



## Full wwPDB EM Validation Report ⓘ

Oct 24, 2022 – 06:18 PM JST

PDB ID : 7W6T  
EMDB ID : EMD-32335  
Title : CryoEM structure of human KChIP1-Kv4.3-DPP6 complex  
Authors : Ma, D.M.; Guo, J.T.  
Deposited on : 2021-12-02  
Resolution : 3.85 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](mailto: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>.

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

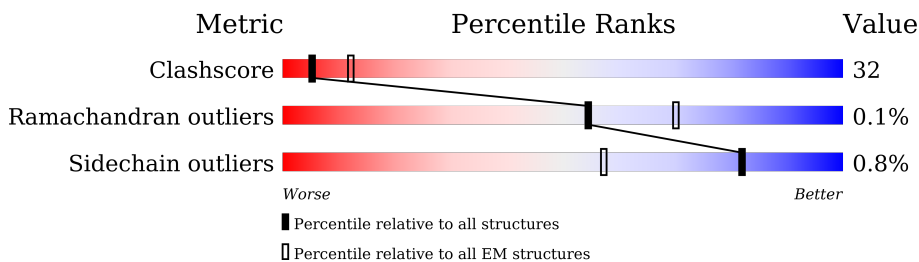
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.85 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	228	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 19%, orange 40%, yellow 38%, green 21%, grey 0%);"></span> 19% 40% 38% 21%
1	C	228	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 29%, yellow 49%, green 21%, grey 0%);"></span> 5% 29% 49% 21%
1	E	228	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 17%, orange 40%, yellow 39%, green 21%, grey 0%);"></span> 17% 40% 39% 21%
1	G	228	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 10%, orange 38%, yellow 40%, green 21%, grey 0%);"></span> 10% 38% 40% 21%
2	B	636	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, green 34%, yellow 34%, grey 32%);"></span> 34% 34% 32%
2	D	636	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, green 31%, yellow 37%, grey 32%);"></span> 31% 37% 32%
2	F	636	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, green 36%, yellow 32%, grey 32%);"></span> 36% 32% 32%
2	H	636	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, green 35%, yellow 32%, grey 32%);"></span> 35% 32% 32%

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Mol	Chain	Length	Quality of chain
3	I	873	
3	J	873	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 31768 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 Kv channel-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	179	1474	942	240	284	8	0	0
1	C	179	1474	942	240	284	8	0	0
1	E	179	1474	942	240	284	8	0	0
1	G	179	1474	942	240	284	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9NZI2
C	0	SER	-	expression tag	UNP Q9NZI2
E	0	SER	-	expression tag	UNP Q9NZI2
G	0	SER	-	expression tag	UNP Q9NZI2

- Molecule 2 is a protein called Isoform 2 of Potassium voltage-gated channel subfamily D member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	430	3456	2245	579	607	25	0	0
2	D	430	3456	2245	579	607	25	0	0
2	F	430	3456	2245	579	607	25	0	0
2	H	430	3456	2245	579	607	25	0	0

- Molecule 3 is a protein called Dipeptidyl aminopeptidase-like protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	749	Total	C	N	O	S	0	0
			6024	3842	1025	1134	23		
3	J	749	Total	C	N	O	S	0	0
			6024	3842	1025	1134	23		

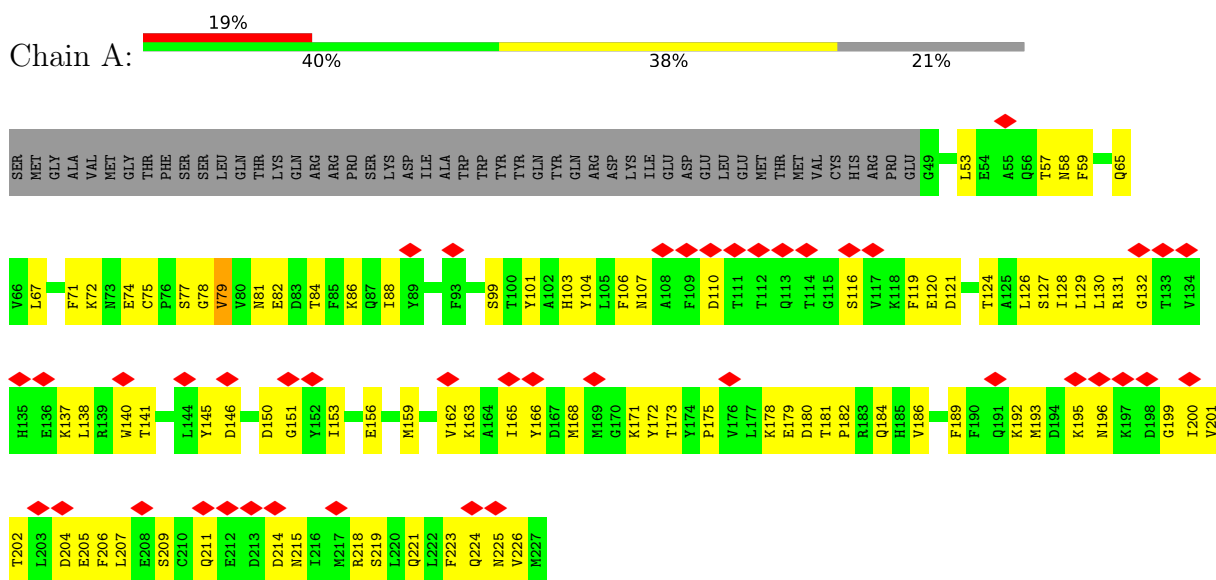
There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	805	LEU	-	expression tag	UNP E9PWX1
I	806	GLU	-	expression tag	UNP E9PWX1
I	807	GLY	-	expression tag	UNP E9PWX1
I	808	GLY	-	expression tag	UNP E9PWX1
I	809	SER	-	expression tag	UNP E9PWX1
I	810	SER	-	expression tag	UNP E9PWX1
I	811	ASP	-	expression tag	UNP E9PWX1
I	812	TYR	-	expression tag	UNP E9PWX1
I	813	LYS	-	expression tag	UNP E9PWX1
I	814	ASP	-	expression tag	UNP E9PWX1
I	815	ASP	-	expression tag	UNP E9PWX1
I	816	ASP	-	expression tag	UNP E9PWX1
I	817	ASP	-	expression tag	UNP E9PWX1
I	818	LYS	-	expression tag	UNP E9PWX1
J	805	LEU	-	expression tag	UNP E9PWX1
J	806	GLU	-	expression tag	UNP E9PWX1
J	807	GLY	-	expression tag	UNP E9PWX1
J	808	GLY	-	expression tag	UNP E9PWX1
J	809	SER	-	expression tag	UNP E9PWX1
J	810	SER	-	expression tag	UNP E9PWX1
J	811	ASP	-	expression tag	UNP E9PWX1
J	812	TYR	-	expression tag	UNP E9PWX1
J	813	LYS	-	expression tag	UNP E9PWX1
J	814	ASP	-	expression tag	UNP E9PWX1
J	815	ASP	-	expression tag	UNP E9PWX1
J	816	ASP	-	expression tag	UNP E9PWX1
J	817	ASP	-	expression tag	UNP E9PWX1
J	818	LYS	-	expression tag	UNP E9PWX1

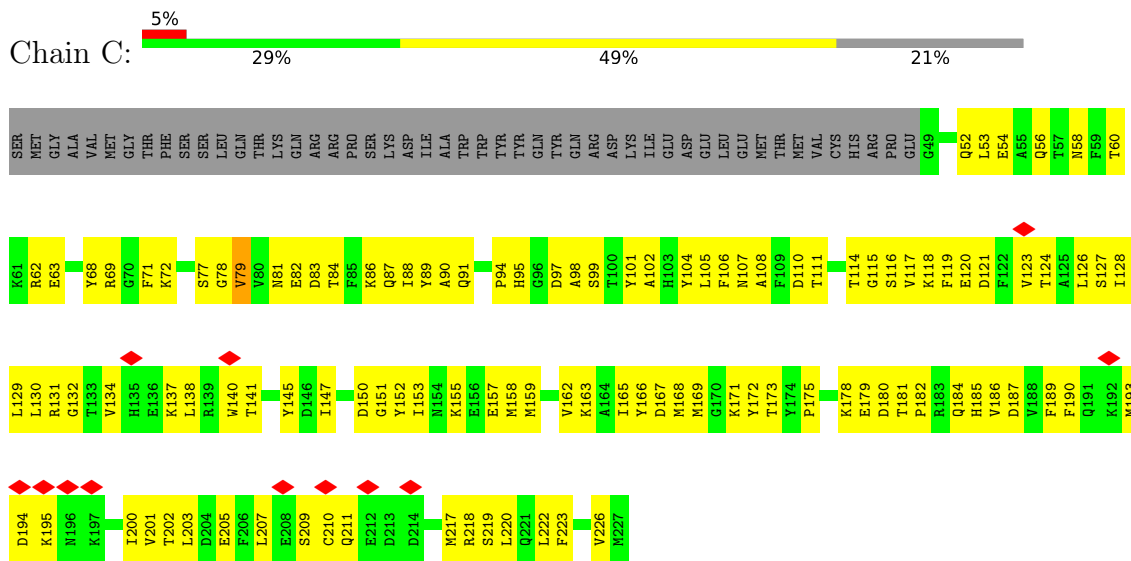
### 3 Residue-property plots

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

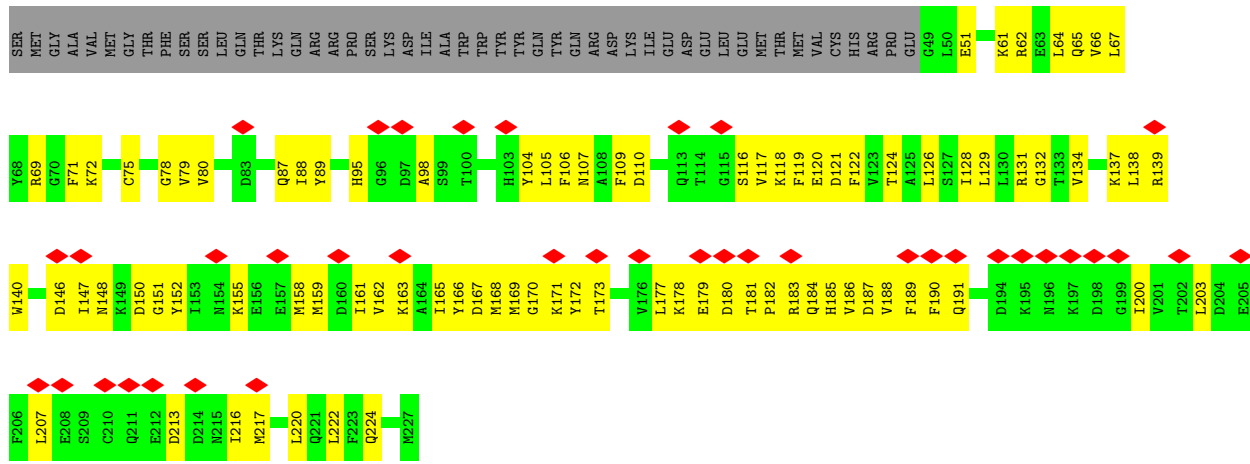
- Molecule 1: Kv channel-interacting protein 1



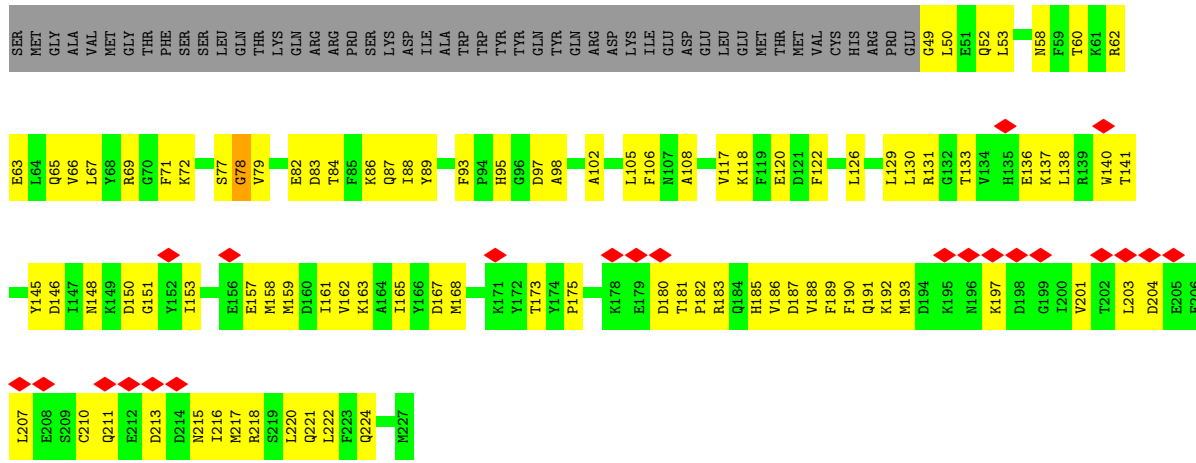
- Molecule 1: Kv channel-interacting protein 1



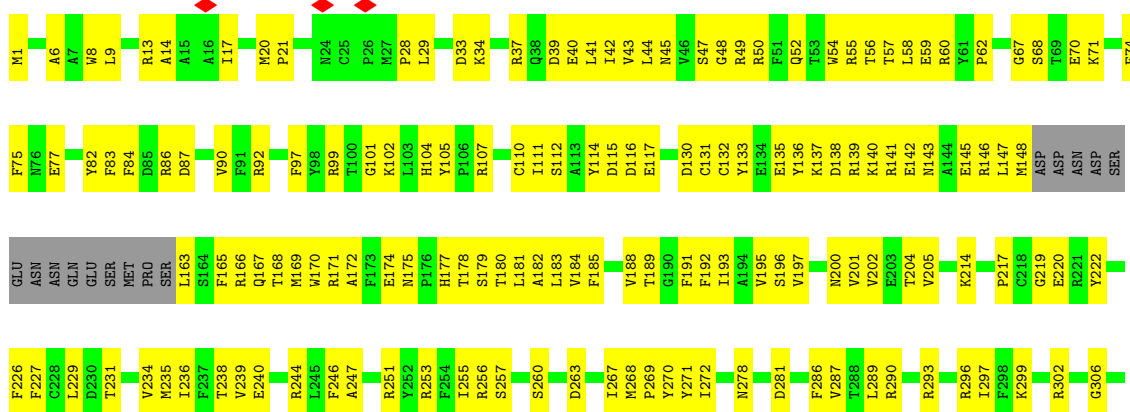
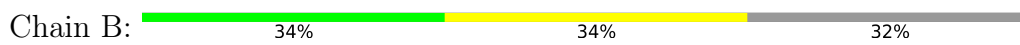
- Molecule 1: Kv channel-interacting protein 1



• Molecule 1: Kv channel-interacting protein 1



• Molecule 2: Isoform 2 of Potassium voltage-gated channel subfamily D member 3



I309	S407	S470	ARG	GLN
L310	R408	L471	ILE	ILE
G311	I409	I472	THR	THR
Y312	Y410	E473	THR	THR
T313	H411	S474	ALA	ALA
L314	H414	H475	LYS	LYS
K315	R415	H476	THR	THR
E320	K418	H477	HIS	THR
L324	R419	H478	ILE	ILE
M330	R420	L479	PRO	PRO
A331	A421	L480	PRO	PRO
I332	K424	H481	ASN	ASN
I333	R425	L482	PRO	PRO
I334	A426	L483	ALA	ALA
V338	LEU	E484	LEU	LEU
Y341	ARG	T487	ARG	ARG
S347	ILE	HIS	GLU	GLU
A348	ARG	GLU	ILE	ILE
I354	VAL	PHE	ARG	ARG
F358	VAL	ILE	GLN	GLN
I362	ALA	ASP	PRO	PRO
M365	LYS	GLU	LEU	LEU
L368	THR	LEU	GLN	GLN
G369	GLY	MET	THR	THR
Y370	THR	TYR	ASN	ASN
G371	HIS	GLU	ILE	ILE
D372	SER	GLU	GLN	GLN
M373	SER	GLY	ASN	ASN
K381	LEU	THR	THR	THR
I382	LEU	LEU	VAL	VAL
S385	LEU	ARG	LYS	LYS
I386	LEU	SER	SER	SER
C387	LEU	PRO	LEU	LEU
S388	LEU	PRO	ASN	ASN
V392	THR	THR	LYS	LYS
L397	THR	ASP	ALA	ALA
P398	PRO	ASP	ASP	ASP
V399	GLU	GLY	GLY	GLY
P400	GLU	PRO	ARG	ARG
V401	GLU	LEU	LEU	LEU
I402	HIS	THR	PRO	PRO
V403	THR	THR	ASN	ASN
N404	GLY	THR	CYS	CYS
N405	LYS	THR	LYS	LYS
F406	THR	SER	THR	THR

• Molecule 2: Isoform 2 of Potassium voltage-gated channel subfamily D member 3

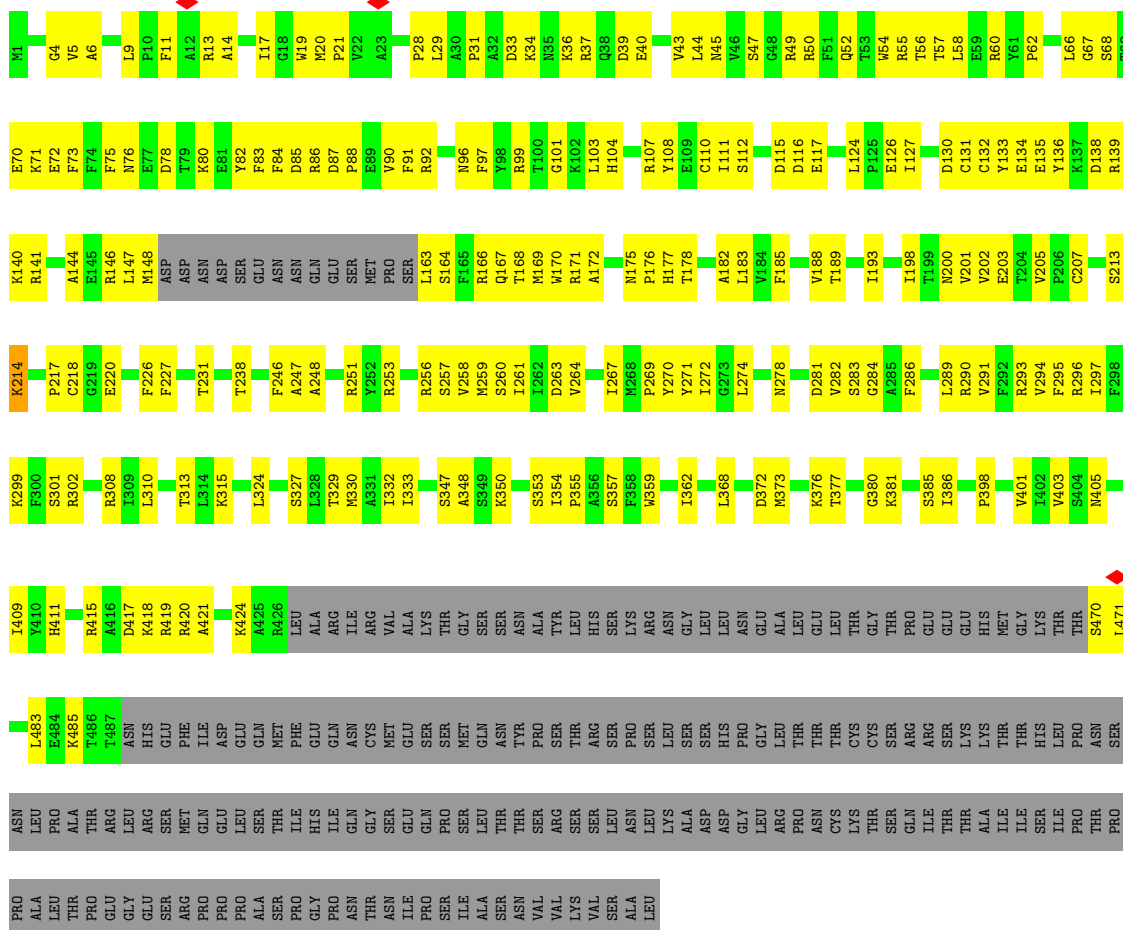


M1	K71	E145	V205	D281	P375	ASN	SER	SER	VAL
A2	E72	R146	P206	F286	K376	GLY	THR	ARG	VAL
A3	F75	L147	G212	Y286	T377	LEU	THR	SER	LYS
G4	M76	M148	S213	R290	G384	LEU	ARG	SER	VAL
A7	T79	ASP	K214	V291	S385	ASN	SER	LEU	ALA
F11	K80	ASN	L216	F292	I386	ALA	SER	LEU	LYS
A12	E81	ASP	E220	R293	C387	LEU	SER	LEU	ALA
R13	K82	SER	L216	V294	S388	LEU	SER	LEU	ALA
Y82	F83	ASP	E220	R295	L389	GLU	SER	LEU	ASP
R13	F83	ASN	L216	R296	S390	THR	HIS	THR	ASP
V19	F84	ASN	Y222	R296	G391	GLY	HIS	THR	ASP
M20	D85	GLN	F226	K299	V392	THR	GLY	THR	GLY
P21	R86	GLU	F227	F300	L393	PRO	LEU	THR	PRO
V22	D87	SER	F227	S301	V394	GLU	LEU	THR	PRO
A23	A23	MET	C228	R302	S397	THR	THR	THR	PRO
C25	F90	PRO	L223	H303	L397	GLU	THR	THR	ASN
F26	R91	SER	D230	S304	P398	GLU	THR	THR	CYS
M27	R92	LEU	T231	O305	V399	GLY	THR	THR	CYS
P28	C93	S164	V234	G306	P400	GLY	THR	THR	SER
L29	F94	F165	M235	L307	V401	LYS	THR	THR	ARG
A30	L95	R166	M236	R308	R408	ARG	THR	THR	ARG
F31	N96	Q167	I236	H309	L409	THR	THR	THR	ILE
A32	F97	T168	E240	T313	Y410	THR	THR	THR	THR
D33	N98	M169	E240	S319	H411	LYS	THR	THR	LYS
K34	R99	H170	E240	S319	Q412	THR	THR	THR	THR
G101	T100	R171	E240	G322	E473	THR	THR	THR	THR
N35	G101	A172	L242	G322	S474	HIS	THR	THR	HIS
K36	K102	F173	L243	F323	Q475	LEU	THR	THR	LEU
R37	L103	E174	R244	F323	H476	PRO	THR	THR	PRO
Q38	H104	M175	L245	F326	H477	ASN	THR	THR	ASN
D39	Y105	F176	F246	F326	K418	THR	THR	THR	THR
E40	P106	H177	A247	F326	R419	ASN	THR	THR	ASN
V43	R107	T178	A248	F326	A420	LEU	THR	THR	LEU
L44	E109	S179	Y252	F326	R421	PRO	THR	THR	PRO
N45	C110	T180	Y252	F326	Q422	ALA	THR	THR	ALA
V46	I111	L181	R256	F326	T486	THR	THR	THR	THR
S47	S112	A182	R256	F326	T487	ARG	THR	THR	ARG
Q48	A113	L183	S257	F326	A425	LEU	THR	THR	LEU
R49	Y114	F184	V258	F326	R426	GLU	THR	THR	GLU
R50	D115	F185	M259	F326	ALA	ARG	THR	THR	ARG
F51	D116	Y186	S260	F326	ILE	ILE	THR	THR	ILE
Q52	E117	Y187	L261	F326	ARG	ARG	THR	THR	ARG
T53	L118	T188	D262	F326	THR	THR	THR	THR	THR
W54	D130	G190	V265	F326	VAL	VAL	THR	THR	VAL
R55	C131	F191	A266	F326	ALA	ALA	THR	THR	ALA
T56	C132	F192	L267	F326	LYS	LYS	THR	THR	LYS
E59	Y133	A194	M268	F326	THR	THR	THR	THR	THR
R60	E134	V195	P269	F326	GLY	GLY	THR	THR	GLY
Y61	E135	S196	Y270	F326	SER	SER	THR	THR	SER
T64	D138	V197	V271	F326	THR	THR	THR	THR	THR
L65	R139	T198	L272	F326	ASN	ASN	THR	THR	ASN
L66	K140	T199	G273	F326	ALA	ALA	THR	THR	ALA
G67	R141	M200	L274	F326	THR	THR	THR	THR	THR
S68	R141	V201	T277	F326	LEU	LEU	THR	THR	LEU
M143	E142	E202	M278	F326	HIS	HIS	THR	THR	HIS
T204	M143	E203	T278	F326	LYS	LYS	THR	THR	LYS
A144	A144	T204		F326	ARG	ARG	THR	THR	ARG

