17
4	G	69	SER	N-CA-C	-5.43	103.52	111.17
4	G	85	ASN	CA-CB-CG	-5.36	107.24	112.60
4	G	87	ALA	CA-C-N	5.34	127.69	120.38
4	G	87	ALA	C-N-CA	5.34	127.69	120.38
4	H	87	ALA	CA-C-N	5.34	127.69	120.38
4	H	87	ALA	C-N-CA	5.34	127.69	120.38
3	F	322	GLU	CB-CG-CD	5.33	121.66	112.60
4	H	76	TRP	N-CA-C	5.31	122.11	110.80
3	E	322	GLU	CB-CG-CD	5.29	121.59	112.60
4	G	66	TYR	N-CA-C	-5.26	101.39	109.76
3	E	1685	MET	CB-CG-SD	-5.25	96.96	112.70
3	F	1685	MET	CB-CG-SD	-5.25	96.96	112.70
4	G	76	TRP	N-CA-C	5.25	121.98	110.80
4	G	68	GLN	CA-CB-CG	5.24	124.58	114.10
4	H	66	TYR	N-CA-C	-5.24	101.43	109.76
4	H	68	GLN	CA-CB-CG	5.21	124.52	114.10
1	A	665	THR	CA-C-N	-5.12	113.42	122.48
1	A	665	THR	C-N-CA	-5.12	113.42	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	75	SER	CB-CA-C	-5.04	100.39	110.42
4	H	77	ASP	OD1-CG-OD2	-5.04	110.81	122.90
4	G	77	ASP	OD1-CG-OD2	-5.04	110.82	122.90
4	H	75	SER	CB-CA-C	-5.04	100.40	110.42

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	80	ILE	CA
4	G	85	ASN	CA
4	H	80	ILE	CA
4	H	85	ASN	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	367	GLY	Peptide
3	F	367	GLY	Peptide
4	G	34	HIS	Mainchain
4	G	36	VAL	Mainchain
4	G	69	SER	Mainchain
4	G	70	VAL	Mainchain
4	G	77	ASP	Sidechain
4	G	85	ASN	Mainchain
4	H	34	HIS	Mainchain
4	H	36	VAL	Mainchain
4	H	69	SER	Mainchain
4	H	70	VAL	Mainchain
4	H	77	ASP	Sidechain
4	H	85	ASN	Mainchain

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	16337	0	15369	550	0
1	B	16304	0	15298	524	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2465	0	2351	109	0
2	D	2465	0	2351	110	0
3	E	8931	0	9083	381	0
3	F	8931	0	9083	395	0
4	G	842	0	695	85	0
4	H	842	0	695	96	0
All	All	57117	0	54925	2180	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 19.

All (2180) 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)
4:H:67:ALA:O	4:H:68:GLN:CG	1.78	1.31
4:G:67:ALA:O	4:G:68:GLN:CG	1.78	1.30
4:H:87:ALA:O	4:H:90:LEU:N	1.71	1.21
4:G:87:ALA:O	4:G:90:LEU:N	1.71	1.21
4:G:67:ALA:O	4:G:68:GLN:CD	1.86	1.18
4:H:67:ALA:O	4:H:68:GLN:CD	1.86	1.18
4:G:32:ILE:HD12	4:G:34:HIS:CD2	1.79	1.17
4:H:32:ILE:HD12	4:H:34:HIS:CD2	1.79	1.17
3:F:68:CYS:SG	4:H:67:ALA:HA	1.89	1.11
4:H:67:ALA:O	4:H:68:GLN:NE2	1.84	1.10
4:G:67:ALA:O	4:G:68:GLN:NE2	1.84	1.09
3:F:151:ARG:HH12	4:H:31:LEU:HA	1.21	1.06
4:G:67:ALA:O	4:G:68:GLN:CB	1.94	1.05
4:G:32:ILE:HD12	4:G:34:HIS:HD2	1.18	0.99
3:F:1619:LEU:HD22	3:F:1636:LEU:HG	1.46	0.98
4:H:32:ILE:HD12	4:H:34:HIS:HD2	1.18	0.98
4:H:67:ALA:O	4:H:68:GLN:CB	1.94	0.98
3:E:1619:LEU:HD22	3:E:1636:LEU:HG	1.46	0.98
4:G:36:VAL:CG1	4:G:37:ASP:H	1.77	0.96
4:G:70:VAL:HG12	4:G:72:ILE:HD11	1.48	0.95
4:H:36:VAL:CG1	4:H:37:ASP:H	1.77	0.94
1:A:1480:ARG:NH1	1:A:1481:MET:SD	2.41	0.93
4:H:70:VAL:HG12	4:H:72:ILE:HD11	1.48	0.93
1:A:1097:LEU:HG	1:A:1138:THR:HG21	1.53	0.91
3:E:828:LEU:HD11	3:E:886:LEU:HD11	1.53	0.91
3:F:322:GLU:OE1	3:F:322:GLU:N	2.06	0.89
1:B:779:LEU:HD12	1:B:798:VAL:HG23	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:828:LEU:HD11	3:F:886:LEU:HD11	1.53	0.88
3:E:322:GLU:OE1	3:E:322:GLU:N	2.06	0.88
4:H:88:GLN:OE1	4:H:88:GLN:N	2.08	0.87
4:H:68:GLN:O	4:H:71:ASP:N	2.07	0.87
1:A:1925:GLU:HA	1:A:1928:LYS:HE2	1.57	0.87
4:G:68:GLN:O	4:G:71:ASP:N	2.07	0.86
1:A:2057:MET:HA	1:A:2060:ARG:HE	1.37	0.86
4:G:36:VAL:HG13	4:G:37:ASP:H	1.41	0.86
4:H:67:ALA:O	4:H:68:GLN:HG2	1.74	0.86
4:G:87:ALA:O	4:G:91:GLU:N	2.10	0.85
3:E:68:CYS:SG	4:G:67:ALA:HA	2.15	0.85
4:G:88:GLN:OE1	4:G:88:GLN:N	2.08	0.85
4:G:88:GLN:O	4:G:89:ARG:C	2.07	0.85
4:H:87:ALA:O	4:H:91:GLU:N	2.10	0.84
4:G:77:ASP:OD1	4:G:77:ASP:N	2.08	0.84
3:E:972:LEU:HD11	3:E:985:LEU:HD11	1.60	0.84
3:F:972:LEU:HD11	3:F:985:LEU:HD11	1.60	0.84
1:A:1194:MET:HE3	1:B:665:THR:HB	1.60	0.84
3:F:1522:TYR:HB2	3:F:1650:ILE:HD13	1.59	0.84
4:H:77:ASP:OD1	4:H:77:ASP:N	2.08	0.84
4:G:67:ALA:O	4:G:68:GLN:HG2	1.74	0.83
4:H:36:VAL:HG13	4:H:37:ASP:H	1.40	0.83
3:E:1522:TYR:HB2	3:E:1650:ILE:HD13	1.59	0.83
1:B:1764:ILE:HG23	1:B:1769:ILE:HD11	1.60	0.83
2:C:27:TRP:HB3	2:C:34:CYS:HA	1.61	0.83
4:H:88:GLN:O	4:H:89:ARG:C	2.07	0.82
1:A:1130:PRO:HA	1:A:1133:LYS:HD2	1.59	0.82
4:H:36:VAL:HG13	4:H:37:ASP:N	1.93	0.82
4:G:36:VAL:HG13	4:G:37:ASP:N	1.93	0.82
4:H:68:GLN:HG3	4:H:72:ILE:H	1.44	0.82
4:H:68:GLN:CG	4:H:72:ILE:H	1.92	0.82
4:G:68:GLN:CG	4:G:72:ILE:H	1.92	0.81
1:A:1467:MET:HE1	1:A:1476:LEU:HB3	1.62	0.81
1:A:631:THR:HA	1:A:682:ARG:HE	1.45	0.81
1:B:1101:GLN:HA	1:B:1141:ARG:NH1	1.95	0.81
4:G:68:GLN:HG3	4:G:72:ILE:H	1.44	0.81
2:D:27:TRP:HB3	2:D:34:CYS:HA	1.61	0.81
1:B:676:LEU:HB3	1:B:710:LEU:HD22	1.62	0.81
1:B:2329:MET:HE1	1:B:2404:MET:HB2	1.63	0.81
3:E:151:ARG:HH12	4:G:31:LEU:HA	1.46	0.80
1:A:779:LEU:HD12	1:A:798:VAL:HG23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:VAL:O	1:A:672:ARG:NH2	2.14	0.80
1:A:1184:LEU:HD11	1:A:1187:LYS:HB2	1.64	0.79
4:H:36:VAL:CG1	4:H:37:ASP:N	2.46	0.79
3:F:385:PRO:HG2	3:F:878:LEU:HD12	1.65	0.79
1:B:666:ASP:O	1:B:672:ARG:NH1	2.16	0.78
3:F:724:ALA:H	3:F:729:ARG:NH2	1.81	0.78
3:F:1623:LEU:HD13	3:F:1632:HIS:HB2	1.65	0.78
3:E:724:ALA:H	3:E:729:ARG:NH2	1.81	0.78
3:E:1666:ARG:HG3	3:E:1668:PRO:HD2	1.66	0.78
2:D:303:GLU:O	2:D:305:LYS:NZ	2.17	0.78
3:E:1434:ASN:O	3:E:1438:GLN:NE2	2.16	0.78
3:F:151:ARG:NH2	4:H:32:ILE:O	2.17	0.78
3:F:1434:ASN:O	3:F:1438:GLN:NE2	2.16	0.78
1:B:686:HIS:O	1:B:689:GLN:NE2	2.18	0.77
4:H:34:HIS:C	4:H:36:VAL:H	1.92	0.77
1:A:957:ARG:HH22	1:A:960:ARG:HD3	1.49	0.77
3:E:807:ARG:HD2	3:E:880:ILE:HG13	1.66	0.77
2:C:303:GLU:O	2:C:305:LYS:NZ	2.17	0.77
1:B:2072:GLN:HE22	3:F:251:GLU:HG3	1.48	0.77
1:A:1433:LEU:HG	1:A:1437:MET:HE1	1.65	0.77
3:E:1623:LEU:HD13	3:E:1632:HIS:HB2	1.65	0.77
1:A:1123:ASP:HA	1:A:1161:ARG:NH2	2.00	0.76
3:E:385:PRO:HG2	3:E:878:LEU:HD12	1.66	0.76
3:F:1666:ARG:HG3	3:F:1668:PRO:HD2	1.66	0.76
1:B:1444:GLU:O	1:B:1446:GLN:NE2	2.19	0.76
1:B:1266:GLN:HA	1:B:1269:TRP:HB2	1.67	0.76
1:B:1141:ARG:HD2	1:B:1141:ARG:C	2.11	0.76
1:B:1709:ARG:HH22	1:B:1711:ILE:HB	1.48	0.76
4:G:34:HIS:C	4:G:36:VAL:H	1.92	0.76
1:A:2511:ARG:HB3	1:A:2515:HIS:HA	1.67	0.76
3:F:131:ARG:NH2	3:F:1653:TYR:OH	2.18	0.76
1:A:952:MET:HE1	1:A:989:PHE:HB3	1.69	0.75
3:E:721:LEU:HD12	3:E:722:THR:HG23	1.68	0.75
1:A:2024:HIS:HB2	1:A:2111:ILE:HD11	1.68	0.75
1:A:1296:SER:H	1:A:1301:ARG:HH22	1.33	0.75
1:B:1097:LEU:HD11	1:B:1135:ALA:HA	1.69	0.75
3:F:807:ARG:HD2	3:F:880:ILE:HG13	1.66	0.75
1:A:824:ILE:HG21	1:A:844:LEU:HD21	1.68	0.75
3:F:779:GLU:HA	3:F:807:ARG:HH22	1.51	0.75
3:E:721:LEU:HD21	3:E:754:LEU:HD12	1.69	0.74
3:E:438:LEU:HD12	3:E:439:PRO:HD2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:87:ALA:O	4:H:90:LEU:CA	2.36	0.74
1:A:2296:GLY:O	1:A:2385:ASN:ND2	2.20	0.74
1:B:1423:LEU:O	1:B:1425:GLN:NE2	2.21	0.74
3:F:721:LEU:HD12	3:F:722:THR:HG23	1.68	0.74
1:B:709:GLU:OE1	1:B:759:HIS:ND1	2.20	0.74
3:F:438:LEU:HD12	3:F:439:PRO:HD2	1.69	0.73
3:E:779:GLU:HA	3:E:807:ARG:HH22	1.51	0.73
1:B:1717:MET:HG3	1:B:1754:LEU:HD13	1.69	0.73
3:E:131:ARG:NH2	3:E:1653:TYR:OH	2.18	0.73
1:B:2432:MET:HE2	1:B:2496:LYS:HB2	1.70	0.73
3:E:537:VAL:O	3:E:576:ARG:NH2	2.22	0.73
1:A:1954:GLY:O	1:A:1958:HIS:ND1	2.21	0.73
3:F:721:LEU:HD21	3:F:754:LEU:HD12	1.69	0.72
4:G:87:ALA:O	4:G:90:LEU:CA	2.36	0.72
4:G:87:ALA:C	4:G:89:ARG:N	2.34	0.72
1:B:747:GLY:HA2	1:B:750:LYS:HE2	1.70	0.72
3:F:537:VAL:O	3:F:576:ARG:NH2	2.22	0.72
4:H:32:ILE:CD1	4:H:34:HIS:HD2	1.99	0.72
1:A:1227:GLU:HB3	1:A:1231:ILE:HD11	1.71	0.72
1:B:742:GLU:OE2	1:B:743:HIS:ND1	2.23	0.72
3:F:634:LEU:HD21	3:F:688:LEU:HD11	1.72	0.72
1:A:2253:TYR:HB2	1:A:2302:LEU:HD13	1.71	0.72
3:E:343:THR:HG22	3:E:345:GLU:H	1.55	0.72
3:E:384:ARG:NH2	3:E:878:LEU:O	2.23	0.72
3:E:634:LEU:HD21	3:E:688:LEU:HD11	1.72	0.72
1:A:1211:VAL:HG22	3:E:553:THR:HG21	1.72	0.72
1:B:1737:GLN:HA	1:B:1740:LYS:HE2	1.72	0.72
1:A:2015:GLU:OE1	1:A:2018:ARG:NH1	2.24	0.71
1:A:1955:ARG:O	1:A:1959:GLN:NE2	2.23	0.71
3:F:384:ARG:NH2	3:F:878:LEU:O	2.23	0.71
1:A:2136:LEU:HD23	1:A:2153:ILE:HD11	1.71	0.71
1:A:736:GLN:OE1	1:B:1112:HIS:NE2	2.23	0.71
1:A:1481:MET:HG2	1:A:1515:MET:HE2	1.71	0.71
1:A:1712:ASP:OD2	1:A:1716:HIS:NE2	2.23	0.71
1:B:1044:MET:O	1:B:1049:GLN:NE2	2.23	0.71
1:A:2431:LEU:HD12	1:A:2432:MET:HG2	1.73	0.71
3:F:691:LEU:HD21	3:F:694:GLN:HB2	1.72	0.71
1:B:2332:TYR:O	1:B:2507:LYS:NZ	2.23	0.70
3:F:343:THR:HG22	3:F:345:GLU:H	1.55	0.70
1:B:2137:GLU:HA	1:B:2152:ARG:HD3	1.72	0.70
3:E:916:LYS:HE3	3:E:919:GLU:OE2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:32:ILE:CD1	4:G:34:HIS:HD2	1.99	0.70
1:B:994:MET:HE1	1:B:1030:TYR:HB3	1.73	0.70
1:A:1087:SER:O	1:A:1090:ARG:NH1	2.23	0.70
3:F:548:TRP:HA	3:F:551:ILE:HD12	1.73	0.70
3:E:579:TYR:HA	3:E:582:LYS:HD3	1.73	0.70
3:F:916:LYS:HE3	3:F:919:GLU:OE2	1.91	0.70
2:D:46:ASN:ND2	2:D:88:ILE:O	2.24	0.70
3:F:379:HIS:HD2	3:F:381:ALA:H	1.39	0.70
2:C:137:HIS:HD1	2:C:139:ASN:H	1.40	0.70
1:A:1002:ARG:HG2	1:A:1037:LEU:HD11	1.73	0.69
3:E:379:HIS:HD2	3:E:381:ALA:H	1.39	0.69
3:E:959:CYS:SG	3:E:960:GLU:N	2.65	0.69
3:F:579:TYR:HA	3:F:582:LYS:HD3	1.73	0.69
4:H:85:ASN:C	4:H:86:THR:HG23	2.17	0.69
3:E:1440:LYS:NZ	3:E:1441:ASP:O	2.23	0.69
3:E:1520:CYS:HB3	3:E:1523:CYS:HB2	1.74	0.69
4:H:23:ASP:OD1	4:H:24:THR:N	2.25	0.69
1:B:2321:THR:HG23	1:B:2387:MET:HE2	1.75	0.69
3:F:40:GLU:OE1	3:F:59:HIS:ND1	2.26	0.69
3:F:151:ARG:NH1	4:H:31:LEU:HA	2.03	0.69
1:B:662:VAL:O	1:B:672:ARG:NH2	2.25	0.69
1:B:1955:ARG:O	1:B:1959:GLN:NE2	2.25	0.69
1:B:2249:LEU:HD12	1:B:2302:LEU:HD21	1.74	0.69
3:E:101:ALA:HB2	3:E:142:GLU:HG3	1.74	0.69
3:E:691:LEU:HD21	3:E:694:GLN:HB2	1.72	0.69
3:E:548:TRP:HA	3:E:551:ILE:HD12	1.73	0.69
4:G:23:ASP:OD1	4:G:24:THR:N	2.25	0.69
1:A:1185:GLY:N	1:A:1226:GLU:OE1	2.26	0.69
3:F:101:ALA:HB2	3:F:142:GLU:HG3	1.74	0.69
3:F:567:ASP:O	3:F:571:HIS:ND1	2.25	0.69
3:F:1520:CYS:HB3	3:F:1523:CYS:HB2	1.74	0.69
1:B:1211:VAL:HG22	3:F:553:THR:HG21	1.75	0.69
3:E:172:VAL:HA	3:E:1667:LEU:HD11	1.74	0.69
1:B:1141:ARG:HD2	1:B:1142:LEU:N	2.08	0.69
1:B:1282:GLU:HG3	1:B:1286:ARG:HE	1.58	0.69
3:E:812:PRO:HA	3:E:815:PHE:HB3	1.73	0.69
3:F:172:VAL:HA	3:F:1667:LEU:HD11	1.74	0.69
4:G:34:HIS:C	4:G:36:VAL:N	2.51	0.69
1:A:824:ILE:HA	1:A:827:MET:HE3	1.75	0.68
2:D:137:HIS:HD1	2:D:139:ASN:H	1.40	0.68
1:A:1595:MET:HE1	1:A:1636:ILE:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:82:GLU:HG2	3:F:1528:ILE:HD11	1.76	0.68
1:A:1000:VAL:O	1:A:1004:CYS:N	2.26	0.68
1:B:2264:GLU:O	1:B:2268:MET:HG3	1.93	0.68
2:C:46:ASN:ND2	2:C:88:ILE:O	2.24	0.68
2:D:260:ILE:HG12	2:D:273:MET:HE3	1.75	0.68
3:E:46:ALA:O	3:E:47:ARG:HG2	1.94	0.68
3:F:535:SER:HA	3:F:547:ASN:HD21	1.59	0.68
3:F:812:PRO:HA	3:F:815:PHE:HB3	1.73	0.68
4:H:85:ASN:O	4:H:85:ASN:ND2	2.27	0.68
1:A:693:LEU:HD11	1:A:725:PHE:HD1	1.58	0.68
1:B:1677:LEU:HD21	1:B:1690:PRO:HG3	1.76	0.68
1:B:885:ILE:HD11	1:B:1568:ARG:HB3	1.76	0.68
3:E:535:SER:HA	3:E:547:ASN:HD21	1.59	0.68
3:F:959:CYS:SG	3:F:960:GLU:N	2.65	0.68
4:G:85:ASN:C	4:G:86:THR:HG23	2.17	0.68
1:B:1499:GLU:HG3	1:B:1500:LYS:HG2	1.75	0.68
4:G:85:ASN:ND2	4:G:85:ASN:O	2.27	0.68
1:B:2191:ASP:OD1	1:B:2193:ARG:NE	2.27	0.68
4:H:87:ALA:C	4:H:89:ARG:N	2.34	0.68
1:A:624:ARG:HB3	1:A:628:ARG:HH22	1.58	0.67
1:B:1924:VAL:O	1:B:1928:LYS:NZ	2.22	0.67
2:D:12:PRO:HB3	2:D:323:SER:HB3	1.77	0.67
3:E:40:GLU:OE1	3:E:59:HIS:ND1	2.26	0.67
1:A:970:MET:HG3	1:A:1306:LEU:HD13	1.75	0.67
1:B:772:MET:HG2	1:B:776:LEU:HD23	1.75	0.67
1:B:1345:LEU:HD21	1:B:1386:ARG:HG3	1.77	0.67
3:F:238:PRO:HD3	3:F:960:GLU:OE1	1.95	0.67
1:A:1133:LYS:HZ2	1:A:1169:LEU:HD21	1.59	0.67
3:E:82:GLU:HG2	3:E:1528:ILE:HD11	1.76	0.67
3:E:322:GLU:HA	3:E:325:ARG:HG2	1.76	0.67
3:E:364:LEU:HD11	3:E:700:LEU:HD11	1.77	0.67
1:B:1558:SER:O	1:B:1561:GLN:NE2	2.27	0.67
4:G:34:HIS:O	4:G:36:VAL:N	2.28	0.67
1:A:1737:GLN:HA	1:A:1740:LYS:HE2	1.75	0.67
1:A:734:LEU:HD11	3:F:453:MET:HE3	1.76	0.67
1:B:1315:ARG:NH2	1:B:1352:GLU:OE2	2.27	0.67
3:F:1440:LYS:NZ	3:F:1441:ASP:O	2.23	0.67
4:H:34:HIS:O	4:H:36:VAL:N	2.28	0.67
1:A:772:MET:HE1	1:A:812:GLU:HB3	1.76	0.67
1:A:1264:ASN:O	1:A:1267:LYS:NZ	2.26	0.67
3:E:756:VAL:HG21	3:E:790:MET:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:MET:HE2	1:B:1058:GLN:HE22	1.60	0.67
1:B:1263:ILE:O	1:B:1267:LYS:NZ	2.27	0.67
2:C:260:ILE:HG12	2:C:273:MET:HE3	1.75	0.67
3:E:238:PRO:HD3	3:E:960:GLU:OE1	1.95	0.67
1:A:954:ALA:HB2	1:A:1317:LEU:HD21	1.77	0.66
1:A:1026:HIS:HA	1:A:1028:ARG:HH11	1.59	0.66
1:B:702:ASP:HB3	1:B:708:ARG:HH12	1.60	0.66
1:B:1096:LEU:O	1:B:1100:ILE:HG12	1.95	0.66
4:H:86:THR:C	4:H:89:ARG:H	2.03	0.66
1:A:2345:MET:HE2	1:A:2356:ILE:HD13	1.78	0.66
3:E:567:ASP:O	3:E:571:HIS:ND1	2.25	0.66
3:F:46:ALA:O	3:F:47:ARG:HG2	1.94	0.66
3:F:322:GLU:HA	3:F:325:ARG:HG2	1.76	0.66
4:H:91:GLU:OE1	4:H:95:LYS:NZ	2.28	0.66
1:A:1004:CYS:O	1:A:1009:ARG:NH2	2.28	0.66
4:H:86:THR:O	4:H:90:LEU:N	2.29	0.66
1:A:1069:LEU:HD13	3:E:467:LEU:HD12	1.77	0.66
1:A:1627:GLN:NE2	1:A:1632:ASP:OD2	2.28	0.66
1:A:2008:GLN:HB3	1:A:2136:LEU:HD11	1.77	0.66
3:F:719:LYS:O	3:F:723:ALA:N	2.25	0.66
4:G:86:THR:O	4:G:90:LEU:N	2.29	0.66
1:A:630:LEU:HD12	1:A:652:VAL:HG23	1.78	0.66
1:B:440:LEU:O	1:B:444:VAL:N	2.28	0.66
1:B:1306:LEU:HD23	1:B:1313:MET:HE3	1.77	0.66
1:A:1072:PRO:HA	1:A:1075:ILE:HD12	1.77	0.66
1:A:1103:PHE:HD2	1:A:1107:LEU:HD23	1.60	0.66
2:C:12:PRO:HB3	2:C:323:SER:HB3	1.76	0.66
3:F:756:VAL:HG21	3:F:790:MET:HE1	1.77	0.66
1:A:1044:MET:O	1:A:1049:GLN:NE2	2.28	0.66
1:A:2345:MET:HE3	1:A:2354:LEU:HD22	1.78	0.66
1:B:2246:LEU:HD22	1:B:2341:PRO:HB3	1.78	0.66
4:G:91:GLU:OE1	4:G:95:LYS:NZ	2.28	0.66
1:B:2057:MET:HA	1:B:2060:ARG:HE	1.61	0.65
1:B:2338:ASP:OD1	1:B:2340:HIS:ND1	2.26	0.65
1:B:1115:LEU:HA	1:B:1118:ILE:HD12	1.78	0.65
1:B:2511:ARG:NH2	1:B:2515:HIS:O	2.28	0.65
3:F:364:LEU:HD11	3:F:700:LEU:HD11	1.77	0.65
4:G:85:ASN:C	4:G:86:THR:CG2	2.60	0.65
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.79	0.65
3:E:582:LYS:O	3:E:585:SER:OG	2.13	0.65
3:E:719:LYS:O	3:E:723:ALA:N	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1318:PHE:HE2	1:B:1360:LEU:HD22	1.61	0.65
2:C:279:SER:OG	2:C:281:ASP:OD1	2.14	0.65
3:F:68:CYS:SG	4:H:67:ALA:CA	2.78	0.65
1:A:1877:LEU:O	1:A:1881:THR:HG23	1.97	0.65
1:A:2204:LEU:HD22	1:A:2417:VAL:HG21	1.78	0.65
1:B:2037:LEU:HD11	1:B:2047:MET:HB3	1.79	0.65
3:E:188:ILE:HA	3:E:191:ILE:HG22	1.79	0.65
2:D:279:SER:OG	2:D:281:ASP:OD1	2.14	0.65
1:A:680:ASP:OD2	1:A:682:ARG:NH1	2.30	0.65
1:A:1171:SER:HA	1:A:1174:MET:HE2	1.79	0.65
1:B:1467:MET:HE1	1:B:1476:LEU:HB3	1.77	0.65
1:B:1647:HIS:NE2	1:B:1676:LEU:O	2.30	0.65
2:D:48:LEU:HG	2:D:319:ALA:HB2	1.79	0.64
3:F:569:GLN:HG2	3:F:572:ARG:HH21	1.62	0.64
4:G:77:ASP:O	4:G:78:PHE:HB2	1.97	0.64
3:E:212:LEU:O	3:E:215:VAL:HG22	1.97	0.64
1:A:1501:TRP:O	1:A:1509:GLN:NE2	2.25	0.64
1:B:1005:ASP:HA	1:B:1009:ARG:HH12	1.61	0.64
3:E:41:ILE:HB	3:E:87:CYS:SG	2.37	0.64
3:E:531:ASN:HB3	3:E:554:ILE:HD11	1.79	0.64
3:F:188:ILE:HA	3:F:191:ILE:HG22	1.78	0.64
4:H:77:ASP:O	4:H:78:PHE:HB2	1.97	0.64
3:E:959:CYS:H	3:E:965:ARG:NH1	1.96	0.64
3:F:212:LEU:O	3:F:215:VAL:HG22	1.96	0.64
1:A:885:ILE:HD11	1:A:1568:ARG:HB3	1.79	0.64
3:F:41:ILE:HB	3:F:87:CYS:SG	2.37	0.64
3:F:531:ASN:HB3	3:F:554:ILE:HD11	1.79	0.64
1:A:1028:ARG:HD3	1:A:1029:PRO:HD3	1.80	0.64
1:A:1101:GLN:HB3	1:A:1141:ARG:HH11	1.63	0.64
1:A:1523:LEU:O	1:A:1525:GLN:NE2	2.30	0.64
1:A:1613:GLU:OE1	1:A:1616:ARG:NH2	2.30	0.64
3:F:959:CYS:H	3:F:965:ARG:NH1	1.96	0.64
1:B:1285:ARG:NH1	1:B:1311:ASN:OD1	2.29	0.64
1:B:2253:TYR:HB2	1:B:2302:LEU:HD13	1.80	0.64
4:H:85:ASN:C	4:H:86:THR:CG2	2.60	0.63
2:C:48:LEU:HG	2:C:319:ALA:HB2	1.79	0.63
4:G:86:THR:C	4:G:89:ARG:H	2.03	0.63
1:B:1271:ALA:HB3	1:B:1274:ARG:HH11	1.63	0.63
3:E:569:GLN:HG2	3:E:572:ARG:HH21	1.62	0.63
3:E:893:CYS:HB2	3:E:942:LEU:HD21	1.81	0.63
3:F:533:ARG:NH1	3:F:534:ASP:OD1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:LYS:O	1:A:736:GLN:HG2	1.98	0.63
1:B:878:GLN:NE2	1:B:1569:ASP:OD2	2.31	0.63
1:B:998:LEU:HA	1:B:1001:ILE:HG22	1.81	0.63
3:F:694:GLN:HB3	3:F:697:LEU:HD13	1.81	0.63
1:A:2536:GLU:OE1	1:A:2536:GLU:N	2.29	0.63
1:B:2318:THR:O	1:B:2322:ARG:HG3	1.99	0.63
1:B:2519:LEU:HB3	1:B:2523:THR:HB	1.81	0.63
3:E:694:GLN:HB3	3:E:697:LEU:HD13	1.81	0.63
1:A:1096:LEU:O	1:A:1100:ILE:HG12	1.99	0.62
1:A:1375:ARG:HH12	1:A:1382:LEU:HD22	1.63	0.62
3:E:533:ARG:NH1	3:E:534:ASP:OD1	2.31	0.62
4:G:68:GLN:O	4:G:69:SER:C	2.42	0.62
4:H:68:GLN:O	4:H:69:SER:C	2.42	0.62
1:A:747:GLY:HA2	1:A:750:LYS:HD2	1.81	0.62
1:A:2512:ASP:OD1	1:A:2513:PHE:N	2.31	0.62
3:E:36:ASP:OD1	3:E:39:ARG:NH1	2.32	0.62
3:E:332:TYR:HE2	3:E:340:PRO:HD3	1.64	0.62
3:F:875:HIS:HB3	3:F:877:TYR:HE2	1.64	0.62
1:A:733:MET:O	1:A:736:GLN:N	2.32	0.62
1:B:1031:MET:HA	1:B:1034:ILE:HD12	1.81	0.62
3:F:893:CYS:HB2	3:F:942:LEU:HD21	1.81	0.62
1:A:727:MET:SD	3:F:447:HIS:NE2	2.73	0.62
1:A:2246:LEU:HD22	1:A:2341:PRO:HB3	1.81	0.62
1:B:601:GLN:HB2	1:B:604:ARG:HH21	1.63	0.62
1:B:1877:LEU:O	1:B:1881:THR:HG23	1.99	0.62
2:C:198:ASN:HB2	2:C:213:LYS:HD3	1.81	0.62
3:F:562:LEU:HD13	3:F:570:LEU:HD22	1.82	0.62
3:F:971:VAL:O	3:F:975:ILE:HG12	1.99	0.62
2:C:296:LEU:HB2	2:C:306:ARG:HB2	1.81	0.62
1:A:1478:LEU:HA	1:A:1481:MET:HE2	1.81	0.62
3:E:971:VAL:O	3:E:975:ILE:HG12	1.99	0.62
1:A:2333:ILE:HD11	1:A:2508:LEU:HD22	1.82	0.62
4:H:88:GLN:O	4:H:89:ARG:O	2.18	0.62
1:A:1890:ARG:O	1:A:1893:SER:OG	2.14	0.62
1:B:1087:SER:O	1:B:1090:ARG:NH1	2.32	0.62
3:F:582:LYS:O	3:F:585:SER:OG	2.13	0.62
1:A:1072:PRO:HG3	1:A:1110:TYR:OH	2.00	0.61
3:F:36:ASP:OD1	3:F:39:ARG:NH1	2.32	0.61
1:A:1581:GLU:OE1	1:A:1585:ARG:NE	2.33	0.61
1:A:1776:TYR:O	1:A:1780:THR:HG23	2.00	0.61
1:B:839:VAL:O	1:B:843:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:650:GLY:O	3:F:654:THR:OG1	2.18	0.61
3:E:722:THR:C	3:E:729:ARG:HH12	2.08	0.61
3:E:724:ALA:H	3:E:729:ARG:HH22	1.49	0.61
3:F:442:HIS:NE2	3:F:1431:VAL:O	2.27	0.61
1:B:1265:LEU:HB3	1:B:1269:TRP:CD1	2.35	0.61
3:F:332:TYR:HE2	3:F:340:PRO:HD3	1.64	0.61
3:F:722:THR:C	3:F:729:ARG:HH12	2.08	0.61
3:F:907:ARG:HA	3:F:910:ARG:HE	1.66	0.61
4:G:88:GLN:O	4:G:89:ARG:O	2.18	0.61
1:A:1318:PHE:HE2	1:A:1360:LEU:HD22	1.66	0.61
1:A:1467:MET:CE	1:A:1476:LEU:HB3	2.29	0.61
1:A:1966:ARG:HG3	1:A:1967:TYR:HD2	1.64	0.61
1:B:759:HIS:O	1:B:763:ASN:ND2	2.28	0.61
1:B:954:ALA:HB2	1:B:1317:LEU:HD21	1.81	0.61
3:F:148:ARG:HE	4:H:32:ILE:HD11	1.66	0.61
1:A:2311:GLU:OE1	1:A:2311:GLU:N	2.26	0.61
1:B:980:LYS:HA	1:B:1022:PHE:HE1	1.65	0.61
2:C:63:GLN:NE2	2:C:85:ASN:O	2.32	0.61
3:E:505:HIS:NE2	3:E:743:ASN:O	2.32	0.61
3:F:249:GLU:OE1	3:F:249:GLU:N	2.33	0.61
3:F:563:ARG:HH11	3:F:616:GLU:H	1.47	0.61
1:A:752:GLN:O	1:A:756:MET:HG2	2.01	0.61
1:A:1082:PHE:HB3	1:A:1121:LEU:HD21	1.83	0.61
1:A:1271:ALA:HB3	1:A:1274:ARG:HH11	1.65	0.61
1:A:2137:GLU:HA	1:A:2152:ARG:HH11	1.66	0.61
1:B:2018:ARG:NH2	1:B:2063:GLN:OE1	2.34	0.61
3:E:442:HIS:NE2	3:E:1431:VAL:O	2.27	0.61
1:B:1164:ASP:OD2	1:B:1201:ARG:NH1	2.33	0.61
3:F:118:GLN:NE2	3:F:119:LYS:HG3	2.15	0.61
1:A:1005:ASP:HA	1:A:1009:ARG:HH12	1.65	0.61
1:A:1709:ARG:HE	1:A:1711:ILE:HB	1.66	0.61
1:B:601:GLN:OE1	1:B:604:ARG:NH2	2.33	0.61
1:B:2397:ARG:NH1	1:B:2526:GLU:OE2	2.33	0.61
3:F:72:HIS:NE2	3:F:112:GLN:HG3	2.16	0.61
1:A:1375:ARG:HH22	1:A:1382:LEU:HB2	1.65	0.61
1:B:1038:MET:HE3	1:B:1074:LEU:HD11	1.81	0.61
2:D:296:LEU:HB2	2:D:306:ARG:HB2	1.82	0.61
3:F:128:LEU:HD22	3:F:131:ARG:HH12	1.66	0.61
1:B:2072:GLN:NE2	3:F:251:GLU:HG3	2.15	0.60
2:D:198:ASN:HB2	2:D:213:LYS:HD3	1.82	0.60
2:D:248:ARG:NE	2:D:250:SER:OG	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:668:CYS:SG	3:F:669:HIS:N	2.74	0.60
3:F:726:ASP:OD1	3:F:727:ALA:N	2.35	0.60
4:H:34:HIS:C	4:H:36:VAL:N	2.51	0.60
3:E:118:GLN:NE2	3:E:119:LYS:HG3	2.15	0.60
3:E:563:ARG:HH11	3:E:616:GLU:H	1.47	0.60
1:A:1793:TRP:O	1:A:1797:ASN:ND2	2.34	0.60
1:A:2080:GLU:O	1:A:2083:GLU:HG3	2.01	0.60
1:B:1701:MET:HA	1:B:1704:MET:HE3	1.82	0.60
1:B:1777:SER:O	1:B:1780:THR:OG1	2.16	0.60
1:B:2161:GLN:OE1	1:B:2162:VAL:N	2.34	0.60
3:E:72:HIS:NE2	3:E:112:GLN:HG3	2.16	0.60
3:E:875:HIS:HB3	3:E:877:TYR:HE2	1.64	0.60
1:A:2018:ARG:NH2	1:A:2063:GLN:OE1	2.35	0.60
2:D:63:GLN:NE2	2:D:85:ASN:O	2.32	0.60
2:D:197:TRP:CD1	2:D:212:PRO:HA	2.37	0.60
3:E:128:LEU:HD22	3:E:131:ARG:HH12	1.65	0.60
3:E:562:LEU:HD13	3:E:570:LEU:HD22	1.82	0.60
1:A:1031:MET:O	1:A:1034:ILE:HB	2.02	0.60
1:B:1440:PHE:HB3	1:B:1442:GLU:OE1	2.02	0.60
3:E:249:GLU:OE1	3:E:249:GLU:N	2.33	0.60
3:E:726:ASP:OD1	3:E:727:ALA:N	2.34	0.60
3:F:1637:LEU:HD21	4:H:93:LEU:HD21	1.82	0.60
2:C:248:ARG:NE	2:C:250:SER:OG	2.34	0.60
3:E:369:VAL:HG13	3:E:494:LEU:HD11	1.84	0.60
3:E:1538:SER:O	3:E:1607:MET:N	2.35	0.60
3:F:733:THR:HG21	3:F:766:ILE:HG23	1.84	0.60
1:A:2187:LYS:O	1:A:2234:SER:OG	2.14	0.60
1:B:1191:PHE:HA	1:B:1194:MET:HE1	1.83	0.60
1:B:1889:PHE:CE2	1:B:1926:GLY:HA3	2.36	0.60
2:C:173:ILE:HA	2:C:189:ASN:HA	1.84	0.60
1:A:2199:MET:HE3	1:A:2225:TYR:H	1.65	0.60
3:E:668:CYS:SG	3:E:669:HIS:N	2.74	0.60
3:E:1650:ILE:HD12	3:E:1685:MET:HE2	1.84	0.60
3:F:109:TYR:O	3:F:112:GLN:NE2	2.34	0.60
4:H:5:ASP:OD1	4:H:6:ASN:N	2.34	0.60
4:H:81:ARG:HH11	4:H:81:ARG:CG	2.15	0.60
1:A:1950:ARG:HB3	1:A:1953:VAL:HG12	1.83	0.59
3:F:1538:SER:O	3:F:1607:MET:N	2.35	0.59
1:B:2199:MET:HE3	1:B:2224:ARG:HB3	1.83	0.59
1:B:2279:THR:OG1	1:B:2281:MET:SD	2.51	0.59
1:B:1338:ILE:HG12	1:B:1372:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:733:THR:HG21	3:E:766:ILE:HG23	1.84	0.59
4:G:81:ARG:HH11	4:G:81:ARG:CG	2.15	0.59
1:A:1921:GLU:HG2	1:A:1922:ALA:N	2.17	0.59
1:B:957:ARG:HA	1:B:957:ARG:CZ	2.31	0.59
1:B:1004:CYS:O	1:B:1009:ARG:NH2	2.32	0.59
1:A:937:ASN:HB2	1:A:946:PHE:CE2	2.38	0.59
1:A:1805:LYS:HA	1:A:1808:ASN:HD21	1.67	0.59
1:B:1171:SER:HA	1:B:1174:MET:HE2	1.83	0.59
1:B:1787:TYR:CE1	1:B:1895:SER:HB3	2.37	0.59
2:C:197:TRP:CD1	2:C:212:PRO:HA	2.37	0.59
2:D:80:SER:OG	4:H:105:ASN:OD1	2.20	0.59
2:D:246:ILE:HB	2:D:256:THR:HB	1.84	0.59
3:E:907:ARG:HA	3:E:910:ARG:HE	1.66	0.59
3:F:505:HIS:NE2	3:F:743:ASN:O	2.32	0.59
1:A:2338:ASP:OD1	1:A:2340:HIS:ND1	2.31	0.59
3:E:109:TYR:O	3:E:112:GLN:NE2	2.34	0.59
3:E:415:SER:OG	3:E:416:ASP:N	2.35	0.59
3:E:663:ILE:H	3:E:663:ILE:HD12	1.66	0.59
3:F:663:ILE:H	3:F:663:ILE:HD12	1.66	0.59
4:G:5:ASP:OD1	4:G:6:ASN:N	2.34	0.59
4:H:86:THR:C	4:H:89:ARG:N	2.60	0.59
1:B:2024:HIS:HB2	1:B:2111:ILE:HD11	1.84	0.59
2:D:173:ILE:HA	2:D:189:ASN:HA	1.84	0.59
3:F:332:TYR:HE1	3:F:426:LEU:HB2	1.68	0.59
1:A:709:GLU:OE1	1:A:759:HIS:ND1	2.36	0.59
1:A:757:LEU:HD12	1:A:760:LEU:HD11	1.85	0.59
1:A:1889:PHE:CE1	1:A:1906:VAL:HG21	2.38	0.59
2:C:39:GLN:O	2:C:68:TYR:OH	2.21	0.59
3:E:332:TYR:HE1	3:E:426:LEU:HB2	1.68	0.59
1:A:1477:MET:O	1:A:1480:ARG:HD3	2.03	0.58
1:A:2121:LEU:HD12	1:A:2126:VAL:HG21	1.85	0.58
1:A:1901:GLN:HE21	1:A:1905:ARG:HH12	1.50	0.58
1:B:1416:LEU:O	1:B:1420:ASN:ND2	2.36	0.58
3:F:724:ALA:H	3:F:729:ARG:HH22	1.49	0.58
4:H:68:GLN:HG3	4:H:72:ILE:N	2.16	0.58
1:A:1382:LEU:O	1:A:1385:GLU:HB3	2.04	0.58
3:E:175:ASP:HB2	3:E:1666:ARG:HH21	1.69	0.58
3:E:854:TYR:HD1	4:G:13:HIS:HD1	1.51	0.58
3:F:1650:ILE:HD12	3:F:1685:MET:HE2	1.84	0.58
4:H:68:GLN:O	4:H:68:GLN:HG2	2.03	0.58
2:C:299:VAL:HG13	2:C:300:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:ARG:NH2	1:A:1216:ILE:HG23	2.19	0.58
1:B:994:MET:HE1	1:B:1030:TYR:CB	2.34	0.58
1:B:1905:ARG:O	1:B:1908:THR:OG1	2.19	0.58
1:B:2298:ASP:H	1:B:2382:MET:HE1	1.67	0.58
2:C:246:ILE:HB	2:C:256:THR:HB	1.84	0.58
3:F:148:ARG:NE	4:H:32:ILE:HD11	2.19	0.58
3:F:175:ASP:HB2	3:F:1666:ARG:HH21	1.69	0.58
3:F:369:VAL:HG13	3:F:494:LEU:HD11	1.84	0.58
3:F:890:LYS:HD2	3:F:938:TRP:CE2	2.39	0.58
1:A:662:VAL:HA	1:A:665:THR:HG22	1.86	0.58
1:A:1950:ARG:HD3	1:A:1951:PRO:HD2	1.86	0.58
2:D:299:VAL:HG13	2:D:300:GLU:HG2	1.85	0.58
1:A:671:ILE:O	1:A:675:VAL:HG12	2.03	0.58
1:A:1615:ILE:HA	1:A:1618:ILE:HG12	1.86	0.58
1:A:1892:ILE:HG23	1:A:1902:ASP:OD2	2.04	0.58
1:B:2209:LEU:HD11	1:B:2220:LEU:HB2	1.86	0.58
4:G:66:TYR:C	4:G:66:TYR:CD2	2.81	0.58
4:H:66:TYR:C	4:H:66:TYR:CD2	2.81	0.58
1:A:1282:GLU:HG2	1:A:1286:ARG:HE	1.69	0.57
1:B:1212:LEU:O	1:B:1216:ILE:HG12	2.04	0.57
3:E:890:LYS:HD2	3:E:938:TRP:CE2	2.39	0.57
4:H:68:GLN:HG2	4:H:72:ILE:H	1.67	0.57
1:B:1970:GLN:HB2	1:B:2144:TYR:CZ	2.40	0.57
4:G:68:GLN:O	4:G:68:GLN:HG2	2.04	0.57
1:A:2182:PHE:HB3	1:A:2184:PHE:HE1	1.68	0.57
2:D:13:VAL:HG13	2:D:28:GLN:HG3	1.86	0.57
3:F:716:ILE:O	3:F:720:ILE:HG12	2.05	0.57
1:B:1382:LEU:O	1:B:1385:GLU:HG3	2.05	0.57
1:B:1720:PHE:CD2	1:B:1724:MET:HE1	2.39	0.57
3:F:537:VAL:HG11	3:F:573:PHE:CD1	2.40	0.57
4:G:68:GLN:O	4:G:71:ASP:CB	2.52	0.57
1:A:1097:LEU:HD21	1:A:1135:ALA:HA	1.85	0.57
1:B:2195:ASP:OD1	1:B:2358:PHE:HB2	2.04	0.57
2:C:123:ARG:NH1	2:C:160:ASP:OD1	2.37	0.57
2:D:123:ARG:NH1	2:D:160:ASP:OD1	2.37	0.57
2:D:137:HIS:ND1	2:D:139:ASN:OD1	2.37	0.57
3:F:784:LEU:O	3:F:788:ILE:HG12	2.05	0.57
3:F:893:CYS:SG	3:F:894:HIS:N	2.78	0.57
4:H:4:LEU:HA	4:H:9:ILE:HD11	1.87	0.57
1:A:586:LEU:HD12	1:A:625:THR:HG21	1.86	0.57
1:A:1377:ASP:OD1	1:A:1406:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:VAL:HG13	2:C:28:GLN:HG3	1.86	0.57
3:E:527:ALA:HA	3:E:530:ILE:HD12	1.87	0.57
1:A:1213:ILE:HA	1:A:1216:ILE:HG12	1.86	0.57
1:B:1788:LYS:H	1:B:1788:LYS:HD2	1.69	0.57
2:C:242:GLN:NE2	2:C:267:GLU:OE2	2.29	0.57
3:E:959:CYS:H	3:E:965:ARG:HH12	1.51	0.57
4:H:68:GLN:O	4:H:71:ASP:CB	2.53	0.57
3:F:737:ARG:NH1	3:F:772:ASP:OD1	2.31	0.57
4:H:87:ALA:C	4:H:90:LEU:H	2.13	0.57
1:A:584:LEU:O	1:A:588:THR:HG23	2.04	0.57
1:A:874:THR:OG1	1:A:875:GLU:OE1	2.21	0.57
1:A:1921:GLU:HA	1:A:1924:VAL:HG22	1.86	0.57
1:A:2332:TYR:O	1:A:2507:LYS:NZ	2.37	0.57
1:B:1101:GLN:HA	1:B:1141:ARG:HH11	1.67	0.57
1:B:1521:TRP:CE3	1:B:1638:MET:HE2	2.40	0.57
3:E:151:ARG:NH2	4:G:32:ILE:O	2.38	0.57
3:E:537:VAL:HG11	3:E:573:PHE:CD1	2.40	0.57
3:E:737:ARG:NH1	3:E:772:ASP:OD1	2.31	0.57
3:F:115:SER:O	3:F:118:GLN:NE2	2.38	0.57
1:A:1153:SER:OG	1:B:701:ASN:O	2.23	0.57
1:A:2408:ARG:HH12	1:A:2509:THR:HA	1.70	0.57
1:B:1954:GLY:O	1:B:1958:HIS:ND1	2.38	0.57
3:E:115:SER:O	3:E:118:GLN:NE2	2.38	0.57
4:G:68:GLN:HG3	4:G:72:ILE:N	2.17	0.57
1:A:857:PRO:HA	1:A:860:LYS:HB2	1.86	0.56
1:A:1414:GLU:OE2	1:A:1452:LYS:NZ	2.37	0.56
1:B:1116:PRO:HB2	1:B:1117:PRO:HD3	1.87	0.56
1:A:1190:ILE:HG13	1:A:1191:PHE:HD1	1.70	0.56
1:A:589:LEU:HD21	1:A:629:LEU:HD11	1.85	0.56
1:A:854:VAL:HG22	1:A:855:VAL:HG13	1.87	0.56
1:B:1194:MET:N	1:B:1194:MET:SD	2.79	0.56
2:C:171:VAL:HG21	2:C:189:ASN:HD22	1.70	0.56
3:E:396:LEU:O	3:E:400:ILE:HG12	2.05	0.56
3:E:539:GLN:OE1	3:E:539:GLN:N	2.38	0.56
3:E:680:SER:HA	3:E:683:GLN:NE2	2.21	0.56
3:E:687:ASN:O	3:E:690:SER:OG	2.23	0.56
3:E:939:GLY:O	3:E:943:LEU:HD12	2.06	0.56
3:E:1512:LEU:HD23	3:E:1515:HIS:HB2	1.87	0.56
3:E:1615:GLU:OE1	3:E:1618:ARG:NH2	2.38	0.56
4:H:64:TYR:O	4:H:64:TYR:HD1	1.88	0.56
1:A:2044:VAL:HG23	1:A:2045:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2169:PRO:HB3	1:B:2187:LYS:HD2	1.87	0.56
1:B:2345:MET:HE3	1:B:2354:LEU:HD22	1.87	0.56
3:E:557:TRP:CD2	3:E:558:PRO:HD2	2.41	0.56
3:F:527:ALA:HA	3:F:530:ILE:HD12	1.87	0.56
4:G:87:ALA:C	4:G:90:LEU:N	2.61	0.56
1:A:779:LEU:CD1	1:A:798:VAL:HG23	2.35	0.56
1:A:1000:VAL:HA	1:A:1003:VAL:HG12	1.88	0.56
1:A:1112:HIS:CE1	1:A:1113:LEU:HD23	2.41	0.56
1:A:2037:LEU:HD22	1:A:2047:MET:HB3	1.87	0.56
1:B:974:ALA:O	1:B:978:ILE:HG12	2.06	0.56
1:B:1645:SER:HB3	1:B:1648:GLU:HG3	1.87	0.56
2:C:247:TRP:HZ3	2:C:254:LEU:HG	1.71	0.56
3:E:784:LEU:O	3:E:788:ILE:HG12	2.04	0.56
3:F:919:GLU:H	3:F:919:GLU:CD	2.13	0.56
1:A:1360:LEU:O	1:A:1364:MET:HG2	2.05	0.56
1:A:1633:TRP:HA	1:A:1636:ILE:HD12	1.87	0.56
1:A:2024:HIS:NE2	1:A:2025:GLU:OE2	2.39	0.56
1:B:1505:ASN:OD1	1:B:1506:ASP:N	2.35	0.56
3:E:893:CYS:SG	3:E:894:HIS:N	2.77	0.56
3:E:904:GLU:O	3:E:907:ARG:HD3	2.05	0.56
3:F:151:ARG:NH1	4:H:31:LEU:HD23	2.20	0.56
3:F:209:ASN:C	3:F:209:ASN:OD1	2.48	0.56
3:F:939:GLY:O	3:F:943:LEU:HD12	2.06	0.56
1:A:2497:ALA:O	1:A:2500:ILE:HG12	2.06	0.56
1:B:1122:PHE:HA	1:B:1132:ARG:HG2	1.88	0.56
1:B:1140:ASP:HA	1:B:1176:THR:HG23	1.88	0.56
1:B:1463:TYR:HE2	1:B:1479:GLY:HA3	1.71	0.56
2:C:137:HIS:ND1	2:C:139:ASN:OD1	2.38	0.56
3:E:737:ARG:HG2	3:E:773:ILE:HD12	1.87	0.56
1:A:1681:PRO:HA	1:A:1684:GLN:HG3	1.87	0.56
1:B:1103:PHE:HD2	1:B:1107:LEU:HD23	1.71	0.56
3:E:716:ILE:O	3:E:720:ILE:HG12	2.05	0.56
3:E:724:ALA:O	3:E:729:ARG:NH2	2.39	0.56
1:A:1806:HIS:O	1:A:1809:GLN:NE2	2.39	0.56
1:B:1119:VAL:HA	1:B:1122:PHE:CE1	2.40	0.56
2:D:247:TRP:HZ3	2:D:254:LEU:HG	1.71	0.56
3:E:568:GLU:OE1	3:E:568:GLU:N	2.37	0.56
3:F:680:SER:HA	3:F:683:GLN:NE2	2.21	0.56
4:G:4:LEU:HA	4:G:9:ILE:HD11	1.87	0.56
1:A:1108:ASP:OD1	1:A:1109:ASP:N	2.40	0.55
1:A:1111:LEU:HD22	1:A:1151:TYR:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1463:TYR:O	1:B:1467:MET:HG2	2.05	0.55
3:F:556:LYS:HE3	3:F:607:GLN:HE22	1.71	0.55
3:F:557:TRP:CD2	3:F:558:PRO:HD2	2.41	0.55
4:G:68:GLN:HG2	4:G:72:ILE:H	1.67	0.55
1:A:2204:LEU:O	1:A:2207:THR:OG1	2.15	0.55
3:F:687:ASN:O	3:F:690:SER:OG	2.23	0.55
4:G:86:THR:C	4:G:89:ARG:N	2.60	0.55
4:G:87:ALA:C	4:G:90:LEU:H	2.13	0.55
1:A:712:ILE:HA	1:A:715:VAL:HG22	1.88	0.55
1:A:1164:ASP:OD2	1:A:1201:ARG:NH1	2.39	0.55
1:A:1892:ILE:HD11	1:A:1930:ILE:HG21	1.87	0.55
3:E:209:ASN:C	3:E:209:ASN:OD1	2.48	0.55
3:E:228:ILE:HG13	3:E:232:LEU:HD23	1.89	0.55
3:E:958:GLN:N	3:E:965:ARG:HH12	2.04	0.55
3:F:904:GLU:O	3:F:907:ARG:HD3	2.05	0.55
4:G:64:TYR:O	4:G:64:TYR:HD1	1.88	0.55
1:B:1712:ASP:O	1:B:1716:HIS:ND1	2.40	0.55
2:D:39:GLN:O	2:D:68:TYR:OH	2.21	0.55
3:F:396:LEU:O	3:F:400:ILE:HG12	2.05	0.55
3:F:724:ALA:O	3:F:729:ARG:NH2	2.39	0.55
3:F:830:LYS:HA	3:F:833:ARG:HG2	1.89	0.55
1:A:633:SER:O	1:A:644:VAL:N	2.40	0.55
1:A:819:GLU:OE2	1:A:819:GLU:N	2.35	0.55
1:A:1397:LEU:O	1:A:1401:GLU:HG2	2.06	0.55
1:A:2074:TYR:HB3	1:A:2078:LEU:HD23	1.88	0.55
3:E:940:LEU:HD21	3:E:984:ILE:HD11	1.89	0.55
1:A:673:TYR:HE1	1:A:710:LEU:HD22	1.71	0.55
1:A:1521:TRP:CE3	1:A:1638:MET:HE2	2.42	0.55
1:A:1889:PHE:CE2	1:A:1926:GLY:HA3	2.42	0.55
3:E:118:GLN:HA	3:E:121:LEU:HG	1.89	0.55
1:A:1433:LEU:HD22	1:A:1453:LEU:HD13	1.87	0.55
1:A:2361:CYS:HG	1:A:2362:PHE:HD1	1.52	0.55
1:B:1200:VAL:HG12	1:B:1203:ARG:HH22	1.71	0.55
1:B:2329:MET:HE3	1:B:2404:MET:HE2	1.88	0.55
1:A:1888:PHE:HD1	1:A:1902:ASP:OD1	1.89	0.55
1:B:2027:TRP:CZ2	1:B:2078:LEU:HD22	2.41	0.55
2:D:193:ASN:HB3	2:D:215:LYS:HE2	1.89	0.55
3:F:128:LEU:O	3:F:131:ARG:HG2	2.07	0.55
3:F:958:GLN:N	3:F:965:ARG:HH12	2.04	0.55
3:F:1512:LEU:HD23	3:F:1515:HIS:HB2	1.87	0.55
1:B:702:ASP:H	1:B:708:ARG:CZ	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:LEU:HD21	2:D:140:GLN:HG3	1.89	0.55
3:E:438:LEU:HD23	3:E:443:SER:HB2	1.89	0.55
3:E:919:GLU:CD	3:E:919:GLU:H	2.13	0.55
3:F:275:GLU:H	3:F:275:GLU:CD	2.15	0.55
3:F:437:ILE:O	3:F:437:ILE:HG22	2.07	0.55
3:F:737:ARG:HG2	3:F:773:ILE:HD12	1.87	0.55
3:F:911:THR:O	3:F:911:THR:OG1	2.25	0.55
3:E:556:LYS:HE3	3:E:607:GLN:HE22	1.71	0.55
3:E:911:THR:O	3:E:911:THR:OG1	2.25	0.55
3:F:136:GLN:NE2	3:F:181:ASP:OD1	2.39	0.55
1:A:1129:LEU:HD23	1:A:1168:GLU:OE2	2.08	0.54
1:A:1375:ARG:HG3	1:A:1376:ASP:N	2.23	0.54
1:B:2024:HIS:NE2	1:B:2025:GLU:OE2	2.40	0.54
2:D:94:HIS:ND1	2:D:140:GLN:HG2	2.22	0.54
3:F:332:TYR:CE1	3:F:426:LEU:HD12	2.42	0.54
3:F:959:CYS:H	3:F:965:ARG:HH12	1.51	0.54
1:A:1489:GLU:OE1	1:A:1491:GLY:N	2.40	0.54
1:B:2329:MET:CE	1:B:2404:MET:HE2	2.38	0.54
3:E:332:TYR:CE1	3:E:426:LEU:HD12	2.42	0.54
3:F:228:ILE:HG13	3:F:232:LEU:HD23	1.89	0.54
1:A:769:ARG:NH2	1:A:808:VAL:O	2.41	0.54
1:A:1193:PRO:HG2	1:A:1194:MET:SD	2.47	0.54
1:A:1970:GLN:HB2	1:A:2144:TYR:CZ	2.43	0.54
1:A:2408:ARG:NH1	1:A:2508:LEU:O	2.40	0.54
1:A:2426:LEU:HG	1:A:2427:LEU:HD22	1.90	0.54
1:B:705:PHE:CZ	1:B:756:MET:HE3	2.43	0.54
1:B:2520:ASP:CG	1:B:2522:PRO:HD2	2.32	0.54
2:C:106:ASP:OD1	2:C:107:CYS:N	2.39	0.54
3:E:136:GLN:NE2	3:E:181:ASP:OD1	2.39	0.54
3:F:94:ASN:HD21	3:F:99:VAL:HG11	1.71	0.54
1:B:769:ARG:NH2	1:B:812:GLU:OE2	2.38	0.54
1:B:820:LEU:O	1:B:824:ILE:HG12	2.07	0.54
1:B:1444:GLU:OE2	1:B:1446:GLN:NE2	2.40	0.54
3:E:62:ASN:O	3:E:66:LEU:HG	2.08	0.54
3:F:62:ASN:O	3:F:66:LEU:HG	2.08	0.54
3:F:336:ARG:HH12	3:F:874:PRO:HD3	1.73	0.54
3:F:387:LEU:H	3:F:387:LEU:HD12	1.72	0.54
1:B:1521:TRP:HB2	1:B:1529:MET:HE2	1.89	0.54
3:E:387:LEU:HD12	3:E:387:LEU:H	1.72	0.54
3:E:628:LYS:HA	3:E:631:VAL:HG12	1.89	0.54
3:F:399:PHE:HB3	3:F:404:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:ALA:HB3	1:A:1274:ARG:NH1	2.22	0.54
1:A:1383:LEU:HB3	1:A:1399:TYR:HE1	1.73	0.54
1:A:1465:LYS:HD3	1:A:1465:LYS:C	2.33	0.54
1:B:819:GLU:HA	1:B:822:ILE:HG12	1.88	0.54
1:B:931:THR:HB	1:B:935:LEU:HD12	1.90	0.54
1:B:1615:ILE:HA	1:B:1618:ILE:HG12	1.90	0.54
2:C:94:HIS:ND1	2:C:140:GLN:HG2	2.22	0.54
1:A:1889:PHE:CD2	1:A:1926:GLY:HA3	2.42	0.54
1:B:1633:TRP:HA	1:B:1636:ILE:HG22	1.88	0.54
1:B:2285:GLU:HG3	2:D:272:TRP:CZ2	2.43	0.54
3:E:437:ILE:HG22	3:E:437:ILE:O	2.07	0.54
3:E:912:PRO:HG2	3:E:914:LEU:HD11	1.90	0.54
3:F:568:GLU:OE1	3:F:568:GLU:N	2.37	0.54
3:F:940:LEU:HD21	3:F:984:ILE:HD11	1.89	0.54
1:B:2000:GLU:OE1	1:B:2000:GLU:N	2.40	0.54
1:B:2204:LEU:HD22	1:B:2417:VAL:HG21	1.90	0.54
3:F:628:LYS:HA	3:F:631:VAL:HG12	1.89	0.54
1:A:2279:THR:OG1	1:A:2281:MET:SD	2.60	0.54
1:B:1181:VAL:HG23	1:B:1212:LEU:HD13	1.89	0.54
1:B:1401:GLU:HG3	1:B:1405:GLN:NE2	2.23	0.54
3:E:225:GLU:O	3:E:229:THR:HG23	2.07	0.54
3:E:807:ARG:HG3	3:E:880:ILE:HG21	1.90	0.54
3:E:1515:HIS:HE2	3:E:1651:CYS:HG	1.49	0.54
3:F:820:GLU:OE2	3:F:821:ARG:HD3	2.08	0.54
3:F:912:PRO:HG2	3:F:914:LEU:HD11	1.90	0.54
1:A:2000:GLU:OE1	1:A:2000:GLU:N	2.41	0.54
3:E:485:ARG:HH12	3:E:488:LYS:HE3	1.73	0.54
3:F:118:GLN:HA	3:F:121:LEU:HG	1.89	0.54
3:F:807:ARG:HG3	3:F:880:ILE:HG21	1.90	0.54
1:A:700:LEU:O	1:A:708:ARG:NE	2.25	0.53
1:A:1348:GLN:O	1:A:1386:ARG:NH2	2.40	0.53
2:C:136:LEU:HD21	2:C:140:GLN:HG3	1.89	0.53
3:E:526:GLU:HG2	3:E:527:ALA:H	1.73	0.53
3:F:225:GLU:O	3:F:229:THR:HG23	2.07	0.53
3:F:415:SER:OG	3:F:416:ASP:N	2.36	0.53
3:F:438:LEU:HD23	3:F:443:SER:HB2	1.90	0.53
1:A:2426:LEU:HD23	1:A:2426:LEU:H	1.72	0.53
1:B:2316:ARG:NE	1:B:2349:LEU:O	2.38	0.53
2:C:193:ASN:HB3	2:C:215:LYS:HE2	1.90	0.53
2:D:171:VAL:HG21	2:D:189:ASN:HD22	1.70	0.53
3:E:830:LYS:HA	3:E:833:ARG:HG2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:961:VAL:HB	3:E:964:ILE:HD12	1.90	0.53
4:H:87:ALA:C	4:H:90:LEU:N	2.61	0.53
1:A:1440:PHE:HB3	1:A:1442:GLU:OE1	2.09	0.53
1:B:938:MET:SD	1:B:2306:LYS:HA	2.49	0.53
1:B:1508:THR:O	1:B:1512:MET:HG2	2.09	0.53
1:B:1948:THR:HG21	1:B:1953:VAL:HG13	1.90	0.53
1:B:1960:LEU:O	1:B:1964:ILE:HG12	2.08	0.53