• Molecule 2: Isoform 2 of Potassium voltage-gated channel subfamily D member 3

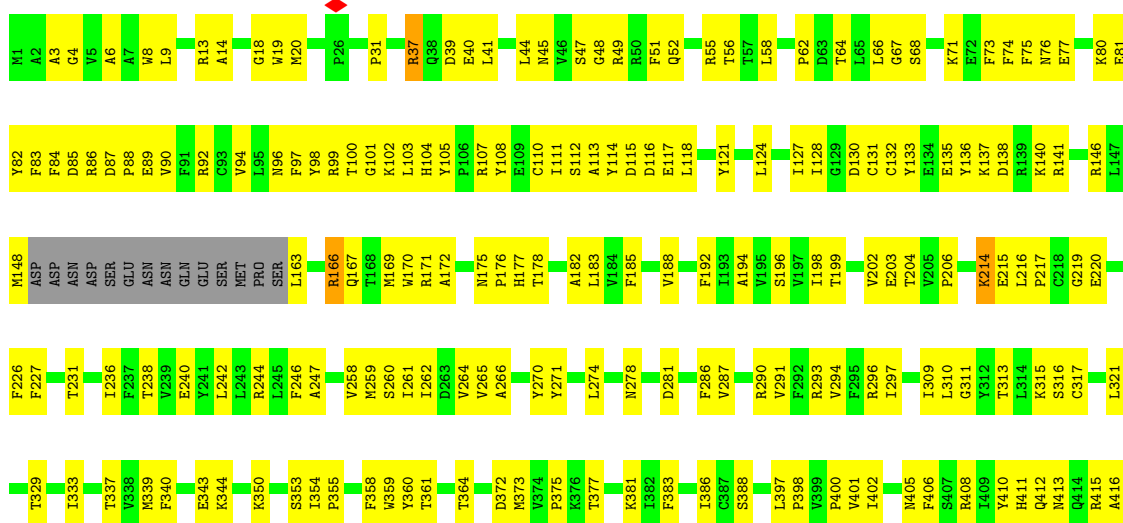


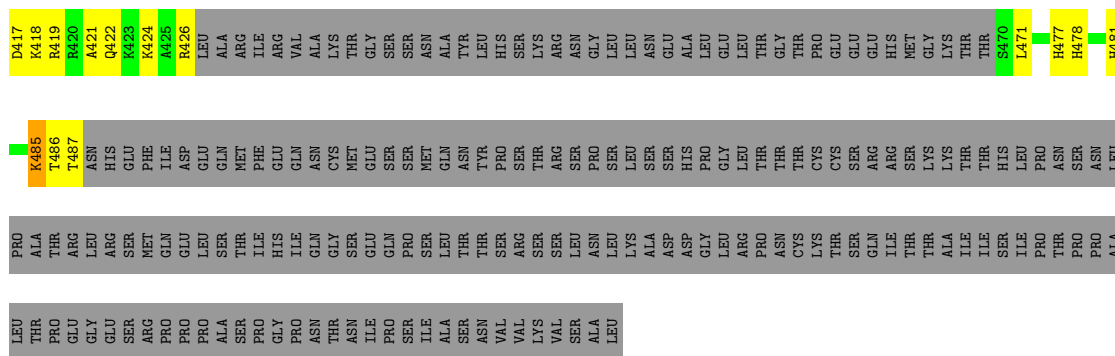
Chain F: 36% 32% 32%



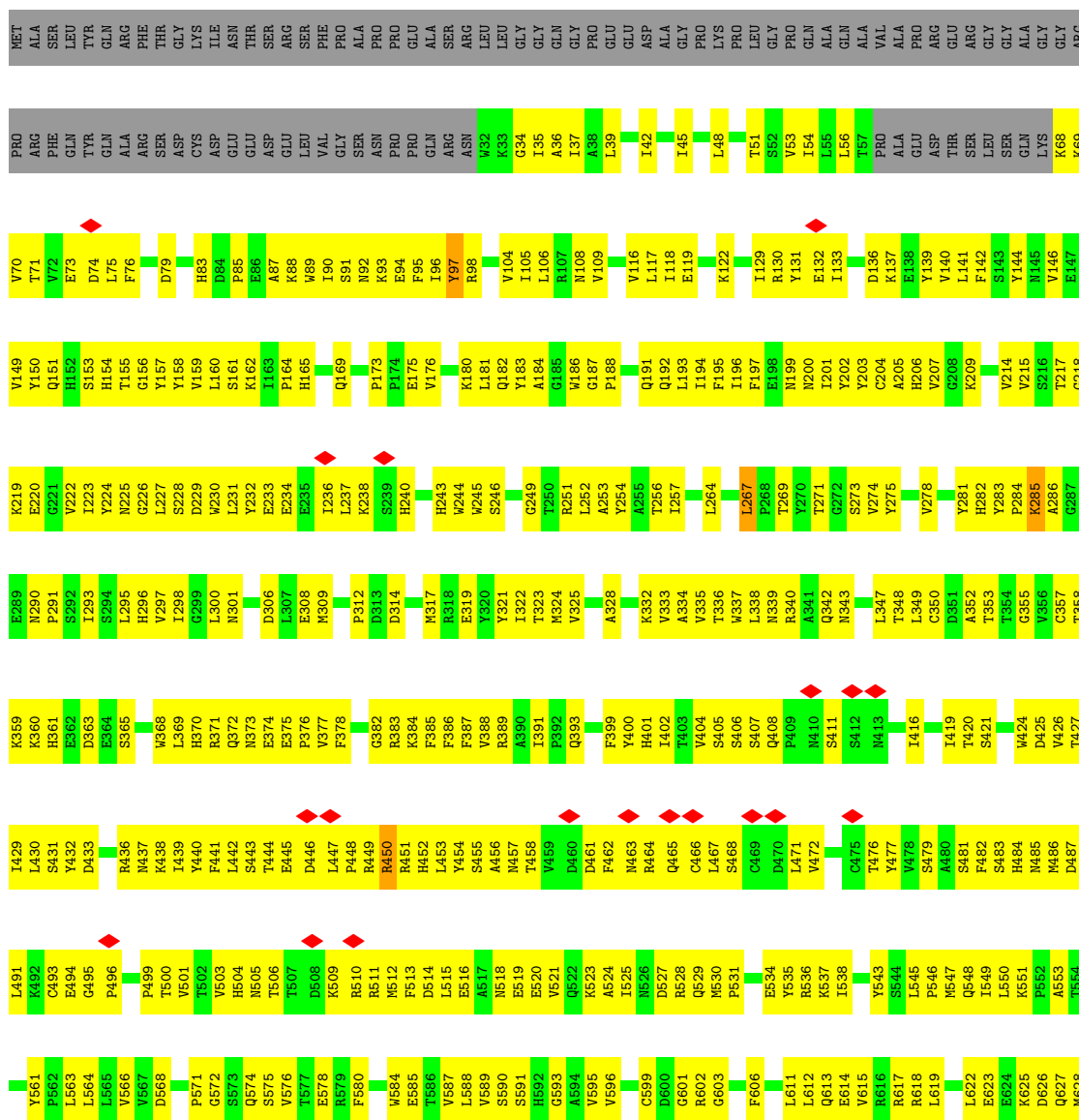
• Molecule 2: Isoform 2 of Potassium voltage-gated channel subfamily D member 3

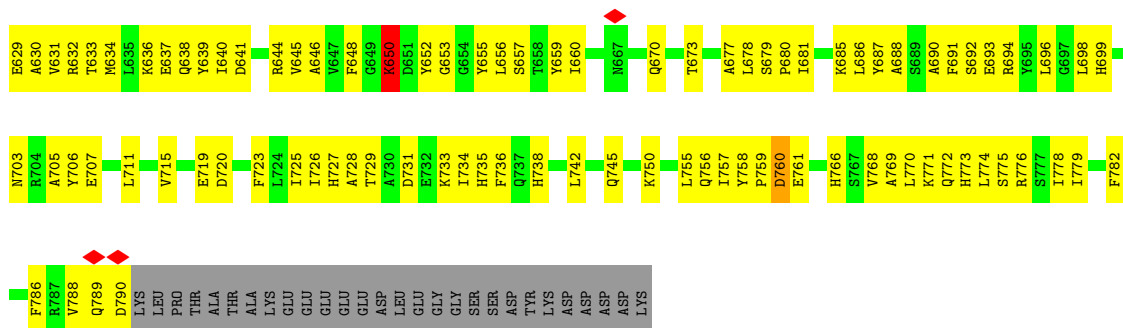
Chain H: 35% 32% 32%



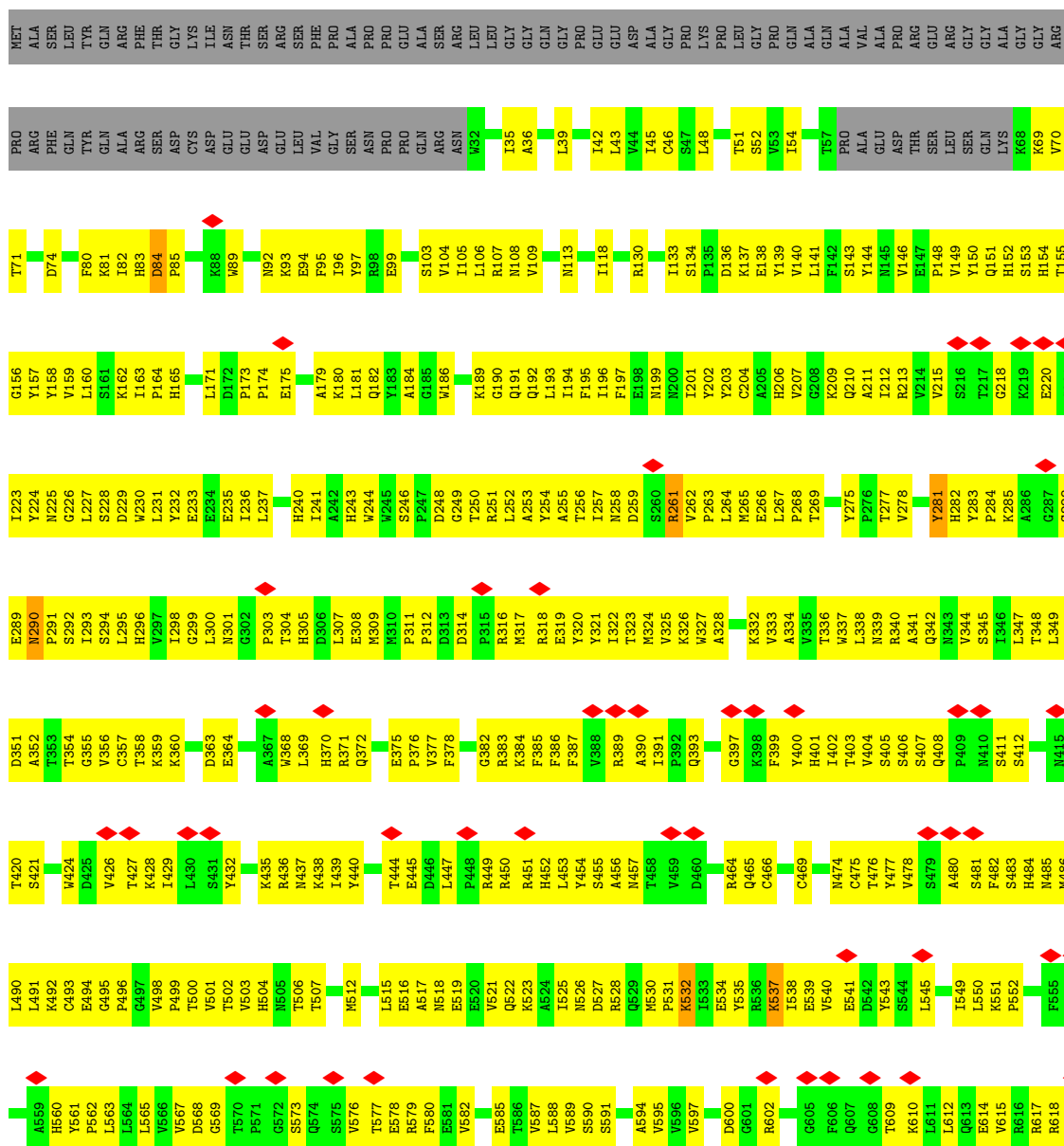


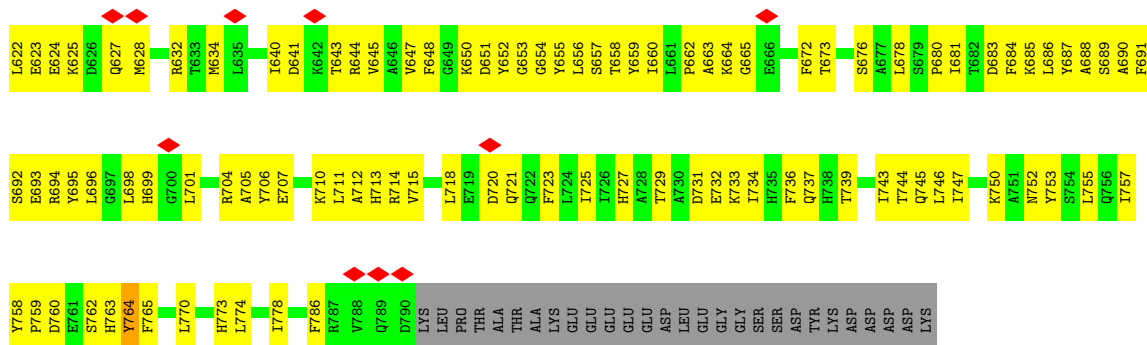
● Molecule 3: Dipeptidyl aminopeptidase-like protein 6





• Molecule 3: Dipeptidyl aminopeptidase-like protein 6





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	263176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	-1100	Depositor
Maximum defocus (nm)	-1300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.080	Depositor
Minimum map value	-0.457	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.0956	Depositor
Map size ( $\text{\AA}$ )	273.78003, 273.78003, 273.78003	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.014, 1.014, 1.014	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.26	0/1506	0.44	0/2032
1	C	0.28	0/1506	0.47	0/2032
1	E	0.28	0/1506	0.48	0/2032
1	G	0.27	0/1506	0.47	0/2032
2	B	0.39	0/3544	0.47	0/4800
2	D	0.37	0/3544	0.46	0/4800
2	F	0.37	0/3544	0.47	0/4800
2	H	0.38	0/3544	0.47	0/4800
3	I	0.35	0/6171	0.54	0/8370
3	J	0.35	0/6171	0.53	0/8370
All	All	0.35	0/32542	0.50	0/44068