1:B:2392:LEU:HD23	1:B:2392:LEU:H	1.73	0.53
3:E:94:ASN:HD21	3:E:99:VAL:HG11	1.71	0.53
1:A:1374:LEU:HB2	1:A:1378:ASN:C	2.33	0.53
1:A:2165:SER:OG	1:A:2166:LYS:N	2.41	0.53
3:E:128:LEU:O	3:E:131:ARG:HG2	2.07	0.53
3:E:151:ARG:HA	3:E:154:ILE:HG12	1.89	0.53
3:E:473:LEU:HA	3:E:476:LEU:HD12	1.90	0.53
3:E:820:GLU:OE2	3:E:821:ARG:HD3	2.08	0.53
3:E:1623:LEU:HD11	3:E:1629:THR:HG23	1.90	0.53
1:A:1111:LEU:HD22	1:A:1151:TYR:CE2	2.43	0.53
1:A:1402:LEU:HA	1:A:1405:GLN:OE1	2.08	0.53
3:E:275:GLU:H	3:E:275:GLU:CD	2.15	0.53
3:E:357:ARG:NH2	3:E:358:PHE:O	2.41	0.53
3:E:399:PHE:HB3	3:E:404:LEU:HD13	1.89	0.53
3:F:473:LEU:HA	3:F:476:LEU:HD12	1.91	0.53
3:F:526:GLU:HG2	3:F:527:ALA:H	1.73	0.53
1:B:751:GLU:HB2	1:B:794:VAL:HG12	1.90	0.53
1:B:980:LYS:HA	1:B:1022:PHE:CE1	2.43	0.53
1:B:1115:LEU:HD21	1:B:1155:ILE:HD11	1.90	0.53
1:B:1235:ARG:HD2	1:B:1236:MET:SD	2.48	0.53
1:B:1950:ARG:HD3	1:B:1951:PRO:HD2	1.90	0.53
3:E:521:LEU:HB3	3:E:557:TRP:HZ2	1.74	0.53
3:F:1615:GLU:OE1	3:F:1618:ARG:NH2	2.38	0.53
1:A:725:PHE:HE2	3:F:1001:TRP:CD2	2.27	0.53
1:A:1901:GLN:NE2	1:A:1905:ARG:HH22	2.06	0.53
1:B:1296:SER:HA	1:B:1301:ARG:HH22	1.74	0.53
1:B:2204:LEU:O	1:B:2207:THR:OG1	2.18	0.53
1:B:2514:SER:OG	1:B:2516:ASP:OD1	2.24	0.53
3:E:240:THR:HA	3:E:243:TYR:CD2	2.44	0.53
3:E:540:HIS:HB2	3:E:542:GLU:OE1	2.08	0.53
4:H:93:LEU:HA	4:H:96:GLU:HG3	1.91	0.53
1:A:1876:THR:HA	1:A:1879:MET:HG3	1.90	0.53
1:B:654:ASP:O	1:B:657:SER:OG	2.24	0.53
3:E:309:ILE:HD11	3:E:399:PHE:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:537:VAL:HG11	3:E:573:PHE:HD1	1.74	0.53
3:F:151:ARG:HA	3:F:154:ILE:HG12	1.90	0.53
3:F:259:ASP:OD1	3:F:261:HIS:N	2.40	0.53
3:F:309:ILE:HD11	3:F:399:PHE:HE1	1.74	0.53
3:F:540:HIS:HB2	3:F:542:GLU:OE1	2.08	0.53
3:F:788:ILE:O	3:F:791:LYS:NZ	2.35	0.53
3:F:830:LYS:HE2	3:F:835:TYR:CE2	2.44	0.53
4:G:69:SER:O	4:G:71:ASP:N	2.41	0.53
4:H:69:SER:O	4:H:71:ASP:N	2.41	0.53
1:A:1269:TRP:O	1:A:1271:ALA:N	2.42	0.53
1:A:1585:ARG:HH11	1:A:1585:ARG:HG2	1.74	0.53
1:B:970:MET:SD	1:B:970:MET:N	2.75	0.53
3:E:186:ALA:O	3:E:190:ILE:HG12	2.08	0.53
3:F:357:ARG:NH2	3:F:358:PHE:O	2.41	0.53
3:F:971:VAL:HA	3:F:974:LEU:HD12	1.91	0.53
3:F:1513:GLN:HG2	3:F:1614:LYS:HE3	1.91	0.53
4:G:87:ALA:O	4:G:89:ARG:C	2.48	0.53
1:A:2026:MET:HE1	1:A:2057:MET:HE2	1.91	0.52
1:B:1000:VAL:HA	1:B:1003:VAL:HG22	1.91	0.52
1:B:1046:THR:HG23	1:B:1048:ILE:H	1.74	0.52
1:B:2105:TYR:CE1	1:B:2109:ARG:HD2	2.44	0.52
1:B:952:MET:HE1	1:B:979:PHE:HE1	1.74	0.52
3:E:273:LEU:O	3:E:276:ASP:HB2	2.10	0.52
3:E:1513:GLN:HG2	3:E:1614:LYS:HE3	1.91	0.52
3:E:1522:TYR:OH	3:E:1532:GLN:O	2.25	0.52
3:F:105:ARG:HA	3:F:108:ARG:NH1	2.24	0.52
3:F:521:LEU:HB3	3:F:557:TRP:HZ2	1.74	0.52
1:A:1804:TYR:O	1:A:1808:ASN:ND2	2.42	0.52
1:B:1950:ARG:HB3	1:B:1953:VAL:HG12	1.91	0.52
3:F:556:LYS:HE3	3:F:607:GLN:OE1	2.10	0.52
3:F:1649:ASP:OD1	3:F:1649:ASP:N	2.42	0.52
4:G:27:CYS:O	4:G:31:LEU:HG	2.08	0.52
1:A:2511:ARG:NH1	1:A:2518:THR:OG1	2.42	0.52
3:F:151:ARG:HH12	4:H:31:LEU:HD23	1.74	0.52
3:F:485:ARG:HH12	3:F:488:LYS:HE3	1.73	0.52
1:A:693:LEU:HD11	1:A:725:PHE:CD1	2.42	0.52
1:A:705:PHE:HA	1:A:708:ARG:HG2	1.91	0.52
1:A:974:ALA:O	1:A:978:ILE:HG12	2.09	0.52
1:A:2392:LEU:HD23	1:A:2392:LEU:H	1.73	0.52
1:B:1889:PHE:CE1	1:B:1906:VAL:HG21	2.44	0.52
3:E:105:ARG:HA	3:E:108:ARG:CZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:186:ALA:O	3:F:190:ILE:HG12	2.08	0.52
4:H:27:CYS:O	4:H:31:LEU:HG	2.08	0.52
1:A:729:PHE:HB3	1:A:733:MET:HE1	1.92	0.52
1:A:1960:LEU:O	1:A:1964:ILE:HG12	2.08	0.52
3:E:259:ASP:OD1	3:E:261:HIS:N	2.40	0.52
3:E:894:HIS:O	3:E:898:VAL:HG13	2.10	0.52
3:F:961:VAL:HB	3:F:964:ILE:HD12	1.90	0.52
1:A:1049:GLN:HA	1:A:1052:ILE:HG22	1.92	0.52
1:B:772:MET:HE1	1:B:812:GLU:CB	2.39	0.52
1:B:1402:LEU:HA	1:B:1405:GLN:OE1	2.10	0.52
1:B:1546:TYR:HA	1:B:1549:VAL:HG12	1.91	0.52
2:C:58:ALA:HB2	2:C:67:MET:HE2	1.92	0.52
3:F:249:GLU:HG2	3:F:250:LEU:N	2.25	0.52
1:A:2520:ASP:CG	1:A:2522:PRO:HD2	2.35	0.52
1:B:1001:ILE:HD12	1:B:1004:CYS:SG	2.50	0.52
1:B:1108:ASP:OD1	1:B:1109:ASP:N	2.42	0.52
1:B:1654:LEU:HD21	1:B:1696:VAL:HG12	1.92	0.52
1:B:2136:LEU:HG	1:B:2137:GLU:H	1.75	0.52
1:B:2340:HIS:CD2	1:B:2342:SER:HB2	2.44	0.52
2:D:219:HIS:NE2	2:D:237:THR:OG1	2.26	0.52
3:E:249:GLU:HG2	3:E:250:LEU:N	2.25	0.52
3:E:336:ARG:HH12	3:E:874:PRO:HD3	1.73	0.52
3:E:556:LYS:HE3	3:E:607:GLN:OE1	2.10	0.52
3:F:75:GLU:HG2	3:F:76:LYS:H	1.74	0.52
3:F:240:THR:HA	3:F:243:TYR:CD2	2.44	0.52
3:F:537:VAL:HG11	3:F:573:PHE:HD1	1.74	0.52
3:F:1522:TYR:OH	3:F:1532:GLN:O	2.24	0.52
1:A:878:GLN:O	1:A:882:ARG:HG3	2.10	0.52
1:A:1222:LEU:HB2	3:E:495:ASP:OD2	2.10	0.52
1:B:663:GLY:C	1:B:672:ARG:HH21	2.18	0.52
3:E:105:ARG:HA	3:E:108:ARG:NH1	2.24	0.52
3:F:105:ARG:HA	3:F:108:ARG:CZ	2.40	0.52
1:A:536:GLN:HA	1:A:594:PHE:HE1	1.74	0.52
1:A:1031:MET:HE1	1:A:1059:ILE:HG23	1.92	0.52
1:A:2076:ARG:HB2	3:E:248:VAL:HB	1.92	0.52
1:B:681:GLU:HG2	1:B:684:ASP:HB2	1.92	0.52
1:B:1072:PRO:HG3	1:B:1110:TYR:OH	2.10	0.52
1:B:1620:TRP:O	1:B:1624:GLN:HG2	2.10	0.52
1:B:2371:PHE:CD2	1:B:2542:TYR:HD1	2.28	0.52
3:E:696:HIS:O	3:E:700:LEU:HD12	2.10	0.52
3:F:724:ALA:N	3:F:729:ARG:NH2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1765:ASN:OD1	1:A:1766:GLU:N	2.40	0.51
1:B:736:GLN:O	1:B:739:THR:OG1	2.19	0.51
1:B:1060:VAL:HG21	1:B:1103:PHE:HE1	1.74	0.51
2:C:40:HIS:NE2	2:C:66:ARG:HD3	2.25	0.51
3:E:971:VAL:HA	3:E:974:LEU:HD12	1.91	0.51
3:F:37:ASN:O	3:F:41:ILE:HG12	2.10	0.51
3:F:696:HIS:O	3:F:700:LEU:HD12	2.10	0.51
1:A:2371:PHE:CD2	1:A:2542:TYR:HD1	2.28	0.51
1:B:733:MET:O	1:B:737:ILE:HD12	2.10	0.51
1:B:1114:LEU:O	1:B:1117:PRO:HD2	2.10	0.51
1:B:1955:ARG:HG2	1:B:1959:GLN:HE22	1.75	0.51
2:C:286:VAL:HG22	2:C:296:LEU:HG	1.92	0.51
3:E:116:ILE:HA	3:E:119:LYS:HE2	1.91	0.51
3:E:493:HIS:O	3:E:497:ILE:HG12	2.10	0.51
3:E:830:LYS:HE2	3:E:835:TYR:CE2	2.44	0.51
3:E:1668:PRO:O	3:E:1671:ARG:HD3	2.11	0.51
3:F:273:LEU:O	3:F:276:ASP:HB2	2.10	0.51
3:F:493:HIS:O	3:F:497:ILE:HG12	2.10	0.51
4:G:93:LEU:HA	4:G:96:GLU:HG3	1.91	0.51
1:A:654:ASP:O	1:A:657:SER:OG	2.28	0.51
1:A:727:MET:HA	1:A:730:LEU:HD12	1.92	0.51
1:A:1161:ARG:CZ	1:A:1162:THR:HB	2.40	0.51
1:B:1112:HIS:CE1	1:B:1113:LEU:HD23	2.46	0.51
1:B:2037:LEU:HD21	1:B:2050:VAL:HG21	1.93	0.51
2:C:92:GLY:HA3	2:C:101:TYR:CZ	2.46	0.51
3:E:526:GLU:OE1	3:E:526:GLU:N	2.26	0.51
1:A:1709:ARG:HH21	1:A:1711:ILE:HB	1.75	0.51
1:B:947:TYR:CE1	1:B:1324:SER:HB2	2.45	0.51
1:B:1110:TYR:O	1:B:1113:LEU:HG	2.10	0.51
1:B:1129:LEU:HD11	1:B:1169:LEU:HD21	1.92	0.51
1:B:1221:THR:OG1	3:F:495:ASP:OD1	2.28	0.51
1:B:1921:GLU:O	1:B:1924:VAL:HG22	2.11	0.51
1:B:2426:LEU:O	1:B:2429:TRP:NE1	2.43	0.51
3:E:37:ASN:O	3:E:41:ILE:HG12	2.10	0.51
3:F:44:ASN:ND2	3:F:59:HIS:HB3	2.26	0.51
1:A:1619:TRP:HB3	1:A:1640:ARG:NH1	2.25	0.51
1:A:2105:TYR:CE2	1:A:2109:ARG:HD2	2.45	0.51
1:A:2362:PHE:CD2	1:A:2500:ILE:HD12	2.46	0.51
1:B:684:ASP:OD1	1:B:717:ARG:NH1	2.43	0.51
1:B:1765:ASN:H	1:B:1768:THR:HG22	1.76	0.51
2:C:86:LYS:HD2	2:C:106:ASP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:878:LEU:HD11	3:E:974:LEU:HD21	1.93	0.51
3:E:1649:ASP:OD1	3:E:1649:ASP:N	2.42	0.51
3:F:1623:LEU:HD11	3:F:1629:THR:HG23	1.90	0.51
1:A:992:GLN:OE1	1:A:992:GLN:N	2.41	0.51
1:A:1112:HIS:ND1	1:B:740:GLU:OE2	2.43	0.51
1:B:1343:LEU:O	1:B:1347:SER:OG	2.16	0.51
1:B:1985:THR:HA	1:B:1988:HIS:CE1	2.46	0.51
1:B:2318:THR:HG22	1:B:2322:ARG:HD2	1.93	0.51
1:A:2079:MET:HE1	3:E:245:ARG:NH1	2.25	0.51
2:D:40:HIS:NE2	2:D:66:ARG:HD3	2.25	0.51
3:E:75:GLU:HG2	3:E:76:LYS:H	1.75	0.51
3:F:539:GLN:OE1	3:F:539:GLN:N	2.38	0.51
3:F:706:ASP:OD1	3:F:707:TYR:N	2.44	0.51
1:A:1129:LEU:HB3	1:A:1133:LYS:NZ	2.26	0.51
1:A:1490:TRP:HE3	1:A:1519:ALA:HA	1.75	0.51
1:A:2105:TYR:O	1:A:2109:ARG:HG3	2.10	0.51
1:B:613:SER:O	1:B:619:ARG:NH1	2.36	0.51
1:B:1069:LEU:HD22	3:F:467:LEU:HD12	1.91	0.51
1:B:1107:LEU:HD12	1:B:1107:LEU:O	2.11	0.51
1:B:1920:ASN:O	1:B:1924:VAL:HG13	2.11	0.51
2:C:20:TYR:HA	2:C:44:GLN:NE2	2.26	0.51
3:F:116:ILE:HA	3:F:119:LYS:HE2	1.92	0.51
3:F:894:HIS:O	3:F:898:VAL:HG13	2.10	0.51
4:H:28:GLU:HA	4:H:31:LEU:HB2	1.93	0.51
1:A:719:SER:HA	1:A:726:VAL:HG11	1.92	0.51
1:A:1921:GLU:HG2	1:A:1922:ALA:H	1.74	0.51
1:B:703:GLN:HG2	1:B:704:VAL:HG13	1.93	0.51
1:B:742:GLU:HG2	3:E:459:PHE:CE2	2.46	0.51
1:B:775:ILE:O	1:B:779:LEU:HD23	2.11	0.51
1:B:1222:LEU:HB2	3:F:495:ASP:OD2	2.11	0.51
1:B:1330:ASN:H	1:B:1333:GLN:NE2	2.09	0.51
1:B:1921:GLU:O	1:B:1925:GLU:OE1	2.29	0.51
2:D:20:TYR:HA	2:D:44:GLN:NE2	2.26	0.51
2:D:92:GLY:HA3	2:D:101:TYR:CZ	2.46	0.51
3:E:131:ARG:HB2	3:E:1674:GLN:NE2	2.26	0.51
3:E:1487:MET:HG3	3:E:1492:ILE:HD13	1.92	0.51
3:F:274:LYS:O	3:F:277:ARG:N	2.44	0.51
4:H:87:ALA:O	4:H:89:ARG:C	2.49	0.51
1:A:2340:HIS:CD2	1:A:2342:SER:HB2	2.46	0.51
1:B:666:ASP:HB3	1:B:672:ARG:HH12	1.75	0.51
1:B:1075:ILE:O	1:B:1079:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1098:ALA:HA	1:B:1101:GLN:HG3	1.94	0.51
1:B:1637:LEU:HD21	1:B:1653:TRP:CE2	2.46	0.51
2:C:145:VAL:O	2:C:152:ILE:HD12	2.11	0.51
3:F:226:ALA:O	3:F:229:THR:OG1	2.29	0.51
3:F:1668:PRO:O	3:F:1671:ARG:HD3	2.11	0.51
1:A:1218:LYS:HE2	3:E:556:LYS:HD2	1.94	0.50
1:A:1480:ARG:HA	1:A:1483:CYS:SG	2.51	0.50
1:A:2509:THR:HB	1:A:2511:ARG:HG3	1.92	0.50
1:B:2133:CYS:C	1:B:2135:ASP:H	2.20	0.50
2:C:219:HIS:NE2	2:C:237:THR:OG1	2.27	0.50
2:D:58:ALA:HB2	2:D:67:MET:HE2	1.92	0.50
3:E:706:ASP:OD1	3:E:707:TYR:N	2.44	0.50
4:G:28:GLU:HA	4:G:31:LEU:HB2	1.93	0.50
1:A:1583:TYR:HE1	1:A:1590:MET:HE1	1.76	0.50
1:A:1785:SER:O	1:A:1785:SER:OG	2.29	0.50
1:A:2285:GLU:HG3	2:C:272:TRP:CZ2	2.46	0.50
1:A:2311:GLU:H	1:A:2311:GLU:CD	2.14	0.50
1:B:772:MET:HE1	1:B:812:GLU:HB3	1.92	0.50
1:B:1207:GLN:H	1:B:1207:GLN:CD	2.18	0.50
1:B:2094:VAL:O	1:B:2098:THR:HG23	2.11	0.50
1:B:2536:GLU:H	1:B:2536:GLU:CD	2.19	0.50
3:E:663:ILE:O	3:E:667:SER:N	2.44	0.50
3:E:710:ASP:C	3:E:710:ASP:OD1	2.54	0.50
3:E:1689:ALA:HA	3:E:1692:VAL:HG22	1.92	0.50
1:A:894:LEU:O	1:A:1583:TYR:OH	2.24	0.50
1:A:955:LEU:HD22	1:A:971:VAL:HG23	1.93	0.50
1:A:957:ARG:NE	1:A:957:ARG:HA	2.26	0.50
1:A:2169:PRO:HB3	1:A:2187:LYS:HD2	1.93	0.50
1:A:2519:LEU:HB3	1:A:2523:THR:HB	1.93	0.50
3:F:710:ASP:C	3:F:710:ASP:OD1	2.54	0.50
1:A:1546:TYR:HA	1:A:1549:VAL:HG12	1.93	0.50
1:A:1985:THR:HA	1:A:1988:HIS:CE1	2.46	0.50
2:D:80:SER:O	4:H:105:ASN:HA	2.10	0.50
2:D:106:ASP:OD1	2:D:107:CYS:N	2.39	0.50
3:F:875:HIS:HB3	3:F:877:TYR:CE2	2.46	0.50
3:F:878:LEU:HD11	3:F:974:LEU:HD21	1.93	0.50
3:F:1641:GLU:HB3	4:H:90:LEU:HD11	1.94	0.50
1:A:1190:ILE:HG13	1:A:1191:PHE:CD1	2.47	0.50
1:A:1697:THR:O	1:A:1701:MET:HG2	2.12	0.50
1:A:2156:ILE:HG12	1:A:2174:LEU:HD22	1.93	0.50
1:B:677:ALA:HA	1:B:710:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:ILE:HG13	1:B:823:ILE:N	2.26	0.50
1:B:2284:VAL:O	1:B:2287:PHE:N	2.44	0.50
2:C:43:SER:OG	2:C:44:GLN:N	2.45	0.50
3:F:547:ASN:ND2	3:F:550:LEU:HD22	2.26	0.50
3:F:945:GLU:OE1	3:F:945:GLU:N	2.43	0.50
3:F:1689:ALA:HA	3:F:1692:VAL:HG22	1.92	0.50
1:A:1924:VAL:HG12	1:A:1956:LEU:HD11	1.93	0.50
1:B:1765:ASN:O	1:B:1769:ILE:HG12	2.12	0.50
2:D:43:SER:OG	2:D:44:GLN:N	2.45	0.50
2:D:286:VAL:HG22	2:D:296:LEU:HG	1.92	0.50
3:E:547:ASN:ND2	3:E:550:LEU:HD22	2.26	0.50
3:F:831:TRP:CD1	3:F:882:LEU:HD13	2.47	0.50
3:F:1650:ILE:CD1	3:F:1685:MET:HE2	2.42	0.50
1:A:151:ARG:O	1:A:155:TRP:N	2.43	0.50
1:A:578:ASP:O	1:A:581:SER:N	2.44	0.50
1:A:1110:TYR:HD1	1:A:1113:LEU:HD21	1.76	0.50
1:A:2195:ASP:HA	1:A:2198:VAL:HG22	1.94	0.50
1:B:810:GLY:O	1:B:811:LEU:HG	2.12	0.50
1:B:957:ARG:HA	1:B:957:ARG:NE	2.27	0.50
1:B:1526:TRP:HA	1:B:1529:MET:HB2	1.93	0.50
1:B:1776:TYR:O	1:B:1780:THR:HG23	2.12	0.50
1:B:2182:PHE:HB3	1:B:2184:PHE:HE1	1.77	0.50
3:E:831:TRP:CD1	3:E:882:LEU:HD13	2.47	0.50
3:F:131:ARG:HB2	3:F:1674:GLN:NE2	2.26	0.50
3:F:189:ALA:HB2	4:H:18:HIS:HD1	1.77	0.50
3:F:663:ILE:O	3:F:667:SER:N	2.44	0.50
4:G:92:ARG:HH22	4:G:93:LEU:HB3	1.77	0.50
1:A:1107:LEU:HD12	1:A:1107:LEU:O	2.11	0.50
1:A:1561:GLN:OE1	1:A:1561:GLN:N	2.45	0.50
1:B:814:ARG:HG2	1:B:814:ARG:HH11	1.77	0.50
1:B:1759:LEU:HD21	1:B:1772:VAL:HG11	1.94	0.50
2:C:110:ARG:HB3	2:C:124:ILE:HG22	1.94	0.50
3:E:44:ASN:ND2	3:E:59:HIS:HB3	2.26	0.50
3:E:788:ILE:O	3:E:791:LYS:NZ	2.35	0.50
3:F:357:ARG:NH2	3:F:359:GLN:OE1	2.45	0.50
1:A:610:PHE:HA	1:A:619:ARG:HG2	1.93	0.50
1:A:957:ARG:HA	1:A:957:ARG:CZ	2.42	0.50
1:A:1277:LYS:NZ	1:A:1281:LEU:HD11	2.26	0.50
1:A:2074:TYR:O	1:A:2078:LEU:HD23	2.11	0.50
1:B:785:ASP:OD1	1:B:785:ASP:N	2.45	0.50
1:B:825:MET:HE1	1:B:861:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1326:TRP:O	1:B:1334:GLN:NE2	2.45	0.50
1:B:1912:ASP:OD1	1:B:1913:TYR:N	2.44	0.50
1:B:2266:ARG:HH11	1:B:2266:ARG:HG3	1.77	0.50
2:D:145:VAL:O	2:D:152:ILE:HD12	2.11	0.50
3:E:357:ARG:NH2	3:E:359:GLN:OE1	2.45	0.50
3:E:386:ASP:HA	3:E:876:VAL:O	2.12	0.50
4:H:16:GLN:O	4:H:20:THR:HG22	2.12	0.50
4:H:76:TRP:CD1	4:H:76:TRP:C	2.85	0.50
1:A:624:ARG:O	1:A:627:SER:OG	2.20	0.49
1:B:1900:LEU:O	1:B:1903:THR:OG1	2.29	0.49
2:D:110:ARG:HB3	2:D:124:ILE:HG22	1.94	0.49
2:D:298:CYS:H	2:D:305:LYS:NZ	2.10	0.49
3:E:1511:GLY:HA2	3:E:1610:ILE:HG12	1.94	0.49
3:F:1511:GLY:HA2	3:F:1610:ILE:HG12	1.94	0.49
1:A:658:LYS:HB3	1:A:658:LYS:HZ3	1.76	0.49
1:A:1367:SER:OG	1:A:1368:ASP:N	2.45	0.49
1:A:2329:MET:HA	1:A:2329:MET:HE3	1.94	0.49
1:B:1401:GLU:OE1	1:B:2389:VAL:HB	2.12	0.49
1:B:2022:LEU:HB3	1:B:2025:GLU:OE1	2.12	0.49
3:E:274:LYS:O	3:E:277:ARG:N	2.44	0.49
3:E:802:LEU:O	3:E:806:LEU:HD23	2.12	0.49
3:E:830:LYS:HE2	3:E:835:TYR:CZ	2.47	0.49
3:E:853:THR:HA	3:E:855:ARG:NH1	2.27	0.49
3:F:103:GLY:O	3:F:107:LEU:HD23	2.12	0.49
3:F:766:ILE:O	3:F:769:GLU:HG3	2.12	0.49
3:F:774:LEU:HD22	3:F:804:LEU:HD21	1.94	0.49
3:F:1682:PHE:HD1	3:F:1685:MET:HE3	1.77	0.49
4:G:16:GLN:O	4:G:20:THR:HG22	2.12	0.49
1:A:1087:SER:HB3	1:A:1090:ARG:HA	1.94	0.49
1:A:1292:LEU:HG	1:A:1304:TRP:HB2	1.92	0.49
1:A:2194:GLN:HG3	1:A:2421:PHE:HZ	1.77	0.49
1:B:1903:THR:O	1:B:1907:LEU:HD23	2.12	0.49
3:E:774:LEU:HD22	3:E:804:LEU:HD21	1.94	0.49
3:E:903:THR:HA	3:E:906:CYS:SG	2.52	0.49
3:F:1487:MET:HG3	3:F:1492:ILE:HD13	1.92	0.49
1:A:1285:ARG:NE	1:A:1311:ASN:OD1	2.37	0.49
1:B:620:MET:O	1:B:624:ARG:HG2	2.13	0.49
1:B:825:MET:HE1	1:B:861:TYR:CG	2.47	0.49
1:B:1053:ILE:O	1:B:1057:GLU:HG3	2.12	0.49
1:B:2025:GLU:OE1	1:B:2025:GLU:N	2.44	0.49
2:C:19:GLY:O	2:C:44:GLN:NE2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:LYS:HD2	2:D:106:ASP:HB3	1.93	0.49
2:D:229:SER:HA	2:D:278:PHE:HD2	1.77	0.49
3:E:129:ILE:O	3:E:133:ILE:HG13	2.13	0.49
3:E:786:ALA:O	3:E:789:GLN:HG3	2.12	0.49
3:E:1607:MET:SD	3:E:1608:CYS:N	2.86	0.49
3:F:236:ASN:HD21	3:F:961:VAL:HG13	1.76	0.49
3:F:332:TYR:HE1	3:F:426:LEU:HD12	1.77	0.49
3:F:830:LYS:HE2	3:F:835:TYR:CZ	2.47	0.49
1:A:677:ALA:HA	1:A:710:LEU:HD21	1.93	0.49
1:A:705:PHE:CE1	1:A:752:GLN:HB3	2.47	0.49
1:A:824:ILE:HG21	1:A:844:LEU:CD2	2.41	0.49
1:A:2022:LEU:HD21	1:A:2066:LYS:HE3	1.94	0.49
1:B:1910:TRP:HZ2	1:B:1956:LEU:HB3	1.76	0.49
1:B:2079:MET:HE1	3:F:245:ARG:NH1	2.28	0.49
1:B:2245:THR:HA	1:B:2345:MET:HG2	1.95	0.49
2:C:298:CYS:H	2:C:305:LYS:NZ	2.10	0.49
3:F:386:ASP:HA	3:F:876:VAL:O	2.12	0.49
3:F:724:ALA:HB1	3:F:728:CYS:HB2	1.94	0.49
3:F:853:THR:HA	3:F:855:ARG:NH1	2.28	0.49
1:A:1677:LEU:HD11	1:A:1690:PRO:HG2	1.94	0.49
1:B:774:PRO:HA	1:B:777:LYS:HG2	1.94	0.49
1:B:882:ARG:HA	1:B:885:ILE:HG12	1.95	0.49
2:C:229:SER:HA	2:C:278:PHE:HD2	1.77	0.49
3:E:236:ASN:HD21	3:E:961:VAL:HG13	1.76	0.49
3:E:717:LEU:HD23	3:E:721:LEU:HD23	1.94	0.49
3:F:903:THR:HA	3:F:906:CYS:SG	2.52	0.49
3:F:991:ASP:OD1	3:F:992:ALA:N	2.45	0.49
1:A:1008:ILE:HD12	1:A:1008:ILE:H	1.78	0.49
1:A:1359:ASN:HA	1:A:1362:GLU:HG2	1.94	0.49
1:A:2330:VAL:O	1:A:2333:ILE:HG22	2.12	0.49
1:B:821:PHE:O	1:B:825:MET:HG2	2.12	0.49
1:B:1135:ALA:O	1:B:1138:THR:HG22	2.13	0.49
1:B:1527:ASP:N	1:B:1527:ASP:OD1	2.46	0.49
2:D:19:GLY:O	2:D:44:GLN:NE2	2.38	0.49
3:E:1442:ILE:HD12	3:E:1443:PRO:HD2	1.95	0.49
3:F:129:ILE:O	3:F:133:ILE:HG13	2.12	0.49
3:F:1607:MET:SD	3:F:1608:CYS:N	2.86	0.49
1:A:825:MET:O	1:A:829:GLN:N	2.43	0.49
1:A:1921:GLU:O	1:A:1924:VAL:N	2.45	0.49
1:B:702:ASP:CG	1:B:703:GLN:H	2.19	0.49
3:E:150:VAL:HA	3:E:153:MET:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:726:ASP:HA	3:E:729:ARG:HG2	1.95	0.49
3:E:1650:ILE:CD1	3:E:1685:MET:HE2	2.42	0.49
1:A:691:GLU:CD	1:A:691:GLU:H	2.20	0.49
1:A:1119:VAL:HA	1:A:1122:PHE:CE1	2.48	0.49
1:A:1921:GLU:O	1:A:1922:ALA:C	2.56	0.49
1:B:1020:VAL:HG13	1:B:1027:ILE:HD13	1.94	0.49
2:C:189:ASN:ND2	2:C:193:ASN:HB2	2.27	0.49
3:E:766:ILE:O	3:E:769:GLU:HG3	2.12	0.49
3:F:802:LEU:O	3:F:806:LEU:HD23	2.12	0.49
4:G:76:TRP:C	4:G:76:TRP:CD1	2.85	0.49
1:A:1971:ALA:HB2	1:A:2144:TYR:HE2	1.78	0.49
1:B:886:ARG:NH1	1:B:1568:ARG:HH22	2.11	0.49
1:B:1157:HIS:C	1:B:1161:ARG:HE	2.20	0.49
1:B:1417:ILE:HD12	1:B:1453:LEU:HD11	1.93	0.49
1:B:1433:LEU:HG	1:B:1437:MET:HE1	1.95	0.49
1:B:1971:ALA:HB2	1:B:2144:TYR:HE2	1.78	0.49
3:E:103:GLY:O	3:E:107:LEU:HD23	2.12	0.49
3:F:726:ASP:HA	3:F:729:ARG:HG2	1.95	0.49
4:H:92:ARG:HH22	4:H:93:LEU:HB3	1.77	0.49
1:A:663:GLY:O	1:A:672:ARG:NH1	2.46	0.48
1:A:856:GLU:N	1:A:857:PRO:HD2	2.28	0.48
1:A:1049:GLN:O	1:A:1052:ILE:HG22	2.12	0.48
1:A:1277:LYS:HZ1	1:A:1281:LEU:HD11	1.78	0.48
1:A:1374:LEU:HD12	1:A:1379:GLY:HA3	1.95	0.48
1:A:1587:TYR:HE2	1:A:1627:GLN:NE2	2.11	0.48
1:A:1948:THR:HG21	1:A:1953:VAL:HG13	1.95	0.48
1:B:1267:LYS:H	1:B:1267:LYS:HD2	1.77	0.48
1:B:1349:ASP:HA	1:B:1386:ARG:HH22	1.78	0.48
1:B:1364:MET:HA	1:B:1364:MET:HE3	1.95	0.48
3:F:522:LYS:O	3:F:559:ASN:HB2	2.13	0.48
1:A:727:MET:O	1:A:730:LEU:N	2.46	0.48
1:A:878:GLN:NE2	1:A:1569:ASP:OD2	2.46	0.48
1:B:1184:LEU:HD23	1:B:1188:TYR:HB2	1.94	0.48
1:B:1218:LYS:HD2	3:F:556:LYS:HD2	1.95	0.48
3:E:1682:PHE:HD1	3:E:1685:MET:HE3	1.77	0.48
3:F:786:ALA:O	3:F:789:GLN:HG3	2.12	0.48
1:A:859:ARG:HB3	1:A:902:ASN:ND2	2.27	0.48
1:A:1296:SER:H	1:A:1301:ARG:NH2	2.07	0.48
1:A:1614:ILE:O	1:A:1618:ILE:HG23	2.13	0.48
1:B:1101:GLN:CA	1:B:1141:ARG:NH1	2.71	0.48
1:B:1294:ASP:OD1	1:B:1294:ASP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2243:CYS:SG	1:B:2345:MET:HB3	2.53	0.48
2:C:100:MET:SD	2:C:112:TRP:HB2	2.53	0.48
2:C:200:THR:HG22	2:C:202:GLY:H	1.78	0.48
2:D:189:ASN:ND2	2:D:193:ASN:HB2	2.28	0.48
3:E:332:TYR:HE1	3:E:426:LEU:HD12	1.76	0.48
3:E:547:ASN:HB2	3:E:550:LEU:HD13	1.94	0.48
3:E:724:ALA:N	3:E:729:ARG:NH2	2.57	0.48
1:A:1889:PHE:HE1	1:A:1906:VAL:HG21	1.78	0.48
3:E:730:LEU:O	3:E:734:LYS:HG2	2.13	0.48
3:F:309:ILE:HD11	3:F:399:PHE:CE1	2.49	0.48
1:B:1056:ILE:HA	1:B:1059:ILE:HG12	1.94	0.48
1:B:1097:LEU:HD22	1:B:1134:ALA:HB1	1.96	0.48
2:D:100:MET:SD	2:D:112:TRP:HB2	2.53	0.48
2:D:200:THR:HG22	2:D:202:GLY:H	1.78	0.48
3:E:522:LYS:O	3:E:559:ASN:HB2	2.13	0.48
3:F:150:VAL:HA	3:F:153:MET:HG2	1.95	0.48
3:F:523:ASP:OD1	3:F:527:ALA:HB3	2.13	0.48
1:A:661:VAL:O	1:A:665:THR:HG22	2.14	0.48
1:A:2082:GLN:HA	1:A:2085:CYS:SG	2.54	0.48
1:B:952:MET:SD	1:B:989:PHE:HB3	2.53	0.48
2:D:78:ILE:HG13	2:D:79:ILE:HD12	1.95	0.48
3:E:115:SER:HA	3:E:118:GLN:HE21	1.78	0.48
3:E:325:ARG:HB3	3:E:419:ILE:CD1	2.43	0.48
1:A:977:PHE:O	1:A:980:LYS:HG3	2.13	0.48
1:A:1181:VAL:HG23	1:A:1212:LEU:HD23	1.95	0.48
1:A:1263:ILE:N	1:A:1265:LEU:HD22	2.28	0.48
1:B:1619:TRP:HB3	1:B:1640:ARG:NH1	2.29	0.48
1:B:1778:ALA:HA	1:B:1781:GLU:CD	2.38	0.48
1:B:2362:PHE:HD1	1:B:2500:ILE:HG21	1.79	0.48
3:E:309:ILE:HD11	3:E:399:PHE:CE1	2.49	0.48
3:E:523:ASP:OD1	3:E:527:ALA:HB3	2.13	0.48
3:E:945:GLU:N	3:E:945:GLU:OE1	2.43	0.48
3:F:118:GLN:HE22	3:F:119:LYS:HG3	1.79	0.48
3:F:345:GLU:OE1	3:F:347:ILE:HG22	2.14	0.48
3:F:547:ASN:HB2	3:F:550:LEU:HD13	1.94	0.48
3:F:1526:ILE:HA	3:F:1531:PHE:HB2	1.96	0.48
1:A:1132:ARG:NH2	1:A:1162:THR:OG1	2.47	0.48
1:A:1192:ILE:HG13	1:A:1193:PRO:HD3	1.96	0.48
1:B:1111:LEU:HG	1:B:1151:TYR:HE2	1.77	0.48
1:B:1152:ALA:O	1:B:1156:ILE:HG12	2.14	0.48
1:B:1374:LEU:H	1:B:1378:ASN:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2411:LYS:O	1:B:2415:MET:HB2	2.14	0.48
2:C:56:MET:HE2	2:C:67:MET:HB3	1.96	0.48
2:C:293:LEU:HB2	2:C:308:TYR:O	2.14	0.48
3:E:557:TRP:CG	3:E:558:PRO:HD2	2.49	0.48
3:E:724:ALA:HB1	3:E:728:CYS:HB2	1.95	0.48
3:F:730:LEU:O	3:F:734:LYS:HG2	2.13	0.48
3:F:750:TRP:O	3:F:753:GLU:HG2	2.14	0.48
3:F:975:ILE:HG12	3:F:975:ILE:H	1.33	0.48
1:B:856:GLU:N	1:B:857:PRO:HD2	2.28	0.48
1:B:1112:HIS:HB3	1:B:1151:TYR:OH	2.14	0.48
1:B:1953:VAL:O	1:B:1957:ILE:HG13	2.14	0.48
1:B:2311:GLU:HG2	1:B:2312:VAL:N	2.28	0.48
2:D:177:HIS:CD2	2:D:227:ARG:HH22	2.32	0.48
3:E:875:HIS:HB3	3:E:877:TYR:CE2	2.46	0.48
3:E:991:ASP:OD1	3:E:992:ALA:N	2.45	0.48
3:E:1526:ILE:HA	3:E:1531:PHE:HB2	1.96	0.48
3:F:250:LEU:HD23	3:F:301:LEU:HD21	1.96	0.48
1:A:1559:LEU:HA	1:A:1562:GLN:NE2	2.29	0.48
1:A:1936:LEU:HA	1:A:1939:ILE:HD11	1.95	0.48
1:A:2228:ILE:HG13	1:A:2228:ILE:O	2.13	0.48
1:B:1345:LEU:HD22	1:B:1382:LEU:HD21	1.95	0.48
1:B:1521:TRP:CD2	1:B:1638:MET:HE2	2.49	0.48
1:B:2191:ASP:HB3	1:B:2430:ARG:HH12	1.79	0.48
3:E:1640:LYS:HA	3:E:1647:PHE:CE2	2.49	0.48
3:F:115:SER:HA	3:F:118:GLN:HE21	1.78	0.48
3:F:325:ARG:HB3	3:F:419:ILE:CD1	2.43	0.48
1:A:952:MET:HE1	1:A:989:PHE:CB	2.41	0.47
1:B:1889:PHE:CD2	1:B:1926:GLY:HA3	2.49	0.47
1:B:2341:PRO:HG2	1:B:2549:TRP:HE3	1.79	0.47
2:C:19:GLY:HA2	2:C:316:VAL:HG12	1.95	0.47
3:E:221:SER:CB	3:E:286:MET:HE1	2.44	0.47
3:E:345:GLU:OE1	3:E:347:ILE:HG22	2.14	0.47
3:E:650:GLY:O	3:E:654:THR:OG1	2.18	0.47
3:F:717:LEU:HD23	3:F:721:LEU:HD23	1.94	0.47
3:F:1442:ILE:HD12	3:F:1443:PRO:HD2	1.95	0.47
1:B:1701:MET:O	1:B:1704:MET:HG2	2.14	0.47
1:B:1888:PHE:O	1:B:1891:SER:OG	2.28	0.47
1:B:2093:ASN:ND2	1:B:2095:LYS:HE2	2.29	0.47
2:D:242:GLN:NE2	2:D:267:GLU:OE2	2.29	0.47
3:E:505:HIS:HB3	3:E:508:ARG:HH22	1.78	0.47
3:F:167:ASN:ND2	3:F:1660:LEU:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:557:TRP:CG	3:F:558:PRO:HD2	2.49	0.47
4:H:68:GLN:HG2	4:H:71:ASP:H	1.79	0.47
1:A:742:GLU:HG3	1:A:743:HIS:N	2.29	0.47
1:B:854:VAL:HG22	1:B:855:VAL:HG13	1.97	0.47
1:B:1910:TRP:NE1	1:B:1953:VAL:HG23	2.29	0.47
1:B:1974:TYR:O	1:B:1978:VAL:HG23	2.15	0.47
3:E:89:ARG:HA	3:E:92:LEU:HD13	1.96	0.47
3:E:567:ASP:C	3:E:571:HIS:HD1	2.20	0.47
3:E:1642:LYS:NZ	3:E:1643:TYR:OH	2.48	0.47
1:A:669:PRO:HA	1:A:672:ARG:CG	2.44	0.47
1:B:1276:SER:OG	1:B:1277:LYS:N	2.47	0.47
2:C:57:ILE:HG22	2:C:68:TYR:O	2.15	0.47
2:C:230:PRO:HG2	2:C:282:SER:OG	2.14	0.47
2:D:19:GLY:HA2	2:D:316:VAL:HG12	1.95	0.47
2:D:100:MET:HE1	2:D:102:THR:HB	1.97	0.47
3:F:1640:LYS:HA	3:F:1647:PHE:CE2	2.49	0.47
1:A:733:MET:O	1:A:737:ILE:HD12	2.15	0.47
1:A:1966:ARG:HG3	1:A:1967:TYR:CD2	2.47	0.47
1:B:691:GLU:O	1:B:694:GLN:HG2	2.14	0.47
1:B:705:PHE:CE2	1:B:752:GLN:HB3	2.50	0.47
1:B:1222:LEU:HD23	1:B:1225:GLU:OE2	2.14	0.47
1:B:1313:MET:SD	1:B:1314:ALA:N	2.87	0.47
1:B:1701:MET:HE2	1:B:1717:MET:HE2	1.97	0.47
2:C:138:PRO:HB3	2:C:180:PRO:HA	1.97	0.47
2:D:56:MET:HE2	2:D:67:MET:HB3	1.96	0.47
2:D:138:PRO:HB3	2:D:180:PRO:HA	1.97	0.47
2:D:177:HIS:CG	2:D:227:ARG:HH12	2.33	0.47
2:D:293:LEU:HB2	2:D:308:TYR:O	2.14	0.47
3:E:125:VAL:HG23	3:E:128:LEU:HD12	1.96	0.47
3:F:80:HIS:HB3	3:F:82:GLU:OE1	2.15	0.47
3:F:89:ARG:HA	3:F:92:LEU:HD13	1.96	0.47
3:F:119:LYS:HA	3:F:122:LYS:HZ2	1.80	0.47
3:F:1668:PRO:O	3:F:1671:ARG:NH1	2.48	0.47
4:G:81:ARG:CG	4:G:81:ARG:NH1	2.76	0.47
1:A:968:HIS:HA	1:A:971:VAL:HG12	1.96	0.47
1:A:1521:TRP:CD2	1:A:1638:MET:HE2	2.50	0.47
1:A:1994:ILE:O	1:A:1998:MET:HG3	2.14	0.47
1:A:2057:MET:O	1:A:2060:ARG:HG2	2.14	0.47
1:B:29:LEU:O	1:B:82:GLU:N	2.47	0.47
1:B:1132:ARG:HH22	1:B:1165:GLN:NE2	2.12	0.47
1:B:2308:PRO:HG2	1:B:2312:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:ILE:HG13	2:C:79:ILE:HD12	1.96	0.47
3:E:1668:PRO:O	3:E:1671:ARG:NH1	2.48	0.47
3:F:108:ARG:HH21	3:F:145:GLN:HB3	1.80	0.47
3:F:221:SER:CB	3:F:286:MET:HE1	2.44	0.47
3:F:505:HIS:HB3	3:F:508:ARG:HH22	1.78	0.47
3:F:894:HIS:HA	3:F:897:GLU:HG3	1.97	0.47
1:A:701:ASN:HA	1:A:708:ARG:NH2	2.29	0.47
1:A:775:ILE:O	1:A:779:LEU:HD23	2.14	0.47
1:A:2321:THR:HG23	1:A:2387:MET:SD	2.54	0.47
1:B:1044:MET:O	1:B:1044:MET:HE3	2.14	0.47
1:B:1707:SER:OG	1:B:1708:ALA:N	2.45	0.47
1:B:1798:PHE:CE2	1:B:1802:LEU:HD11	2.48	0.47
1:B:1798:PHE:CE1	1:B:1909:LEU:HD21	2.49	0.47
1:B:1901:GLN:O	1:B:1905:ARG:HG3	2.13	0.47
1:B:2123:LEU:HD21	1:B:2160:LEU:HG	1.96	0.47
2:D:230:PRO:HG2	2:D:282:SER:OG	2.14	0.47
3:E:118:GLN:HE22	3:E:119:LYS:HG3	1.79	0.47
3:E:625:ASP:HA	3:E:628:LYS:NZ	2.30	0.47
3:E:750:TRP:O	3:E:753:GLU:HG2	2.14	0.47
3:F:374:LYS:HA	3:F:741:ARG:HH12	1.79	0.47
1:A:1391:ARG:HA	1:A:1393:TYR:CZ	2.49	0.47
1:A:1905:ARG:HA	1:A:1908:THR:HG22	1.96	0.47
1:A:2264:GLU:O	1:A:2268:MET:HG3	2.15	0.47
3:E:374:LYS:HA	3:E:741:ARG:HH12	1.78	0.47
3:E:894:HIS:HA	3:E:897:GLU:HG3	1.97	0.47
3:F:125:VAL:HG23	3:F:128:LEU:HD12	1.96	0.47
1:B:795:ILE:HA	1:B:798:VAL:HG12	1.97	0.47
1:B:1541:HIS:NE2	1:B:1571:LEU:HB2	2.29	0.47
1:B:1725:GLN:O	1:B:1729:GLN:NE2	2.48	0.47
1:B:1753:LYS:HB3	1:B:1757:TRP:CH2	2.49	0.47
1:B:2509:THR:HG23	1:B:2511:ARG:HG3	1.96	0.47
2:C:177:HIS:CD2	2:C:227:ARG:HH22	2.32	0.47
2:C:245:LYS:HE2	2:C:247:TRP:CH2	2.50	0.47
3:E:83:ASP:OD1	3:E:84:ILE:N	2.48	0.47
3:E:250:LEU:HD23	3:E:301:LEU:HD21	1.96	0.47
3:E:730:LEU:HA	3:E:733:THR:HG22	1.96	0.47
3:F:625:ASP:HA	3:F:628:LYS:NZ	2.30	0.47
1:A:1445:ILE:O	1:A:1445:ILE:HG13	2.15	0.47
1:A:1611:ARG:O	1:A:1615:ILE:HG12	2.14	0.47
1:B:944:ASP:OD1	1:B:944:ASP:N	2.45	0.47
1:B:1001:ILE:HA	1:B:1004:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:ARG:CZ	2:C:118:ASN:H	2.28	0.47
2:D:57:ILE:HG22	2:D:68:TYR:O	2.15	0.47
3:E:167:ASN:ND2	3:E:1660:LEU:O	2.47	0.47
3:F:549:ASN:O	3:F:553:THR:HG23	2.14	0.47
1:A:703:GLN:HE22	1:B:1157:HIS:HB2	1.80	0.46
1:A:2021:ILE:HG12	1:A:2026:MET:HB2	1.97	0.46
2:C:267:GLU:O	2:C:270:ARG:HG3	2.15	0.46
2:D:232:SER:O	2:D:232:SER:OG	2.33	0.46
3:E:244:VAL:CG2	3:E:249:GLU:HG3	2.45	0.46
3:E:259:ASP:OD1	3:E:260:PHE:N	2.48	0.46
3:F:75:GLU:HG2	3:F:76:LYS:N	2.31	0.46
3:F:249:GLU:H	3:F:249:GLU:CD	2.21	0.46
3:F:1641:GLU:CB	4:H:90:LEU:HD11	2.45	0.46
1:A:1526:TRP:HA	1:A:1529:MET:HB2	1.97	0.46
1:A:1921:GLU:O	1:A:1924:VAL:HG22	2.15	0.46
1:B:663:GLY:CA	1:B:672:ARG:HH21	2.29	0.46
1:B:672:ARG:O	1:B:676:LEU:HD23	2.15	0.46
1:B:881:ARG:HD3	1:B:1572:ASP:OD2	2.15	0.46
2:D:12:PRO:C	2:D:54:ARG:HH12	2.23	0.46
3:E:108:ARG:HH21	3:E:145:GLN:HB3	1.80	0.46
3:E:119:LYS:HA	3:E:122:LYS:HZ2	1.79	0.46
3:E:738:VAL:HG13	3:E:739:LEU:HD22	1.97	0.46
3:E:1668:PRO:HA	3:E:1671:ARG:NE	2.30	0.46
3:E:1672:PHE:O	3:E:1675:GLU:HG3	2.15	0.46
3:F:83:ASP:OD1	3:F:84:ILE:N	2.48	0.46
3:F:189:ALA:HB2	4:H:18:HIS:ND1	2.29	0.46
3:F:1668:PRO:HA	3:F:1671:ARG:NE	2.30	0.46
1:A:727:MET:HE1	1:A:731:ARG:CZ	2.46	0.46
1:B:937:ASN:HB2	1:B:946:PHE:CE1	2.50	0.46
1:B:945:GLU:C	1:B:948:PRO:HD2	2.40	0.46
2:C:94:HIS:HB2	2:C:99:TRP:CE2	2.50	0.46
2:C:177:HIS:CG	2:C:227:ARG:HH12	2.33	0.46
3:E:905:LEU:H	3:E:905:LEU:HG	1.34	0.46
3:F:840:VAL:HA	3:F:843:ILE:HG22	1.98	0.46
4:G:67:ALA:O	4:G:68:GLN:HB3	2.05	0.46
1:A:819:GLU:HA	1:A:822:ILE:HG12	1.97	0.46
1:A:1155:ILE:C	1:A:1158:PRO:HD2	2.40	0.46
1:A:1882:VAL:N	1:A:1883:PRO:HD2	2.31	0.46
1:A:2191:ASP:OD1	1:A:2192:LEU:N	2.48	0.46
1:A:2427:LEU:HD12	1:A:2430:ARG:HH22	1.79	0.46
1:B:624:ARG:HG2	1:B:624:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1564:ILE:O	1:B:1568:ARG:HG2	2.15	0.46
1:B:1918:ASP:O	1:B:1921:GLU:HG3	2.15	0.46
2:C:12:PRO:C	2:C:54:ARG:HH12	2.23	0.46
2:C:100:MET:HE1	2:C:102:THR:HB	1.97	0.46
3:E:549:ASN:O	3:E:553:THR:HG23	2.15	0.46
3:E:972:LEU:HD23	3:E:990:TRP:CZ3	2.51	0.46
4:G:68:GLN:HG2	4:G:71:ASP:H	1.79	0.46
4:G:87:ALA:O	4:G:90:LEU:C	2.59	0.46
1:A:1986:ALA:HA	1:A:1989:ASN:HD21	1.80	0.46
1:B:1691:THR:HG21	1:B:1723:THR:HG21	1.97	0.46
1:B:1902:ASP:OD1	1:B:1903:THR:N	2.48	0.46
1:B:2121:LEU:HB3	1:B:2126:VAL:HG21	1.98	0.46
1:B:2175:MET:HE1	1:B:2181:GLU:HG3	1.98	0.46
2:C:183:SER:O	2:C:199:LEU:HB3	2.15	0.46
3:E:80:HIS:HB3	3:E:82:GLU:OE1	2.14	0.46
4:H:81:ARG:CG	4:H:81:ARG:NH1	2.76	0.46
1:A:1463:TYR:CE2	1:A:1479:GLY:HA3	2.51	0.46
1:A:1559:LEU:HA	1:A:1562:GLN:HE22	1.81	0.46
1:A:2427:LEU:HD12	1:A:2430:ARG:NH2	2.31	0.46
1:B:2023:TRP:O	1:B:2026:MET:HG2	2.15	0.46
1:B:2408:ARG:HH12	1:B:2510:GLY:N	2.13	0.46
3:F:151:ARG:HH22	4:H:31:LEU:C	2.23	0.46
3:F:259:ASP:OD1	3:F:260:PHE:N	2.48	0.46
1:A:673:TYR:CE1	1:A:710:LEU:HD22	2.51	0.46
1:B:886:ARG:HG3	1:B:886:ARG:HH11	1.79	0.46
2:C:227:ARG:O	2:C:235:LEU:HA	2.16	0.46
2:D:28:GLN:O	2:D:30:HIS:ND1	2.49	0.46
2:D:267:GLU:O	2:D:270:ARG:HG3	2.15	0.46
3:E:1653:TYR:HD1	3:E:1677:PHE:CD2	2.34	0.46
3:F:244:VAL:CG2	3:F:249:GLU:HG3	2.45	0.46
1:B:1215:ARG:HH22	1:B:1225:GLU:CB	2.28	0.46
1:B:1614:ILE:O	1:B:1618:ILE:HG23	2.15	0.46
1:B:1947:ASP:OD1	1:B:1987:ARG:NH2	2.37	0.46
2:D:117:ARG:CZ	2:D:118:ASN:H	2.28	0.46
3:E:119:LYS:HA	3:E:122:LYS:NZ	2.31	0.46
3:E:178:GLN:O	3:E:180:ARG:NH1	2.49	0.46
3:F:131:ARG:HB2	3:F:1674:GLN:HE21	1.81	0.46
3:F:556:LYS:HE3	3:F:607:GLN:NE2	2.31	0.46
3:F:1642:LYS:NZ	3:F:1643:TYR:OH	2.48	0.46
3:F:1672:PHE:O	3:F:1675:GLU:HG3	2.15	0.46
1:A:1125:PRO:HB3	1:A:1165:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1561:GLN:NE2	1:B:1562:GLN:HG3	2.31	0.46
1:B:2276:ASP:OD1	1:B:2276:ASP:N	2.48	0.46
2:C:60:ALA:HB1	2:C:88:ILE:HG21	1.97	0.46
2:D:48:LEU:H	2:D:48:LEU:HD23	1.81	0.46
3:F:178:GLN:O	3:F:180:ARG:NH1	2.49	0.46
3:F:730:LEU:HA	3:F:733:THR:HG22	1.96	0.46
1:A:785:ASP:OD2	1:A:785:ASP:N	2.49	0.46
1:A:997:PHE:HE2	1:A:1016:LEU:HD22	1.79	0.46
1:A:1754:LEU:HA	1:A:1754:LEU:HD23	1.80	0.46
1:B:90:ILE:O	1:B:94:ILE:N	2.35	0.46
1:B:827:MET:HB3	1:B:827:MET:HE2	1.77	0.46
1:B:1208:ARG:NH1	1:B:1212:LEU:HG	2.31	0.46
2:C:196:VAL:HG11	2:C:252:PHE:CZ	2.51	0.46
3:E:840:VAL:HA	3:E:843:ILE:HG22	1.98	0.46
1:A:1067:PHE:HB3	1:A:1106:ASN:OD1	2.15	0.45
1:A:2432:MET:SD	1:A:2496:LYS:HE3	2.56	0.45
1:B:652:VAL:HA	1:B:655:VAL:HG22	1.97	0.45
1:B:972:VAL:O	1:B:975:ILE:HG22	2.16	0.45
1:B:1904:LEU:O	1:B:1908:THR:HG23	2.16	0.45
1:B:2162:VAL:HG22	1:B:2170:ARG:HG3	1.98	0.45
1:B:2498:ILE:O	1:B:2501:ILE:HG22	2.16	0.45
2:C:28:GLN:O	2:C:30:HIS:ND1	2.49	0.45
2:D:94:HIS:HB2	2:D:99:TRP:CE2	2.50	0.45
2:D:183:SER:O	2:D:199:LEU:HB3	2.15	0.45
2:D:227:ARG:O	2:D:235:LEU:HA	2.16	0.45
2:D:245:LYS:HE2	2:D:247:TRP:CH2	2.50	0.45
3:E:140:GLU:N	3:E:140:GLU:OE1	2.49	0.45
3:E:505:HIS:HB3	3:E:508:ARG:NH2	2.31	0.45
3:F:119:LYS:HA	3:F:122:LYS:NZ	2.31	0.45
3:F:567:ASP:C	3:F:571:HIS:HD1	2.20	0.45
4:H:64:TYR:O	4:H:64:TYR:CD1	2.68	0.45
1:A:669:PRO:HA	1:A:672:ARG:HG3	1.97	0.45
1:A:1171:SER:HA	1:A:1174:MET:HG2	1.98	0.45
1:A:1265:LEU:HG	1:A:1269:TRP:HZ3	1.80	0.45
1:B:737:ILE:HA	1:B:740:GLU:OE1	2.16	0.45
1:B:1125:PRO:HA	1:B:1132:ARG:NH1	2.31	0.45
1:B:1374:LEU:HB2	1:B:1378:ASN:C	2.41	0.45
1:B:1747:MET:HE2	1:B:1782:HIS:CD2	2.51	0.45
1:B:2218:LYS:HE3	1:B:2322:ARG:HH21	1.81	0.45
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.98	0.45
3:E:556:LYS:HE3	3:E:607:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:738:VAL:HG13	3:F:739:LEU:HD22	1.97	0.45
4:H:35:ASP:OD1	4:H:35:ASP:C	2.60	0.45
4:H:87:ALA:O	4:H:90:LEU:C	2.59	0.45
1:B:1098:ALA:HA	1:B:1101:GLN:NE2	2.31	0.45
1:B:1178:SER:HA	1:B:1181:VAL:HG22	1.98	0.45
3:E:108:ARG:NH2	3:E:145:GLN:HB3	2.32	0.45
3:E:249:GLU:H	3:E:249:GLU:CD	2.21	0.45
3:F:133:ILE:O	3:F:143:ARG:NE	2.50	0.45
3:F:140:GLU:OE1	3:F:140:GLU:N	2.49	0.45
1:A:985:LYS:HE2	1:A:985:LYS:HA	1.98	0.45
1:B:445:ARG:O	1:B:449:LYS:N	2.49	0.45
1:B:689:GLN:HB2	1:B:692:ASN:OD1	2.16	0.45
1:B:869:LEU:HA	1:B:872:LEU:HD13	1.98	0.45
1:B:2340:HIS:HD2	1:B:2342:SER:HB2	1.81	0.45
2:C:48:LEU:HD23	2:C:48:LEU:H	1.81	0.45
3:E:226:ALA:O	3:E:229:THR:OG1	2.29	0.45
3:E:458:SER:OG	3:E:460:ASP:OD1	2.35	0.45
3:F:526:GLU:OE1	3:F:526:GLU:N	2.26	0.45
3:F:972:LEU:HD23	3:F:990:TRP:CZ3	2.51	0.45
4:G:78:PHE:HD2	4:G:78:PHE:HA	1.50	0.45
1:A:746:ILE:HB	1:A:749:ILE:HD13	1.98	0.45
1:A:801:THR:O	1:A:805:LEU:HD23	2.16	0.45
1:A:1115:LEU:HG	1:A:1154:ARG:HH21	1.82	0.45
1:A:2341:PRO:HG2	1:A:2549:TRP:HE3	1.81	0.45
1:A:2525:VAL:O	1:A:2529:ILE:HG12	2.17	0.45
1:B:656:LEU:HA	1:B:659:LEU:HD23	1.98	0.45
2:D:60:ALA:HB1	2:D:88:ILE:HG21	1.97	0.45
3:E:930:LEU:HD13	3:E:933:ILE:HD11	1.99	0.45
3:E:1515:HIS:CD2	3:E:1651:CYS:HG	2.32	0.45
3:F:118:GLN:O	3:F:122:LYS:NZ	2.50	0.45
3:F:165:VAL:O	3:F:169:LEU:HD23	2.17	0.45
3:F:668:CYS:HG	3:F:669:HIS:CG	2.35	0.45
3:F:1653:TYR:HD1	3:F:1677:PHE:CD2	2.34	0.45
1:A:700:LEU:HD11	1:A:715:VAL:HG11	1.98	0.45
1:A:857:PRO:O	1:A:861:TYR:N	2.47	0.45
1:A:1401:GLU:OE1	1:A:2389:VAL:HB	2.16	0.45
1:A:2510:GLY:HA2	1:A:2524:GLN:OE1	2.17	0.45
1:B:1595:MET:HE1	1:B:1636:ILE:HA	1.98	0.45
2:D:200:THR:HG21	2:D:208:THR:HA	1.98	0.45
2:D:200:THR:HG23	2:D:209:GLN:OE1	2.16	0.45