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
3	I	0	4
3	J	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	78	GLY	Peptide
3	I	267	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	I	285	LYS	Peptide
3	I	650	LYS	Peptide
3	I	760	ASP	Peptide
3	J	281	TYR	Peptide
3	J	651	ASP	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1474	0	1415	72	0
1	C	1474	0	1415	104	0
1	E	1474	0	1415	73	0
1	G	1474	0	1415	75	0
2	B	3456	0	3462	200	0
2	D	3456	0	3462	226	0
2	F	3456	0	3462	182	0
2	H	3456	0	3462	192	0
3	I	6024	0	5922	528	0
3	J	6024	0	5922	516	0
All	All	31768	0	31352	2013	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (2013) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:VAL:O	1:C:189:PHE:HB3	1.60	1.01
1:A:186:VAL:O	1:A:189:PHE:HB3	1.61	0.99
3:J:265:MET:HB2	3:J:283:TYR:HB2	1.42	0.98
3:J:92:ASN:HA	3:J:484:HIS:HB2	1.50	0.94
3:J:264:LEU:HA	3:J:282:HIS:HA	1.51	0.92
1:E:105:LEU:O	1:E:109:PHE:HB2	1.70	0.90
3:J:589:VAL:HA	3:J:594:ALA:H	1.36	0.88
3:J:224:TYR:HB3	3:J:227:LEU:HB2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:274:VAL:HB	3:J:285:LYS:HE2	1.55	0.87
3:J:174:PRO:HB3	3:J:210:GLN:HE21	1.40	0.87
3:J:693:GLU:HG2	3:J:699:HIS:H	1.38	0.86
3:J:490:LEU:HA	3:J:503:VAL:HA	1.55	0.86
3:I:393:GLN:HG3	3:I:399:PHE:HB2	1.58	0.86
3:I:90:ILE:HG13	3:I:96:ILE:HG23	1.57	0.86
3:J:257:ILE:HG22	3:J:291:PRO:HB2	1.56	0.85
3:J:326:LYS:HB2	3:J:375:GLU:HB3	1.57	0.85
3:I:228:SER:HB2	3:I:240:HIS:HA	1.55	0.85
3:J:252:LEU:HD23	3:J:298:ILE:HD11	1.58	0.83
2:B:407:SER:O	2:B:411:HIS:ND1	2.12	0.83
3:I:653:GLY:O	3:I:657:SER:N	2.11	0.82
3:J:428:LYS:NZ	3:J:429:ILE:O	2.11	0.82
3:J:218:GLY:HA2	3:J:223:ILE:HG22	1.59	0.82
3:I:328:ALA:HB1	3:I:382:GLY:HA2	1.60	0.82
2:F:130:ASP:HA	2:F:133:TYR:HB2	1.63	0.81
3:J:253:ALA:HB1	3:J:295:LEU:HD11	1.62	0.81
2:B:405:ASN:HD22	2:B:408:ARG:HH21	1.25	0.81
3:I:485:ASN:ND2	3:I:487:ASP:OD2	2.14	0.80
3:I:371:ARG:NH2	3:I:374:GLU:OE1	2.14	0.80
2:B:130:ASP:HA	2:B:133:TYR:HB2	1.62	0.80
3:I:286:ALA:HB3	3:I:685:LYS:HA	1.64	0.80
2:F:170:TRP:HB2	2:F:247:ALA:HB1	1.63	0.80
3:I:231:LEU:HD21	3:I:690:ALA:HB2	1.63	0.80
3:I:232:TYR:HB3	3:I:237:LEU:HD12	1.63	0.80
2:B:110:CYS:HG	2:D:104:HIS:HD1	1.29	0.79
2:B:163:LEU:N	2:B:167:GLN:OE1	2.16	0.78
3:J:94:GLU:HA	3:J:108:ASN:HA	1.63	0.78
3:J:36:ALA:HA	3:J:39:LEU:HD12	1.66	0.78
2:H:97:PHE:O	2:H:101:GLY:N	2.14	0.78
2:B:112:SER:HB2	2:D:104:HIS:HE1	1.49	0.78
2:H:75:PHE:HA	2:H:82:TYR:HA	1.66	0.78
3:J:340:ARG:NH2	3:J:693:GLU:OE1	2.17	0.78
2:F:139:ARG:HE	2:H:107:ARG:HH21	1.31	0.77
3:J:490:LEU:HG	3:J:503:VAL:HG22	1.66	0.77
1:G:215:ASN:HA	1:G:218:ARG:HE	1.49	0.77
3:J:194:ILE:HG21	3:J:252:LEU:HD22	1.67	0.77
2:D:87:ASP:OD1	2:F:92:ARG:NH1	2.18	0.77
3:J:391:ILE:O	3:J:393:GLN:NE2	2.18	0.77
2:B:50:ARG:NH1	2:H:48:GLY:O	2.18	0.77
3:J:201:ILE:HG21	3:J:252:LEU:HD21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:HG22	1:C:175:PRO:HD2	1.66	0.77
3:I:141:LEU:HB2	3:I:186:TRP:HE1	1.49	0.77
3:I:371:ARG:NH1	3:I:426:VAL:O	2.18	0.77
2:H:166:ARG:NH2	2:H:246:PHE:O	2.17	0.76
3:I:199:ASN:ND2	3:I:223:ILE:O	2.19	0.76
3:I:365:SER:OG	3:I:613:GLN:NE2	2.17	0.76
3:I:537:LYS:HA	3:I:546:PRO:HA	1.68	0.76
3:J:94:GLU:OE2	3:J:137:LYS:NZ	2.19	0.76
3:I:761:GLU:OE2	3:I:766:HIS:N	2.19	0.76
3:J:466:CYS:SG	3:J:469:CYS:N	2.58	0.76
2:D:481:HIS:O	2:D:485:LYS:NZ	2.17	0.76
3:J:435:LYS:NZ	3:J:487:ASP:OD1	2.18	0.76
2:B:370:TYR:OH	2:D:364:THR:OG1	2.03	0.75
3:I:568:ASP:HA	3:I:650:LYS:HE3	1.68	0.75
2:B:110:CYS:SG	2:D:104:HIS:ND1	2.59	0.75
3:I:249:GLY:O	3:I:301:ASN:ND2	2.19	0.75
2:B:175:ASN:HB3	2:B:178:THR:HG23	1.66	0.75
3:I:338:LEU:HD21	3:I:342:GLN:HG2	1.68	0.75
3:J:707:GLU:HA	3:J:710:LYS:HG2	1.69	0.75
3:J:384:LYS:HA	3:J:406:SER:HA	1.66	0.75
3:I:149:VAL:H	3:I:154:HIS:HA	1.51	0.74
3:I:506:THR:O	3:I:509:LYS:NZ	2.17	0.74
3:J:436:ARG:HH22	3:J:487:ASP:HA	1.52	0.74
3:I:499:PRO:O	3:I:518:ASN:ND2	2.20	0.74
2:F:248:ALA:HB3	2:F:251:ARG:HG2	1.69	0.74
2:H:64:THR:OG1	2:H:98:TYR:OH	2.04	0.74
3:I:384:LYS:HA	3:I:406:SER:HA	1.68	0.74
3:I:447:LEU:HD12	3:I:448:PRO:HD2	1.67	0.74
2:F:146:ARG:NH1	2:H:131:CYS:O	2.20	0.74
3:I:231:LEU:HD23	3:I:236:ILE:HD11	1.69	0.74
2:D:92:ARG:NH2	2:D:93:CYS:SG	2.60	0.74
3:J:285:LYS:N	3:J:288:SER:OG	2.20	0.74
3:J:402:ILE:HG13	3:J:426:VAL:HG21	1.69	0.74
2:D:240:GLU:OE2	2:D:244:ARG:NH1	2.21	0.73
3:J:550:LEU:HD22	3:J:589:VAL:HG21	1.70	0.73
3:J:715:VAL:HG11	3:J:745:GLN:HB2	1.69	0.73
3:J:148:PRO:HA	3:J:154:HIS:HA	1.70	0.73
3:J:436:ARG:HB3	3:J:438:LYS:HG3	1.70	0.73
3:I:511:ARG:NH1	3:I:514:ASP:OD1	2.21	0.73
3:J:609:THR:HA	3:J:612:LEU:HB3	1.69	0.73
2:B:163:LEU:O	2:B:171:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:172:ALA:HB1	2:H:182:ALA:HB2	1.70	0.73
3:I:105:ILE:HG23	3:I:116:VAL:HA	1.70	0.73
3:I:678:LEU:HA	3:I:726:ILE:HB	1.69	0.73
3:J:489:PHE:O	3:J:504:HIS:N	2.21	0.73
2:H:146:ARG:O	2:H:419:ARG:NH1	2.21	0.73
3:I:184:ALA:HA	3:I:195:PHE:HA	1.70	0.73
3:I:678:LEU:HD12	3:I:726:ILE:HG21	1.69	0.73
3:I:448:PRO:O	3:I:451:ARG:NH1	2.21	0.73
3:J:341:ALA:HA	3:J:698:LEU:HD21	1.70	0.73
2:D:130:ASP:HA	2:D:133:TYR:HB2	1.69	0.73
3:I:575:SER:OG	3:I:599:CYS:N	2.21	0.73
3:J:449:ARG:NE	3:J:578:GLU:OE1	2.22	0.73
3:J:351:ASP:O	3:J:355:GLY:N	2.21	0.72
2:B:77:GLU:OE1	1:C:62:ARG:NH1	2.22	0.72
2:H:203:GLU:OE2	2:H:293:ARG:NH2	2.21	0.72
3:I:232:TYR:HA	3:I:236:ILE:HB	1.71	0.72
3:J:371:ARG:NH2	3:J:427:THR:O	2.21	0.72
3:I:561:TYR:N	3:I:639:TYR:O	2.23	0.72
2:B:105:TYR:N	2:B:132:CYS:SG	2.63	0.71
1:A:79:VAL:HB	1:A:116:SER:HB3	1.70	0.71
2:B:92:ARG:NH1	2:H:87:ASP:OD1	2.17	0.71
3:I:525:ILE:HG23	3:I:530:MET:HG3	1.72	0.71
2:D:75:PHE:HA	2:D:82:TYR:HA	1.72	0.71
3:J:401:HIS:NE2	3:J:424:TRP:O	2.24	0.71
2:B:177:HIS:HD2	2:B:183:LEU:HD21	1.56	0.71
2:D:72:GLU:HA	2:D:75:PHE:HB3	1.71	0.71
3:I:685:LYS:NZ	3:I:707:GLU:OE2	2.21	0.71
1:E:118:LYS:HG3	1:E:120:GLU:H	1.53	0.71
3:I:187:GLY:HA3	3:I:192:GLN:HG3	1.70	0.71
1:A:175:PRO:HG3	2:H:487:THR:HG22	1.73	0.71
2:H:105:TYR:N	2:H:132:CYS:SG	2.62	0.71
3:J:332:LYS:HD3	3:J:349:LEU:HD11	1.73	0.71
3:J:222:VAL:HA	3:J:282:HIS:HE1	1.56	0.71
2:D:166:ARG:NH1	2:D:166:ARG:O	2.22	0.71
3:I:73:GLU:HA	3:I:76:PHE:HD2	1.56	0.71
1:C:126:LEU:HD11	2:D:11:PHE:HD1	1.56	0.70
3:I:427:THR:HG21	3:I:451:ARG:HE	1.55	0.70
2:D:104:HIS:O	2:D:114:TYR:OH	2.09	0.70
3:I:653:GLY:HA2	3:I:656:LEU:HB2	1.72	0.70
2:F:172:ALA:HB1	2:F:182:ALA:HB2	1.72	0.70
3:I:729:THR:HA	3:I:736:PHE:HD1	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:170:TRP:HB2	2:H:247:ALA:HB1	1.74	0.70
3:I:449:ARG:NH1	3:I:535:TYR:HB3	2.07	0.70
3:I:455:SER:N	3:I:465:GLN:O	2.24	0.70
3:J:333:VAL:O	3:J:350:CYS:N	2.25	0.70
2:D:48:GLY:O	2:F:50:ARG:NH1	2.25	0.70
2:D:293:ARG:HG2	2:D:296:ARG:HH22	1.56	0.70
3:I:454:TYR:HA	3:I:466:CYS:HA	1.74	0.70
3:J:285:LYS:O	3:J:689:SER:OG	2.06	0.70
1:E:166:TYR:HA	1:E:169:MET:HG3	1.74	0.69
2:F:403:VAL:HG11	2:H:400:PRO:HG2	1.74	0.69
3:I:130:ARG:HH22	3:I:141:LEU:HB3	1.57	0.69
2:D:114:TYR:O	2:D:118:LEU:HG	1.93	0.69
3:J:265:MET:N	3:J:281:TYR:O	2.24	0.69
2:H:412:GLN:NE2	2:H:413:ASN:OD1	2.25	0.69
3:J:371:ARG:HH12	3:J:427:THR:HA	1.57	0.69
1:C:217:MET:HA	1:C:220:LEU:HD12	1.75	0.69
3:I:770:LEU:O	3:I:774:LEU:N	2.22	0.69
3:J:729:THR:HA	3:J:736:PHE:CD1	2.27	0.69
3:I:283:TYR:O	3:J:275:TYR:OH	2.11	0.69
2:B:42:ILE:HD12	2:B:58:LEU:HD12	1.74	0.69
2:D:163:LEU:O	2:D:171:ARG:NH1	2.26	0.69
3:I:83:HIS:O	3:I:518:ASN:ND2	2.25	0.69
3:J:290:ASN:ND2	3:J:319:GLU:HG2	2.07	0.69
3:I:564:LEU:HD13	3:I:588:LEU:HD21	1.74	0.69
1:A:65:GLN:HG2	2:H:73:PHE:HA	1.75	0.69
3:I:98:ARG:HG3	3:I:104:VAL:HG22	1.75	0.69
3:I:156:GLY:HA2	3:I:180:LYS:HG2	1.73	0.69
3:J:232:TYR:O	3:J:236:ILE:N	2.24	0.69
2:F:166:ARG:HH11	2:F:167:GLN:HG3	1.58	0.68
3:I:160:LEU:HD13	3:I:207:VAL:HG13	1.75	0.68
3:I:599:CYS:SG	3:I:627:GLN:NE2	2.66	0.68
2:H:135:GLU:OE1	2:H:135:GLU:N	2.22	0.68
2:B:382:ILE:O	2:B:385:SER:OG	2.11	0.68
3:J:390:ALA:HA	3:J:400:TYR:HA	1.75	0.68
3:J:650:LYS:HB2	3:J:678:LEU:HB3	1.75	0.68
1:E:222:LEU:HD22	2:F:31:PRO:HD3	1.74	0.68
3:I:406:SER:OG	3:I:408:GLN:NE2	2.26	0.68
3:J:293:ILE:HG21	3:J:322:ILE:H	1.58	0.68
3:J:319:GLU:OE2	3:J:340:ARG:NH1	2.26	0.68
2:B:39:ASP:OD2	2:B:55:ARG:N	2.27	0.68
3:I:350:CYS:HA	3:I:357:CYS:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:439:ILE:N	3:J:456:ALA:O	2.26	0.68
3:J:625:LYS:O	3:J:632:ARG:NH2	2.27	0.68
2:F:246:PHE:O	2:F:251:ARG:NH2	2.27	0.68
1:C:138:LEU:HD21	1:C:220:LEU:HD11	1.74	0.68
3:I:549:ILE:HG23	3:I:595:VAL:HG13	1.76	0.68
2:D:60:ARG:NH2	2:D:61:TYR:OH	2.27	0.67
2:H:317:CYS:SG	2:H:405:ASN:ND2	2.67	0.67
3:I:245:TRP:HA	3:I:252:LEU:HA	1.76	0.67
3:J:678:LEU:HD11	3:J:774:LEU:HD11	1.76	0.67
2:H:90:VAL:HG11	2:H:117:GLU:HG3	1.77	0.67
2:H:321:LEU:HD11	2:H:402:ILE:HD11	1.76	0.67
3:J:192:GLN:NE2	3:J:249:GLY:O	2.27	0.67
3:J:568:ASP:O	3:J:653:GLY:N	2.27	0.67
2:D:68:SER:O	2:D:71:LYS:NZ	2.27	0.67
2:D:343:GLU:OE1	2:D:377:THR:OG1	2.12	0.67
1:G:162:VAL:HA	1:G:165:ILE:HD12	1.75	0.67
2:H:175:ASN:HB3	2:H:178:THR:HG23	1.77	0.67
3:I:347:LEU:HD23	3:I:361:HIS:HB3	1.76	0.67
3:J:196:ILE:HG12	3:J:201:ILE:HG23	1.76	0.67
3:J:419:ILE:HG22	3:J:420:THR:HG23	1.77	0.67
1:C:147:ILE:N	1:C:157:GLU:OE2	2.28	0.67
2:H:130:ASP:HA	2:H:133:TYR:HB2	1.76	0.67
3:I:452:HIS:NE2	3:I:476:THR:O	2.28	0.67
3:J:199:ASN:HB3	3:J:224:TYR:HA	1.75	0.67
3:J:386:PHE:HA	3:J:404:VAL:HA	1.75	0.67
2:B:170:TRP:HB2	2:B:247:ALA:HB1	1.77	0.67
3:I:53:VAL:HA	3:I:56:LEU:HB2	1.76	0.67
3:I:383:ARG:O	3:I:407:SER:N	2.26	0.67
3:I:402:ILE:HB	3:I:420:THR:HG23	1.77	0.67
3:J:94:GLU:HB3	3:J:106:LEU:HD11	1.77	0.67
1:E:159:MET:O	1:E:163:LYS:HG2	1.94	0.67
3:I:181:LEU:HA	3:I:197:PHE:HD2	1.60	0.67
3:J:130:ARG:NH2	3:J:184:ALA:O	2.28	0.67
3:I:349:LEU:N	3:I:358:THR:O	2.28	0.66
3:I:769:ALA:O	3:I:772:GLN:NE2	2.28	0.66
2:B:196:SER:O	2:B:200:ASN:ND2	2.29	0.66
3:I:455:SER:O	3:I:465:GLN:N	2.27	0.66
2:F:68:SER:O	2:F:71:LYS:NZ	2.26	0.66
3:I:750:LYS:HG2	3:J:773:HIS:HE1	1.60	0.66
2:D:170:TRP:HB2	2:D:247:ALA:HB1	1.77	0.66
2:D:259:MET:SD	2:D:302:ARG:NH1	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:427:THR:HG21	3:I:451:ARG:NE	2.09	0.66
3:I:442:LEU:HD11	3:I:479:SER:HA	1.77	0.66
3:J:130:ARG:NH1	3:J:143:SER:OG	2.27	0.66
2:D:203:GLU:OE1	2:D:290:ARG:NH2	2.29	0.66
3:J:231:LEU:HD21	3:J:689:SER:HB2	1.78	0.66
2:H:55:ARG:HA	2:H:58:LEU:HD12	1.78	0.66
3:I:297:VAL:HG11	3:I:352:ALA:HB1	1.77	0.66
3:I:348:THR:HG22	3:I:359:LYS:HG3	1.77	0.66
3:I:472:VAL:HG22	3:I:511:ARG:HH21	1.61	0.66
3:J:684:PHE:HB3	3:J:692:SER:HA	1.77	0.66
3:I:70:VAL:HG22	3:I:528:ARG:HB3	1.77	0.66
2:D:44:LEU:HD13	2:D:82:TYR:HB2	1.77	0.66
1:E:79:VAL:HG22	1:E:118:LYS:HA	1.78	0.66
3:J:231:LEU:HB2	3:J:284:PRO:HG3	1.76	0.65
2:D:372:ASP:OD1	2:D:373:MET:N	2.29	0.65
3:I:275:TYR:OH	3:J:283:TYR:O	2.11	0.65
3:J:303:PRO:O	3:J:305:HIS:ND1	2.29	0.65
2:B:138:ASP:HB2	2:B:139:ARG:NH2	2.11	0.65
1:C:194:ASP:HA	1:C:205:GLU:HG2	1.77	0.65
2:D:226:PHE:HA	2:D:229:LEU:HD12	1.79	0.65
2:F:146:ARG:NH2	2:H:135:GLU:OE2	2.29	0.65
3:I:226:GLY:O	3:I:243:HIS:ND1	2.29	0.65
3:J:342:GLN:O	3:J:369:LEU:N	2.24	0.65
2:B:34:LYS:HE3	2:H:471:LEU:HD13	1.77	0.65
2:B:487:THR:HG22	1:C:175:PRO:HG3	1.79	0.65
1:E:162:VAL:HA	1:E:165:ILE:HD12	1.78	0.65
3:I:615:VAL:HG12	3:I:622:LEU:HB2	1.77	0.65
3:J:48:LEU:O	3:J:52:SER:N	2.30	0.65
3:J:263:PRO:O	3:J:283:TYR:N	2.22	0.65
3:J:532:LYS:HE3	3:J:551:LYS:HB2	1.77	0.65
3:J:587:VAL:O	3:J:591:SER:OG	2.10	0.65
2:B:145:GLU:O	2:B:419:ARG:NH2	2.30	0.65
2:B:146:ARG:NH1	2:D:134:GLU:OE1	2.30	0.65
3:I:371:ARG:HD2	3:I:606:PHE:HE1	1.61	0.65
3:J:727:HIS:O	3:J:757:ILE:HA	1.96	0.65
2:F:166:ARG:HH21	2:F:251:ARG:HH21	1.44	0.65
3:I:729:THR:OG1	3:I:760:ASP:N	2.29	0.65
3:J:146:VAL:HG12	3:J:148:PRO:HD3	1.79	0.65
2:H:214:LYS:NZ	2:H:220:GLU:OE2	2.26	0.65
3:I:254:TYR:OH	3:I:306:ASP:OD2	2.13	0.65
3:J:174:PRO:HD3	3:J:211:ALA:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:228:SER:HA	3:J:257:ILE:HD13	1.79	0.65
2:F:207:CYS:HB3	2:F:218:CYS:HB2	1.78	0.65
3:I:715:VAL:HG11	3:I:745:GLN:HB3	1.79	0.65
3:J:231:LEU:HD13	3:J:284:PRO:HG2	1.79	0.65
3:J:262:VAL:HG22	3:J:284:PRO:HB3	1.77	0.65
2:B:70:GLU:OE1	1:C:68:TYR:OH	2.15	0.64
2:D:19:TRP:O	2:D:23:ALA:N	2.30	0.64
2:D:353:SER:H	2:D:356:ALA:HB3	1.61	0.64
2:H:45:ASN:HB3	2:H:83:PHE:HA	1.77	0.64
2:H:421:ALA:HA	2:H:424:LYS:HD2	1.79	0.64
3:J:455:SER:N	3:J:465:GLN:O	2.24	0.64
2:B:193:ILE:HD12	2:B:299:LYS:HB2	1.79	0.64
3:I:687:TYR:HE1	3:I:691:PHE:HB3	1.62	0.64
3:J:350:CYS:HA	3:J:357:CYS:HA	1.79	0.64
1:G:159:MET:HA	1:G:162:VAL:HG12	1.77	0.64
3:J:349:LEU:O	3:J:358:THR:N	2.26	0.64
3:J:489:PHE:HE2	3:J:491:LEU:HD12	1.63	0.64
3:I:776:ARG:HH11	3:J:750:LYS:HZ3	1.45	0.64
3:J:263:PRO:HD2	3:J:284:PRO:HA	1.78	0.64
3:I:244:TRP:CE2	3:I:325:VAL:HB	2.33	0.64
3:I:518:ASN:HB3	3:I:521:VAL:HB	1.78	0.64
3:J:328:ALA:HB3	3:J:332:LYS:O	1.98	0.64
2:B:97:PHE:O	2:B:101:GLY:N	2.21	0.64
3:I:201:ILE:HD12	3:I:215:VAL:HB	1.80	0.64
2:F:107:ARG:O	2:F:139:ARG:NH1	2.31	0.64
3:I:419:ILE:HG12	3:I:462:PHE:CG	2.33	0.64
3:J:202:TYR:HA	3:J:213:ARG:HA	1.78	0.64
3:J:729:THR:HA	3:J:736:PHE:HD1	1.63	0.64
2:D:187:TYR:HB2	3:J:39:LEU:HD21	1.79	0.64
1:E:152:TYR:HB3	1:E:200:ILE:HD11	1.79	0.64
2:H:337:THR:HA	2:H:354:ILE:HD11	1.79	0.64
3:J:236:ILE:HG22	3:J:237:LEU:HD23	1.78	0.64
3:J:258:ASN:O	3:J:261:ARG:NH1	2.30	0.64
2:D:86:ARG:O	2:F:99:ARG:NH1	2.31	0.64
3:J:316:ARG:HD2	3:J:344:VAL:HG21	1.79	0.64
3:J:96:ILE:HA	3:J:106:LEU:HA	1.80	0.63
3:J:320:TYR:HE2	3:J:322:ILE:HG13	1.61	0.63