3:E:75:GLU:HG2	3:E:76:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:292:PHE:O	3:E:391:TYR:OH	2.35	0.45
3:E:578:LEU:O	3:E:582:LYS:HG3	2.16	0.45
3:F:439:PRO:HB2	3:F:991:ASP:OD2	2.17	0.45
3:F:1515:HIS:CD2	3:F:1651:CYS:HG	2.33	0.45
1:A:666:ASP:H	1:A:672:ARG:NH2	2.15	0.45
1:B:666:ASP:CG	1:B:667:PRO:HD2	2.41	0.45
1:B:1461:VAL:O	1:B:1465:LYS:HG2	2.17	0.45
1:B:1480:ARG:HA	1:B:1483:CYS:SG	2.56	0.45
3:E:368:PHE:CD2	3:E:369:VAL:HG23	2.52	0.45
3:E:724:ALA:HB1	3:E:728:CYS:CB	2.47	0.45
3:E:750:TRP:O	3:E:754:LEU:HD23	2.17	0.45
3:E:954:LYS:NZ	3:E:958:GLN:HG3	2.32	0.45
3:E:1681:GLN:OE1	3:E:1683:LEU:N	2.50	0.45
3:F:368:PHE:CD2	3:F:369:VAL:HG23	2.52	0.45
3:F:670:PRO:O	3:F:673:VAL:HG12	2.17	0.45
3:F:724:ALA:HB1	3:F:728:CYS:CB	2.47	0.45
3:F:1617:LEU:HA	3:F:1620:VAL:HG12	1.98	0.45
4:G:66:TYR:HD2	4:G:66:TYR:O	2.00	0.45
4:H:80:ILE:HD12	4:H:81:ARG:H	1.82	0.45
1:A:1129:LEU:HB3	1:A:1133:LYS:HZ1	1.80	0.45
1:A:1228:ASP:O	1:A:1231:ILE:HG12	2.16	0.45
1:A:1669:ALA:O	1:A:1673:LEU:HD23	2.17	0.45
1:B:1472:ASP:HB2	1:B:1476:LEU:HD22	1.98	0.45
1:B:1520:ALA:HB3	1:B:1529:MET:SD	2.56	0.45
1:B:1561:GLN:HE22	1:B:1562:GLN:HG3	1.81	0.45
1:B:2188:GLY:O	1:B:2190:GLU:HG3	2.17	0.45
1:B:2416:ALA:HA	1:B:2419:GLU:HG2	1.98	0.45
2:C:200:THR:HG23	2:C:209:GLN:OE1	2.16	0.45
3:E:439:PRO:HB2	3:E:991:ASP:OD2	2.17	0.45
1:A:175:LEU:O	1:A:179:VAL:N	2.49	0.45
1:A:603:VAL:O	1:A:606:CYS:HB2	2.17	0.45
1:A:669:PRO:O	1:A:672:ARG:HB2	2.17	0.45
1:A:1350:ILE:H	1:A:1350:ILE:HD12	1.82	0.45
1:A:1423:LEU:O	1:A:1425:GLN:HG2	2.16	0.45
1:A:1901:GLN:HE22	1:A:2412:ASP:HB3	1.81	0.45
1:A:1974:TYR:O	1:A:1978:VAL:HG23	2.17	0.45
1:A:2191:ASP:CG	1:A:2193:ARG:HE	2.22	0.45
1:B:811:LEU:O	1:B:814:ARG:HG3	2.16	0.45
1:B:1916:TRP:O	1:B:1919:VAL:N	2.50	0.45
1:B:1986:ALA:HA	1:B:1989:ASN:HD21	1.81	0.45
2:C:200:THR:HG21	2:C:208:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:VAL:HG11	2:D:252:PHE:CZ	2.52	0.45
3:F:285:LYS:HG3	3:F:330:VAL:HG22	1.99	0.45
3:F:292:PHE:O	3:F:391:TYR:OH	2.35	0.45
4:G:81:ARG:HH11	4:G:81:ARG:HG3	1.80	0.45
1:A:1113:LEU:HD12	1:A:1114:LEU:N	2.32	0.45
1:B:1467:MET:HE1	1:B:1476:LEU:C	2.41	0.45
2:C:94:HIS:HB2	2:C:99:TRP:CD2	2.52	0.45
3:E:118:GLN:O	3:E:122:LYS:NZ	2.50	0.45
3:E:131:ARG:HB2	3:E:1674:GLN:HE21	1.81	0.45
3:E:165:VAL:O	3:E:169:LEU:HD23	2.17	0.45
3:E:1617:LEU:HA	3:E:1620:VAL:HG12	1.98	0.45
3:F:108:ARG:NH2	3:F:145:GLN:HB3	2.32	0.45
3:F:114:SER:O	3:F:117:LEU:HG	2.18	0.45
3:F:150:VAL:HA	3:F:153:MET:HE3	1.99	0.45
3:F:578:LEU:O	3:F:582:LYS:HG3	2.16	0.45
3:F:583:PRO:O	3:F:586:LYS:HD2	2.17	0.45
1:A:1285:ARG:O	1:A:1289:LEU:HG	2.17	0.44
1:A:2008:GLN:OE1	1:A:2137:GLU:HB2	2.16	0.44
1:A:2095:LYS:HE2	1:A:2095:LYS:HB3	1.69	0.44
1:B:1265:LEU:HB3	1:B:1269:TRP:HD1	1.78	0.44
1:B:1282:GLU:HG3	1:B:1286:ARG:NE	2.28	0.44
1:B:1542:ASP:OD1	1:B:1543:GLY:N	2.51	0.44
1:B:1709:ARG:HH11	1:B:1709:ARG:HA	1.82	0.44
1:B:1768:THR:O	1:B:1772:VAL:HG23	2.16	0.44
1:B:1910:TRP:CD1	1:B:1953:VAL:HG23	2.52	0.44
2:C:20:TYR:HA	2:C:44:GLN:HE22	1.81	0.44
2:D:242:GLN:O	2:D:261:LYS:NZ	2.49	0.44
3:E:583:PRO:O	3:E:586:LYS:HD2	2.18	0.44
3:F:1628:SER:O	3:F:1628:SER:OG	2.29	0.44
1:A:725:PHE:HE2	3:F:1001:TRP:CE3	2.35	0.44
1:A:1901:GLN:HG2	1:A:1905:ARG:NH2	2.32	0.44
1:B:601:GLN:O	1:B:604:ARG:NH2	2.50	0.44
1:B:776:LEU:HD12	1:B:777:LYS:N	2.33	0.44
1:B:857:PRO:HA	1:B:860:LYS:HG2	1.99	0.44
1:B:1000:VAL:O	1:B:1004:CYS:N	2.47	0.44
1:B:1193:PRO:HG2	1:B:1194:MET:SD	2.58	0.44
2:C:51:THR:OG1	2:C:53:ASP:OD1	2.27	0.44
2:D:20:TYR:HA	2:D:44:GLN:HE22	1.81	0.44
2:D:94:HIS:HB2	2:D:99:TRP:CD2	2.52	0.44
3:E:906:CYS:O	3:E:909:VAL:HG12	2.17	0.44
3:F:379:HIS:CD2	3:F:381:ALA:H	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:593:LEU:HD22	3:F:653:THR:HA	2.00	0.44
3:F:954:LYS:NZ	3:F:958:GLN:HG3	2.32	0.44
1:A:693:LEU:HA	1:A:696:LEU:HB2	2.00	0.44
1:B:1974:TYR:O	1:B:1977:THR:HG22	2.17	0.44
1:B:2015:GLU:OE1	1:B:2127:SER:OG	2.35	0.44
3:F:240:THR:HA	3:F:243:TYR:HD2	1.81	0.44
3:F:381:ALA:C	3:F:997:ARG:HH22	2.26	0.44
3:F:458:SER:OG	3:F:460:ASP:OD1	2.35	0.44
3:F:750:TRP:O	3:F:754:LEU:HD23	2.17	0.44
3:F:1681:GLN:OE1	3:F:1683:LEU:N	2.50	0.44
1:A:2385:ASN:OD1	1:A:2386:ALA:N	2.51	0.44
1:B:1907:LEU:HD21	1:B:1935:TRP:HZ3	1.83	0.44
1:B:2024:HIS:HB2	1:B:2111:ILE:CD1	2.45	0.44
2:C:168:GLU:HG3	2:C:171:VAL:HG11	1.99	0.44
2:D:137:HIS:CG	2:D:138:PRO:HD2	2.52	0.44
3:E:114:SER:O	3:E:117:LEU:HG	2.18	0.44
3:E:325:ARG:HB3	3:E:419:ILE:HD11	1.99	0.44
3:F:161:PHE:CD1	3:F:162:PRO:HD2	2.52	0.44
4:G:64:TYR:O	4:G:64:TYR:CD1	2.69	0.44
4:H:81:ARG:HH11	4:H:81:ARG:HG3	1.80	0.44
1:A:1313:MET:SD	1:A:1314:ALA:N	2.90	0.44
1:A:1974:TYR:O	1:A:1977:THR:HG22	2.18	0.44
1:B:937:ASN:ND2	1:B:941:LEU:O	2.43	0.44
1:B:1004:CYS:HB2	1:B:1008:ILE:HD11	2.00	0.44
1:B:1136:LEU:HD21	1:B:1173:ALA:HA	2.00	0.44
1:B:1414:GLU:OE2	1:B:1452:LYS:NZ	2.49	0.44
1:B:1972:LEU:O	1:B:1976:LEU:HG	2.17	0.44
2:C:80:SER:OG	4:G:105:ASN:OD1	2.34	0.44
2:D:136:LEU:HD12	2:D:142:GLU:O	2.18	0.44
3:E:133:ILE:O	3:E:143:ARG:NE	2.50	0.44
3:E:346:PHE:CZ	3:E:475:CYS:HB3	2.53	0.44
3:E:668:CYS:HG	3:E:669:HIS:CG	2.35	0.44
3:E:949:ILE:HB	3:E:950:PRO:HD3	2.00	0.44
3:F:93:LEU:HD13	3:F:1686:HIS:CE1	2.52	0.44
3:F:505:HIS:HB3	3:F:508:ARG:NH2	2.32	0.44
3:F:623:LEU:HD23	3:F:675:MET:HG2	1.99	0.44
4:G:80:ILE:HD12	4:G:81:ARG:H	1.82	0.44
1:A:701:ASN:O	1:B:1153:SER:OG	2.36	0.44
1:A:1721:VAL:O	1:A:1725:GLN:HG2	2.17	0.44
1:A:2336:LEU:HD21	1:A:2339:ARG:NH1	2.32	0.44
1:A:2408:ARG:HH12	1:A:2509:THR:CA	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1924:VAL:HG12	1:B:1956:LEU:HD11	1.98	0.44
1:B:2093:ASN:HD21	1:B:2095:LYS:HE2	1.83	0.44
2:C:137:HIS:CG	2:C:138:PRO:HD2	2.52	0.44
2:D:259:SER:OG	2:D:261:LYS:HE2	2.18	0.44
3:E:150:VAL:HA	3:E:153:MET:HE3	1.99	0.44
3:E:295:TRP:CE2	3:E:966:GLY:HA3	2.53	0.44
3:E:332:TYR:CE1	3:E:426:LEU:HB2	2.51	0.44
3:E:441:SER:O	3:E:444:HIS:ND1	2.48	0.44
3:F:295:TRP:CE2	3:F:966:GLY:HA3	2.53	0.44
4:H:81:ARG:H	4:H:81:ARG:HG2	1.59	0.44
1:A:723:PRO:HA	1:A:726:VAL:HG12	1.98	0.44
1:A:988:GLN:HG3	1:A:989:PHE:CE1	2.52	0.44
1:A:1194:MET:HA	1:A:1197:LYS:NZ	2.33	0.44
1:A:1216:ILE:HG13	1:A:1217:VAL:N	2.32	0.44
1:A:1277:LYS:O	1:A:1281:LEU:HG	2.17	0.44
1:B:671:ILE:O	1:B:675:VAL:HG12	2.18	0.44
1:B:733:MET:O	1:B:736:GLN:N	2.49	0.44
1:B:1141:ARG:C	1:B:1141:ARG:CD	2.86	0.44
1:B:1265:LEU:C	1:B:1269:TRP:HD1	2.25	0.44
1:B:1312:PRO:HA	1:B:1315:ARG:HG3	2.00	0.44
1:B:1669:ALA:O	1:B:1673:LEU:HD23	2.18	0.44
1:B:1878:LEU:O	1:B:1882:VAL:HG23	2.17	0.44
1:B:1882:VAL:N	1:B:1883:PRO:HD2	2.32	0.44
1:B:2105:TYR:O	1:B:2109:ARG:HG3	2.17	0.44
2:D:94:HIS:CD2	2:D:98:ARG:HG3	2.53	0.44
2:D:168:GLU:HG3	2:D:171:VAL:HG11	1.99	0.44
3:E:593:LEU:HD22	3:E:653:THR:HA	2.00	0.44
3:F:82:GLU:OE1	3:F:82:GLU:N	2.48	0.44
3:F:325:ARG:HB3	3:F:419:ILE:HD11	1.99	0.44
1:A:1101:GLN:O	1:A:1141:ARG:NH1	2.48	0.44
1:B:742:GLU:HG2	3:E:459:PHE:HE2	1.82	0.44
1:B:1362:GLU:OE1	1:B:1395:LYS:NZ	2.51	0.44
1:B:1755:GLY:O	1:B:1759:LEU:HD23	2.17	0.44
2:C:11:ASP:OD1	2:C:28:GLN:NE2	2.51	0.44
2:C:259:SER:OG	2:C:261:LYS:HE2	2.18	0.44
3:E:37:ASN:OD1	3:E:38:LEU:N	2.51	0.44
3:E:151:ARG:HH12	4:G:31:LEU:HD23	1.83	0.44
3:E:237:HIS:HB3	3:E:240:THR:HG23	2.00	0.44
3:E:381:ALA:C	3:E:997:ARG:HH22	2.26	0.44
3:F:382:ARG:HG2	3:F:382:ARG:HH11	1.83	0.44
1:A:703:GLN:NE2	1:B:1158:PRO:HD3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2022:LEU:HB3	1:A:2025:GLU:OE1	2.18	0.44
1:B:806:ALA:HA	1:B:813:MET:SD	2.58	0.44
1:B:1196:ASN:O	1:B:1200:VAL:HG13	2.18	0.44
2:C:94:HIS:CD2	2:C:98:ARG:HG3	2.53	0.44
2:C:114:LEU:HB3	2:C:115:ARG:NH2	2.33	0.44
2:D:114:LEU:HB3	2:D:115:ARG:NH2	2.33	0.44
3:E:550:LEU:O	3:E:553:THR:OG1	2.26	0.44
3:E:623:LEU:HD23	3:E:675:MET:HG2	1.99	0.44
3:F:37:ASN:OD1	3:F:38:LEU:N	2.51	0.44
4:G:68:GLN:O	4:G:70:VAL:N	2.51	0.44
4:H:91:GLU:HB3	4:H:95:LYS:NZ	2.33	0.44
1:A:822:ILE:HG13	1:A:823:ILE:N	2.32	0.43
1:A:883:GLU:O	1:A:887:VAL:HG23	2.18	0.43
1:A:937:ASN:HB2	1:A:946:PHE:HE2	1.83	0.43
1:A:2365:ALA:O	1:A:2368:ARG:HG2	2.18	0.43
1:B:624:ARG:NH2	1:B:675:VAL:HA	2.32	0.43
1:B:947:TYR:HB2	1:B:948:PRO:HD3	2.00	0.43
1:B:1214:CYS:SG	3:F:553:THR:HG22	2.58	0.43
1:B:1788:LYS:HD2	1:B:1788:LYS:N	2.33	0.43
1:B:2080:GLU:OE2	1:B:2103:LEU:HD13	2.18	0.43
2:D:11:ASP:OD1	2:D:28:GLN:NE2	2.51	0.43
3:E:74:GLU:O	3:E:78:GLY:N	2.51	0.43
3:E:161:PHE:CD1	3:E:162:PRO:HD2	2.52	0.43
3:E:382:ARG:HG2	3:E:382:ARG:HH11	1.83	0.43
3:F:38:LEU:HB2	3:F:79:PHE:CZ	2.53	0.43
3:F:930:LEU:HD13	3:F:933:ILE:HD11	1.99	0.43
1:A:115:LEU:HA	1:A:167:ALA:HB1	2.00	0.43
1:A:1155:ILE:O	1:A:1159:ILE:HG12	2.17	0.43
1:A:2055:HIS:NE2	1:A:2082:GLN:HB2	2.32	0.43
1:B:1574:GLU:H	1:B:1574:GLU:CD	2.23	0.43
1:B:2123:LEU:HD23	1:B:2158:PRO:C	2.43	0.43
2:C:267:GLU:CG	2:C:270:ARG:H	2.31	0.43
3:E:902:ILE:HD12	3:E:902:ILE:H	1.84	0.43
3:F:763:ASN:HB3	3:F:766:ILE:HD12	2.00	0.43
3:F:949:ILE:HB	3:F:950:PRO:HD3	2.00	0.43
1:A:664:ILE:C	1:A:672:ARG:HH12	2.26	0.43
1:A:1098:ALA:HA	1:A:1101:GLN:HE21	1.83	0.43
1:A:1151:TYR:O	1:A:1155:ILE:HD13	2.19	0.43
1:A:1293:LYS:HE2	1:A:1304:TRP:CZ2	2.54	0.43
1:A:1963:ASP:HA	1:A:1966:ARG:HG2	1.99	0.43
1:B:1116:PRO:HG3	1:B:1154:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:VAL:HB	2:D:153:HIS:HB2	2.01	0.43
3:E:35:SER:O	3:E:39:ARG:HG2	2.18	0.43
3:E:200:GLU:OE2	3:E:243:TYR:HE1	2.01	0.43
4:H:66:TYR:O	4:H:66:TYR:HD2	2.00	0.43
1:A:2099:GLN:NE2	3:E:1664:THR:HG23	2.33	0.43
1:B:610:PHE:HA	1:B:613:SER:HB3	1.99	0.43
1:B:1747:MET:HE2	1:B:1782:HIS:NE2	2.34	0.43
1:B:1875:LYS:HD3	1:B:1875:LYS:N	2.33	0.43
2:C:142:GLU:OE1	2:C:142:GLU:N	2.51	0.43
2:C:145:VAL:HB	2:C:153:HIS:HB2	2.00	0.43
3:E:228:ILE:O	3:E:232:LEU:HD23	2.18	0.43
3:E:670:PRO:O	3:E:673:VAL:HG12	2.17	0.43
3:E:963:SER:O	3:E:967:THR:HG23	2.18	0.43
3:F:200:GLU:OE2	3:F:243:TYR:HE1	2.01	0.43
3:F:906:CYS:O	3:F:909:VAL:HG12	2.17	0.43
3:F:963:SER:O	3:F:967:THR:HG23	2.18	0.43
1:A:675:VAL:O	1:A:678:SER:OG	2.36	0.43
1:A:748:ARG:NH1	1:A:749:ILE:HG13	2.34	0.43
1:A:773:GLU:OE2	3:F:454:ASN:ND2	2.44	0.43
1:A:805:LEU:HA	1:A:808:VAL:HG12	2.00	0.43
1:A:813:MET:O	1:A:817:VAL:HG13	2.17	0.43
1:A:1747:MET:HA	1:A:1750:CYS:SG	2.58	0.43
1:B:1234:HIS:NE2	3:F:348:GLU:OE1	2.46	0.43
1:B:1477:MET:SD	1:B:1477:MET:N	2.90	0.43
1:B:1569:ASP:HA	1:B:1572:ASP:HB3	2.01	0.43
1:B:1578:MET:SD	1:B:1585:ARG:NH2	2.92	0.43
1:B:2274:ASP:OD1	1:B:2274:ASP:N	2.49	0.43
2:D:142:GLU:OE1	2:D:142:GLU:N	2.51	0.43
3:E:38:LEU:HB2	3:E:79:PHE:CZ	2.52	0.43
3:E:770:ALA:HA	3:E:773:ILE:HG22	2.00	0.43
3:F:237:HIS:HB3	3:F:240:THR:HG23	2.00	0.43
3:F:920:ILE:HD12	3:F:964:ILE:HD11	2.00	0.43
1:B:1697:THR:HG23	1:B:1720:PHE:HZ	1.84	0.43
1:B:1724:MET:HE2	1:B:1724:MET:HB2	1.88	0.43
2:D:153:HIS:CD2	2:D:164:GLN:HB3	2.54	0.43
2:D:189:ASN:OD1	2:D:193:ASN:N	2.52	0.43
3:E:93:LEU:HD13	3:E:1686:HIS:CE1	2.53	0.43
3:E:685:LEU:HD23	3:E:688:LEU:HD12	2.01	0.43
3:F:228:ILE:O	3:F:232:LEU:HD23	2.18	0.43
3:F:346:PHE:CZ	3:F:475:CYS:HB3	2.53	0.43
3:F:1518:ASP:CG	3:F:1519:ASN:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LEU:O	1:A:721:MET:HE3	2.19	0.43
1:A:824:ILE:CG2	1:A:844:LEU:HD21	2.44	0.43
1:A:1878:LEU:O	1:A:1882:VAL:HG23	2.18	0.43
1:A:1901:GLN:HG2	1:A:1905:ARG:HH22	1.83	0.43
1:A:1910:TRP:HZ2	1:A:1956:LEU:HB3	1.83	0.43
1:A:2218:LYS:HB3	1:A:2322:ARG:HH21	1.84	0.43
1:B:28:GLY:O	1:B:85:GLY:N	2.52	0.43
1:B:1207:GLN:O	1:B:1211:VAL:HG23	2.18	0.43
2:C:153:HIS:CD2	2:C:164:GLN:HB3	2.54	0.43
3:E:285:LYS:HG3	3:E:330:VAL:HG22	1.99	0.43
3:E:1518:ASP:CG	3:E:1519:ASN:H	2.27	0.43
3:F:521:LEU:HB3	3:F:557:TRP:CZ2	2.54	0.43
4:G:35:ASP:OD1	4:G:35:ASP:C	2.60	0.43
4:G:88:GLN:OE1	4:G:88:GLN:CA	2.65	0.43
1:A:626:CYS:O	1:A:630:LEU:HD23	2.18	0.43
1:A:1555:ASP:HA	1:A:1557:PHE:CE1	2.54	0.43
1:A:1700:TYR:HD1	1:A:1701:MET:HE2	1.84	0.43
1:B:876:GLN:OE1	1:B:876:GLN:N	2.51	0.43
1:B:988:GLN:HG3	1:B:989:PHE:CE1	2.54	0.43
2:C:144:ILE:CG2	2:C:152:ILE:HD11	2.49	0.43
3:E:851:LEU:HD11	4:G:2:ALA:HB2	2.01	0.43
4:G:6:ASN:OD1	4:G:9:ILE:HG12	2.19	0.43
1:A:677:ALA:CA	1:A:710:LEU:HD21	2.48	0.43
1:A:957:ARG:NH2	1:A:960:ARG:HH11	2.17	0.43
1:A:1191:PHE:HA	1:A:1194:MET:HE2	2.01	0.43
1:A:1809:GLN:OE1	1:A:1809:GLN:N	2.47	0.43
1:B:714:THR:HG23	1:B:717:ARG:NH2	2.34	0.43
1:B:1292:LEU:HG	1:B:1304:TRP:HB2	2.01	0.43
2:C:136:LEU:HD12	2:C:142:GLU:O	2.18	0.43
2:C:165:LEU:HD22	2:C:197:TRP:HH2	1.84	0.43
2:D:144:ILE:CG2	2:D:152:ILE:HD11	2.49	0.43
2:D:156:ASP:OD1	2:D:159:THR:OG1	2.34	0.43
3:E:146:ALA:O	3:E:150:VAL:HG23	2.19	0.43
3:E:374:LYS:HA	3:E:741:ARG:NH1	2.34	0.43
3:F:685:LEU:HD23	3:F:688:LEU:HD12	2.01	0.43
4:G:83:ARG:NH2	4:G:83:ARG:HG3	2.34	0.43
1:A:1009:ARG:HA	1:A:1012:LEU:HD12	1.99	0.43
1:A:1116:PRO:HA	1:A:1119:VAL:HG12	2.00	0.43
1:A:1903:THR:O	1:A:1907:LEU:HD23	2.19	0.43
1:B:1098:ALA:HA	1:B:1101:GLN:HE21	1.84	0.43
1:B:1113:LEU:C	1:B:1116:PRO:HD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1157:HIS:HB2	1:B:1158:PRO:HD3	2.01	0.43
1:B:1194:MET:HE2	1:B:1194:MET:HB2	1.80	0.43
1:B:1414:GLU:CD	1:B:1449:TRP:HE1	2.27	0.43
1:B:1752:LEU:HD12	1:B:1776:TYR:CE1	2.54	0.43
1:B:2099:GLN:O	1:B:2103:LEU:HG	2.19	0.43
1:B:2218:LYS:HE3	1:B:2322:ARG:NH2	2.34	0.43
3:E:97:LYS:HA	3:E:100:ARG:HH21	1.84	0.43
3:F:384:ARG:HA	3:F:385:PRO:HD3	1.89	0.43
4:H:68:GLN:O	4:H:70:VAL:N	2.51	0.43
4:H:83:ARG:NH2	4:H:83:ARG:HG3	2.34	0.43
1:A:1184:LEU:HD23	1:A:1188:TYR:HB2	2.01	0.42
1:A:1355:GLN:NE2	1:A:1390:CYS:SG	2.91	0.42
1:A:1500:LYS:HB3	1:A:1500:LYS:HE2	1.80	0.42
1:B:624:ARG:HG2	1:B:624:ARG:NH1	2.33	0.42
1:B:2161:GLN:HB3	1:B:2171:LYS:HD3	2.01	0.42
1:B:2263:ILE:O	1:B:2267:ILE:HG12	2.18	0.42
2:C:200:THR:CG2	2:C:208:THR:HA	2.49	0.42
3:E:431:LEU:HD11	3:E:449:LEU:HD21	2.01	0.42
3:E:521:LEU:HB3	3:E:557:TRP:CZ2	2.54	0.42
3:E:920:ILE:HD12	3:E:964:ILE:HD11	2.00	0.42
3:F:189:ALA:HB2	4:H:18:HIS:CE1	2.54	0.42
3:F:902:ILE:H	3:F:902:ILE:HD12	1.83	0.42
4:H:91:GLU:HB3	4:H:95:LYS:HZ1	1.84	0.42
1:A:688:ALA:HB1	3:F:1003:VAL:HG21	2.01	0.42
1:A:1033:GLU:O	1:A:1036:THR:HG22	2.19	0.42
1:A:1095:LYS:HE2	1:A:1095:LYS:HB3	1.88	0.42
1:A:1119:VAL:HG23	1:A:1122:PHE:CE1	2.54	0.42
1:A:1177:LEU:O	1:A:1181:VAL:HG13	2.19	0.42
1:A:1282:GLU:HG2	1:A:1286:ARG:NE	2.34	0.42
1:A:1989:ASN:OD1	1:A:1990:ALA:N	2.52	0.42
1:A:2411:LYS:O	1:A:2415:MET:HB2	2.19	0.42
1:B:617:GLU:OE2	1:B:618:ILE:HG23	2.19	0.42
1:B:1119:VAL:HA	1:B:1122:PHE:CD1	2.53	0.42
2:D:200:THR:CG2	2:D:208:THR:HA	2.49	0.42
3:F:312:LEU:HD12	3:F:327:LEU:HD11	2.01	0.42
3:F:374:LYS:HA	3:F:741:ARG:NH1	2.34	0.42
3:F:531:ASN:CB	3:F:554:ILE:HD11	2.47	0.42
3:F:550:LEU:O	3:F:553:THR:OG1	2.26	0.42
3:F:624:GLU:HG2	3:F:675:MET:HE1	2.01	0.42
3:F:726:ASP:O	3:F:729:ARG:HB2	2.19	0.42
3:F:916:LYS:NZ	3:F:918:GLU:OE1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1666:ARG:HD3	3:F:1666:ARG:HA	1.84	0.42
1:A:623:ALA:HA	1:A:626:CYS:SG	2.58	0.42
1:A:727:MET:HE3	3:F:447:HIS:O	2.20	0.42
1:A:886:ARG:O	1:A:890:LEU:HD23	2.20	0.42
1:A:944:ASP:OD1	1:A:945:GLU:N	2.50	0.42
1:A:1101:GLN:HB3	1:A:1141:ARG:NH1	2.32	0.42
1:A:1178:SER:O	1:A:1181:VAL:HG22	2.18	0.42
1:A:1920:ASN:O	1:A:1924:VAL:HG13	2.19	0.42
1:A:2182:PHE:HB3	1:A:2184:PHE:CE1	2.50	0.42
1:B:1477:MET:HA	1:B:1480:ARG:HG2	2.01	0.42
1:B:2055:HIS:NE2	1:B:2082:GLN:HB2	2.34	0.42
2:D:48:LEU:HD21	2:D:318:LEU:C	2.44	0.42
3:E:110:LEU:O	3:E:112:GLN:HG2	2.19	0.42
3:E:240:THR:HA	3:E:243:TYR:HD2	1.81	0.42
3:F:146:ALA:O	3:F:150:VAL:HG23	2.19	0.42
3:F:291:THR:HG23	3:F:292:PHE:HD2	1.84	0.42
3:F:735:HIS:ND1	3:F:735:HIS:O	2.52	0.42
1:A:1098:ALA:HA	1:A:1101:GLN:HG3	2.00	0.42
1:A:1119:VAL:HA	1:A:1122:PHE:HE1	1.84	0.42
1:A:1235:ARG:NH2	1:A:1236:MET:SD	2.89	0.42
1:A:2184:PHE:HB3	1:A:2236:LEU:HD11	2.01	0.42
2:D:123:ARG:NH1	2:D:157:LEU:O	2.46	0.42
3:E:735:HIS:ND1	3:E:735:HIS:O	2.52	0.42
3:E:763:ASN:HB3	3:E:766:ILE:HD12	2.00	0.42
3:F:364:LEU:HA	3:F:368:PHE:CD1	2.54	0.42
4:G:4:LEU:HD23	4:G:9:ILE:HD12	2.01	0.42
4:H:6:ASN:OD1	4:H:9:ILE:HG12	2.19	0.42
1:A:1362:GLU:HA	1:A:1365:GLU:HG2	2.01	0.42
1:B:614:GLU:H	1:B:614:GLU:CD	2.28	0.42
1:B:835:ALA:O	1:B:837:ARG:N	2.53	0.42
2:C:189:ASN:OD1	2:C:193:ASN:N	2.52	0.42
2:D:94:HIS:CD2	2:D:96:ASP:H	2.38	0.42
2:D:226:CYS:O	2:D:227:ARG:HD2	2.20	0.42
3:E:222:ARG:NH1	4:G:20:THR:HG21	2.35	0.42
3:E:225:GLU:O	3:E:228:ILE:HG22	2.20	0.42
3:E:1528:ILE:HG12	3:E:1529:LEU:HD22	2.02	0.42
3:F:380:ARG:NH1	3:F:743:ASN:OD1	2.52	0.42
3:F:926:SER:O	3:F:930:LEU:HD23	2.20	0.42
3:F:934:GLY:HA2	3:F:943:LEU:HD13	2.00	0.42
3:F:1528:ILE:HG12	3:F:1529:LEU:HD22	2.02	0.42
1:A:1480:ARG:HH22	1:A:1496:GLN:HE21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:MET:O	1:B:624:ARG:NH1	2.53	0.42
1:B:718:LEU:C	1:B:721:MET:HE3	2.45	0.42
1:B:1193:PRO:O	1:B:1197:LYS:HG2	2.20	0.42
1:B:2209:LEU:HD21	1:B:2220:LEU:HB3	2.00	0.42
2:D:267:GLU:CG	2:D:270:ARG:H	2.31	0.42
3:E:113:ASP:H	3:E:116:ILE:HD12	1.85	0.42
3:E:934:GLY:HA2	3:E:943:LEU:HD13	2.00	0.42
3:F:35:SER:O	3:F:39:ARG:HG2	2.18	0.42
3:F:441:SER:O	3:F:444:HIS:ND1	2.48	0.42
1:A:947:TYR:CE1	1:A:1324:SER:HB3	2.55	0.42
1:A:1120:LYS:HA	1:A:1123:ASP:OD2	2.20	0.42
1:A:1157:HIS:HB2	1:A:1158:PRO:HD3	2.01	0.42
1:A:1738:GLN:H	1:A:1738:GLN:CD	2.28	0.42
1:A:1945:ARG:HG3	1:A:1945:ARG:O	2.19	0.42
1:B:943:LEU:HD12	1:B:944:ASP:N	2.34	0.42
1:B:1226:GLU:O	3:F:485:ARG:NE	2.53	0.42
1:B:1497:CYS:SG	1:B:1515:MET:HE1	2.60	0.42
2:C:53:ASP:OD1	2:C:55:SER:OG	2.37	0.42
2:D:165:LEU:HD22	2:D:197:TRP:HH2	1.84	0.42
3:E:526:GLU:HG2	3:E:527:ALA:N	2.34	0.42
3:F:332:TYR:CE1	3:F:426:LEU:HB2	2.51	0.42
4:G:91:GLU:HB3	4:G:95:LYS:NZ	2.33	0.42
4:H:66:TYR:CD2	4:H:66:TYR:O	2.73	0.42
1:A:929:TYR:O	1:A:933:GLU:HG2	2.20	0.42
1:A:970:MET:O	1:A:973:GLN:HG2	2.20	0.42
1:A:1520:ALA:HB3	1:A:1529:MET:HG2	2.02	0.42
1:A:1595:MET:HE1	1:A:1636:ILE:CA	2.45	0.42
1:A:1972:LEU:O	1:A:1976:LEU:HG	2.19	0.42
1:A:2021:ILE:HG23	1:A:2021:ILE:O	2.20	0.42
1:B:705:PHE:O	1:B:708:ARG:HB2	2.19	0.42
1:B:1192:ILE:HG13	1:B:1193:PRO:HD3	2.01	0.42
1:B:1701:MET:HE1	1:B:1717:MET:HA	2.02	0.42
3:E:291:THR:HG23	3:E:292:PHE:HD2	1.84	0.42
3:E:312:LEU:HD12	3:E:327:LEU:HD11	2.01	0.42
3:E:907:ARG:O	3:E:911:THR:HG23	2.20	0.42
3:E:926:SER:O	3:E:930:LEU:HD23	2.20	0.42
3:F:526:GLU:HG2	3:F:527:ALA:N	2.34	0.42
3:F:609:THR:HG21	3:F:662:PHE:CD1	2.55	0.42
1:A:718:LEU:C	1:A:721:MET:HE3	2.45	0.42
1:A:1414:GLU:CD	1:A:1449:TRP:HE1	2.27	0.42
1:A:1500:LYS:HD2	1:A:1503:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:ASP:N	1:A:1527:ASP:OD1	2.51	0.42
1:A:1752:LEU:HD12	1:A:1776:TYR:CE1	2.54	0.42
1:B:1709:ARG:NH2	1:B:1711:ILE:HB	2.26	0.42
1:B:1793:TRP:O	1:B:1797:ASN:ND2	2.53	0.42
2:D:221:ARG:HG3	2:D:222:TYR:H	1.85	0.42
3:E:296:ALA:O	3:E:300:ASN:ND2	2.38	0.42
3:E:726:ASP:HA	3:E:729:ARG:CG	2.49	0.42
3:F:135:ILE:HG21	3:F:139:ASN:HD21	1.85	0.42
3:F:770:ALA:HA	3:F:773:ILE:HG22	2.00	0.42
1:A:773:GLU:HA	1:A:776:LEU:HG	2.02	0.42
1:A:1038:MET:SD	1:A:1056:ILE:HD11	2.59	0.42
1:A:1174:MET:HE3	1:A:1206:HIS:ND1	2.35	0.42
1:A:1234:HIS:NE2	3:E:348:GLU:OE1	2.50	0.42
1:A:1293:LYS:HA	1:A:1304:TRP:CG	2.55	0.42
1:A:1620:TRP:HE3	1:A:1652:THR:HG22	1.85	0.42
1:A:1884:ALA:O	1:A:1888:PHE:CD2	2.73	0.42
1:A:1921:GLU:O	1:A:1925:GLU:OE1	2.38	0.42
1:A:2203:GLY:O	1:A:2207:THR:HG23	2.19	0.42
1:B:704:VAL:CG2	1:B:707:ILE:HD12	2.49	0.42
1:B:1569:ASP:OD1	1:B:1570:LEU:N	2.53	0.42
1:B:1697:THR:HG23	1:B:1720:PHE:CZ	2.55	0.42
1:B:2015:GLU:OE1	1:B:2018:ARG:NH1	2.53	0.42
1:B:2512:ASP:OD1	1:B:2512:ASP:N	2.52	0.42
2:C:48:LEU:HD21	2:C:318:LEU:C	2.44	0.42
2:C:94:HIS:CD2	2:C:96:ASP:H	2.38	0.42
2:D:48:LEU:HD22	2:D:317:CYS:SG	2.60	0.42
3:E:150:VAL:O	3:E:153:MET:HG2	2.19	0.42
3:E:336:ARG:NH1	3:E:874:PRO:HD3	2.35	0.42
3:E:364:LEU:HA	3:E:368:PHE:CD1	2.54	0.42
3:E:624:GLU:HG2	3:E:675:MET:HE1	2.01	0.42
3:F:225:GLU:O	3:F:228:ILE:HG22	2.20	0.42
3:F:389:ASP:HB3	3:F:437:ILE:HG21	2.02	0.42
3:F:663:ILE:HA	3:F:666:LEU:HB3	2.01	0.42
4:H:66:TYR:CE2	4:H:67:ALA:HB3	2.55	0.42
1:A:614:GLU:CD	1:A:614:GLU:H	2.27	0.41
1:A:627:SER:HB2	1:A:678:SER:HB2	2.02	0.41
1:A:1114:LEU:HD12	1:A:1114:LEU:HA	1.83	0.41
1:A:1215:ARG:HH21	1:A:1216:ILE:HG23	1.84	0.41
1:A:1514:ARG:HG3	1:A:1515:MET:N	2.35	0.41
1:A:1910:TRP:NE1	1:A:1953:VAL:HG23	2.35	0.41
1:A:1986:ALA:HA	1:A:1989:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1990:ALA:O	1:A:1994:ILE:HG22	2.20	0.41
1:A:2078:LEU:HA	1:A:2078:LEU:HD13	1.83	0.41
1:B:712:ILE:HD11	1:B:760:LEU:HD21	2.02	0.41
1:B:1072:PRO:HA	1:B:1075:ILE:HG12	2.02	0.41
1:B:1536:ILE:O	1:B:1538:ARG:NH1	2.53	0.41
1:B:1686:ASP:OD1	1:B:1687:HIS:N	2.52	0.41
2:D:199:LEU:H	2:D:199:LEU:HD23	1.85	0.41
3:E:380:ARG:NH1	3:E:743:ASN:OD1	2.52	0.41
3:E:818:LEU:HD21	3:E:823:TYR:HD2	1.84	0.41
3:E:881:HIS:O	3:E:885:GLN:HG2	2.20	0.41
3:F:150:VAL:O	3:F:153:MET:HG2	2.19	0.41
3:F:906:CYS:HA	3:F:909:VAL:HG12	2.02	0.41
3:F:919:GLU:HA	3:F:922:LYS:NZ	2.35	0.41
4:G:81:ARG:H	4:G:81:ARG:HG2	1.59	0.41
1:A:1208:ARG:O	1:A:1212:LEU:HD13	2.21	0.41
1:A:1265:LEU:HG	1:A:1269:TRP:CZ3	2.54	0.41
1:A:1269:TRP:C	1:A:1271:ALA:H	2.25	0.41
1:A:1277:LYS:HG3	1:A:1278:ASP:N	2.35	0.41
1:A:1360:LEU:HD11	1:A:1364:MET:HE2	2.02	0.41
1:A:1416:LEU:HA	1:A:1419:ILE:HG22	2.02	0.41
1:A:2047:MET:HA	1:A:2050:VAL:HB	2.03	0.41
1:A:2086:ARG:HA	1:A:2089:MET:HG3	2.02	0.41
1:B:1045:ASN:HD22	1:B:1045:ASN:C	2.27	0.41
2:C:48:LEU:HD22	2:C:317:CYS:SG	2.60	0.41
2:C:248:ARG:HG2	2:C:250:SER:H	1.86	0.41
3:E:46:ALA:C	3:E:47:ARG:HG2	2.45	0.41
3:E:971:VAL:O	3:E:974:LEU:HB2	2.21	0.41
3:F:46:ALA:C	3:F:47:ARG:HG2	2.46	0.41
3:F:97:LYS:HA	3:F:100:ARG:HH21	1.84	0.41
3:F:153:MET:HA	3:F:156:VAL:HG12	2.02	0.41
3:F:881:HIS:O	3:F:885:GLN:HG2	2.20	0.41
3:F:907:ARG:O	3:F:911:THR:HG23	2.20	0.41
3:F:962:LEU:O	3:F:965:ARG:HB2	2.19	0.41
4:G:66:TYR:CE2	4:G:67:ALA:HB3	2.55	0.41
1:A:621:GLU:OE2	1:A:624:ARG:NH1	2.50	0.41
1:A:737:ILE:O	1:A:740:GLU:HB3	2.19	0.41
1:A:1020:VAL:HG13	1:A:1027:ILE:HD13	2.03	0.41
1:A:1607:LEU:HD23	1:A:1607:LEU:HA	1.85	0.41
1:B:1069:LEU:HD13	3:F:467:LEU:HD12	2.02	0.41
3:E:82:GLU:OE1	3:E:82:GLU:N	2.48	0.41
3:E:556:LYS:CE	3:E:607:GLN:HE22	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:336:ARG:NH1	3:F:874:PRO:HD3	2.34	0.41
3:F:431:LEU:HD11	3:F:449:LEU:HD21	2.01	0.41
3:F:726:ASP:HA	3:F:729:ARG:CG	2.49	0.41
3:F:900:ASN:O	3:F:903:THR:HG22	2.20	0.41
4:H:80:ILE:HD12	4:H:81:ARG:N	2.35	0.41
1:A:660:LEU:O	1:A:664:ILE:HG12	2.20	0.41
1:A:854:VAL:HG13	1:A:855:VAL:N	2.35	0.41
1:A:1717:MET:HG3	1:A:1757:TRP:HZ3	1.85	0.41
1:A:2052:GLU:HB3	1:A:2053:PRO:HD3	2.03	0.41
1:A:2169:PRO:HB2	1:A:2185:LEU:HD11	2.02	0.41
1:B:1274:ARG:HA	1:B:1279:ASP:CG	2.45	0.41
1:B:1322:PHE:CD2	1:B:1360:LEU:HD11	2.55	0.41
2:C:248:ARG:NH1	2:C:253:SER:OG	2.53	0.41
2:D:34:CYS:HB3	2:D:308:TYR:OH	2.21	0.41
2:D:248:ARG:NH1	2:D:253:SER:OG	2.53	0.41
3:E:115:SER:CA	3:E:118:GLN:HE21	2.33	0.41
3:E:663:ILE:HA	3:E:666:LEU:HB3	2.01	0.41
3:E:726:ASP:O	3:E:729:ARG:HB2	2.19	0.41
3:E:900:ASN:O	3:E:903:THR:HG22	2.20	0.41
3:E:962:LEU:O	3:E:965:ARG:HB2	2.19	0.41
3:F:620:GLN:O	3:F:624:GLU:HG3	2.21	0.41
3:F:971:VAL:O	3:F:974:LEU:HB2	2.21	0.41
4:H:4:LEU:HD23	4:H:9:ILE:HD12	2.01	0.41
1:A:1154:ARG:HG2	1:B:702:ASP:HA	2.01	0.41
1:A:1609:PRO:HA	1:A:1612:ARG:NE	2.36	0.41
1:A:2345:MET:O	1:A:2353:ILE:HD12	2.20	0.41
1:B:967:HIS:O	1:B:971:VAL:HG23	2.20	0.41
1:B:1031:MET:O	1:B:1034:ILE:HB	2.20	0.41
1:B:1117:PRO:O	1:B:1121:LEU:HD23	2.20	0.41
1:B:1753:LYS:HB3	1:B:1757:TRP:CZ3	2.55	0.41
1:B:2153:ILE:O	1:B:2153:ILE:HG13	2.20	0.41
2:C:199:LEU:HD23	2:C:199:LEU:H	1.85	0.41
2:C:278:PHE:CD1	2:C:285:ILE:HG22	2.56	0.41
3:E:389:ASP:HB3	3:E:437:ILE:HG21	2.03	0.41
3:E:1526:ILE:HD11	3:E:1533:PRO:HA	2.03	0.41
3:F:382:ARG:HG2	3:F:382:ARG:NH1	2.35	0.41
3:F:818:LEU:HD21	3:F:823:TYR:HD2	1.84	0.41
1:A:664:ILE:HG13	1:A:695:ALA:HB1	2.03	0.41
1:A:1060:VAL:HG21	1:A:1103:PHE:HE1	1.85	0.41
1:A:1325:CYS:O	1:A:1329:LEU:HG	2.21	0.41
1:A:2212:ASP:HB3	1:A:2215:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:ARG:NH1	1:B:886:ARG:HG3	2.34	0.41
1:B:1389:LYS:O	1:B:1391:ARG:NH1	2.54	0.41
1:B:1681:PRO:HA	1:B:1684:GLN:HG3	2.02	0.41
1:B:2036:ARG:HG3	1:B:2037:LEU:N	2.36	0.41
1:B:2131:LEU:HD23	1:B:2131:LEU:H	1.85	0.41
1:B:2527:LEU:HD23	1:B:2527:LEU:HA	1.78	0.41
1:B:2534:SER:OG	1:B:2536:GLU:OE1	2.36	0.41
2:C:226:CYS:O	2:C:227:ARG:HD2	2.20	0.41
2:D:278:PHE:CD1	2:D:285:ILE:HG22	2.56	0.41
3:E:379:HIS:CD2	3:E:381:ALA:H	2.28	0.41
3:E:382:ARG:HG2	3:E:382:ARG:NH1	2.35	0.41
3:F:623:LEU:CD2	3:F:675:MET:HG2	2.51	0.41
3:F:628:LYS:O	3:F:631:VAL:HG12	2.21	0.41
3:F:761:ASP:OD1	3:F:762:LYS:N	2.44	0.41
4:G:68:GLN:O	4:G:69:SER:O	2.38	0.41
1:A:835:ALA:O	1:A:837:ARG:N	2.54	0.41
1:A:1031:MET:SD	1:A:1063:LEU:HD11	2.60	0.41
1:A:1098:ALA:HA	1:A:1101:GLN:NE2	2.36	0.41
1:A:1236:MET:SD	1:A:1236:MET:N	2.94	0.41
1:A:1391:ARG:HA	1:A:1393:TYR:CE1	2.56	0.41
1:A:1578:MET:HE2	1:A:1578:MET:HA	2.02	0.41
1:A:1620:TRP:O	1:A:1624:GLN:HG2	2.20	0.41
1:B:708:ARG:O	1:B:712:ILE:HG22	2.21	0.41
1:B:883:GLU:O	1:B:887:VAL:HG23	2.21	0.41
1:B:1220:TYR:CD2	1:B:1221:THR:HG22	2.56	0.41
1:B:1264:ASN:HA	1:B:1267:LYS:NZ	2.36	0.41
1:B:1989:ASN:OD1	1:B:1990:ALA:N	2.52	0.41
2:C:14:ILE:HG13	2:C:321:ASN:H	1.86	0.41
2:C:34:CYS:HB3	2:C:308:TYR:OH	2.20	0.41
2:C:88:ILE:HD12	2:C:104:GLY:HA2	2.03	0.41
2:C:194:CYS:HB2	2:C:216:ILE:CG2	2.51	0.41
3:E:609:THR:HG21	3:E:662:PHE:CD1	2.55	0.41
3:F:43:GLN:OE1	3:F:59:HIS:NE2	2.54	0.41
3:F:110:LEU:O	3:F:112:GLN:HG2	2.19	0.41
4:G:66:TYR:CD2	4:G:66:TYR:O	2.73	0.41
4:G:80:ILE:HD12	4:G:81:ARG:N	2.35	0.41
4:H:68:GLN:O	4:H:69:SER:O	2.38	0.41
1:A:1212:LEU:HG	1:A:1215:ARG:NH1	2.35	0.41
1:A:2281:MET:HE3	1:A:2281:MET:HB3	1.92	0.41
1:B:1083:MET:SD	1:B:1083:MET:N	2.94	0.41
1:B:1200:VAL:HA	1:B:1203:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	2.03	0.41
1:B:2339:ARG:O	1:B:2378:ARG:HD3	2.21	0.41
2:C:98:ARG:HA	2:C:115:ARG:NH2	2.36	0.41
2:C:156:ASP:OD1	2:C:159:THR:OG1	2.34	0.41
2:D:177:HIS:ND1	2:D:228:PHE:HD2	2.19	0.41
3:E:336:ARG:NH1	3:E:873:ARG:HA	2.36	0.41
3:E:548:TRP:CD1	3:E:597:LYS:HE3	2.56	0.41
3:E:613:LEU:HA	3:E:616:GLU:OE2	2.20	0.41
3:F:481:GLU:O	3:F:484:LYS:HG2	2.21	0.41
3:F:824:VAL:HG23	3:F:825:ALA:H	1.86	0.41
1:A:242:GLU:HA	1:A:365:LEU:HA	2.02	0.41
1:A:664:ILE:CA	1:A:672:ARG:HH12	2.34	0.41
1:A:731:ARG:HG2	3:F:453:MET:HE2	2.03	0.41
1:A:858:TYR:CD1	1:A:894:LEU:HD22	2.56	0.41
1:A:1208:ARG:H	1:A:1208:ARG:HG2	1.63	0.41
1:A:1504:VAL:HG22	1:A:1508:THR:OG1	2.21	0.41
1:A:1874:SER:HA	1:A:1877:LEU:HD12	2.02	0.41
1:A:1917:PRO:HA	1:A:1920:ASN:OD1	2.21	0.41
1:A:1953:VAL:O	1:A:1957:ILE:HG13	2.21	0.41
1:A:1954:GLY:C	1:A:1958:HIS:HD1	2.25	0.41
1:A:2102:ASP:OD1	3:E:1626:SER:OG	2.31	0.41
1:A:2137:GLU:O	1:A:2152:ARG:HD2	2.21	0.41
1:B:680:ASP:OD2	1:B:682:ARG:HD3	2.20	0.41
1:B:777:LYS:HA	1:B:780:ILE:HG12	2.03	0.41
1:B:1123:ASP:OD1	1:B:1123:ASP:N	2.52	0.41
1:B:1280:TRP:CE2	1:B:1348:GLN:HB3	2.56	0.41
1:B:1797:ASN:HB3	1:B:1884:ALA:HB2	2.01	0.41
1:B:2171:LYS:O	1:B:2171:LYS:HG3	2.21	0.41
2:C:177:HIS:ND1	2:C:228:PHE:HD2	2.19	0.41
2:C:248:ARG:NH2	2:C:251:ASN:OD1	2.53	0.41
2:C:305:LYS:HB2	2:C:305:LYS:HE2	1.78	0.41
2:D:46:ASN:N	2:D:60:ALA:O	2.37	0.41
2:D:196:VAL:HB	2:D:214:THR:HB	2.03	0.41
2:D:248:ARG:NH2	2:D:251:ASN:OD1	2.53	0.41
2:D:248:ARG:HG2	2:D:250:SER:H	1.86	0.41
2:D:305:LYS:HE2	2:D:305:LYS:HB2	1.79	0.41
3:E:482:MET:O	3:E:485:ARG:HB3	2.21	0.41
3:E:628:LYS:O	3:E:631:VAL:HG12	2.21	0.41
3:E:779:GLU:HA	3:E:807:ARG:NH2	2.29	0.41
3:E:890:LYS:HD2	3:E:938:TRP:CD2	2.56	0.41
3:E:907:ARG:HA	3:E:910:ARG:NE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1491:GLU:OE1	3:E:1491:GLU:N	2.52	0.41
3:E:1613:ARG:HH22	3:E:1651:CYS:HB2	1.86	0.41
3:F:595:PHE:HB3	3:F:598:ALA:HB2	2.03	0.41
3:F:613:LEU:HA	3:F:616:GLU:OE2	2.20	0.41
3:F:725:THR:O	3:F:729:ARG:HG2	2.21	0.41
3:F:1637:LEU:CD2	4:H:93:LEU:HD21	2.49	0.41
1:A:858:TYR:OH	1:A:891:LEU:HB3	2.21	0.41
1:A:1054:LEU:HD12	1:A:1054:LEU:HA	1.90	0.41
1:A:2064:THR:O	1:A:2068:THR:OG1	2.28	0.41
1:A:2133:CYS:C	1:A:2135:ASP:H	2.29	0.41
1:B:772:MET:HE1	1:B:812:GLU:HB2	2.03	0.41
1:B:1210:ASP:HA	1:B:1213:ILE:HG12	2.02	0.41
1:B:1919:VAL:O	1:B:1923:LEU:HG	2.21	0.41
1:B:1971:ALA:HB2	1:B:2144:TYR:CE2	2.55	0.41
1:B:2165:SER:OG	1:B:2166:LYS:N	2.54	0.41
3:E:167:ASN:CG	3:E:1670:ARG:HH22	2.29	0.41
3:E:818:LEU:HA	3:E:821:ARG:HH21	1.86	0.41
3:E:1636:LEU:HD23	3:E:1636:LEU:HA	1.92	0.41
3:E:1687:GLU:HA	3:E:1690:GLU:HG3	2.03	0.41
3:F:1613:ARG:HH22	3:F:1651:CYS:HB2	1.86	0.41
1:A:544:SER:O	1:A:548:MET:CB	2.69	0.40
1:A:708:ARG:HG3	1:A:708:ARG:HH11	1.86	0.40
1:A:814:ARG:NH1	1:A:851:THR:O	2.54	0.40
1:A:1123:ASP:HA	1:A:1161:ARG:HH22	1.79	0.40
1:A:1149:THR:OG1	1:A:1150:ASP:N	2.54	0.40
1:A:1907:LEU:HD21	1:A:1935:TRP:HZ3	1.86	0.40
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	2.02	0.40
1:B:824:ILE:HG21	1:B:844:LEU:HB2	2.02	0.40
1:B:1095:LYS:HE2	1:B:1095:LYS:HB3	1.91	0.40
1:B:1155:ILE:C	1:B:1158:PRO:HD2	2.45	0.40
1:B:1340:SER:O	1:B:1343:LEU:HG	2.22	0.40
1:B:2285:GLU:HG3	2:D:272:TRP:CE2	2.56	0.40
2:D:14:ILE:HD11	2:D:321:ASN:HB2	2.03	0.40
2:D:88:ILE:HD12	2:D:104:GLY:HA2	2.03	0.40
3:E:36:ASP:HA	3:E:39:ARG:CZ	2.51	0.40
3:E:43:GLN:OE1	3:E:59:HIS:NE2	2.54	0.40
3:E:124:LYS:HA	3:E:124:LYS:HD2	1.82	0.40
3:E:1619:LEU:HD21	3:E:1632:HIS:HB3	2.03	0.40
3:E:1670:ARG:O	3:E:1673:ILE:HG22	2.21	0.40
3:F:115:SER:CA	3:F:118:GLN:HE21	2.33	0.40
3:F:907:ARG:HA	3:F:910:ARG:NE	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1484:ARG:HA	3:F:1484:ARG:HD2	1.87	0.40
4:H:78:PHE:HD2	4:H:78:PHE:HA	1.50	0.40
1:A:430:ARG:HA	1:A:433:ALA:HB3	2.04	0.40
1:A:736:GLN:HB3	1:B:1112:HIS:NE2	2.36	0.40
1:A:1338:ILE:HG22	1:A:1372:LEU:HD21	2.02	0.40
1:A:1613:GLU:N	1:A:1613:GLU:OE2	2.54	0.40
1:A:2085:CYS:O	1:A:2089:MET:HG3	2.21	0.40
1:A:2541:CYS:HG	1:A:2545:TRP:CG	2.39	0.40
1:B:614:GLU:OE1	1:B:614:GLU:N	2.53	0.40
1:B:952:MET:HE1	1:B:979:PHE:CE1	2.55	0.40
1:B:1325:CYS:O	1:B:1329:LEU:HG	2.21	0.40
2:C:49:GLU:OE1	2:C:92:GLY:HA2	2.21	0.40
2:C:221:ARG:HG3	2:C:222:TYR:H	1.85	0.40
2:C:267:GLU:HG2	2:C:269:SER:N	2.37	0.40
3:E:135:ILE:HG21	3:E:139:ASN:HD21	1.85	0.40
3:E:595:PHE:HB3	3:E:598:ALA:HB2	2.03	0.40
3:E:919:GLU:HA	3:E:922:LYS:NZ	2.35	0.40
3:F:321:MET:HA	3:F:321:MET:HE2	2.03	0.40
3:F:336:ARG:NH1	3:F:873:ARG:HA	2.36	0.40
3:F:1521:LEU:HB3	3:F:1650:ILE:HD11	2.03	0.40
1:A:701:ASN:OD1	1:A:708:ARG:NH2	2.54	0.40
1:A:776:LEU:O	1:A:780:ILE:HG12	2.22	0.40
1:A:1217:VAL:HG13	1:A:1218:LYS:HG2	2.03	0.40
1:A:1300:LEU:HD23	1:A:1300:LEU:HA	1.93	0.40
1:A:2066:LYS:HD3	1:A:2125:TYR:CE2	2.57	0.40
1:A:2135:ASP:OD1	1:A:2136:LEU:N	2.55	0.40
1:A:2191:ASP:O	1:A:2192:LEU:HD12	2.20	0.40
1:B:1097:LEU:O	1:B:1101:GLN:HG3	2.21	0.40
1:B:1595:MET:SD	1:B:1639:VAL:HG11	2.61	0.40
1:B:2199:MET:CE	1:B:2225:TYR:H	2.35	0.40
1:B:2538:LEU:HD23	1:B:2538:LEU:HA	1.90	0.40
2:C:107:CYS:HB3	2:C:127:VAL:O	2.21	0.40
2:D:20:TYR:HD2	2:D:44:GLN:NE2	2.20	0.40
3:E:337:LEU:HD21	3:E:429:GLU:HG2	2.04	0.40
3:E:620:GLN:O	3:E:624:GLU:HG3	2.21	0.40
3:F:36:ASP:HA	3:F:39:ARG:CZ	2.51	0.40
3:F:113:ASP:H	3:F:116:ILE:HD12	1.85	0.40
4:G:69:SER:O	4:G:70:VAL:C	2.64	0.40
4:H:92:ARG:NH2	4:H:93:LEU:HB3	2.36	0.40
1:A:2228:ILE:CG1	1:A:2236:LEU:HB3	2.50	0.40
1:B:1434:GLU:HA	1:B:1437:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1442:GLU:OE1	1:B:1442:GLU:N	2.54	0.40
1:B:1501:TRP:CZ2	1:B:1535:MET:HE3	2.57	0.40
1:B:1630:VAL:HG22	1:B:1659:LEU:HD12	2.03	0.40
1:B:2336:LEU:HD21	1:B:2339:ARG:NH1	2.37	0.40
2:D:49:GLU:OE1	2:D:92:GLY:HA2	2.21	0.40
3:E:623:LEU:CD2	3:E:675:MET:HG2	2.51	0.40
3:E:725:THR:O	3:E:729:ARG:HG2	2.21	0.40
3:E:1515:HIS:CE1	3:E:1651:CYS:HG	2.34	0.40
3:F:392:LEU:HD23	3:F:392:LEU:HA	1.82	0.40
3:F:890:LYS:HD2	3:F:938:TRP:CD2	2.56	0.40
1:A:267:ILE:O	1:A:271:LEU:N	2.44	0.40
1:A:649:VAL:HA	1:A:652:VAL:HG12	2.03	0.40
1:A:797:ASN:O	1:A:801:THR:HG23	2.22	0.40
1:A:1338:ILE:HA	1:A:1341:ILE:HG22	2.02	0.40
1:A:1342:GLU:OE1	1:A:1343:LEU:HD22	2.21	0.40
1:B:663:GLY:HA2	1:B:672:ARG:HH21	1.87	0.40
1:B:1357:LEU:HD13	1:B:1357:LEU:HA	1.94	0.40
2:C:20:TYR:HB2	2:C:313:LYS:CB	2.52	0.40
3:E:153:MET:HA	3:E:156:VAL:HG12	2.02	0.40
3:E:906:CYS:HA	3:E:909:VAL:HG12	2.02	0.40
3:F:223:ILE:O	3:F:227:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2143/2674 (80%)	2026 (94%)	117 (6%)	0	100	100
1	B	2145/2674 (80%)	2012 (94%)	133 (6%)	0	100	100
2	C	317/347 (91%)	292 (92%)	25 (8%)	0	100	100
2	D	317/347 (91%)	292 (92%)	25 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	1103/1720 (64%)	1027 (93%)	76 (7%)	0	100	100
3	F	1103/1720 (64%)	1027 (93%)	76 (7%)	0	100	100
4	G	116/538 (22%)	87 (75%)	17 (15%)	12 (10%)	0	2
4	H	116/538 (22%)	87 (75%)	17 (15%)	12 (10%)	0	2
All	All	7360/10558 (70%)	6850 (93%)	486 (7%)	24 (0%)	37	66