2:D:47:SER:HA	2:F:99:ARG:HH22	1.63	0.63
1:E:179:GLU:O	1:E:183:ARG:NH2	2.31	0.63
2:F:76:ASN:O	2:F:80:LYS:N	2.31	0.63
2:F:205:VAL:HG22	2:H:355:PRO:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:340:PHE:O	2:H:344:LYS:N	2.31	0.63
2:H:214:LYS:HZ2	2:H:216:LEU:HA	1.63	0.63
3:I:385:PHE:N	3:I:405:SER:O	2.30	0.63
3:J:712:ALA:HB2	3:J:745:GLN:HG3	1.80	0.63
1:A:72:LYS:HG3	1:A:77:SER:HB3	1.79	0.63
1:A:156:GLU:HA	1:A:159:MET:HE3	1.79	0.63
2:D:138:ASP:OD1	2:D:141:ARG:NH1	2.31	0.63
2:H:103:LEU:HD23	2:H:128:ILE:HG12	1.79	0.63
3:I:334:ALA:HB2	3:I:349:LEU:HD23	1.80	0.63
3:J:241:ILE:HD13	3:J:244:TRP:HE1	1.63	0.63
3:J:481:SER:OG	3:J:490:LEU:HB2	1.99	0.63
1:A:101:TYR:H	1:A:168:MET:HE3	1.63	0.63
1:C:153:ILE:HB	1:C:201:VAL:HG12	1.81	0.63
2:F:148:MET:O	2:F:419:ARG:NH1	2.23	0.63
3:I:236:ILE:O	3:I:373:ASN:ND2	2.30	0.63
3:I:756:GLN:NE2	3:I:758:TYR:OH	2.32	0.63
3:I:439:ILE:N	3:I:456:ALA:O	2.24	0.63
2:D:360:TYR:HB2	2:D:373:MET:HE3	1.79	0.63
2:D:4:GLY:HA3	2:D:56:THR:HB	1.81	0.63
2:D:72:GLU:O	1:E:65:GLN:NE2	2.32	0.63
2:H:62:PRO:HA	2:H:67:GLY:HA3	1.81	0.63
3:I:142:PHE:O	3:I:159:VAL:N	2.31	0.63
1:A:162:VAL:HA	1:A:165:ILE:HG22	1.80	0.62
2:B:135:GLU:O	2:B:139:ARG:NH2	2.32	0.62
1:C:159:MET:HA	1:C:162:VAL:HG22	1.79	0.62
2:D:257:SER:O	2:D:260:SER:OG	2.17	0.62
3:I:430:LEU:HD12	3:I:453:LEU:HD13	1.80	0.62
3:I:482:PHE:HB3	3:I:486:MET:HG3	1.81	0.62
3:J:71:THR:N	3:J:74:ASP:OD2	2.28	0.62
2:B:39:ASP:OD1	2:B:54:TRP:HB3	1.98	0.62
2:B:269:PRO:HA	2:B:272:ILE:HG22	1.79	0.62
2:F:301:SER:O	2:F:308:ARG:NH2	2.32	0.62
2:H:6:ALA:HA	2:H:9:LEU:HD13	1.81	0.62
2:D:64:THR:OG1	2:D:98:TYR:OH	2.14	0.62
3:J:51:THR:HA	3:J:54:ILE:HD12	1.81	0.62
2:B:478:HIS:CE1	1:C:223:PHE:HZ	2.17	0.62
1:C:166:TYR:CD2	1:C:182:PRO:HG3	2.35	0.62
1:E:105:LEU:HB2	1:E:140:TRP:HH2	1.64	0.62
3:I:106:LEU:HB2	3:I:117:LEU:HD11	1.81	0.62
3:J:348:THR:HG22	3:J:359:LYS:HA	1.81	0.62
3:J:482:PHE:HA	3:J:489:PHE:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ASP:OD2	2:B:90:VAL:N	2.31	0.62
2:H:416:ALA:HA	2:H:419:ARG:HH21	1.64	0.62
3:J:498:VAL:HG11	3:J:522:GLN:HB2	1.82	0.62
2:H:68:SER:O	2:H:71:LYS:NZ	2.30	0.62
3:I:156:GLY:N	3:I:181:LEU:O	2.23	0.62
3:I:200:ASN:HB2	3:I:202:TYR:CE2	2.35	0.62
3:I:237:LEU:HD21	3:I:322:ILE:HG22	1.80	0.62
3:I:254:TYR:CE1	3:I:296:HIS:HB2	2.35	0.62
2:D:485:LYS:HE2	2:F:28:PRO:HA	1.82	0.62
1:G:138:LEU:HA	1:G:141:THR:HG22	1.81	0.62
3:I:725:ILE:O	3:I:756:GLN:HB3	1.99	0.62
3:J:134:SER:OG	3:J:190:GLY:O	2.17	0.62
3:J:692:SER:HB2	3:J:706:TYR:HE1	1.64	0.62
2:H:206:PRO:HA	2:H:217:PRO:HA	1.79	0.62
3:I:274:VAL:HG11	3:J:686:LEU:HA	1.80	0.62
3:J:203:TYR:N	3:J:212:ILE:O	2.33	0.62
3:J:224:TYR:O	3:J:256:THR:HA	1.99	0.62
3:J:321:TYR:HB2	3:J:338:LEU:HB3	1.82	0.62
2:D:43:VAL:HG22	2:D:52:GLN:HG2	1.82	0.62
3:I:444:THR:HB	3:I:448:PRO:HA	1.80	0.62
1:C:79:VAL:HG12	1:C:116:SER:HB3	1.81	0.61
2:D:110:CYS:SG	2:F:104:HIS:ND1	2.66	0.61
2:F:421:ALA:HA	2:F:424:LYS:HD2	1.81	0.61
3:I:727:HIS:O	3:I:757:ILE:HA	1.99	0.61
1:G:217:MET:HA	1:G:220:LEU:HD12	1.80	0.61
1:G:222:LEU:HD22	2:H:31:PRO:HD3	1.82	0.61
2:H:39:ASP:HA	2:H:55:ARG:HH21	1.65	0.61
3:I:729:THR:OG1	3:I:760:ASP:OD1	2.14	0.61
3:J:436:ARG:NH1	3:J:486:MET:O	2.27	0.61
3:I:322:ILE:HG12	3:I:335:VAL:HG11	1.81	0.61
3:I:377:VAL:HG21	3:I:429:ILE:HG21	1.82	0.61
3:J:482:PHE:HA	3:J:489:PHE:HB3	1.83	0.61
2:B:166:ARG:HH21	2:B:251:ARG:HH21	1.47	0.61
2:D:47:SER:OG	2:F:99:ARG:NH1	2.28	0.61
2:B:365:MET:HG3	2:B:387:CYS:SG	2.40	0.61
1:G:186:VAL:O	1:G:189:PHE:HB3	2.00	0.61
3:J:232:TYR:HE2	3:J:290:ASN:HB3	1.64	0.61
3:J:246:SER:HA	3:J:327:TRP:HB3	1.83	0.61
1:G:78:GLY:O	1:G:79:VAL:HG23	2.00	0.61
2:H:45:ASN:ND2	2:H:81:GLU:OE1	2.31	0.61
2:H:163:LEU:O	2:H:171:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:348:THR:HA	3:I:359:LYS:HA	1.81	0.61
3:J:295:LEU:HB3	3:J:309:MET:HB2	1.81	0.61
3:I:293:ILE:HD13	3:I:322:ILE:HB	1.82	0.61
3:J:182:GLN:NE2	3:J:220:GLU:OE1	2.34	0.61
3:J:451:ARG:N	3:J:476:THR:O	2.33	0.61
3:J:522:GLN:NE2	3:J:522:GLN:O	2.32	0.61
2:F:72:GLU:O	1:G:65:GLN:NE2	2.33	0.61
3:J:474:ASN:HD21	3:J:496:PRO:HB2	1.66	0.61
3:I:141:LEU:HD13	3:I:193:LEU:HD22	1.81	0.61
3:J:266:GLU:HB2	3:J:278:VAL:HG23	1.83	0.61
3:J:450:ARG:HB3	3:J:476:THR:HB	1.82	0.61
2:D:84:PHE:HB3	2:D:86:ARG:HG2	1.82	0.60
3:I:285:LYS:N	3:I:288:SER:OG	2.33	0.60
3:J:203:TYR:O	3:J:212:ILE:N	2.33	0.60
2:F:138:ASP:OD1	2:F:141:ARG:NH1	2.34	0.60
3:I:408:GLN:OE1	3:I:411:SER:OG	2.18	0.60
3:J:83:HIS:N	3:J:518:ASN:OD1	2.34	0.60
2:B:99:ARG:NE	2:H:85:ASP:OD1	2.23	0.60
2:D:332:ILE:HD11	2:D:362:ILE:HD13	1.83	0.60
2:F:350:LYS:NZ	2:F:372:ASP:O	2.33	0.60
2:H:166:ARG:HH12	2:H:247:ALA:HA	1.66	0.60
3:I:538:ILE:HG21	3:I:630:ALA:HA	1.83	0.60
3:I:619:LEU:HG	3:I:696:LEU:HD21	1.83	0.60
2:B:86:ARG:HH12	2:D:99:ARG:HB3	1.67	0.60
1:C:81:ASN:ND2	1:C:83:ASP:OD2	2.34	0.60
2:D:146:ARG:NH1	2:F:132:CYS:HA	2.17	0.60
3:I:322:ILE:HG23	3:I:335:VAL:HG13	1.81	0.60
3:I:453:LEU:HD21	3:I:482:PHE:HE2	1.66	0.60
2:B:473:GLU:O	2:B:477:HIS:ND1	2.26	0.60
1:C:219:SER:HA	1:C:222:LEU:HG	1.83	0.60
1:E:78:GLY:O	1:E:79:VAL:HG23	2.01	0.60
2:F:87:ASP:OD1	2:H:92:ARG:NH1	2.35	0.60
1:C:138:LEU:HD13	1:C:210:CYS:SG	2.42	0.60
3:I:150:TYR:OH	3:I:224:TYR:OH	2.08	0.60
3:J:624:GLU:HB2	3:J:659:TYR:HD2	1.66	0.60
1:C:187:ASP:HA	1:C:190:PHE:CD2	2.37	0.60
2:F:43:VAL:HG13	2:F:52:GLN:HG2	1.84	0.60
3:J:70:VAL:HG23	3:J:587:VAL:HA	1.84	0.60
3:J:80:PHE:HA	3:J:521:VAL:HG13	1.84	0.60
3:J:130:ARG:HH12	3:J:184:ALA:HB3	1.66	0.60
3:J:175:GLU:OE1	3:J:210:GLN:NE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:288:SER:O	3:J:340:ARG:NH1	2.30	0.60
1:G:93:PHE:HD2	1:G:98:ALA:HB2	1.67	0.59
3:I:153:SER:HB2	3:I:240:HIS:CD2	2.37	0.59
3:J:500:THR:HA	3:J:517:ALA:HA	1.84	0.59
3:J:589:VAL:HG22	3:J:594:ALA:HB3	1.84	0.59
2:H:40:GLU:OE1	2:H:55:ARG:NE	2.34	0.59
3:J:189:LYS:HD2	3:J:248:ASP:HA	1.83	0.59
3:J:527:ASP:O	3:J:528:ARG:NH1	2.35	0.59
2:B:478:HIS:NE2	2:D:29:LEU:O	2.36	0.59
2:D:293:ARG:O	2:D:296:ARG:NH1	2.34	0.59
3:I:342:GLN:OE1	3:I:694:ARG:NE	2.35	0.59
3:I:650:LYS:O	3:I:652:TYR:N	2.32	0.59
1:G:137:LYS:NZ	1:G:224:GLN:OE1	2.36	0.59
3:J:156:GLY:HA2	3:J:180:LYS:NZ	2.17	0.59
3:J:729:THR:OG1	3:J:760:ASP:N	2.27	0.59
2:F:70:GLU:HB2	2:F:73:PHE:HE2	1.67	0.59
2:F:257:SER:O	2:F:260:SER:OG	2.20	0.59
2:H:163:LEU:HA	2:H:167:GLN:HB2	1.85	0.59
3:I:425:ASP:H	3:I:444:THR:HG1	1.47	0.59
3:I:71:THR:N	3:I:74:ASP:OD2	2.29	0.59
3:J:241:ILE:HG21	3:J:244:TRP:NE1	2.18	0.59
1:A:146:ASP:HA	1:A:153:ILE:HD11	1.84	0.59
2:H:110:CYS:SG	2:H:112:SER:OG	2.59	0.59
2:H:286:PHE:O	2:H:290:ARG:HG3	2.01	0.59
3:I:91:SER:HB2	3:I:94:GLU:HG2	1.83	0.59
3:I:129:ILE:HG13	3:I:146:VAL:HG12	1.85	0.59
3:I:568:ASP:OD1	3:I:650:LYS:NZ	2.29	0.59
3:J:491:LEU:O	3:J:502:THR:OG1	2.20	0.59
1:E:213:ASP:HB2	1:E:216:ILE:HG12	1.85	0.59
3:J:652:TYR:HD1	3:J:681:ILE:HB	1.66	0.59
2:D:304:SER:O	2:D:308:ARG:NH2	2.36	0.59
2:H:355:PRO:HA	2:H:358:PHE:CD2	2.37	0.59
3:I:246:SER:OG	3:I:251:ARG:N	2.27	0.59
3:I:295:LEU:O	3:I:309:MET:N	2.27	0.59
3:I:447:LEU:HG	3:I:449:ARG:H	1.67	0.59
3:J:318:ARG:NH1	3:J:319:GLU:OE1	2.36	0.59
2:B:99:ARG:NH1	2:H:86:ARG:O	2.35	0.59
3:I:309:MET:SD	3:I:355:GLY:HA2	2.42	0.59
3:J:97:TYR:N	3:J:105:ILE:O	2.33	0.59
1:C:145:TYR:OH	2:D:22:VAL:HG23	2.02	0.58
2:D:45:ASN:HB3	2:D:83:PHE:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:PHE:HB2	2:D:82:TYR:CD1	2.38	0.58
2:F:134:GLU:N	2:F:134:GLU:OE1	2.31	0.58
3:I:183:TYR:HB3	3:I:196:ILE:HB	1.85	0.58
3:I:246:SER:HB3	3:I:251:ARG:HB2	1.85	0.58
3:I:628:MET:O	3:I:632:ARG:N	2.33	0.58
2:D:177:HIS:CD2	2:D:183:LEU:HD21	2.37	0.58
1:G:130:LEU:O	1:G:224:GLN:HB3	2.02	0.58
2:H:259:MET:HG2	2:H:262:ILE:HD12	1.86	0.58
3:I:449:ARG:HH12	3:I:535:TYR:HB3	1.68	0.58
3:I:650:LYS:HA	3:I:678:LEU:HB3	1.84	0.58
3:I:687:TYR:HD1	3:I:692:SER:HB3	1.69	0.58
3:J:153:SER:OG	3:J:154:HIS:N	2.35	0.58
2:B:196:SER:OG	2:B:296:ARG:NH1	2.35	0.58
1:C:117:VAL:HG13	1:C:118:LYS:H	1.69	0.58
2:D:180:THR:HG23	3:J:35:ILE:HG23	1.85	0.58
2:D:365:MET:HG3	2:D:391:GLY:HA3	1.84	0.58
2:D:475:GLN:HB3	2:F:13:ARG:HH22	1.68	0.58
2:F:39:ASP:OD2	2:F:40:GLU:N	2.36	0.58
2:H:217:PRO:HG2	2:H:220:GLU:HG2	1.84	0.58
3:I:233:GLU:OE2	3:I:240:HIS:HB3	2.02	0.58
2:B:57:THR:OG1	2:H:85:ASP:OD2	2.18	0.58
1:C:189:PHE:O	1:C:193:MET:N	2.28	0.58
3:I:519:GLU:HG2	3:I:520:GLU:H	1.68	0.58
3:I:728:ALA:HA	3:I:758:TYR:H	1.67	0.58
2:B:107:ARG:HH22	2:H:110:CYS:HA	1.68	0.58
2:B:115:ASP:OD2	2:B:140:LYS:NZ	2.36	0.58
1:C:202:THR:HG22	1:C:203:LEU:HD23	1.86	0.58
2:F:92:ARG:HG2	2:F:96:ASN:HD21	1.68	0.58
3:I:312:PRO:HD3	3:I:337:TRP:CD2	2.38	0.58
3:I:387:PHE:HE2	3:I:389:ARG:HD3	1.68	0.58
3:J:244:TRP:O	3:J:327:TRP:HD1	1.87	0.58
1:E:117:VAL:HG13	1:E:118:LYS:H	1.67	0.58
2:F:177:HIS:HD2	2:F:183:LEU:HD11	1.69	0.58
3:I:342:GLN:NE2	3:I:690:ALA:HB1	2.19	0.58
3:I:432:TYR:HH	3:I:437:ASN:HA	1.67	0.58
3:I:455:SER:HB2	3:I:467:LEU:HD21	1.84	0.58
2:H:377:THR:O	2:H:381:LYS:HG3	2.04	0.58
3:I:130:ARG:HH12	3:I:132:GLU:HB2	1.69	0.58
3:J:107:ARG:HA	3:J:113:ASN:O	2.04	0.58
2:B:197:VAL:O	2:B:201:VAL:HG23	2.04	0.58
2:B:421:ALA:HA	2:B:424:LYS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:ASP:OD2	2:D:56:THR:OG1	2.18	0.58
2:D:421:ALA:HA	2:D:424:LYS:HD2	1.86	0.58
2:F:45:ASN:ND2	2:H:52:GLN:OE1	2.36	0.58
2:F:54:TRP:HB2	2:F:57:THR:HG23	1.84	0.58
1:G:105:LEU:HA	1:G:108:ALA:HB3	1.86	0.58
3:J:421:SER:O	3:J:464:ARG:NH1	2.37	0.58
2:B:138:ASP:OD1	2:B:141:ARG:NH1	2.37	0.58
3:I:243:HIS:HA	3:I:254:TYR:HA	1.86	0.58
3:J:228:SER:OG	3:J:233:GLU:HB2	2.02	0.58
1:A:159:MET:HA	1:A:162:VAL:HG22	1.85	0.58
1:C:78:GLY:O	1:C:79:VAL:HG23	2.04	0.58
2:D:177:HIS:HD2	2:D:183:LEU:HD21	1.69	0.58
1:G:173:THR:HG22	1:G:175:PRO:HD2	1.84	0.58
3:J:447:LEU:HD13	3:J:450:ARG:HD2	1.86	0.58
2:B:372:ASP:OD1	2:B:373:MET:N	2.32	0.57
1:C:72:LYS:HE3	1:C:77:SER:HB3	1.86	0.57
3:I:94:GLU:HB3	3:I:108:ASN:HD22	1.68	0.57
3:I:457:ASN:ND2	3:I:463:ASN:OD1	2.35	0.57
3:J:82:ILE:HD11	3:J:580:PHE:HE1	1.69	0.57
3:J:199:ASN:ND2	3:J:220:GLU:HA	2.18	0.57
3:J:620:GLY:N	3:J:623:GLU:OE1	2.32	0.57
2:B:135:GLU:OE1	2:B:135:GLU:N	2.30	0.57
1:C:163:LYS:NZ	1:C:179:GLU:O	2.36	0.57
1:G:131:ARG:NH1	1:G:224:GLN:O	2.37	0.57
3:I:648:PHE:HD2	3:I:782:PHE:HE2	1.52	0.57
2:B:86:ARG:NH1	2:D:99:ARG:HB3	2.19	0.57
2:B:485:LYS:HE2	2:D:19:TRP:HB3	1.84	0.57
3:I:94:GLU:OE2	3:I:137:LYS:NZ	2.37	0.57
3:I:203:TYR:HB2	3:I:300:LEU:HD22	1.87	0.57
2:D:93:CYS:HB3	2:D:103:LEU:HD11	1.86	0.57
3:I:450:ARG:C	3:I:451:ARG:HD2	2.25	0.57
2:B:472:ILE:O	2:B:476:HIS:N	2.36	0.57
1:G:213:ASP:O	1:G:216:ILE:HG12	2.05	0.57
2:H:278:ASN:HA	2:H:281:ASP:HB3	1.86	0.57
3:I:104:VAL:O	3:I:118:ILE:N	2.25	0.57
3:I:140:VAL:N	3:I:161:SER:O	2.35	0.57
3:I:232:TYR:HE2	3:I:291:PRO:HB2	1.70	0.57
2:D:76:ASN:HB3	2:D:79:THR:HG22	1.87	0.57
2:F:227:PHE:O	2:F:231:THR:HG23	2.05	0.57
3:I:693:GLU:HB3	3:I:698:LEU:HD23	1.86	0.57
3:J:230:TRP:CD1	3:J:281:TYR:HE2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:TYR:CD2	1:C:98:ALA:HB1	2.40	0.57
2:H:111:ILE:HD11	2:H:136:TYR:CD1	2.40	0.57
3:I:623:GLU:OE1	3:I:623:GLU:N	2.30	0.57
3:J:295:LEU:HD23	3:J:309:MET:HG3	1.87	0.57
3:J:312:PRO:HD3	3:J:337:TRP:CD1	2.40	0.57
2:B:253:ARG:HH22	2:B:256:ARG:HD2	1.70	0.57
1:C:178:LYS:HD3	1:C:180:ASP:HB2	1.85	0.57
1:G:89:TYR:CD2	1:G:98:ALA:HB1	2.39	0.57
1:C:58:ASN:ND2	1:C:127:SER:O	2.38	0.57
2:D:97:PHE:O	2:D:101:GLY:N	2.38	0.57
1:E:131:ARG:HG2	1:E:224:GLN:HA	1.87	0.57
3:I:219:LYS:HB3	3:I:222:VAL:HB	1.86	0.57
3:J:623:GLU:N	3:J:623:GLU:OE2	2.36	0.57
2:B:68:SER:O	2:B:71:LYS:NZ	2.38	0.56
2:D:142:GLU:OE1	2:D:146:ARG:NH2	2.38	0.56
2:D:235:MET:O	2:D:239:VAL:HG23	2.05	0.56
2:B:172:ALA:HB1	2:B:182:ALA:HB2	1.85	0.56
2:B:39:ASP:OD2	2:B:40:GLU:N	2.38	0.56
3:J:487:ASP:O	3:J:506:THR:N	2.38	0.56
2:B:49:ARG:HG2	2:B:50:ARG:H	1.69	0.56
2:D:146:ARG:HH11	2:F:132:CYS:HA	1.70	0.56
2:D:305:GLN:HA	2:D:308:ARG:NH1	2.21	0.56
2:F:44:LEU:HD12	2:F:84:PHE:HE2	1.69	0.56
2:F:97:PHE:O	2:F:101:GLY:N	2.37	0.56
3:I:227:LEU:HD13	3:I:240:HIS:HE2	1.70	0.56
3:J:146:VAL:HG13	3:J:154:HIS:HB2	1.88	0.56
2:F:286:PHE:O	2:F:289:LEU:HG	2.06	0.56
3:I:336:THR:HA	3:I:347:LEU:HA	1.86	0.56
3:I:445:GLU:OE1	3:I:464:ARG:NE	2.39	0.56
1:C:187:ASP:HA	1:C:190:PHE:HD2	1.71	0.56
2:H:372:ASP:OD1	2:H:373:MET:N	2.39	0.56
3:I:271:THR:HG21	3:I:759:PRO:HB3	1.87	0.56
3:J:762:SER:OG	3:J:763:HIS:N	2.39	0.56
1:A:173:THR:OG1	1:A:175:PRO:O	2.23	0.56
2:B:227:PHE:O	2:B:231:THR:HG23	2.06	0.56
2:H:343:GLU:HG3	2:H:377:THR:HG23	1.87	0.56
3:I:520:GLU:HA	3:I:523:LYS:HB3	1.87	0.56
3:J:752:ASN:OD1	3:J:752:ASN:N	2.39	0.56
2:B:286:PHE:O	2:B:289:LEU:HG	2.06	0.56
2:D:39:ASP:OD2	2:D:54:TRP:HB3	2.06	0.56
2:D:92:ARG:O	2:D:96:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:535:TYR:OH	3:I:578:GLU:HG3	2.06	0.56
3:I:547:MET:HA	3:I:576:VAL:HG21	1.87	0.56
3:I:615:VAL:HA	3:I:622:LEU:HD12	1.87	0.56
3:I:645:VAL:O	3:I:673:THR:N	2.33	0.56
3:J:252:LEU:HB3	3:J:298:ILE:HG13	1.86	0.56
2:D:82:TYR:HB3	2:D:84:PHE:HE2	1.71	0.56
2:F:40:GLU:OE1	2:F:55:ARG:NH2	2.33	0.56
3:I:494:GLU:HA	3:I:499:PRO:HA	1.88	0.56
2:D:481:HIS:CD2	2:F:29:LEU:HB2	2.41	0.56
2:H:39:ASP:OD1	2:H:40:GLU:N	2.37	0.56
2:H:216:LEU:HD23	2:H:220:GLU:HG3	1.87	0.56
3:I:232:TYR:HE1	3:I:322:ILE:H	1.54	0.56
3:I:338:LEU:HD11	3:I:342:GLN:HA	1.87	0.56
3:I:385:PHE:HE1	3:I:407:SER:HB3	1.70	0.56
3:J:267:LEU:HD12	3:J:281:TYR:CE1	2.41	0.56
1:A:181:THR:HA	1:A:184:GLN:HG3	1.88	0.55
2:F:231:THR:HG22	2:F:270:TYR:OH	2.06	0.55