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	35	ASP
4	G	37	ASP
4	G	72	ILE
4	G	74	SER
4	G	78	PHE
4	G	80	ILE
4	G	85	ASN
4	H	35	ASP
4	H	37	ASP
4	H	72	ILE
4	H	74	SER
4	H	78	PHE
4	H	80	ILE
4	H	85	ASN
4	G	36	VAL
4	G	68	GLN
4	H	36	VAL
4	H	68	GLN
4	G	75	SER
4	G	76	TRP
4	H	75	SER
4	H	76	TRP
4	G	70	VAL
4	H	70	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1563/2319 (67%)	1561 (100%)	2 (0%)	88	91
1	B	1552/2319 (67%)	1552 (100%)	0	100	100
2	C	269/290 (93%)	266 (99%)	3 (1%)	65	76
2	D	269/290 (93%)	266 (99%)	3 (1%)	65	76
3	E	987/1550 (64%)	962 (98%)	25 (2%)	42	65
3	F	987/1550 (64%)	962 (98%)	25 (2%)	42	65
4	G	70/479 (15%)	55 (79%)	15 (21%)	1	5
4	H	70/479 (15%)	55 (79%)	15 (21%)	1	5
All	All	5767/9276 (62%)	5679 (98%)	88 (2%)	55	73

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1722	GLN
1	A	1738	GLN
2	C	56	MET
2	C	67	MET
2	C	234	LEU
2	D	56	MET
2	D	67	MET
2	D	234	LEU
3	E	177	LEU
3	E	196	LEU
3	E	208	LEU
3	E	209	ASN
3	E	270	GLU
3	E	322	GLU
3	E	333	ASP
3	E	405	LEU
3	E	430	LEU
3	E	431	LEU
3	E	500	LYS
3	E	710	ASP
3	E	807	ARG
3	E	821	ARG
3	E	826	LYS
3	E	828	LEU
3	E	838	LYS

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Mol	Chain	Res	Type
3	E	905	LEU
3	E	910	ARG
3	E	911	THR
3	E	926	SER
3	E	960	GLU
3	E	975	ILE
3	E	1487	MET
3	E	1621	ILE
3	F	177	LEU
3	F	196	LEU
3	F	208	LEU
3	F	209	ASN
3	F	270	GLU
3	F	322	GLU
3	F	333	ASP
3	F	405	LEU
3	F	430	LEU
3	F	431	LEU
3	F	500	LYS
3	F	710	ASP
3	F	807	ARG
3	F	821	ARG
3	F	826	LYS
3	F	828	LEU
3	F	838	LYS
3	F	905	LEU
3	F	910	ARG
3	F	911	THR
3	F	926	SER
3	F	960	GLU
3	F	975	ILE
3	F	1487	MET
3	F	1621	ILE
4	G	35	ASP
4	G	36	VAL
4	G	64	TYR
4	G	65	VAL
4	G	66	TYR
4	G	68	GLN
4	G	70	VAL
4	G	72	ILE
4	G	73	THR