1:G:95:HIS:ND1	1:G:95:HIS:O	2.39	0.55
3:I:650:LYS:O	3:I:650:LYS:HD2	2.06	0.55
3:J:324:MET:HG3	3:J:376:PRO:HD2	1.87	0.55
2:B:204:THR:OG1	2:D:354:ILE:HG12	2.06	0.55
2:B:324:LEU:HD22	2:B:398:PRO:HG2	1.87	0.55
2:F:135:GLU:N	2:F:135:GLU:OE1	2.39	0.55
3:I:731:ASP:OD1	3:I:733:LYS:N	2.39	0.55
2:B:163:LEU:HA	2:B:167:GLN:HB2	1.88	0.55
1:C:52:GLN:O	1:C:56:GLN:NE2	2.40	0.55
1:C:114:THR:HG22	1:C:115:GLY:H	1.71	0.55
2:D:66:LEU:O	2:D:71:LYS:NZ	2.28	0.55
2:D:198:ILE:O	2:D:202:VAL:HG23	2.06	0.55
2:F:78:ASP:OD2	1:G:62:ARG:NH1	2.28	0.55
2:F:269:PRO:HA	2:F:272:ILE:HG22	1.88	0.55
3:I:83:HIS:ND1	3:I:516:GLU:OE1	2.40	0.55
3:J:266:GLU:HB2	3:J:278:VAL:CG2	2.36	0.55
3:J:370:HIS:CD2	3:J:371:ARG:HG3	2.42	0.55
3:J:696:LEU:HB3	3:J:705:ALA:HB3	1.88	0.55
3:I:360:LYS:NZ	3:I:411:SER:O	2.36	0.55
2:H:114:TYR:O	2:H:118:LEU:HG	2.07	0.55
3:J:617:ARG:NH2	3:J:705:ALA:H	2.05	0.55
1:A:84:THR:O	1:A:88:ILE:HG12	2.07	0.55
1:A:107:ASN:HA	1:A:110:ASP:HB3	1.89	0.55
2:B:49:ARG:HG2	2:B:50:ARG:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:115:ASP:OD2	2:F:140:LYS:NZ	2.39	0.55
2:F:148:MET:O	2:F:420:ARG:NH2	2.39	0.55
3:J:226:GLY:H	3:J:254:TYR:HB2	1.72	0.55
3:J:408:GLN:HB2	3:J:411:SER:HB3	1.87	0.55
2:B:330:MET:O	2:B:334:ILE:HG13	2.07	0.55
1:G:181:THR:OG1	1:G:182:PRO:HD3	2.07	0.55
3:I:155:THR:O	3:I:180:LYS:NZ	2.27	0.55
3:I:687:TYR:CE1	3:I:691:PHE:HB3	2.42	0.55
2:H:163:LEU:HD23	2:H:167:GLN:HB2	1.88	0.55
3:J:614:GLU:O	3:J:618:ARG:NH2	2.37	0.55
3:I:215:VAL:HG13	3:I:217:THR:HG23	1.89	0.55
1:C:101:TYR:HA	1:C:104:TYR:HD2	1.71	0.55
2:D:259:MET:SD	2:D:301:SER:OG	2.56	0.55
1:E:66:VAL:HG23	1:E:69:ARG:HH22	1.72	0.55
2:F:260:SER:O	2:F:264:VAL:HG23	2.07	0.55
3:I:686:LEU:HB2	3:I:738:HIS:CE1	2.42	0.55
3:J:344:VAL:HG22	3:J:364:GLU:HG2	1.88	0.55
3:J:664:LYS:HD3	3:J:665:GLY:O	2.07	0.55
3:I:602:ARG:HH11	3:I:622:LEU:HD22	1.72	0.54
3:J:474:ASN:ND2	3:J:496:PRO:HB2	2.22	0.54
2:D:96:ASN:HA	2:D:99:ARG:HD2	1.90	0.54
2:D:340:PHE:O	2:D:344:LYS:N	2.40	0.54
2:H:477:HIS:O	2:H:481:HIS:ND1	2.25	0.54
3:I:191:GLN:HE21	3:I:206:HIS:HB3	1.73	0.54
3:I:731:ASP:OD1	3:I:734:ILE:N	2.35	0.54
3:J:251:ARG:NH1	3:J:352:ALA:O	2.41	0.54
3:J:261:ARG:HD3	3:J:261:ARG:H	1.73	0.54
2:D:202:VAL:HA	2:D:205:VAL:HG23	1.89	0.54
2:F:324:LEU:HD22	2:F:398:PRO:HG2	1.89	0.54
1:G:89:TYR:HD2	1:G:102:ALA:HB2	1.72	0.54
3:I:347:LEU:HB3	3:I:361:HIS:HB3	1.89	0.54
3:I:534:GLU:HB3	3:I:549:ILE:HB	1.88	0.54
3:J:222:VAL:HA	3:J:282:HIS:CE1	2.40	0.54
2:B:485:LYS:HB2	2:D:25:CYS:SG	2.47	0.54
2:D:227:PHE:O	2:D:231:THR:HG23	2.06	0.54
2:F:163:LEU:O	2:F:171:ARG:NH1	2.40	0.54
3:I:285:LYS:HZ2	3:I:686:LEU:HD22	1.72	0.54
3:I:453:LEU:HD21	3:I:482:PHE:CE2	2.43	0.54
3:J:657:SER:OG	3:J:676:SER:O	2.10	0.54
2:B:44:LEU:HD12	2:B:84:PHE:HE2	1.72	0.54
2:B:201:VAL:O	2:B:204:THR:OG1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:PRO:O	2:D:401:VAL:HG22	2.08	0.54
2:F:203:GLU:HG3	2:F:226:PHE:CD1	2.42	0.54
3:I:632:ARG:HG2	3:I:636:LYS:HE3	1.90	0.54
3:J:327:TRP:HH2	3:J:352:ALA:HB2	1.71	0.54
3:J:393:GLN:HE21	3:J:399:PHE:H	1.56	0.54
1:G:145:TYR:OH	2:H:18:GLY:O	2.19	0.54
3:I:755:LEU:HG	3:I:757:ILE:HG23	1.89	0.54
3:J:257:ILE:HA	3:J:292:SER:O	2.06	0.54
2:B:56:THR:HA	2:B:59:GLU:HG2	1.88	0.54
2:B:131:CYS:O	2:H:146:ARG:NH2	2.41	0.54
2:B:311:GLY:O	2:B:315:LYS:HG2	2.07	0.54
2:B:398:PRO:O	2:B:401:VAL:HG12	2.07	0.54
2:D:426:ARG:NH1	2:F:130:ASP:OD2	2.41	0.54
1:G:53:LEU:HD21	1:G:120:GLU:HB3	1.90	0.54
3:I:68:LYS:HB2	3:I:528:ARG:HG3	1.89	0.54
3:I:433:ASP:OD2	3:I:436:ARG:NH1	2.37	0.54
3:I:433:ASP:HB3	3:I:436:ARG:HB2	1.89	0.54
3:J:383:ARG:HA	3:J:407:SER:HB2	1.89	0.54
3:J:654:GLY:O	3:J:658:THR:HG23	2.08	0.54
2:B:142:GLU:O	2:B:146:ARG:HG3	2.08	0.54
2:B:385:SER:O	2:B:388:SER:OG	2.15	0.54
1:E:66:VAL:HG23	1:E:69:ARG:NH2	2.22	0.54
1:E:163:LYS:O	1:E:167:ASP:N	2.40	0.54
2:H:44:LEU:HD13	2:H:82:TYR:HB2	1.90	0.54
3:I:186:TRP:HA	3:I:193:LEU:HA	1.89	0.54
3:I:529:GLN:HB3	3:I:553:ALA:HB3	1.88	0.54
3:J:378:PHE:CE1	3:J:385:PHE:HB3	2.43	0.54
3:J:645:VAL:H	3:J:673:THR:HG22	1.72	0.54
1:E:104:TYR:HA	1:E:107:ASN:HD21	1.72	0.54
3:I:252:LEU:HD22	3:I:300:LEU:HD11	1.90	0.54
3:I:324:MET:SD	3:I:375:GLU:HG2	2.48	0.54
3:J:478:VAL:HB	3:J:491:LEU:CD2	2.38	0.54
2:D:221:ARG:NH2	2:D:222:TYR:OH	2.41	0.54
3:I:670:GLN:HE22	3:I:720:ASP:HB3	1.72	0.54
1:A:128:ILE:HA	1:A:132:GLY:HA3	1.89	0.53
1:A:225:ASN:ND2	2:B:33:ASP:OD2	2.41	0.53
2:B:136:TYR:HD2	2:B:137:LYS:HD2	1.73	0.53
2:H:417:ASP:OD1	2:H:418:LYS:N	2.41	0.53
3:I:173:PRO:HG2	3:I:197:PHE:CD1	2.43	0.53
3:I:536:ARG:NH2	3:I:639:TYR:OH	2.41	0.53
3:I:538:ILE:HG13	3:I:545:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:250:THR:HG22	3:J:301:ASN:HD22	1.73	0.53
3:J:567:VAL:HB	3:J:627:GLN:NE2	2.23	0.53
2:D:167:GLN:OE1	2:D:167:GLN:N	2.41	0.53
2:F:175:ASN:HB3	2:F:178:THR:HG23	1.89	0.53
3:I:699:HIS:HD2	3:I:706:TYR:CG	2.26	0.53
2:B:146:ARG:NH2	2:D:131:CYS:O	2.40	0.53
2:F:108:TYR:CG	2:H:108:TYR:HE1	2.27	0.53
2:H:116:ASP:OD1	2:H:117:GLU:N	2.41	0.53
2:H:310:LEU:HA	2:H:313:THR:HG22	1.89	0.53
3:J:327:TRP:CH2	3:J:352:ALA:HB2	2.43	0.53
3:J:436:ARG:NH1	3:J:440:TYR:OH	2.41	0.53
1:C:58:ASN:N	1:C:127:SER:OG	2.26	0.53
2:D:278:ASN:HA	2:D:281:ASP:HB2	1.90	0.53
1:G:189:PHE:O	1:G:193:MET:HG2	2.08	0.53
3:I:109:VAL:HG11	3:I:488:PHE:CD1	2.44	0.53
3:I:158:TYR:HB2	3:I:181:LEU:HD12	1.91	0.53
3:I:729:THR:HA	3:I:736:PHE:CD1	2.38	0.53
3:J:265:MET:O	3:J:267:LEU:N	2.41	0.53
3:J:294:SER:HB3	3:J:308:GLU:CD	2.28	0.53
3:J:645:VAL:HG12	3:J:672:PHE:CD1	2.44	0.53
1:A:202:THR:O	1:A:206:PHE:N	2.36	0.53
2:B:112:SER:HB2	2:D:104:HIS:CE1	2.37	0.53
2:B:287:VAL:HA	2:B:290:ARG:HG3	1.90	0.53
2:B:381:LYS:HB3	2:H:359:TRP:CE3	2.43	0.53
1:G:133:THR:HG23	1:G:136:GLU:H	1.74	0.53
2:H:411:HIS:HB3	2:H:415:ARG:NH2	2.23	0.53
3:I:183:TYR:O	3:I:196:ILE:N	2.23	0.53
3:J:436:ARG:NH2	3:J:506:THR:HB	2.23	0.53
3:J:454:TYR:HA	3:J:466:CYS:HA	1.91	0.53
3:J:475:CYS:HA	3:J:495:GLY:O	2.08	0.53
3:J:681:ILE:CG1	3:J:734:ILE:HD12	2.38	0.53
1:A:186:VAL:O	1:A:189:PHE:CB	2.47	0.53
1:E:165:ILE:HG12	2:F:19:TRP:NE1	2.24	0.53
1:E:187:ASP:HA	1:E:190:PHE:CD2	2.43	0.53
2:F:200:ASN:ND2	2:F:293:ARG:HB3	2.23	0.53
3:I:119:GLU:OE1	3:I:165:HIS:NE2	2.42	0.53
3:I:191:GLN:NE2	3:I:207:VAL:H	2.07	0.53
3:I:194:ILE:HG22	3:I:203:TYR:HA	1.90	0.53
3:J:326:LYS:HG3	3:J:377:VAL:HG12	1.91	0.53
3:J:619:LEU:HD11	3:J:695:TYR:HB2	1.91	0.53
2:F:111:ILE:HD11	2:F:136:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:LEU:O	1:G:207:LEU:HG	2.09	0.53
3:I:440:TYR:HA	3:I:454:TYR:O	2.09	0.53
3:I:571:PRO:HD2	3:I:691:PHE:CZ	2.43	0.53
3:J:133:ILE:HD13	3:J:163:ILE:HD11	1.90	0.53
3:J:181:LEU:HD22	3:J:195:PHE:HD2	1.74	0.53
1:A:86:LYS:HD2	1:A:99:SER:HA	1.91	0.53
2:D:240:GLU:O	2:D:244:ARG:HG2	2.09	0.53
1:E:150:ASP:OD1	1:E:151:GLY:N	2.42	0.53
2:F:332:ILE:HD11	2:F:362:ILE:HD13	1.91	0.53
2:F:347:SER:OG	2:F:348:ALA:N	2.42	0.53
3:I:545:LEU:HD13	3:I:601:GLY:HA2	1.91	0.53
3:J:218:GLY:H	3:J:225:ASN:ND2	2.07	0.53
3:J:560:HIS:O	3:J:644:ARG:NH2	2.42	0.53
3:J:628:MET:HG2	3:J:660:ILE:HG23	1.91	0.53
3:J:655:TYR:CZ	3:J:711:LEU:HD21	2.44	0.53
2:D:146:ARG:O	2:D:419:ARG:NH1	2.42	0.53
1:E:134:VAL:O	1:E:138:LEU:HG	2.09	0.53
1:G:191:GLN:HA	1:G:197:LYS:NZ	2.24	0.53
3:I:48:LEU:HD12	3:I:51:THR:HB	1.92	0.53
3:I:139:TYR:CD1	3:I:207:VAL:HG11	2.44	0.53
3:J:99:GLU:HB2	3:J:103:SER:O	2.09	0.53
3:J:230:TRP:CD1	3:J:281:TYR:CE2	2.97	0.53
3:J:307:LEU:HD22	3:J:354:THR:HA	1.89	0.53
3:J:432:TYR:HA	3:J:439:ILE:HG13	1.89	0.53
3:J:532:LYS:N	3:J:551:LYS:O	2.24	0.53
2:B:368:LEU:HD21	2:D:364:THR:HG23	1.90	0.52
2:D:192:PHE:CD2	2:D:236:ILE:HG21	2.43	0.52
3:I:293:ILE:HG12	3:I:322:ILE:HD12	1.91	0.52
3:I:499:PRO:HD3	3:I:580:PHE:CG	2.44	0.52
3:I:588:LEU:O	3:I:593:GLY:N	2.42	0.52
3:J:153:SER:HB2	3:J:240:HIS:HB3	1.91	0.52
1:C:94:PRO:O	1:C:95:HIS:ND1	2.42	0.52
1:C:155:LYS:HA	1:C:190:PHE:HZ	1.73	0.52
1:E:98:ALA:HA	1:E:168:MET:HE1	1.90	0.52
2:H:124:LEU:O	2:H:127:ILE:HG12	2.09	0.52
2:H:240:GLU:O	2:H:244:ARG:HG2	2.09	0.52
3:J:139:TYR:CE2	3:J:207:VAL:HG21	2.43	0.52
3:J:715:VAL:HG21	3:J:745:GLN:HB3	1.91	0.52
2:D:305:GLN:HA	2:D:308:ARG:HH12	1.75	0.52
2:F:58:LEU:O	2:F:67:GLY:HA2	2.09	0.52
2:F:75:PHE:HA	2:F:82:TYR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:GLU:HA	3:I:108:ASN:HA	1.91	0.52
3:I:374:GLU:OE1	3:I:388:VAL:HB	2.09	0.52
3:I:449:ARG:NH1	3:I:546:PRO:HB2	2.23	0.52
3:I:633:THR:O	3:I:637:GLU:N	2.42	0.52
3:J:499:PRO:O	3:J:518:ASN:ND2	2.42	0.52
3:J:648:PHE:HZ	3:J:778:ILE:HD13	1.74	0.52
3:I:230:TRP:HB3	3:I:281:TYR:OH	2.10	0.52
3:I:285:LYS:HD3	3:I:686:LEU:HD22	1.91	0.52
3:I:602:ARG:N	3:I:626:ASP:OD2	2.42	0.52
3:J:314:ASP:HB3	3:J:317:MET:HG2	1.91	0.52
1:C:87:GLN:O	1:C:91:GLN:N	2.34	0.52
2:H:87:ASP:HB3	2:H:90:VAL:HG12	1.90	0.52
2:H:398:PRO:O	2:H:401:VAL:HG12	2.09	0.52
3:I:51:THR:HA	3:I:54:ILE:HD12	1.90	0.52
3:I:149:VAL:N	3:I:153:SER:O	2.43	0.52
3:I:295:LEU:HD23	3:I:309:MET:HG3	1.91	0.52
3:I:340:ARG:NH2	3:I:693:GLU:OE1	2.38	0.52
3:I:531:PRO:HB3	3:I:589:VAL:HG11	1.91	0.52
3:J:42:ILE:H	3:J:42:ILE:HD12	1.75	0.52
3:J:182:GLN:HE22	3:J:199:ASN:H	1.58	0.52
3:J:378:PHE:CD1	3:J:385:PHE:HB3	2.45	0.52
1:C:195:LYS:NZ	1:C:209:SER:HB3	2.25	0.52
2:F:39:ASP:OD2	2:F:55:ARG:N	2.36	0.52
1:G:216:ILE:O	1:G:220:LEU:HG	2.10	0.52
3:I:548:GLN:HB2	3:I:576:VAL:HG13	1.90	0.52
3:J:143:SER:HA	3:J:158:TYR:HD1	1.74	0.52
3:J:327:TRP:CZ3	3:J:333:VAL:HB	2.44	0.52
2:F:88:PRO:HA	2:F:91:PHE:HB3	1.92	0.52
2:H:41:LEU:HB3	2:H:52:GLN:HB3	1.91	0.52
3:I:228:SER:N	3:I:240:HIS:O	2.43	0.52
3:I:297:VAL:HG21	3:I:333:VAL:HG11	1.91	0.52
3:J:563:LEU:HB2	3:J:640:ILE:HD11	1.92	0.52
2:D:259:MET:HA	2:D:262:ILE:HD12	1.91	0.52
2:F:49:ARG:HD2	2:H:49:ARG:HH21	1.75	0.52
2:F:327:SER:O	2:F:330:MET:HG2	2.10	0.52
1:G:71:PHE:HA	2:H:8:TRP:HZ2	1.74	0.52
1:C:202:THR:HG22	1:C:203:LEU:H	1.75	0.52
2:D:386:ILE:O	2:D:390:SER:OG	2.25	0.52
3:I:555:PHE:HZ	3:I:639:TYR:CG	2.28	0.52
3:J:130:ARG:HB2	3:J:143:SER:HB2	1.90	0.52
3:J:193:LEU:HG	3:J:204:CYS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:285:LYS:HD3	3:J:685:LYS:HZ1	1.75	0.52
3:J:328:ALA:CB	3:J:378:PHE:HB2	2.40	0.52
1:A:218:ARG:HH22	2:B:28:PRO:HD2	1.75	0.52
1:C:101:TYR:HA	1:C:104:TYR:CD2	2.45	0.52
2:D:110:CYS:HG	2:F:104:HIS:CE1	2.25	0.52
3:I:439:ILE:O	3:I:456:ALA:N	2.37	0.52
3:I:519:GLU:H	3:I:519:GLU:CD	2.14	0.52
3:I:614:GLU:O	3:I:618:ARG:NH2	2.42	0.52
3:J:615:VAL:HG22	3:J:619:LEU:HD23	1.92	0.52
1:C:128:ILE:O	1:C:137:LYS:HE2	2.10	0.51
1:C:150:ASP:OD1	1:C:151:GLY:N	2.43	0.51
2:D:83:PHE:HE1	2:F:52:GLN:HB2	1.75	0.51
1:G:129:LEU:HD21	1:G:140:TRP:CH2	2.46	0.51
3:I:148:PRO:HA	3:I:154:HIS:HB3	1.92	0.51
3:I:548:GLN:HE21	3:I:550:LEU:HD11	1.74	0.51
3:J:230:TRP:HB2	3:J:282:HIS:HB2	1.91	0.51
2:D:105:TYR:N	2:D:132:CYS:SG	2.83	0.51
2:F:198:ILE:O	2:F:202:VAL:HG23	2.11	0.51
3:I:438:LYS:HD3	3:I:455:SER:OG	2.10	0.51
3:I:471:LEU:HG	3:I:504:HIS:CE1	2.45	0.51
3:J:293:ILE:O	3:J:320:TYR:OH	2.19	0.51
3:J:445:GLU:HB3	3:J:454:TYR:OH	2.10	0.51
2:B:188:VAL:HG22	2:B:192:PHE:CE2	2.45	0.51
3:I:543:TYR:HB3	3:I:611:LEU:HD13	1.91	0.51
3:I:551:LYS:HE2	3:I:555:PHE:CZ	2.46	0.51
3:J:336:THR:HG22	3:J:347:LEU:HA	1.91	0.51
3:J:360:LYS:NZ	3:J:411:SER:OG	2.35	0.51
1:G:217:MET:O	1:G:221:GLN:NE2	2.44	0.51
2:H:227:PHE:O	2:H:231:THR:HG23	2.09	0.51
2:H:311:GLY:O	2:H:315:LYS:HG2	2.10	0.51
3:I:291:PRO:HD2	3:I:321:TYR:HE1	1.74	0.51
3:I:370:HIS:CE1	3:I:572:GLY:HA3	2.45	0.51
3:J:565:LEU:HD21	3:J:627:GLN:HG3	1.92	0.51
2:B:29:LEU:O	2:H:478:HIS:NE2	2.36	0.51
2:B:235:MET:O	2:B:239:VAL:HG23	2.09	0.51
2:F:164:SER:O	2:F:168:THR:OG1	2.29	0.51
2:H:266:ALA:HB1	2:H:296:ARG:HB3	1.93	0.51
2:H:313:THR:HG21	2:H:406:PHE:HD1	1.76	0.51
3:I:295:LEU:HD13	3:I:322:ILE:HD13	1.93	0.51
3:I:378:PHE:HA	3:I:385:PHE:HB3	1.92	0.51
3:I:483:SER:OG	3:I:484:HIS:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:261:ARG:HE	3:J:289:GLU:HG3	1.75	0.51
1:A:196:ASN:ND2	1:A:205:GLU:OE2	2.43	0.51
2:B:192:PHE:CD2	2:B:236:ILE:HG21	2.46	0.51
2:F:45:ASN:O	2:F:83:PHE:HA	2.11	0.51
2:F:286:PHE:CE2	2:F:290:ARG:HD2	2.46	0.51
3:I:117:LEU:HD12	3:I:133:ILE:HD13	1.91	0.51
3:J:218:GLY:H	3:J:225:ASN:HD21	1.57	0.51
3:J:268:PRO:HA	3:J:278:VAL:HG12	1.91	0.51
3:J:436:ARG:HH22	3:J:506:THR:HB	1.76	0.51
2:B:169:MET:HE1	2:B:246:PHE:HD2	1.76	0.51
2:B:246:PHE:O	2:B:251:ARG:NH2	2.42	0.51
3:J:140:VAL:HG13	3:J:163:ILE:HG12	1.92	0.51
3:J:309:MET:SD	3:J:355:GLY:HA2	2.51	0.51
3:J:744:THR:HA	3:J:747:ILE:HD12	1.91	0.51
1:A:124:THR:O	1:A:127:SER:OG	2.28	0.51
2:B:116:ASP:OD1	2:B:117:GLU:N	2.42	0.51
2:B:130:ASP:O	2:H:146:ARG:NH2	2.43	0.51
2:D:197:VAL:O	2:D:201:VAL:HG23	2.11	0.51
1:E:51:GLU:OE2	1:E:61:LYS:NZ	2.42	0.51
2:F:44:LEU:HD13	2:F:82:TYR:HB2	1.93	0.51
3:I:297:VAL:H	3:I:309:MET:HE3	1.76	0.51
3:I:388:VAL:HG13	3:I:401:HIS:N	2.25	0.51
3:J:97:TYR:CE1	3:J:107:ARG:HB2	2.45	0.51
1:A:126:LEU:HD13	2:B:14:ALA:HB2	1.92	0.51
1:C:134:VAL:HG13	1:C:220:LEU:HD13	1.93	0.51
2:F:33:ASP:OD2	2:F:34:LYS:N	2.43	0.51
3:I:122:LYS:NZ	3:I:165:HIS:HA	2.26	0.51
3:I:359:LYS:HD2	3:I:359:LYS:N	2.26	0.51
3:I:490:LEU:HD21	3:I:503:VAL:HG22	1.92	0.51
3:J:693:GLU:HB3	3:J:698:LEU:HA	1.93	0.51
2:B:278:ASN:HA	2:B:281:ASP:HB2	1.94	0.50
2:B:332:ILE:HD11	2:B:362:ILE:HD13	1.93	0.50
3:I:687:TYR:CG	3:I:688:ALA:N	2.79	0.50
3:J:262:VAL:HG21	3:J:291:PRO:HD3	1.92	0.50
3:J:359:LYS:O	3:J:412:SER:HA	2.11	0.50
3:J:531:PRO:HB3	3:J:552:PRO:HA	1.92	0.50
3:J:658:THR:HG22	3:J:723:PHE:CE1	2.46	0.50
3:J:731:ASP:OD1	3:J:732:GLU:N	2.44	0.50