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Mol	Chain	Res	Type
4	G	78	PHE
4	G	80	ILE
4	G	81	ARG
4	G	85	ASN
4	G	88	GLN
4	G	104	LYS
4	H	35	ASP
4	H	36	VAL
4	H	64	TYR
4	H	65	VAL
4	H	66	TYR
4	H	68	GLN
4	H	70	VAL
4	H	72	ILE
4	H	73	THR
4	H	78	PHE
4	H	80	ILE
4	H	81	ARG
4	H	85	ASN
4	H	88	GLN
4	H	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	686	HIS
1	A	846	GLN
1	A	1045	ASN
1	A	1101	GLN
1	A	1165	GLN
1	A	1266	GLN
1	A	1330	ASN
1	A	1355	GLN
1	A	1553	HIS
1	A	1604	GLN
1	A	1627	GLN
1	A	1722	GLN
1	A	1808	ASN
1	A	1886	GLN
1	A	1959	GLN
1	A	2028	HIS
1	A	2099	GLN

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Mol	Chain	Res	Type
1	A	2154	GLN
1	A	2211	ASN
1	A	2515	HIS
1	B	999	ASN
1	B	1084	HIS
1	B	1165	GLN
1	B	1378	ASN
1	B	1525	GLN
1	B	1695	GLN
1	B	1703	ASN
1	B	1727	GLN
1	B	1729	GLN
1	B	1797	ASN
1	B	1901	GLN
1	B	1959	GLN
1	B	1997	ASN
1	B	2028	HIS
1	B	2072	GLN
1	B	2093	ASN
2	C	161	HIS
2	D	161	HIS
3	E	62	ASN
3	E	94	ASN
3	E	137	GLN
3	E	214	ASN
3	E	224	ASN
3	E	264	HIS
3	E	379	HIS
3	E	480	HIS
3	E	499	GLN
3	E	547	ASN
3	E	607	GLN
3	E	783	ASN
3	E	988	HIS
3	E	1674	GLN
3	F	62	ASN
3	F	94	ASN
3	F	137	GLN
3	F	214	ASN
3	F	224	ASN
3	F	264	HIS
3	F	379	HIS

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Mol	Chain	Res	Type
3	F	480	HIS
3	F	499	GLN
3	F	547	ASN
3	F	607	GLN
3	F	783	ASN
3	F	988	HIS
3	F	1674	GLN
4	G	34	HIS
4	G	85	ASN
4	H	34	HIS
4	H	85	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	G	1

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Mol	Chain	Number of breaks
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	85:ASN	C	86:THR	N	1.20
1	H	85:ASN	C	86:THR	N	1.20

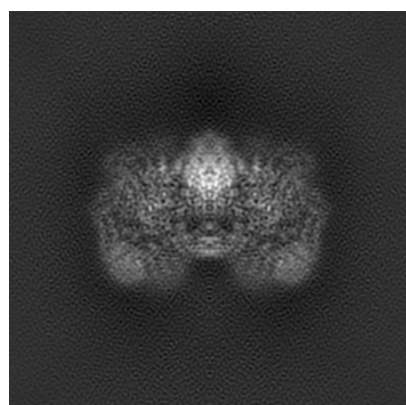
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26213. These allow visual inspection of the internal detail of the map and identification of artifacts.