1:A:71:PHE:HA	2:B:8:TRP:CZ2	2.47	0.50
2:D:131:CYS:SG	2:D:132:CYS:N	2.85	0.50
2:D:205:VAL:HG22	2:F:355:PRO:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:391:GLY:HA2	2:D:394:VAL:HG12	1.93	0.50
1:G:84:THR:HA	1:G:87:GLN:HE21	1.77	0.50
2:H:3:ALA:HB3	2:H:56:THR:HG21	1.93	0.50
3:I:230:TRP:CZ3	3:I:284:PRO:HG3	2.47	0.50
3:I:254:TYR:O	3:I:295:LEU:HD12	2.12	0.50
2:D:191:PHE:O	2:D:195:VAL:HG23	2.11	0.50
2:D:389:LEU:O	2:D:393:LEU:HG	2.11	0.50
1:E:72:LYS:HA	1:E:75:CYS:O	2.12	0.50
1:E:181:THR:O	1:E:185:HIS:N	2.25	0.50
1:G:221:GLN:HB3	1:G:224:GLN:NE2	2.27	0.50
3:I:96:ILE:HD13	3:I:133:ILE:HB	1.93	0.50
3:I:233:GLU:CD	3:I:240:HIS:HB3	2.31	0.50
3:I:646:ALA:HB1	3:I:782:PHE:HE1	1.75	0.50
2:B:411:HIS:HD1	2:B:411:HIS:H	1.60	0.50
2:F:368:LEU:HD11	2:H:388:SER:HB2	1.93	0.50
3:I:93:LYS:O	3:I:109:VAL:HG23	2.12	0.50
3:I:246:SER:HG	3:I:251:ARG:H	1.54	0.50
3:I:644:ARG:HD2	3:I:786:PHE:C	2.32	0.50
3:J:360:LYS:HG3	3:J:407:SER:OG	2.12	0.50
2:B:217:PRO:HG2	2:B:220:GLU:HG2	1.92	0.50
2:D:49:ARG:HG2	2:D:51:PHE:CE2	2.47	0.50
2:D:181:LEU:HA	2:D:184:VAL:HG12	1.94	0.50
3:J:231:LEU:CD1	3:J:688:ALA:HB1	2.42	0.50
3:J:435:LYS:HZ1	3:J:436:ARG:CZ	2.24	0.50
3:J:494:GLU:HA	3:J:499:PRO:HB3	1.92	0.50
3:J:647:VAL:HG22	3:J:648:PHE:H	1.75	0.50
1:C:120:GLU:O	1:C:124:THR:HG23	2.11	0.50
2:D:299:LYS:O	2:D:302:ARG:NH2	2.45	0.50
1:E:146:ASP:OD2	1:E:150:ASP:N	2.44	0.50
3:J:191:GLN:HG3	3:J:206:HIS:CD2	2.46	0.50
3:J:617:ARG:HH22	3:J:704:ARG:H	1.59	0.50
1:A:78:GLY:O	1:A:79:VAL:HG13	2.11	0.50
2:B:163:LEU:HD23	2:B:167:GLN:HB2	1.92	0.50
2:B:309:ILE:HD11	2:B:410:TYR:HA	1.92	0.50
2:D:75:PHE:HB2	2:D:82:TYR:CE1	2.46	0.50
2:F:259:MET:HB3	2:F:302:ARG:NH2	2.26	0.50
3:I:238:LYS:HD2	3:I:373:ASN:HB2	1.94	0.50
3:J:134:SER:HB2	3:J:186:TRP:CG	2.47	0.50
3:J:312:PRO:HG3	3:J:348:THR:HG21	1.94	0.50
3:J:324:MET:CG	3:J:375:GLU:HA	2.42	0.50
1:A:101:TYR:HA	1:A:104:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ARG:NH2	2:B:256:ARG:HD2	2.27	0.50
2:B:257:SER:O	2:B:260:SER:OG	2.28	0.50
1:C:171:LYS:HG3	1:C:172:TYR:HD1	1.76	0.50
2:D:111:ILE:HB	2:D:139:ARG:HB3	1.93	0.50
2:D:175:ASN:HB3	2:D:178:THR:HG23	1.94	0.50
2:D:294:VAL:HG23	2:D:295:PHE:HD2	1.75	0.50
2:F:403:VAL:HG22	2:H:397:LEU:HD23	1.94	0.50
1:G:118:LYS:HG3	1:G:120:GLU:H	1.76	0.50
3:I:70:VAL:HB	3:I:590:SER:OG	2.12	0.50
3:I:477:TYR:HB3	3:I:495:GLY:HA3	1.92	0.50
3:I:773:HIS:HD2	3:J:750:LYS:HG2	1.76	0.50
3:J:289:GLU:HA	3:J:319:GLU:OE2	2.11	0.50
2:B:347:SER:OG	2:B:348:ALA:N	2.45	0.50
1:C:105:LEU:HA	1:C:108:ALA:HB3	1.94	0.50
2:D:20:MET:HB2	2:D:21:PRO:HD3	1.93	0.50
2:F:213:SER:OG	2:F:214:LYS:N	2.45	0.50
3:I:104:VAL:HG21	3:I:131:TYR:CE2	2.47	0.50
3:I:227:LEU:HB3	3:I:240:HIS:CD2	2.46	0.50
3:J:562:PRO:HA	3:J:644:ARG:O	2.11	0.50
1:A:192:LYS:HG3	1:A:193:MET:HG2	1.94	0.49
1:E:139:ARG:HG2	1:E:203:LEU:HD11	1.93	0.49
3:I:564:LEU:HD21	3:I:566:VAL:HG23	1.93	0.49
3:J:644:ARG:HB3	3:J:786:PHE:CD1	2.46	0.49
3:J:654:GLY:HA3	3:J:680:PRO:HB3	1.93	0.49
3:J:743:ILE:HD11	3:J:753:TYR:CE2	2.47	0.49
2:B:107:ARG:HB2	2:H:108:TYR:HB2	1.94	0.49
1:C:106:PHE:O	1:C:110:ASP:N	2.30	0.49
2:F:103:LEU:HD12	2:F:104:HIS:H	1.77	0.49
2:F:372:ASP:OD1	2:F:373:MET:N	2.45	0.49
3:I:389:ARG:CZ	3:I:391:ILE:HG22	2.41	0.49
3:I:537:LYS:HD3	3:I:545:LEU:C	2.32	0.49
1:C:217:MET:HG3	1:C:220:LEU:HD12	1.94	0.49
1:E:222:LEU:HB3	2:F:31:PRO:HD3	1.94	0.49
2:F:259:MET:HB3	2:F:302:ARG:HH22	1.77	0.49
3:I:273:SER:OG	3:I:274:VAL:N	2.45	0.49
3:I:590:SER:OG	3:I:591:SER:N	2.45	0.49
3:J:226:GLY:N	3:J:254:TYR:HB2	2.27	0.49
3:J:264:LEU:HD22	3:J:281:TYR:HA	1.94	0.49
1:C:81:ASN:OD1	1:C:84:THR:HG23	2.13	0.49
2:D:274:LEU:O	2:D:277:THR:HG23	2.12	0.49
3:I:441:PHE:CD2	3:I:443:SER:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:468:SER:HA	3:I:471:LEU:HB2	1.93	0.49
1:A:171:LYS:HG3	1:A:172:TYR:HD1	1.77	0.49
2:B:290:ARG:HB3	2:B:293:ARG:HH22	1.77	0.49
1:C:130:LEU:HD22	1:C:131:ARG:HG2	1.94	0.49
1:E:71:PHE:CZ	1:E:119:PHE:HB2	2.47	0.49
3:I:449:ARG:HA	3:I:574:GLN:OE1	2.13	0.49
3:I:641:ASP:OD2	3:I:644:ARG:NH2	2.44	0.49
3:I:742:LEU:O	3:I:745:GLN:N	2.45	0.49
3:J:452:HIS:CE1	3:J:476:THR:HG22	2.47	0.49
1:A:189:PHE:HE2	1:A:201:VAL:HG21	1.78	0.49
1:C:84:THR:O	1:C:88:ILE:HB	2.12	0.49
1:C:129:LEU:HD11	1:C:140:TRP:CD2	2.48	0.49
2:F:4:GLY:HA3	2:F:56:THR:HB	1.93	0.49
2:F:57:THR:HA	2:F:60:ARG:HD2	1.93	0.49
3:I:227:LEU:HB3	3:I:240:HIS:HD2	1.76	0.49
3:I:290:ASN:ND2	3:I:340:ARG:HG3	2.27	0.49
3:I:293:ILE:HG23	3:I:322:ILE:HG13	1.95	0.49
1:A:71:PHE:CZ	1:A:119:PHE:HB2	2.48	0.49
2:B:234:VAL:HG11	2:B:270:TYR:CD2	2.48	0.49
2:B:240:GLU:O	2:B:244:ARG:HG2	2.12	0.49
2:B:477:HIS:HA	2:B:480:LEU:HB3	1.94	0.49
2:D:113:ALA:HA	2:D:116:ASP:OD2	2.12	0.49
2:F:85:ASP:O	2:F:86:ARG:HD2	2.13	0.49
2:H:103:LEU:HB3	2:H:128:ILE:HA	1.94	0.49
3:I:286:ALA:O	3:I:699:HIS:ND1	2.46	0.49
3:I:376:PRO:HB3	3:I:387:PHE:HB3	1.94	0.49
3:I:726:ILE:HA	3:I:756:GLN:HG2	1.93	0.49
3:I:769:ALA:HA	3:I:772:GLN:HE21	1.78	0.49
3:J:151:GLN:HG2	3:J:152:HIS:CD2	2.48	0.49
1:A:163:LYS:NZ	1:A:179:GLU:O	2.39	0.49
2:B:415:ARG:HA	2:B:418:LYS:HE2	1.93	0.49
1:C:87:GLN:HA	1:C:90:ALA:HB3	1.94	0.49
2:D:87:ASP:HB3	2:D:90:VAL:HG12	1.94	0.49
3:I:89:TRP:CD1	3:I:483:SER:HA	2.48	0.49
3:I:106:LEU:HD11	3:I:137:LYS:HZ3	1.77	0.49
3:I:160:LEU:HD21	3:I:193:LEU:HD21	1.94	0.49
3:I:335:VAL:O	3:I:348:THR:N	2.38	0.49
3:I:401:HIS:HE1	3:I:424:TRP:CE2	2.31	0.49
3:I:733:LYS:O	3:I:734:ILE:HD13	2.12	0.49
3:J:215:VAL:HG11	3:J:254:TYR:CE2	2.48	0.49
3:J:585:GLU:O	3:J:589:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD12	2:B:17:ILE:HB	1.94	0.49
2:B:138:ASP:HA	2:B:141:ARG:HH11	1.77	0.49
1:C:82:GLU:O	1:C:86:LYS:HG2	2.13	0.49
2:D:231:THR:HG22	2:D:270:TYR:OH	2.13	0.49
1:E:128:ILE:HA	1:E:132:GLY:HA3	1.94	0.49
1:G:87:GLN:HG3	1:G:88:ILE:H	1.78	0.49
3:I:440:TYR:CD1	3:I:467:LEU:HD11	2.47	0.49
3:I:563:LEU:HD21	3:I:631:VAL:HG22	1.93	0.49
3:J:153:SER:HA	3:J:240:HIS:HB3	1.94	0.49
3:J:522:GLN:HE21	3:J:526:ASN:HD21	1.60	0.49
3:J:690:ALA:O	3:J:694:ARG:HB2	2.13	0.49
3:I:488:PHE:CD1	3:I:505:ASN:HA	2.48	0.49
3:I:623:GLU:O	3:I:627:GLN:HG2	2.13	0.49
1:A:166:TYR:CE1	2:H:486:THR:HB	2.48	0.48
1:E:126:LEU:HD12	2:F:14:ALA:HB2	1.95	0.48
1:G:79:VAL:HG11	1:G:117:VAL:N	2.29	0.48
2:H:355:PRO:HA	2:H:358:PHE:CE2	2.48	0.48
3:I:328:ALA:HB3	3:I:332:LYS:HD2	1.94	0.48
3:I:402:ILE:HG22	3:I:419:ILE:HB	1.95	0.48
3:I:420:THR:HA	3:I:464:ARG:HH11	1.78	0.48
3:J:246:SER:HA	3:J:327:TRP:CB	2.42	0.48
2:B:354:ILE:HG12	2:H:204:THR:OG1	2.13	0.48
1:C:137:LYS:NZ	1:C:220:LEU:O	2.31	0.48
2:F:146:ARG:HG2	2:F:147:LEU:HD22	1.95	0.48
2:F:271:TYR:HD1	2:F:274:LEU:HD12	1.78	0.48
1:G:66:VAL:HG22	2:H:3:ALA:HB2	1.95	0.48
3:I:95:PHE:CZ	3:I:503:VAL:HG21	2.48	0.48
3:I:218:GLY:CA	3:I:225:ASN:HD22	2.26	0.48
3:I:324:MET:SD	3:I:376:PRO:HD2	2.53	0.48
3:J:201:ILE:HD11	3:J:226:GLY:N	2.29	0.48
3:J:658:THR:HG22	3:J:723:PHE:CZ	2.49	0.48
2:F:176:PRO:HB2	2:F:183:LEU:HD23	1.94	0.48
2:H:198:ILE:O	2:H:202:VAL:HG23	2.13	0.48
3:I:572:GLY:N	3:I:603:GLY:O	2.46	0.48
3:J:156:GLY:HA2	3:J:180:LYS:HZ2	1.79	0.48
3:J:232:TYR:CE2	3:J:290:ASN:HB3	2.47	0.48
3:J:267:LEU:CD2	3:J:268:PRO:HD2	2.44	0.48
2:D:166:ARG:HH12	2:D:247:ALA:HA	1.77	0.48
1:G:87:GLN:HG3	1:G:88:ILE:N	2.28	0.48
1:G:180:ASP:O	1:G:183:ARG:HB3	2.14	0.48
3:I:130:ARG:NH1	3:I:132:GLU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:314:ASP:HB3	3:I:317:MET:HG2	1.93	0.48
3:I:385:PHE:CE1	3:I:407:SER:HB3	2.49	0.48
3:J:648:PHE:CZ	3:J:778:ILE:HD13	2.48	0.48
2:D:290:ARG:HA	2:D:293:ARG:NH1	2.29	0.48
2:F:124:LEU:HG	2:F:126:GLU:H	1.78	0.48
2:H:309:ILE:HD11	2:H:410:TYR:HA	1.96	0.48
3:I:186:TRP:HZ3	3:I:191:GLN:HB2	1.78	0.48
3:I:267:LEU:HD12	3:I:281:TYR:HB3	1.95	0.48
3:I:368:TRP:HE1	3:I:612:LEU:HD21	1.78	0.48
3:I:368:TRP:CH2	3:I:613:GLN:HA	2.48	0.48
3:J:299:GLY:O	3:J:304:THR:HA	2.14	0.48
3:J:437:ASN:O	3:J:457:ASN:HA	2.13	0.48
1:C:107:ASN:HA	1:C:110:ASP:HB3	1.96	0.48
2:D:40:GLU:OE1	2:D:55:ARG:NH2	2.46	0.48
2:F:88:PRO:O	2:F:92:ARG:N	2.46	0.48
2:F:310:LEU:HA	2:F:313:THR:HG22	1.96	0.48
2:F:376:LYS:HA	2:F:381:LYS:HE3	1.96	0.48
2:F:385:SER:OG	2:F:386:ILE:N	2.46	0.48
2:H:169:MET:HG3	2:H:247:ALA:HB2	1.96	0.48
2:H:287:VAL:O	2:H:291:VAL:HG23	2.13	0.48
3:I:377:VAL:N	3:I:386:PHE:O	2.30	0.48
3:J:267:LEU:HD22	3:J:268:PRO:HD2	1.96	0.48
3:J:568:ASP:OD1	3:J:573:SER:OG	2.17	0.48
3:J:576:VAL:HB	3:J:600:ASP:OD2	2.13	0.48
3:J:617:ARG:HH22	3:J:704:ARG:N	2.12	0.48
1:A:129:LEU:HD21	1:A:140:TRP:CD2	2.48	0.48
2:B:43:VAL:HG22	2:B:52:GLN:HG2	1.96	0.48
3:I:94:GLU:HB3	3:I:108:ASN:ND2	2.29	0.48
3:I:503:VAL:O	3:I:512:MET:N	2.45	0.48
3:J:82:ILE:HD11	3:J:580:PHE:CE1	2.49	0.48
3:J:139:TYR:CZ	3:J:207:VAL:HG21	2.49	0.48
3:J:393:GLN:NE2	3:J:399:PHE:O	2.46	0.48
3:J:681:ILE:HG13	3:J:734:ILE:HD12	1.95	0.48
3:J:725:ILE:HB	3:J:755:LEU:HD12	1.95	0.48
1:A:137:LYS:HD2	1:A:221:GLN:NE2	2.29	0.48
1:C:162:VAL:HA	1:C:165:ILE:HD12	1.94	0.48
2:D:47:SER:OG	2:D:86:ARG:O	2.31	0.48
1:E:216:ILE:HD12	2:F:21:PRO:HA	1.95	0.48
2:F:124:LEU:HD23	2:F:127:ILE:HG23	1.95	0.48
2:F:167:GLN:OE1	2:F:167:GLN:N	2.42	0.48
2:F:167:GLN:HB2	2:F:171:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:THR:HG23	1:G:63:GLU:H	1.78	0.48
2:H:177:HIS:HD2	2:H:183:LEU:HD21	1.79	0.48
3:I:148:PRO:HA	3:I:154:HIS:HA	1.95	0.48
3:I:175:GLU:HG2	3:I:176:VAL:HG23	1.96	0.48
3:I:408:GLN:HB2	3:I:411:SER:OG	2.14	0.48
3:J:326:LYS:NZ	3:J:328:ALA:HA	2.29	0.48
3:J:662:PRO:HB3	3:J:718:LEU:HD13	1.96	0.48
2:B:48:GLY:HA3	2:D:52:GLN:N	2.29	0.48
2:B:403:VAL:HG21	2:D:400:PRO:HG2	1.95	0.48
2:F:294:VAL:HG23	2:F:295:PHE:HD2	1.79	0.48
1:G:83:ASP:O	1:G:87:GLN:HG2	2.13	0.48
3:J:85:PRO:HG2	3:J:515:LEU:HD23	1.96	0.48
3:J:489:PHE:HD1	3:J:506:THR:HG1	1.57	0.48
3:J:715:VAL:HG12	3:J:746:LEU:HG	1.96	0.48
2:B:320:GLU:H	2:B:320:GLU:CD	2.18	0.48
1:C:169:MET:HG2	1:C:173:THR:HG23	1.96	0.48
2:D:354:ILE:HB	2:D:355:PRO:HD3	1.95	0.48
2:F:411:HIS:HB3	2:F:415:ARG:NH2	2.29	0.48
1:G:190:PHE:CE1	1:G:201:VAL:HG13	2.49	0.48
3:I:679:SER:HA	3:I:727:HIS:ND1	2.28	0.48
1:A:178:LYS:HG3	1:A:180:ASP:H	1.79	0.47
2:B:191:PHE:O	2:B:195:VAL:HG23	2.14	0.47
1:C:218:ARG:HH22	2:D:30:ALA:HB2	1.79	0.47
2:D:106:PRO:HG2	2:D:109:GLU:CG	2.43	0.47
1:E:110:ASP:CG	1:E:117:VAL:HB	2.35	0.47
3:I:401:HIS:HE1	3:I:424:TRP:CD2	2.31	0.47
3:I:432:TYR:OH	3:I:437:ASN:OD1	2.31	0.47
3:I:468:SER:HA	3:I:471:LEU:HD22	1.96	0.47
3:I:519:GLU:OE1	3:I:519:GLU:N	2.39	0.47
3:J:130:ARG:NH1	3:J:184:ALA:HB3	2.28	0.47
3:J:173:PRO:HB3	3:J:202:TYR:CZ	2.49	0.47
3:J:765:PHE:HD1	3:J:770:LEU:HD23	1.79	0.47
1:A:219:SER:HB3	2:B:20:MET:SD	2.55	0.47
2:F:72:GLU:HB2	1:G:50:LEU:HD23	1.96	0.47
2:F:189:THR:O	2:F:193:ILE:HG13	2.15	0.47
2:H:206:PRO:HB2	2:H:215:GLU:OE1	2.13	0.47
2:H:261:ILE:O	2:H:265:VAL:HG22	2.14	0.47
2:H:316:SER:OG	2:H:405:ASN:ND2	2.45	0.47
2:H:353:SER:OG	2:H:355:PRO:HD2	2.14	0.47
2:H:422:GLN:HE22	2:H:426:ARG:NH2	2.11	0.47
3:I:295:LEU:HB3	3:I:309:MET:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:561:TYR:O	3:I:641:ASP:N	2.37	0.47
3:J:85:PRO:HD2	3:J:492:LYS:HE2	1.95	0.47
2:B:39:ASP:OD1	2:B:56:THR:OG1	2.17	0.47
2:F:291:VAL:O	2:F:294:VAL:HG22	2.14	0.47
1:G:117:VAL:HG13	1:G:118:LYS:H	1.78	0.47
3:I:429:ILE:HD13	3:I:439:ILE:HD11	1.96	0.47
3:I:433:ASP:O	3:I:437:ASN:N	2.47	0.47
3:I:750:LYS:HG2	3:J:773:HIS:CE1	2.46	0.47
3:J:492:LYS:HG2	3:J:501:VAL:HG13	1.97	0.47
2:B:74:PHE:HE1	1:C:69:ARG:HG3	1.79	0.47
2:D:83:PHE:CE1	2:F:52:GLN:HB2	2.50	0.47
3:I:187:GLY:N	3:I:192:GLN:O	2.22	0.47
3:I:339:ASN:ND2	3:I:343:ASN:OD1	2.36	0.47
3:I:441:PHE:HZ	3:I:464:ARG:HD2	1.79	0.47
3:J:84:ASP:OD2	3:J:492:LYS:HD3	2.15	0.47
3:J:295:LEU:N	3:J:308:GLU:OE2	2.46	0.47
3:J:588:LEU:HG	3:J:594:ALA:HB2	1.96	0.47
2:D:166:ARG:NH2	2:D:246:PHE:O	2.47	0.47
2:B:104:HIS:CG	2:B:131:CYS:HG	2.31	0.47
2:B:310:LEU:HA	2:B:313:THR:HG22	1.97	0.47
2:B:483:LEU:HD21	1:C:169:MET:HA	1.96	0.47
2:D:313:THR:HG22	2:D:409:ILE:HD12	1.97	0.47
2:D:397:LEU:HB2	2:D:398:PRO:HD3	1.94	0.47
1:E:186:VAL:O	1:E:189:PHE:HB3	2.14	0.47
3:I:141:LEU:HB2	3:I:186:TRP:NE1	2.24	0.47
3:I:149:VAL:HG23	3:I:155:THR:N	2.29	0.47
3:I:157:TYR:HA	3:I:181:LEU:HG	1.97	0.47
3:I:224:TYR:HB2	3:I:257:ILE:HB	1.97	0.47
3:I:296:HIS:CE1	3:I:308:GLU:HB2	2.49	0.47
3:I:439:ILE:HG23	3:I:456:ALA:HB3	1.97	0.47
3:I:637:GLU:OE2	3:I:638:GLN:N	2.48	0.47
3:J:244:TRP:HZ3	3:J:325:VAL:HB	1.80	0.47
3:J:259:ASP:HB3	3:J:282:HIS:CD2	2.50	0.47
3:J:537:LYS:NZ	3:J:539:GLU:HB2	2.29	0.47
3:J:684:PHE:HA	3:J:687:TYR:HB3	1.97	0.47
2:B:184:VAL:HG23	3:I:39:LEU:HD23	1.96	0.47
2:B:479:LEU:HA	2:B:482:CYS:HB3	1.97	0.47
2:D:116:ASP:OD1	2:D:117:GLU:N	2.47	0.47
2:D:183:LEU:HD22	2:D:187:TYR:CE2	2.49	0.47
2:D:214:LYS:HZ2	2:D:216:LEU:HA	1.80	0.47
2:D:252:TYR:OH	2:D:256:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:261:ILE:H	2:H:261:ILE:HD12	1.80	0.47
3:I:139:TYR:HA	3:I:162:LYS:HA	1.97	0.47
3:I:388:VAL:HG21	3:I:426:VAL:HG11	1.96	0.47
3:I:535:TYR:CZ	3:I:578:GLU:HG3	2.50	0.47
3:I:726:ILE:HA	3:I:756:GLN:HB3	1.97	0.47
3:J:104:VAL:HB	3:J:118:ILE:HB	1.97	0.47
3:J:148:PRO:HB3	3:J:153:SER:O	2.15	0.47
3:J:235:GLU:O	3:J:236:ILE:HD13	2.15	0.47
3:J:391:ILE:HG13	3:J:393:GLN:HE22	1.79	0.47
2:B:111:ILE:HD12	2:B:114:TYR:HB3	1.96	0.47
2:F:116:ASP:OD1	2:F:117:GLU:N	2.48	0.47
1:G:150:ASP:OD2	1:G:151:GLY:N	2.48	0.47
2:H:131:CYS:SG	2:H:132:CYS:N	2.88	0.47
2:H:196:SER:O	2:H:199:THR:HG22	2.15	0.47
3:I:450:ARG:HH21	3:I:578:GLU:HG2	1.80	0.47
1:A:215:ASN:O	1:A:218:ARG:NH2	2.48	0.47