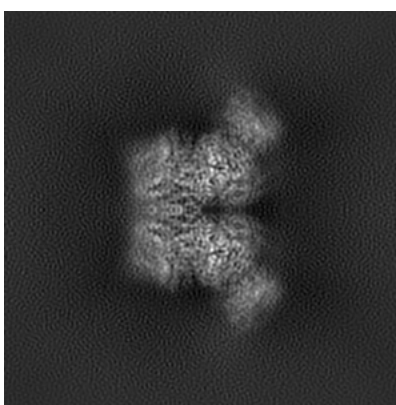
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

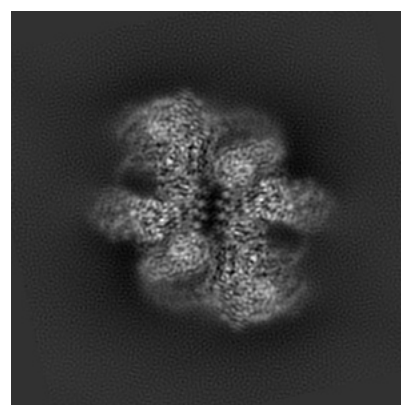
6.1.1 Primary map



X



Y

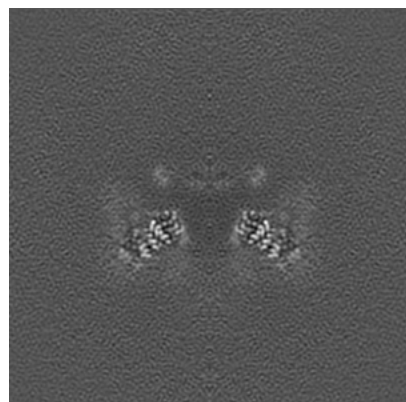


Z

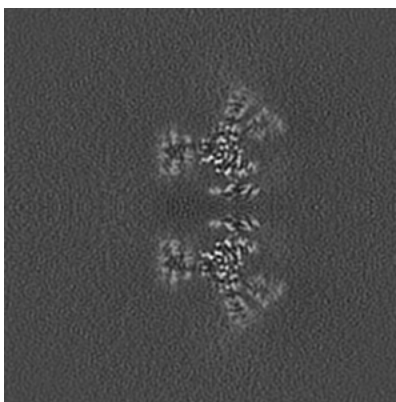
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

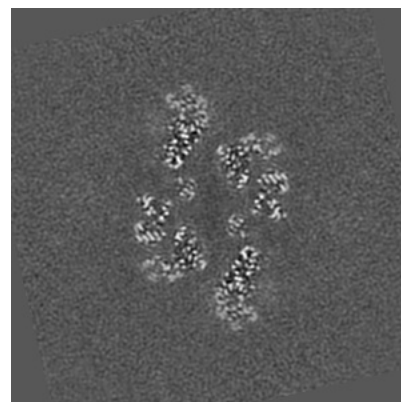
6.2.1 Primary map



X Index: 162



Y Index: 162

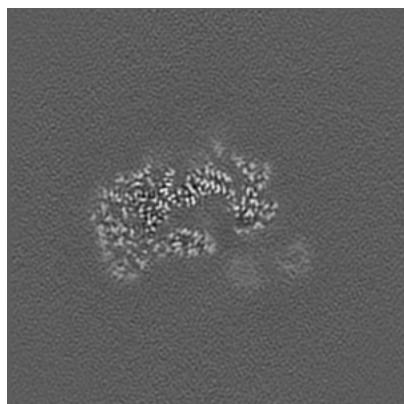


Z Index: 162

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

6.3 Largest variance slices [i](#)

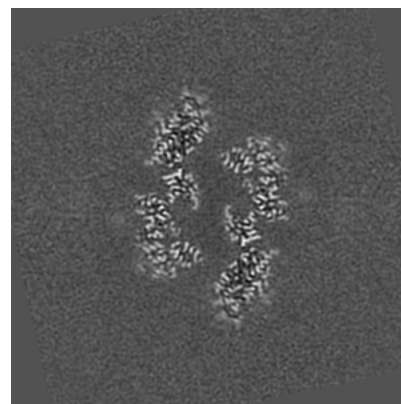
6.3.1 Primary map



X Index: 190



Y Index: 157

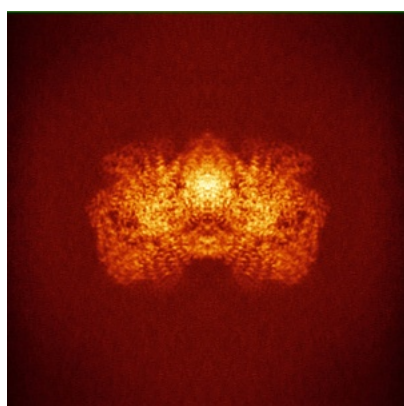


Z Index: 167

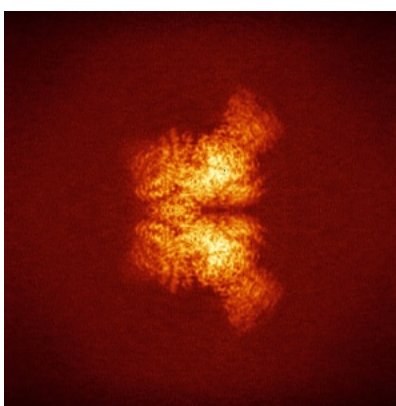
The images above show the largest variance slices of the map in three orthogonal directions.

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

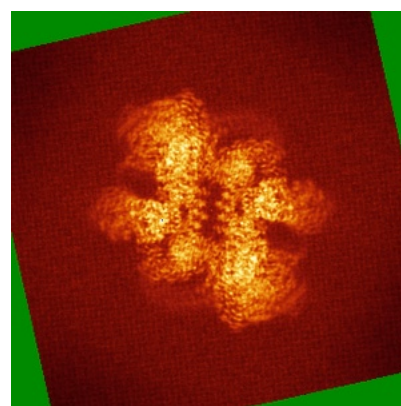
6.4.1 Primary map



X



Y

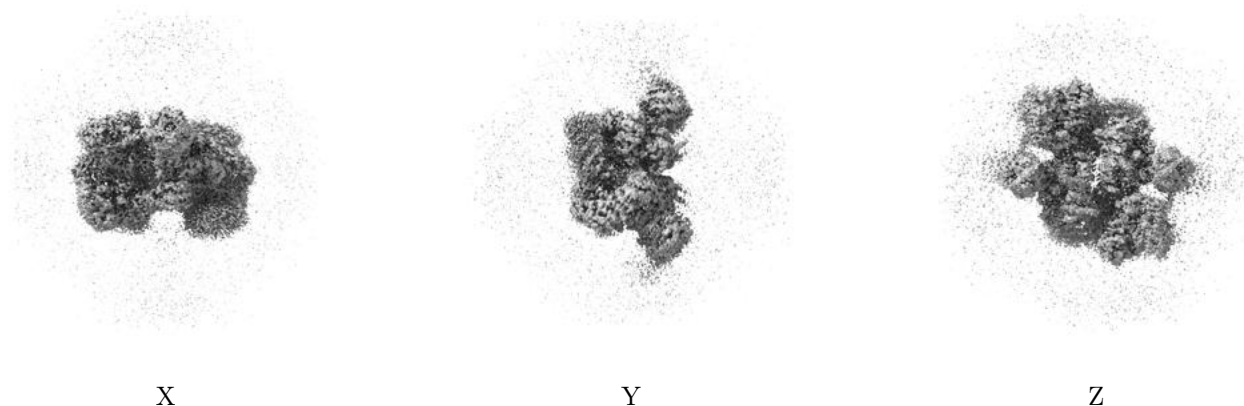


Z

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 2.64. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

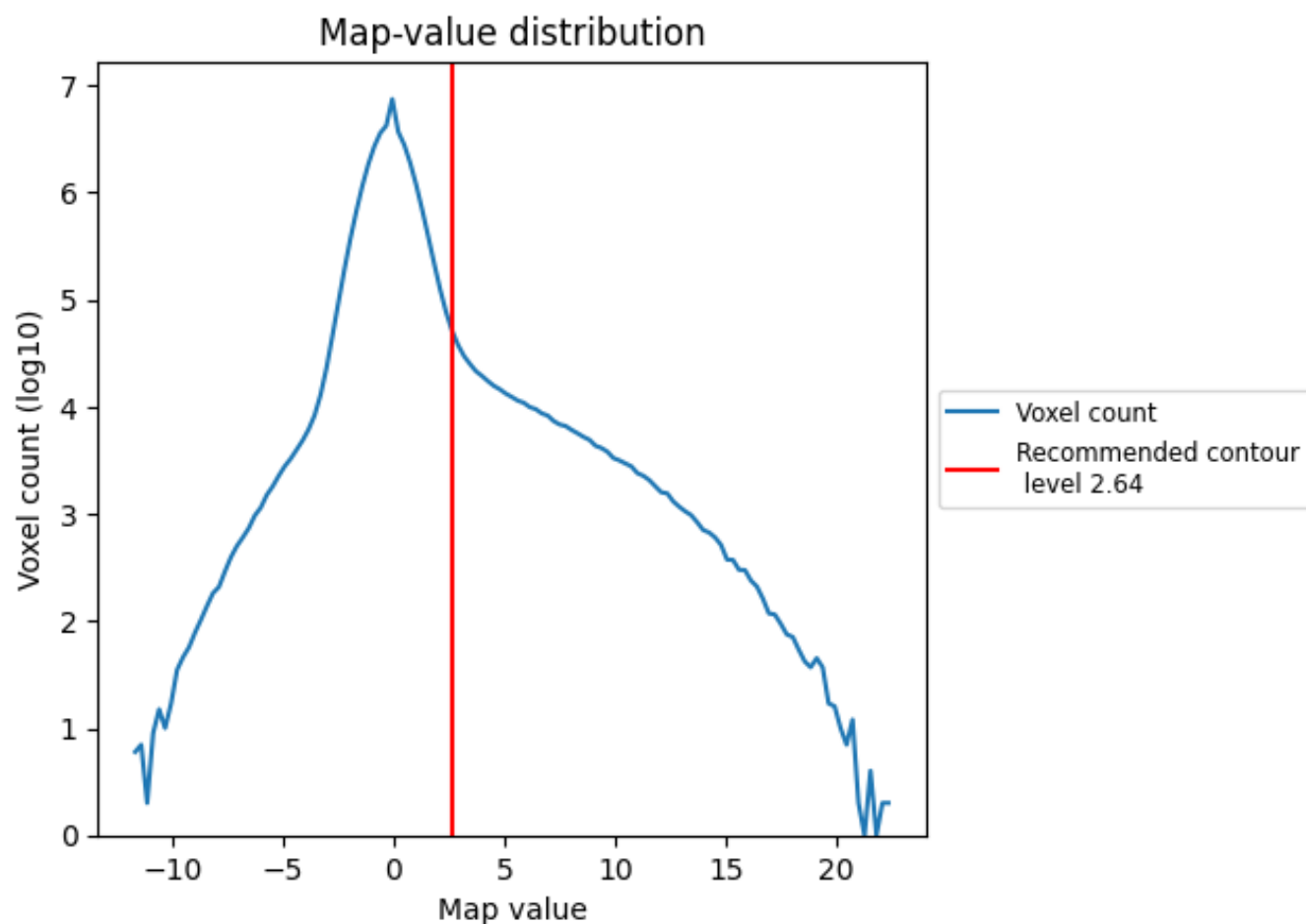
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

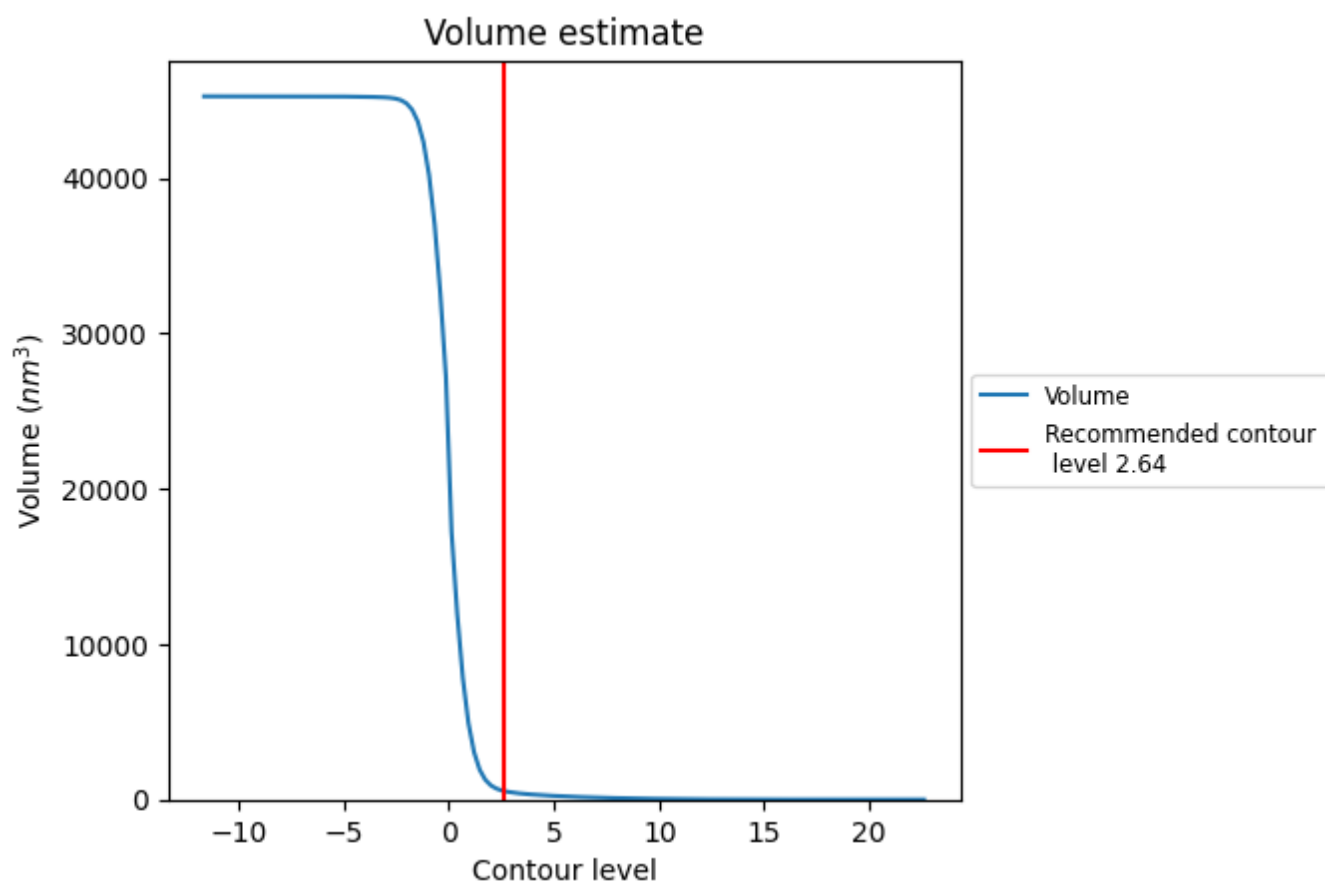
This section contains the results of statistical analysis of the map.

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.

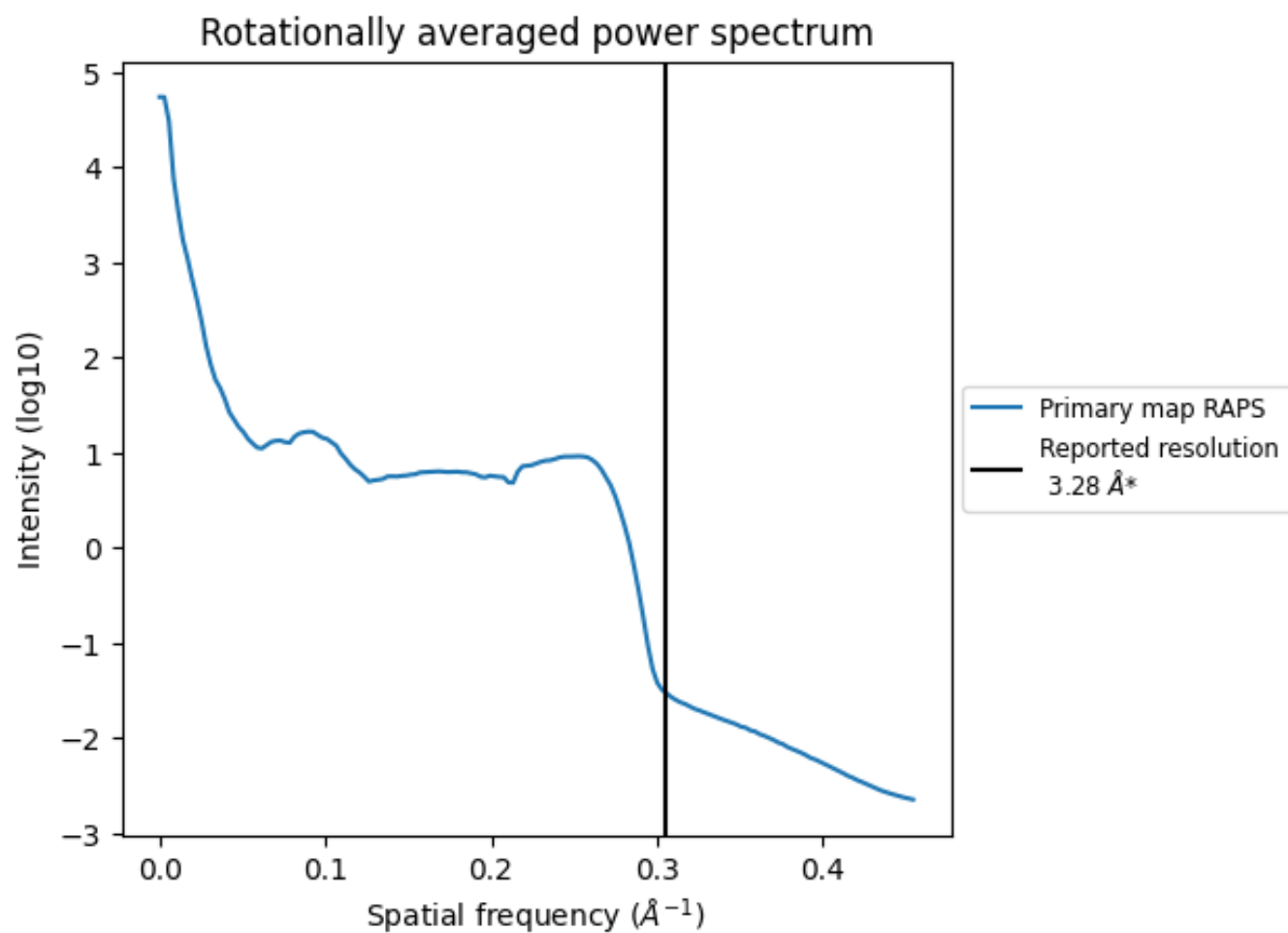
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 548 nm³; this corresponds to an approximate mass of 495 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 0.305 Å⁻¹

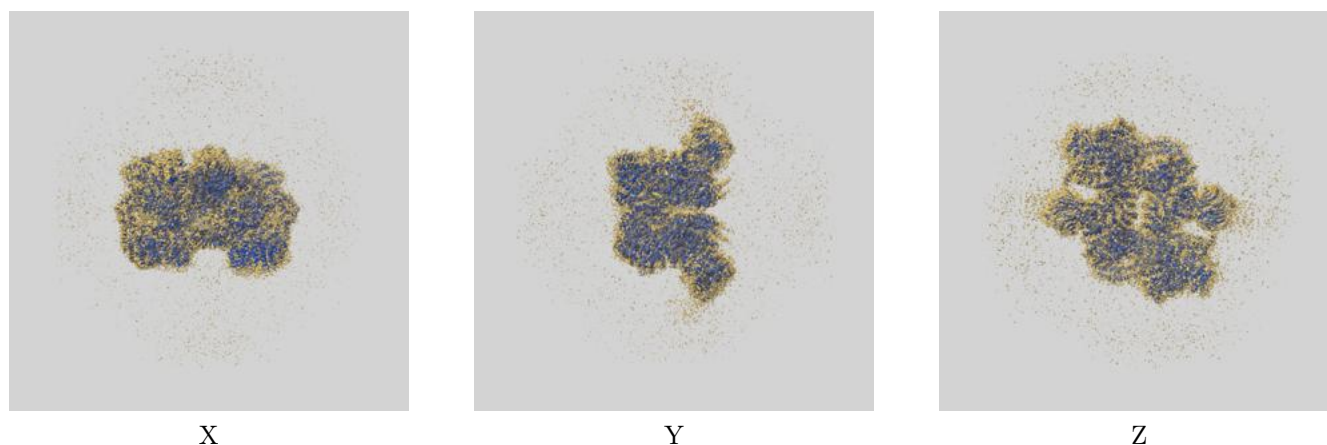
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

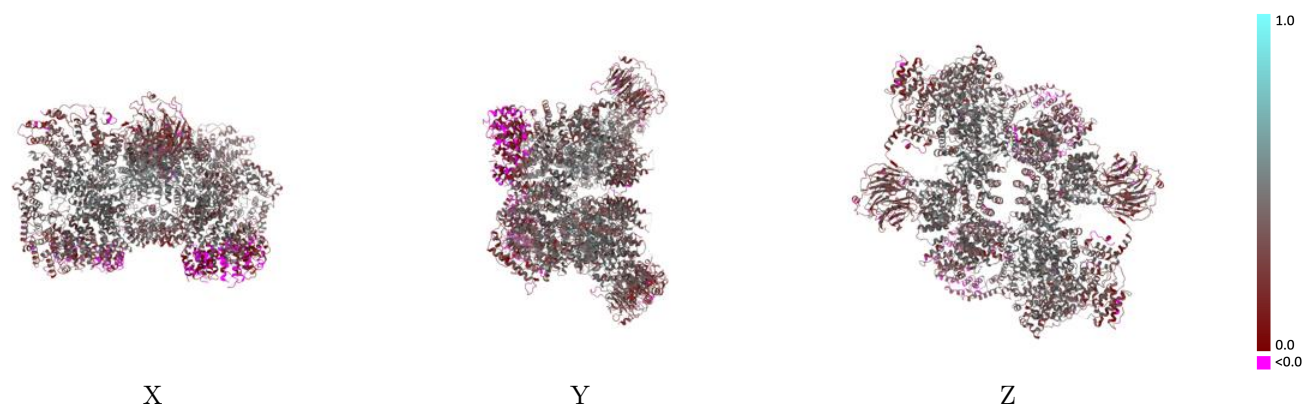
This section contains information regarding the fit between EMDB map EMD-26213 and PDB model 7TZO. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



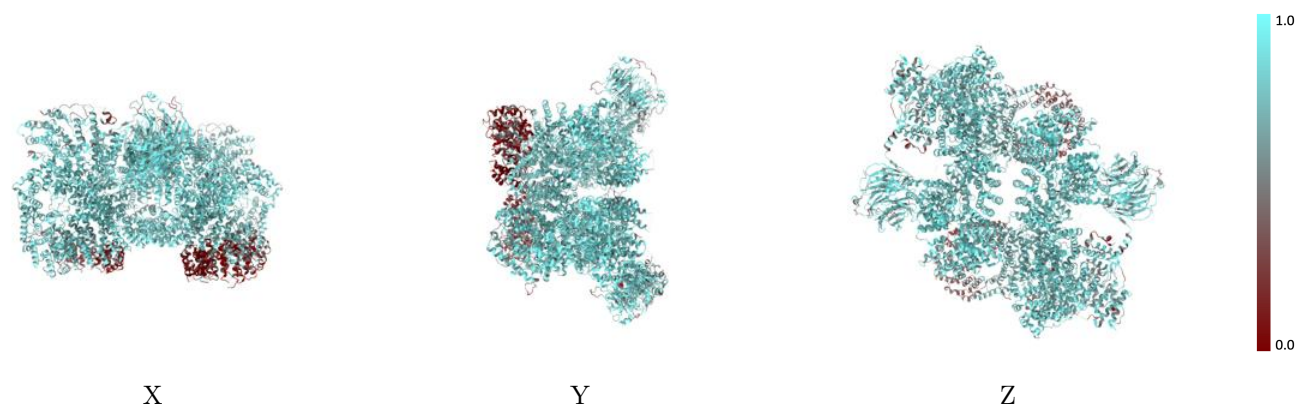
The images above show the 3D surface view of the map at the recommended contour level 2.64 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



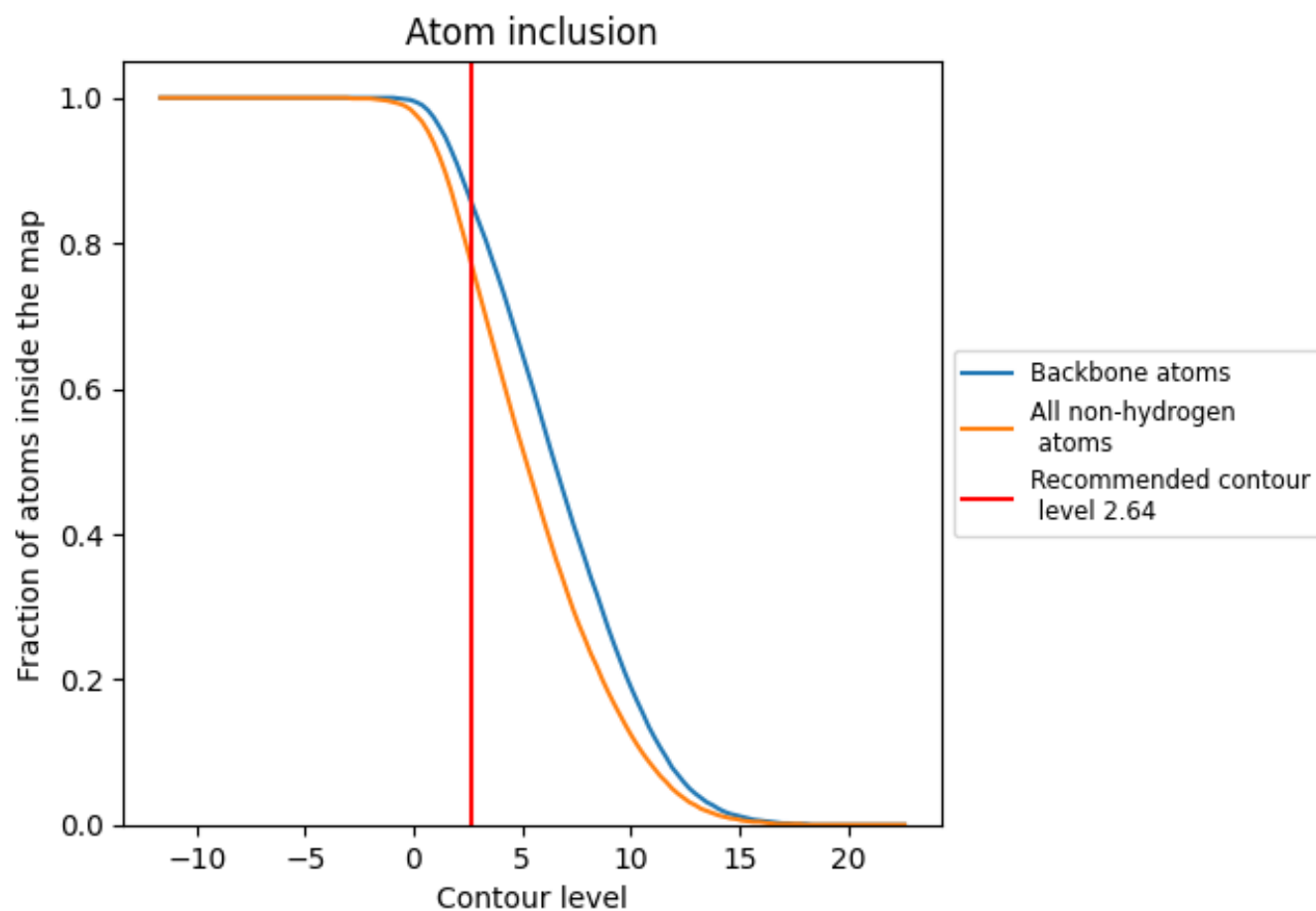
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.64).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (2.64) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.3530
A	0.7620	0.3570
B	0.7660	0.3630
C	0.7690	0.2750
D	0.7720	0.2860
E	0.8010	0.3650
F	0.7980	0.3600
G	0.7110	0.3150
H	0.7100	0.3180

1.0

0.0

<0.0