2:D:399:VAL:CG1	2:D:400:PRO:HD3	2.45	0.47
2:F:66:LEU:HD21	2:F:84:PHE:CZ	2.49	0.47
2:H:86:ARG:NH2	2:H:117:GLU:OE2	2.48	0.47
3:I:230:TRP:O	3:I:234:GLU:HB2	2.15	0.47
3:I:617:ARG:HE	3:I:617:ARG:HB3	1.55	0.47
3:J:95:PHE:CZ	3:J:503:VAL:HG21	2.50	0.47
3:J:261:ARG:NH2	3:J:290:ASN:O	2.48	0.47
1:A:145:TYR:HE2	2:B:21:PRO:HB2	1.79	0.47
2:B:470:SER:O	2:B:471:LEU:HG	2.15	0.47
2:D:196:SER:O	2:D:200:ASN:ND2	2.48	0.47
2:D:267:ILE:HG13	2:D:268:MET:N	2.30	0.47
1:G:72:LYS:HE3	1:G:77:SER:HB3	1.96	0.47
3:I:385:PHE:O	3:I:405:SER:N	2.44	0.47
3:I:426:VAL:HG13	3:I:441:PHE:CD2	2.50	0.47
3:J:721:GLN:OE1	3:J:721:GLN:N	2.30	0.47
2:D:216:LEU:HD23	2:D:220:GLU:HG3	1.98	0.46
2:D:326:PHE:O	2:D:330:MET:HG2	2.14	0.46
1:E:134:VAL:HG21	1:E:217:MET:CE	2.45	0.46
2:H:166:ARG:NH1	2:H:247:ALA:HA	2.28	0.46
3:I:427:THR:H	3:I:443:SER:HA	1.80	0.46
3:I:726:ILE:HA	3:I:756:GLN:CG	2.45	0.46
1:A:137:LYS:O	1:A:141:THR:HG23	2.15	0.46
2:D:184:VAL:HG23	3:J:39:LEU:HG	1.97	0.46
2:D:339:MET:HE1	2:D:375:PRO:HB3	1.98	0.46
2:D:412:GLN:NE2	2:D:413:ASN:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:PHE:HB2	1:E:191:GLN:NE2	2.29	0.46
2:F:377:THR:OG1	2:F:380:GLY:N	2.49	0.46
2:H:37:ARG:HG2	2:H:55:ARG:HH22	1.80	0.46
2:H:343:GLU:OE2	2:H:375:PRO:HA	2.15	0.46
3:I:158:TYR:HD2	3:I:181:LEU:HD12	1.80	0.46
3:I:193:LEU:HD12	3:I:193:LEU:O	2.16	0.46
3:I:670:GLN:HE21	3:I:719:GLU:HG3	1.81	0.46
3:J:241:ILE:HG22	3:J:243:HIS:H	1.80	0.46
3:J:519:GLU:HA	3:J:522:GLN:HB3	1.98	0.46
3:J:650:LYS:HE3	3:J:678:LEU:HD23	1.97	0.46
3:J:655:TYR:CE2	3:J:711:LEU:HD21	2.50	0.46
1:C:53:LEU:HD11	1:C:120:GLU:HB3	1.96	0.46
2:D:343:GLU:OE2	2:D:377:THR:N	2.47	0.46
2:F:398:PRO:O	2:F:401:VAL:HG22	2.14	0.46
2:H:44:LEU:HB2	2:H:51:PHE:HB2	1.96	0.46
3:I:461:ASP:OD1	3:I:461:ASP:N	2.48	0.46
3:J:694:ARG:HB3	3:J:695:TYR:CE2	2.51	0.46
2:B:48:GLY:HA3	2:D:51:PHE:HA	1.98	0.46
3:I:88:LYS:HZ2	3:I:481:SER:HB3	1.80	0.46
3:J:288:SER:O	3:J:689:SER:OG	2.33	0.46
3:J:713:HIS:CE1	3:J:714:ARG:HH11	2.33	0.46
2:B:293:ARG:O	2:B:296:ARG:NE	2.40	0.46
2:F:290:ARG:HA	2:F:293:ARG:NH1	2.30	0.46
3:I:431:SER:HB3	3:I:482:PHE:HB2	1.97	0.46
3:I:536:ARG:NH2	3:I:637:GLU:OE1	2.34	0.46
3:J:109:VAL:HG13	3:J:512:MET:HG3	1.98	0.46
3:J:174:PRO:HD2	3:J:202:TYR:CD1	2.50	0.46
3:J:201:ILE:HD12	3:J:215:VAL:HG21	1.98	0.46
3:J:283:TYR:OH	3:J:686:LEU:O	2.33	0.46
3:J:493:CYS:SG	3:J:494:GLU:N	2.88	0.46
2:D:167:GLN:O	2:D:171:ARG:HG3	2.16	0.46
2:D:278:ASN:HA	2:D:281:ASP:CB	2.45	0.46
2:D:410:TYR:O	2:D:414:GLN:HG2	2.15	0.46
2:D:473:GLU:O	2:D:477:HIS:HB2	2.16	0.46
1:E:180:ASP:O	1:E:183:ARG:HB2	2.15	0.46
1:G:117:VAL:HG13	1:G:118:LYS:N	2.30	0.46
3:I:144:TYR:CE1	3:I:157:TYR:HB2	2.50	0.46
3:I:188:PRO:HD3	3:I:245:TRP:CD2	2.50	0.46
3:I:275:TYR:CZ	3:J:285:LYS:HG3	2.51	0.46
3:I:388:VAL:HG21	3:I:426:VAL:CG1	2.46	0.46
3:J:186:TRP:CZ3	3:J:193:LEU:HD23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:549:ILE:HG12	3:J:597:VAL:HG22	1.98	0.46
1:A:81:ASN:O	1:A:84:THR:OG1	2.32	0.46
1:A:218:ARG:HH12	2:B:28:PRO:HD2	1.81	0.46
2:B:414:GLN:O	2:B:418:LYS:HG3	2.15	0.46
1:E:146:ASP:CG	1:E:151:GLY:H	2.18	0.46
2:F:92:ARG:O	2:F:96:ASN:ND2	2.49	0.46
1:G:153:ILE:HG23	1:G:157:GLU:HG2	1.97	0.46
2:H:361:THR:O	2:H:364:THR:OG1	2.24	0.46
3:I:419:ILE:HG23	3:I:462:PHE:HB3	1.97	0.46
3:I:476:THR:H	3:I:496:PRO:HD3	1.81	0.46
3:I:656:LEU:O	3:I:660:ILE:N	2.48	0.46
3:I:775:SER:HA	3:I:778:ILE:HB	1.97	0.46
3:J:164:PRO:HG2	3:J:165:HIS:CD2	2.50	0.46
3:J:326:LYS:HD2	3:J:377:VAL:HA	1.96	0.46
2:B:166:ARG:HH21	2:B:251:ARG:NH2	2.14	0.46
1:C:207:LEU:O	1:C:211:GLN:NE2	2.49	0.46
1:E:166:TYR:HA	1:E:169:MET:CG	2.44	0.46
2:F:86:ARG:HH12	2:H:99:ARG:HB3	1.80	0.46
1:G:129:LEU:HD11	1:G:140:TRP:CD2	2.50	0.46
1:G:189:PHE:HE2	1:G:201:VAL:HG21	1.79	0.46
2:H:138:ASP:OD1	2:H:141:ARG:NH1	2.48	0.46
3:I:775:SER:O	3:I:779:ILE:HG12	2.16	0.46
3:J:218:GLY:N	3:J:225:ASN:HD21	2.13	0.46
3:J:342:GLN:OE1	3:J:694:ARG:NE	2.37	0.46
3:J:450:ARG:NE	3:J:476:THR:HG21	2.31	0.46
1:A:223:PHE:HD2	2:B:17:ILE:HD11	1.80	0.46
1:C:118:LYS:NZ	1:C:120:GLU:OE1	2.36	0.46
2:D:142:GLU:O	2:D:145:GLU:HG3	2.16	0.46
3:I:95:PHE:CE2	3:I:515:LEU:HD11	2.51	0.46
3:I:181:LEU:HD23	3:I:197:PHE:CD2	2.51	0.46
3:I:293:ILE:HG21	3:I:322:ILE:H	1.81	0.46
3:I:419:ILE:HA	3:I:462:PHE:HB3	1.97	0.46
3:I:711:LEU:O	3:I:715:VAL:N	2.26	0.46
3:J:285:LYS:HD3	3:J:685:LYS:NZ	2.29	0.46
3:J:485:ASN:HD21	3:J:488:PHE:HE2	1.60	0.46
1:A:162:VAL:HG23	1:A:182:PRO:HB3	1.98	0.46
1:A:207:LEU:O	1:A:211:GLN:HG2	2.16	0.46
2:B:179:SER:OG	2:B:180:THR:N	2.49	0.46
2:B:183:LEU:HD13	3:I:35:ILE:HG21	1.98	0.46
2:B:475:GLN:HB3	2:D:13:ARG:NH2	2.31	0.46
2:D:134:GLU:OE1	2:D:134:GLU:N	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:GLU:C	1:E:182:PRO:HD2	2.36	0.46
2:F:62:PRO:HA	2:F:67:GLY:C	2.36	0.46
2:F:263:ASP:O	2:F:267:ILE:HG12	2.15	0.46
2:H:355:PRO:HA	2:H:358:PHE:HD2	1.79	0.46
3:I:451:ARG:HD2	3:I:451:ARG:N	2.30	0.46
3:J:689:SER:O	3:J:692:SER:OG	2.27	0.46
2:F:357:SER:O	2:F:357:SER:OG	2.33	0.45
1:G:67:LEU:HD21	1:G:122:PHE:HE2	1.80	0.45
3:I:199:ASN:ND2	3:I:218:GLY:HA3	2.30	0.45
3:I:252:LEU:O	3:I:298:ILE:N	2.45	0.45
3:I:439:ILE:HG22	3:I:456:ALA:O	2.16	0.45
3:I:488:PHE:HD1	3:I:505:ASN:HA	1.82	0.45
1:A:138:LEU:HD13	1:A:138:LEU:HA	1.82	0.45
2:B:143:ASN:O	2:B:147:LEU:HG	2.17	0.45
2:B:475:GLN:HB3	2:D:13:ARG:HH22	1.82	0.45
2:D:193:ILE:O	2:D:197:VAL:HG13	2.16	0.45
2:D:365:MET:HG3	2:D:391:GLY:CA	2.46	0.45
1:E:148:ASN:ND2	1:E:152:TYR:O	2.35	0.45
2:F:201:VAL:HG13	2:H:354:ILE:HG21	1.97	0.45
2:H:58:LEU:HD22	2:H:66:LEU:HD12	1.98	0.45
2:H:260:SER:O	2:H:264:VAL:HG13	2.17	0.45
2:H:261:ILE:HA	2:H:264:VAL:HG22	1.99	0.45
3:I:139:TYR:CB	3:I:207:VAL:HG21	2.47	0.45
3:J:645:VAL:HB	3:J:672:PHE:HA	1.97	0.45
1:A:131:ARG:HA	1:A:224:GLN:HB3	1.98	0.45
1:A:150:ASP:OD1	1:A:151:GLY:N	2.48	0.45
2:B:229:LEU:HA	2:B:229:LEU:HD23	1.72	0.45
1:E:171:LYS:HG3	1:E:172:TYR:N	2.31	0.45
3:J:393:GLN:HG3	3:J:399:PHE:HB2	1.97	0.45
3:J:501:VAL:HG23	3:J:516:GLU:O	2.17	0.45
1:A:130:LEU:O	1:A:224:GLN:HB3	2.17	0.45
1:C:138:LEU:HA	1:C:141:THR:HG22	1.97	0.45
2:D:221:ARG:HG2	2:D:222:TYR:CE1	2.51	0.45
2:D:306:GLY:O	2:D:309:ILE:HG22	2.16	0.45
2:F:200:ASN:HA	2:F:203:GLU:OE2	2.17	0.45
2:H:238:THR:O	2:H:242:LEU:HG	2.17	0.45
3:I:148:PRO:HA	3:I:154:HIS:CB	2.46	0.45
3:I:245:TRP:CE3	3:I:249:GLY:HA2	2.51	0.45
3:I:467:LEU:HB3	3:I:489:PHE:CZ	2.51	0.45
2:B:97:PHE:HA	2:B:102:LYS:O	2.17	0.45
2:D:115:ASP:OD2	2:D:140:LYS:NZ	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:LYS:HD3	2:F:36:LYS:HA	1.71	0.45
1:G:215:ASN:HB3	1:G:218:ARG:HH21	1.82	0.45
3:I:136:ASP:OD1	3:I:136:ASP:N	2.43	0.45
3:I:543:TYR:CB	3:I:611:LEU:HD13	2.46	0.45
3:I:648:PHE:CD2	3:I:782:PHE:HE2	2.32	0.45
3:J:400:TYR:O	3:J:426:VAL:N	2.46	0.45
1:A:74:GLU:HG2	2:B:8:TRP:HE1	1.81	0.45
1:A:192:LYS:HE3	1:A:192:LYS:HB2	1.75	0.45
2:D:163:LEU:N	2:D:167:GLN:OE1	2.50	0.45
1:G:82:GLU:O	1:G:86:LYS:HG2	2.17	0.45
2:H:133:TYR:O	2:H:136:TYR:HB3	2.16	0.45
2:H:217:PRO:HD2	2:H:220:GLU:OE2	2.16	0.45
2:H:397:LEU:HB2	2:H:398:PRO:HD3	1.98	0.45
3:I:97:TYR:O	3:I:105:ILE:N	2.45	0.45
3:I:389:ARG:O	3:I:400:TYR:HA	2.16	0.45
3:I:457:ASN:O	3:I:462:PHE:HA	2.17	0.45
3:J:403:THR:HA	3:J:418:SER:HA	1.98	0.45
3:J:450:ARG:HB3	3:J:452:HIS:NE2	2.32	0.45
3:J:602:ARG:NH2	3:J:622:LEU:HB3	2.32	0.45
3:J:619:LEU:HG	3:J:696:LEU:HD21	1.98	0.45
1:C:222:LEU:O	2:D:31:PRO:HG3	2.17	0.45
2:D:106:PRO:HG2	2:D:109:GLU:HG3	1.98	0.45
2:D:266:ALA:HB1	2:D:296:ARG:HB3	1.97	0.45
2:F:87:ASP:HB2	2:H:96:ASN:HD21	1.82	0.45
2:F:294:VAL:O	2:F:297:ILE:N	2.47	0.45
2:F:359:TRP:HA	2:F:359:TRP:CE3	2.52	0.45
2:H:86:ARG:HH21	2:H:117:GLU:CD	2.20	0.45
2:H:113:ALA:HA	2:H:116:ASP:OD2	2.17	0.45
2:H:485:LYS:HD2	2:H:486:THR:HG23	1.98	0.45
3:I:73:GLU:HA	3:I:76:PHE:CD2	2.43	0.45
3:I:227:LEU:HD13	3:I:240:HIS:NE2	2.31	0.45
3:I:623:GLU:O	3:I:626:ASP:HB2	2.17	0.45
3:J:182:GLN:NE2	3:J:199:ASN:H	2.15	0.45
3:J:363:ASP:O	3:J:369:LEU:HD11	2.16	0.45
3:J:494:GLU:OE2	3:J:579:ARG:NH2	2.39	0.45
1:C:129:LEU:HD21	1:C:140:TRP:CH2	2.52	0.45
1:E:95:HIS:O	1:E:170:GLY:HA2	2.16	0.45
2:H:192:PHE:CD2	2:H:236:ILE:HG21	2.51	0.45
3:I:505:ASN:HB2	3:I:512:MET:SD	2.57	0.45
3:J:209:LYS:HG2	3:J:210:GLN:O	2.16	0.45
3:J:328:ALA:HB2	3:J:378:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:500:THR:HG23	3:J:517:ALA:HB2	1.98	0.45
3:J:540:VAL:HG22	3:J:541:GLU:H	1.81	0.45
3:J:617:ARG:HH12	3:J:704:ARG:HB3	1.80	0.45
2:B:62:PRO:HA	2:B:67:GLY:C	2.38	0.45
2:B:92:ARG:HH11	2:H:88:PRO:HG2	1.82	0.45
1:C:86:LYS:HD3	1:C:102:ALA:HB3	1.97	0.45
1:C:114:THR:HG22	1:C:115:GLY:N	2.32	0.45
2:D:230:ASP:O	2:D:234:VAL:HG12	2.17	0.45
2:F:140:LYS:HB2	2:F:140:LYS:HE2	1.60	0.45
3:I:71:THR:O	3:I:587:VAL:HG22	2.17	0.45
3:I:323:THR:HG21	3:I:372:GLN:HB3	1.98	0.45
3:J:215:VAL:HG12	3:J:225:ASN:ND2	2.31	0.45
3:J:493:CYS:HB3	3:J:500:THR:O	2.16	0.45
3:J:589:VAL:HG13	3:J:594:ALA:O	2.17	0.45
2:B:75:PHE:HB2	2:B:82:TYR:CE1	2.52	0.45
2:B:163:LEU:O	2:B:168:THR:OG1	2.26	0.45
2:B:170:TRP:O	2:B:174:GLU:OE1	2.35	0.45
2:B:181:LEU:HA	2:B:184:VAL:HG12	1.99	0.45
2:F:111:ILE:HG13	2:F:115:ASP:OD2	2.17	0.45
2:H:4:GLY:HA3	2:H:56:THR:HB	1.98	0.45
2:H:76:ASN:N	2:H:81:GLU:O	2.41	0.45
3:I:146:VAL:HA	3:I:155:THR:O	2.17	0.45
3:I:771:LYS:HD2	3:I:771:LYS:HA	1.81	0.45
3:J:89:TRP:HH2	3:J:109:VAL:HG23	1.82	0.45
3:J:96:ILE:HD11	3:J:104:VAL:HG12	1.99	0.45
3:J:160:LEU:HG	3:J:171:LEU:HB2	1.99	0.45
2:B:131:CYS:HB2	2:H:110:CYS:SG	2.57	0.44
2:D:76:ASN:O	2:D:80:LYS:N	2.50	0.44
1:E:62:ARG:HD2	1:E:62:ARG:HA	1.85	0.44
1:E:64:LEU:O	1:E:67:LEU:HG	2.17	0.44
1:E:150:ASP:OD1	1:E:152:TYR:N	2.42	0.44
2:F:175:ASN:OD1	2:F:177:HIS:HB2	2.16	0.44
2:F:271:TYR:HA	2:F:274:LEU:HD12	1.98	0.44
3:J:153:SER:CB	3:J:240:HIS:HB3	2.47	0.44
3:J:269:THR:HB	3:J:277:THR:O	2.17	0.44
2:B:131:CYS:SG	2:B:132:CYS:N	2.90	0.44
2:B:263:ASP:O	2:B:267:ILE:HG12	2.17	0.44
1:C:82:GLU:HB3	1:C:86:LYS:HE2	1.98	0.44
2:D:108:TYR:O	2:F:107:ARG:NH1	2.50	0.44
1:E:159:MET:HA	1:E:162:VAL:HG12	1.99	0.44
2:F:70:GLU:HB2	2:F:73:PHE:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:283:SER:HA	2:F:286:PHE:CE1	2.52	0.44
2:F:329:THR:O	2:F:333:ILE:HG12	2.18	0.44
2:F:417:ASP:OD1	2:F:418:LYS:N	2.50	0.44
1:G:146:ASP:OD2	1:G:151:GLY:N	2.45	0.44
2:H:419:ARG:CZ	2:H:419:ARG:HB2	2.46	0.44
1:C:117:VAL:HG13	1:C:118:LYS:N	2.31	0.44
1:C:171:LYS:HG3	1:C:172:TYR:N	2.33	0.44
2:D:408:ARG:NH2	2:D:409:ILE:HG12	2.33	0.44
2:H:39:ASP:OD2	2:H:56:THR:N	2.30	0.44
2:H:176:PRO:HB2	2:H:183:LEU:HD23	1.99	0.44
3:I:323:THR:O	3:I:373:ASN:ND2	2.51	0.44
3:J:163:ILE:HA	3:J:164:PRO:HA	1.78	0.44
3:J:229:ASP:OD2	3:J:259:ASP:N	2.49	0.44
3:J:522:GLN:NE2	3:J:526:ASN:OD1	2.50	0.44
3:J:622:LEU:HA	3:J:625:LYS:HD2	1.99	0.44
3:J:650:LYS:CB	3:J:678:LEU:HB3	2.44	0.44
2:B:99:ARG:NH1	2:H:47:SER:OG	2.51	0.44
2:D:309:ILE:O	2:D:313:THR:HG23	2.17	0.44
1:G:58:ASN:ND2	1:G:131:ARG:O	2.51	0.44
3:I:789:GLN:HG2	3:I:790:ASP:N	2.31	0.44
3:J:133:ILE:HG23	3:J:139:TYR:O	2.17	0.44
3:J:136:ASP:OD2	3:J:191:GLN:HB3	2.17	0.44
3:J:408:GLN:HB2	3:J:411:SER:CB	2.46	0.44
3:J:602:ARG:CZ	3:J:622:LEU:HB3	2.47	0.44
3:J:698:LEU:HD12	3:J:701:LEU:HD12	1.99	0.44
1:A:75:CYS:O	1:A:77:SER:N	2.46	0.44
1:C:190:PHE:O	1:C:194:ASP:N	2.47	0.44
2:F:193:ILE:HG21	2:F:299:LYS:HB2	2.00	0.44
1:G:181:THR:O	1:G:185:HIS:N	2.38	0.44
3:I:182:GLN:NE2	3:I:196:ILE:HG22	2.32	0.44
3:I:419:ILE:HG12	3:I:462:PHE:CD1	2.52	0.44
3:J:155:THR:HG22	3:J:180:LYS:HE3	2.00	0.44
3:J:317:MET:HE1	3:J:339:ASN:HB3	1.99	0.44
2:B:219:GLY:HA2	2:B:226:PHE:HD2	1.82	0.44
2:B:306:GLY:HA3	2:D:323:PHE:CE1	2.53	0.44
2:D:180:THR:HG23	3:J:35:ILE:HG12	1.99	0.44
1:E:137:LYS:HD3	1:E:220:LEU:HG	1.98	0.44
1:E:146:ASP:OD1	1:E:152:TYR:N	2.50	0.44
1:E:165:ILE:HG12	2:F:19:TRP:CE2	2.53	0.44
2:F:108:TYR:CD2	2:H:108:TYR:HE1	2.36	0.44
2:F:176:PRO:O	2:F:183:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:PHE:HD2	1:G:190:PHE:CD2	2.36	0.44
3:I:244:TRP:CD2	3:I:325:VAL:HB	2.53	0.44
3:I:472:VAL:HG22	3:I:511:ARG:NH2	2.30	0.44
3:I:699:HIS:HB2	3:I:706:TYR:CZ	2.53	0.44
3:J:360:LYS:HD3	3:J:360:LYS:HA	1.70	0.44
3:J:393:GLN:N	3:J:397:GLY:O	2.49	0.44
3:J:537:LYS:O	3:J:538:ILE:HD13	2.18	0.44
3:J:590:SER:OG	3:J:591:SER:N	2.50	0.44
1:A:67:LEU:HD23	2:B:1:MET:H3	1.81	0.44
2:B:388:SER:O	2:B:392:VAL:HG23	2.18	0.44
2:D:470:SER:O	2:D:471:LEU:HG	2.18	0.44
1:E:185:HIS:HA	1:E:188:VAL:HG12	2.00	0.44
2:F:293:ARG:HG2	2:F:296:ARG:NH2	2.33	0.44
3:I:230:TRP:O	3:I:234:GLU:OE1	2.36	0.44
3:I:369:LEU:HB2	3:I:372:GLN:NE2	2.33	0.44
3:I:496:PRO:HA	3:I:578:GLU:O	2.18	0.44
2:F:200:ASN:HD21	2:F:293:ARG:HB3	1.83	0.44
2:F:253:ARG:NH2	2:F:256:ARG:HD2	2.32	0.44
2:F:263:ASP:OD1	2:F:302:ARG:NH1	2.51	0.44
2:H:286:PHE:CD2	2:H:290:ARG:HD2	2.52	0.44
2:H:411:HIS:HB3	2:H:415:ARG:HH22	1.83	0.44
3:I:87:ALA:O	3:I:490:LEU:HD13	2.18	0.44
3:I:274:VAL:CB	3:J:285:LYS:HE2	2.39	0.44
3:I:472:VAL:HG13	3:I:511:ARG:NH2	2.33	0.44
3:J:440:TYR:HB3	3:J:453:LEU:HD11	2.00	0.44
1:C:101:TYR:HB3	1:C:168:MET:HE1	2.00	0.44
2:D:165:PHE:O	2:D:169:MET:HG2	2.18	0.44
2:D:214:LYS:NZ	2:D:216:LEU:HA	2.33	0.44
2:F:17:ILE:HA	2:F:20:MET:HG2	2.00	0.44
2:H:185:PHE:HA	2:H:188:VAL:HG12	2.00	0.44
3:I:89:TRP:HZ2	3:I:490:LEU:N	2.16	0.44
3:I:193:LEU:N	3:I:204:CYS:O	2.48	0.44
3:I:494:GLU:HB3	3:I:499:PRO:HG3	1.98	0.44
3:I:696:LEU:HD22	3:I:705:ALA:HB1	2.00	0.44
3:J:162:LYS:HB3	3:J:165:HIS:O	2.17	0.44
3:J:226:GLY:HA2	3:J:254:TYR:HB2	1.99	0.44
3:J:324:MET:SD	3:J:376:PRO:HD2	2.58	0.44
3:J:684:PHE:HB2	3:J:706:TYR:CD1	2.53	0.44
2:B:111:ILE:HD12	2:B:111:ILE:HA	1.77	0.43
2:B:405:ASN:ND2	2:B:408:ARG:HH21	2.04	0.43
1:C:97:ASP:HB3	1:C:167:ASP:OD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:PRO:HD3	2:F:353:SER:HB3	1.99	0.43
1:E:106:PHE:HZ	1:E:116:SER:HA	1.83	0.43
2:F:146:ARG:O	2:F:419:ARG:NH1	2.51	0.43
2:F:282:VAL:HG22	2:F:284:GLY:H	1.82	0.43
2:H:94:VAL:HG21	2:H:121:TYR:CD2	2.52	0.43
2:H:360:TYR:CZ	2:H:364:THR:HG21	2.53	0.43
3:I:215:VAL:HG21	3:I:254:TYR:CE1	2.53	0.43
3:I:220:GLU:H	3:I:220:GLU:HG2	1.59	0.43
3:I:244:TRP:HB2	3:I:253:ALA:HB3	2.00	0.43
3:I:333:VAL:HG13	3:I:333:VAL:O	2.18	0.43
3:J:130:ARG:HH22	3:J:184:ALA:HB3	1.83	0.43
3:J:228:SER:HA	3:J:257:ILE:CD1	2.46	0.43
3:J:320:TYR:CE2	3:J:322:ILE:HG13	2.49	0.43
3:J:354:THR:HG23	3:J:356:VAL:HG12	1.99	0.43
3:J:436:ARG:NH2	3:J:487:ASP:HA	2.26	0.43
1:A:202:THR:H	1:A:205:GLU:HB3	1.84	0.43
1:A:204:ASP:OD1	1:A:205:GLU:N	2.51	0.43
2:B:165:PHE:O	2:B:169:MET:HG2	2.18	0.43
2:D:95:LEU:O	2:D:99:ARG:HG3	2.18	0.43
2:H:199:THR:O	2:H:203:GLU:HG3	2.18	0.43
3:I:48:LEU:HA	3:I:51:THR:HB	1.99	0.43
3:I:69:LYS:HB3	3:I:591:SER:HA	2.00	0.43
3:I:79:ASP:O	3:I:521:VAL:HG22	2.18	0.43
3:I:92:ASN:HB3	3:I:485:ASN:CG	2.38	0.43
3:I:441:PHE:HD2	3:I:443:SER:HB3	1.82	0.43
2:B:193:ILE:HD11	2:B:297:ILE:HA	2.00	0.43
1:C:181:THR:OG1	1:C:182:PRO:HD3	2.18	0.43
2:F:144:ALA:O	2:F:148:MET:HG3	2.18	0.43
1:G:69:ARG:NH2	2:H:56:THR:OG1	2.52	0.43
1:G:183:ARG:NH2	1:G:187:ASP:OD2	2.51	0.43
3:I:146:VAL:CG2	3:I:154:HIS:HB2	2.49	0.43
3:I:501:VAL:O	3:I:515:LEU:HB2	2.18	0.43
3:J:93:LYS:HG2	3:J:488:PHE:CE2	2.53	0.43
3:J:312:PRO:HD3	3:J:337:TRP:NE1	2.34	0.43
3:J:337:TRP:HZ2	3:J:357:CYS:SG	2.41	0.43
3:J:731:ASP:OD1	3:J:734:ILE:N	2.51	0.43
2:B:354:ILE:HG22	2:B:358:PHE:CE1	2.53	0.43
2:B:485:LYS:HD2	2:B:486:THR:HG23	2.00	0.43
1:C:158:MET:O	1:C:162:VAL:HG13	2.18	0.43
2:D:108:TYR:CD2	2:F:108:TYR:HE1	2.36	0.43
2:D:359:TRP:HD1	2:D:373:MET:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:MET:HA	1:E:161:ILE:HD12	2.00	0.43
2:F:238:THR:HG21	2:F:271:TYR:OH	2.18	0.43
2:F:258:VAL:HA	2:F:261:ILE:HD12	1.99	0.43
1:G:82:GLU:HG3	1:G:106:PHE:CG	2.54	0.43
3:I:158:TYR:OH	3:I:183:TYR:HA	2.18	0.43
3:I:312:PRO:HG2	3:I:317:MET:HB2	2.00	0.43
3:I:432:TYR:CE1	3:I:437:ASN:HA	2.53	0.43
3:I:448:PRO:C	3:I:574:GLN:HE22	2.21	0.43
3:I:531:PRO:HA	3:I:551:LYS:O	2.18	0.43
3:I:571:PRO:HD2	3:I:691:PHE:HZ	1.84	0.43
3:J:477:TYR:OH	3:J:578:GLU:N	2.28	0.43
1:A:121:ASP:HA	1:A:124:THR:OG1	2.18	0.43
2:D:144:ALA:O	2:D:148:MET:HG2	2.18	0.43
1:E:147:ILE:HD11	1:E:161:ILE:HD11	2.00	0.43
2:F:33:ASP:OD2	2:F:36:LYS:NZ	2.41	0.43
2:F:90:VAL:HG21	2:F:117:GLU:HG3	2.00	0.43
3:I:104:VAL:HB	3:I:118:ILE:HD12	2.00	0.43
3:I:312:PRO:HD3	3:I:337:TRP:CE2	2.53	0.43
3:J:140:VAL:HG13	3:J:163:ILE:CG1	2.48	0.43
3:J:144:TYR:HE1	3:J:159:VAL:HG23	1.82	0.43
1:C:77:SER:O	1:C:77:SER:OG	2.32	0.43
2:D:260:SER:O	2:D:264:VAL:HG13	2.18	0.43
1:E:109:PHE:CZ	1:E:122:PHE:HA	2.53	0.43
2:H:137:LYS:HB3	2:H:141:ARG:NH2	2.33	0.43
3:I:122:LYS:NZ	3:I:164:PRO:O	2.34	0.43
3:I:251:ARG:HB3	3:I:297:VAL:HG13	2.01	0.43
3:J:45:ILE:HG13	3:J:46:CYS:N	2.33	0.43
3:J:232:TYR:CE2	3:J:291:PRO:HD2	2.53	0.43
3:J:283:TYR:HE2	3:J:285:LYS:HG2	1.81	0.43
3:J:597:VAL:HG21	3:J:634:MET:SD	2.59	0.43
1:A:53:LEU:HD12	1:A:120:GLU:HG2	2.00	0.43
1:A:57:THR:HG22	1:A:58:ASN:N	2.34	0.43
2:D:135:GLU:HA	2:D:138:ASP:OD2	2.17	0.43
2:D:185:PHE:O	2:D:189:THR:HG22	2.18	0.43
2:H:294:VAL:O	2:H:297:ILE:HG22	2.19	0.43
3:I:75:LEU:HD11	3:I:584:TRP:HA	2.01	0.43
3:I:401:HIS:CG	3:I:421:SER:HA	2.54	0.43
3:J:151:GLN:HG3	3:J:764:TYR:HE2	1.84	0.43
3:J:153:SER:CA	3:J:240:HIS:HB3	2.48	0.43
3:J:226:GLY:CA	3:J:254:TYR:HB2	2.48	0.43
3:J:309:MET:O	3:J:337:TRP:HH2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:540:VAL:HG12	3:J:543:TYR:O	2.19	0.43
2:B:50:ARG:HD2	2:B:52:GLN:NE2	2.34	0.43
1:C:79:VAL:HG22	1:C:118:LYS:HA	1.99	0.43
2:D:109:GLU:C	2:F:107:ARG:HH22	2.22	0.43
2:D:359:TRP:HB3	2:D:373:MET:HE1	2.00	0.43
2:H:19:TRP:HB2	2:H:20:MET:CE	2.48	0.43
2:H:286:PHE:CE2	2:H:290:ARG:HD2	2.54	0.43
3:I:149:VAL:O	3:I:150:TYR:HD1	2.02	0.43
3:I:254:TYR:HE2	3:I:256:THR:OG1	2.01	0.43
3:J:231:LEU:HD23	3:J:290:ASN:HA	2.01	0.43
3:J:255:ALA:CB	3:J:257:ILE:HD11	2.49	0.43
3:J:316:ARG:NE	3:J:344:VAL:HG11	2.34	0.43
3:J:522:GLN:O	3:J:526:ASN:ND2	2.52	0.43
3:J:582:VAL:O	3:J:582:VAL:HG13	2.18	0.43
1:A:57:THR:HG22	1:A:59:PHE:H	1.83	0.43
2:B:49:ARG:HB2	2:D:49:ARG:HH21	1.83	0.43
2:D:96:ASN:HA	2:D:99:ARG:HH11	1.84	0.43
2:F:185:PHE:O	2:F:189:THR:HG22	2.19	0.43
2:H:177:HIS:CD2	2:H:183:LEU:HD21	2.54	0.43
3:I:95:PHE:HE1	3:I:109:VAL:HG22	1.83	0.43
3:I:151:GLN:NE2	3:I:233:GLU:HG2	2.34	0.43
3:I:447:LEU:HD23	3:I:450:ARG:HD3	2.01	0.43
3:I:572:GLY:HA2	3:I:612:LEU:HD13	2.00	0.43
3:J:213:ARG:HE	3:J:213:ARG:HB3	1.68	0.43
3:J:334:ALA:HB2	3:J:378:PHE:CE2	2.54	0.43
2:B:42:ILE:HD11	2:B:55:ARG:HG3	2.00	0.43
1:C:128:ILE:HA	1:C:132:GLY:HA3	2.01	0.43
2:H:148:MET:O	2:H:419:ARG:NH1	2.36	0.43
3:I:96:ILE:HG21	3:I:133:ILE:HG21	1.99	0.43
3:I:140:VAL:HG12	3:I:161:SER:O	2.19	0.43
3:I:476:THR:N	3:I:496:PRO:HD3	2.34	0.43
3:I:484:HIS:CD2	3:I:484:HIS:H	2.35	0.43
3:I:564:LEU:HD13	3:I:588:LEU:CD2	2.45	0.43
3:J:312:PRO:HB3	3:J:348:THR:HG21	2.01	0.43
3:J:478:VAL:HB	3:J:491:LEU:HD22	2.00	0.43
3:J:655:TYR:HB2	3:J:681:ILE:O	2.19	0.43
2:B:222:TYR:CD1	2:B:222:TYR:N	2.87	0.42
2:B:299:LYS:HE2	2:B:299:LYS:HB3	1.78	0.42
1:C:111:THR:OG1	1:C:121:ASP:OD2	2.30	0.42
1:E:168:MET:HB3	1:E:168:MET:HE2	1.77	0.42
2:F:68:SER:OG	2:F:70:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:PHE:HD1	2:F:82:TYR:CZ	2.36	0.42
1:G:146:ASP:OD2	1:G:150:ASP:N	2.52	0.42
2:H:115:ASP:OD2	2:H:140:LYS:NZ	2.49	0.42
2:H:339:MET:SD	2:H:383:PHE:HB2	2.59	0.42
2:H:358:PHE:O	2:H:361:THR:N	2.51	0.42
3:I:585:GLU:CD	3:I:596:VAL:HG11	2.39	0.42
3:I:637:GLU:HG3	3:I:640:ILE:HG12	2.01	0.42
3:I:644:ARG:HB3	3:I:786:PHE:HD1	1.84	0.42
3:I:679:SER:N	3:I:726:ILE:O	2.41	0.42
3:J:139:TYR:CZ	3:J:162:LYS:HE3	2.54	0.42
3:J:347:LEU:H	3:J:347:LEU:HD12	1.84	0.42
3:J:424:TRP:HB2	3:J:444:THR:OG1	2.19	0.42
3:J:686:LEU:HD13	3:J:737:GLN:O	2.18	0.42
1:A:57:THR:HG23	1:A:127:SER:HB3	2.01	0.42
1:A:130:LEU:O	1:A:137:LYS:NZ	2.52	0.42
2:B:47:SER:OG	2:D:99:ARG:NH2	2.52	0.42
2:B:251:ARG:O	2:B:255:ILE:HG12	2.19	0.42
2:B:268:MET:HG3	2:B:269:PRO:HD3	2.01	0.42
2:B:334:ILE:O	2:B:338:VAL:HG22	2.18	0.42
1:C:219:SER:HB3	2:D:20:MET:SD	2.60	0.42
2:D:366:THR:O	2:D:366:THR:HG22	2.18	0.42
1:E:71:PHE:CZ	1:E:80:VAL:HG13	2.54	0.42
1:E:117:VAL:HG13	1:E:118:LYS:N	2.33	0.42
2:F:6:ALA:HA	2:F:9:LEU:HD13	2.01	0.42
2:F:411:HIS:HB3	2:F:415:ARG:HH22	1.84	0.42
2:H:405:ASN:OD1	2:H:408:ARG:NH2	2.38	0.42
3:I:150:TYR:HH	3:I:281:TYR:HH	1.58	0.42
3:I:224:TYR:CD1	3:I:229:ASP:HA	2.53	0.42
3:I:319:GLU:CD	3:I:340:ARG:HD2	2.40	0.42
3:I:442:LEU:HD22	3:I:451:ARG:HB3	2.01	0.42
3:I:451:ARG:HD3	3:I:477:TYR:CE1	2.53	0.42
3:I:524:ALA:HA	3:I:527:ASP:OD2	2.18	0.42
3:J:203:TYR:CG	3:J:300:LEU:HD22	2.54	0.42
3:J:244:TRP:CZ3	3:J:325:VAL:HB	2.54	0.42
3:J:567:VAL:HG13	3:J:653:GLY:HA2	2.02	0.42
3:J:589:VAL:HA	3:J:594:ALA:N	2.19	0.42
2:B:148:MET:O	2:B:419:ARG:NH1	2.39	0.42
2:B:219:GLY:HA2	2:B:226:PHE:CD2	2.53	0.42
1:C:54:GLU:OE2	1:C:60:THR:HA	2.20	0.42
1:C:166:TYR:HD2	1:C:182:PRO:HG3	1.84	0.42
2:D:242:LEU:HD13	2:D:242:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ASP:HA	1:E:124:THR:HG22	2.00	0.42
2:F:217:PRO:HG2	2:F:220:GLU:HG2	2.01	0.42
2:H:104:HIS:O	2:H:114:TYR:OH	2.37	0.42
3:I:450:ARG:NH2	3:I:578:GLU:HG2	2.33	0.42
3:I:493:CYS:N	3:I:500:THR:O	2.41	0.42
3:I:602:ARG:NH1	3:I:622:LEU:HD22	2.33	0.42
3:J:94:GLU:OE2	3:J:106:LEU:HD21	2.20	0.42
3:J:231:LEU:O	3:J:235:GLU:HB2	2.19	0.42
3:J:259:ASP:HB2	3:J:282:HIS:CE1	2.54	0.42
3:J:285:LYS:H	3:J:288:SER:CB	2.30	0.42
3:J:307:LEU:HD13	3:J:352:ALA:O	2.19	0.42
3:J:344:VAL:HG13	3:J:364:GLU:HG2	2.00	0.42
1:A:189:PHE:CE1	1:A:193:MET:HG3	2.54	0.42
2:B:290:ARG:HA	2:B:293:ARG:NH1	2.33	0.42
2:B:382:ILE:O	2:B:386:ILE:HG13	2.19	0.42
1:E:89:TYR:HB2	2:F:11:PHE:HE2	1.84	0.42
2:F:483:LEU:HD23	2:F:483:LEU:HA	1.86	0.42
1:G:158:MET:HG3	1:G:186:VAL:HG13	2.02	0.42
2:H:45:ASN:O	2:H:84:PHE:N	2.42	0.42
3:I:160:LEU:O	3:I:169:GLN:N	2.43	0.42
3:I:199:ASN:HB3	3:I:218:GLY:O	2.19	0.42
3:I:203:TYR:CE1	3:I:205:ALA:HB2	2.54	0.42
3:I:230:TRP:CE3	3:I:231:LEU:HB2	2.55	0.42
3:I:290:ASN:HD22	3:I:340:ARG:HG3	1.85	0.42
3:I:370:HIS:CG	3:I:371:ARG:H	2.37	0.42
3:J:251:ARG:HD3	3:J:352:ALA:HB1	2.02	0.42
3:J:253:ALA:HA	3:J:296:HIS:O	2.19	0.42
3:J:326:LYS:HB2	3:J:375:GLU:CB	2.39	0.42
3:J:348:THR:HB	3:J:357:CYS:HB3	2.01	0.42
3:J:704:ARG:O	3:J:707:GLU:HG3	2.20	0.42
2:B:45:ASN:O	2:B:83:PHE:HA	2.20	0.42
1:C:63:GLU:HG2	2:D:1:MET:H1	1.84	0.42
1:C:71:PHE:CZ	1:C:119:PHE:HB2	2.54	0.42
2:D:418:LYS:NZ	2:D:422:GLN:HB2	2.34	0.42
2:F:146:ARG:HD3	2:H:130:ASP:O	2.20	0.42
2:H:75:PHE:CZ	2:H:80:LYS:HA	2.54	0.42
3:I:201:ILE:O	3:I:214:VAL:HG22	2.20	0.42
3:I:269:THR:H	3:I:278:VAL:HG12	1.83	0.42
3:I:538:ILE:HB	3:I:629:GLU:HG3	2.02	0.42
3:I:703:ASN:O	3:I:707:GLU:N	2.40	0.42
3:I:742:LEU:HD12	3:I:742:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:92:ASN:O	3:J:483:SER:HB2	2.19	0.42
3:J:197:PHE:HB3	3:J:202:TYR:HE2	1.84	0.42
3:J:368:TRP:HD1	3:J:369:LEU:O	2.02	0.42
3:J:369:LEU:HD13	3:J:372:GLN:NE2	2.35	0.42
2:B:185:PHE:O	2:B:189:THR:HG22	2.20	0.42
2:D:49:ARG:HG2	2:D:51:PHE:CZ	2.54	0.42
2:F:34:LYS:H	2:F:36:LYS:NZ	2.17	0.42
2:H:219:GLY:HA2	2:H:226:PHE:CD2	2.55	0.42
3:I:36:ALA:HA	3:I:39:LEU:HG	2.01	0.42
3:I:402:ILE:HD13	3:I:439:ILE:HD13	2.00	0.42
3:J:42:ILE:O	3:J:45:ILE:HG12	2.20	0.42
3:J:157:TYR:CE1	3:J:180:LYS:HG3	2.53	0.42
3:J:228:SER:HB3	3:J:233:GLU:HG3	2.01	0.42
3:J:264:LEU:HD23	3:J:282:HIS:CD2	2.54	0.42
3:J:289:GLU:CD	3:J:290:ASN:H	2.23	0.42
3:J:733:LYS:HG2	3:J:734:ILE:HD13	2.00	0.42
3:J:770:LEU:O	3:J:774:LEU:N	2.39	0.42
2:B:135:GLU:O	2:B:139:ARG:HG2	2.20	0.42
2:B:478:HIS:HA	2:D:29:LEU:HD23	2.02	0.42
2:D:170:TRP:CZ3	2:D:248:ALA:HA	2.55	0.42
2:D:286:PHE:O	2:D:290:ARG:HG3	2.20	0.42
2:D:309:ILE:HD11	2:D:410:TYR:HA	2.02	0.42
1:G:188:VAL:O	1:G:192:LYS:HE2	2.20	0.42
2:H:9:LEU:O	2:H:13:ARG:HG3	2.19	0.42
2:H:49:ARG:HA	2:H:49:ARG:HD2	1.86	0.42
3:I:229:ASP:HB3	3:I:257:ILE:HD13	2.02	0.42
3:I:271:THR:OG1	3:I:760:ASP:OD2	2.32	0.42
3:I:361:HIS:NE2	3:I:363:ASP:OD2	2.52	0.42
3:I:363:ASP:OD1	3:I:389:ARG:HD2	2.20	0.42
3:J:499:PRO:HB2	3:J:518:ASN:HD21	1.84	0.42
3:J:569:GLY:C	3:J:652:TYR:HB3	2.40	0.42
2:D:70:GLU:H	2:D:70:GLU:HG2	1.68	0.42
1:E:134:VAL:HG21	1:E:217:MET:HE1	2.00	0.42
1:E:159:MET:O	1:E:162:VAL:HG12	2.20	0.42
1:G:207:LEU:O	1:G:211:GLN:HG2	2.20	0.42
2:H:62:PRO:HA	2:H:67:GLY:CA	2.49	0.42
3:I:146:VAL:HG22	3:I:154:HIS:HB2	2.02	0.42
3:I:264:LEU:HA	3:I:282:HIS:CD2	2.55	0.42
3:I:283:TYR:CD2	3:I:284:PRO:HD2	2.53	0.42
3:I:284:PRO:HG2	3:I:688:ALA:HA	2.01	0.42
3:I:360:LYS:HD3	3:I:360:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:378:PHE:CD1	3:I:385:PHE:HB3	2.55	0.42
3:I:471:LEU:HD11	3:I:509:LYS:O	2.19	0.42
3:I:768:VAL:O	3:I:771:LYS:N	2.53	0.42
3:J:248:ASP:OD1	3:J:249:GLY:N	2.52	0.42
1:C:123:VAL:HA	1:C:126:LEU:HB2	2.01	0.42
1:C:195:LYS:HZ3	1:C:209:SER:HB3	1.84	0.42
2:F:47:SER:OG	2:H:99:ARG:NH2	2.41	0.42
2:F:87:ASP:HB2	2:H:96:ASN:ND2	2.35	0.42
2:H:238:THR:HG21	2:H:271:TYR:OH	2.19	0.42
3:I:141:LEU:HD22	3:I:186:TRP:CD1	2.54	0.42
3:J:257:ILE:HG13	3:J:293:ILE:HA	2.01	0.42
3:J:340:ARG:NE	3:J:693:GLU:OE2	2.39	0.42
3:J:364:GLU:H	3:J:389:ARG:NH2	2.17	0.42
3:J:720:ASP:C	3:J:752:ASN:HD21	2.23	0.42
2:D:92:ARG:HG2	2:D:96:ASN:HD21	1.85	0.42
2:D:95:LEU:HG	2:D:99:ARG:CZ	2.49	0.42
2:D:222:TYR:CD1	2:D:222:TYR:N	2.88	0.42
2:D:291:VAL:O	2:D:293:ARG:N	2.53	0.42
1:G:49:GLY:HA3	1:G:52:GLN:HG2	2.02	0.42
3:I:85:PRO:HB3	3:I:516:GLU:HG2	2.01	0.42
3:I:228:SER:HB2	3:I:240:HIS:CA	2.40	0.42
3:I:656:LEU:HA	3:I:659:TYR:HB3	2.02	0.42
3:J:348:THR:OG1	3:J:357:CYS:HB3	2.20	0.42
3:J:477:TYR:CZ	3:J:577:THR:HB	2.55	0.42
1:A:181:THR:OG1	1:A:182:PRO:HD3	2.20	0.41
2:B:52:GLN:O	2:H:47:SER:HA	2.20	0.41
2:B:240:GLU:OE2	2:B:302:ARG:NH2	2.52	0.41
1:C:153:ILE:HA	1:C:157:GLU:OE1	2.20	0.41
2:D:168:THR:HA	2:D:171:ARG:NE	2.35	0.41
2:D:388:SER:OG	2:D:389:LEU:N	2.53	0.41
2:H:350:LYS:HE3	2:H:372:ASP:O	2.20	0.41
3:I:205:ALA:HB3	3:I:209:LYS:HD3	2.02	0.41
3:I:336:THR:OG1	3:I:347:LEU:HD13	2.20	0.41
3:I:368:TRP:CZ2	3:I:613:GLN:HA	2.55	0.41
3:J:83:HIS:CG	3:J:84:ASP:N	2.88	0.41
3:J:391:ILE:HG12	3:J:401:HIS:HB2	2.01	0.41
3:J:628:MET:CE	3:J:663:ALA:HB3	2.50	0.41
1:A:199:GLY:O	1:A:200:ILE:HD13	2.20	0.41
1:A:223:PHE:HD1	2:B:13:ARG:HH11	1.68	0.41
2:B:6:ALA:HB1	2:B:9:LEU:HD12	2.02	0.41
1:C:153:ILE:HG23	1:C:157:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:THR:HB	1:C:184:GLN:HE21	1.86	0.41
1:C:223:PHE:HD1	1:C:226:VAL:HG21	1.84	0.41
2:D:146:ARG:HD2	2:F:131:CYS:O	2.20	0.41
2:D:291:VAL:O	2:D:294:VAL:HG22	2.20	0.41
2:H:103:LEU:HD12	2:H:103:LEU:HA	1.80	0.41
3:I:571:PRO:HD2	3:I:691:PHE:CE1	2.55	0.41
3:I:625:LYS:HA	3:I:628:MET:HB2	2.01	0.41
3:I:655:TYR:HB2	3:I:681:ILE:HB	2.02	0.41
3:J:81:LYS:HE2	3:J:81:LYS:HB3	1.88	0.41
3:J:251:ARG:HG2	3:J:299:GLY:HA2	2.02	0.41
3:J:252:LEU:HB3	3:J:298:ILE:CG1	2.50	0.41
3:J:311:PRO:HA	3:J:337:TRP:CE2	2.55	0.41
3:J:318:ARG:HD2	3:J:319:GLU:HB2	2.01	0.41
1:A:218:ARG:NH2	2:B:28:PRO:HD2	2.35	0.41
2:B:181:LEU:O	2:B:184:VAL:HG12	2.20	0.41
2:D:164:SER:OG	2:D:165:PHE:N	2.53	0.41
2:F:278:ASN:HA	2:F:281:ASP:HB2	2.02	0.41
1:G:158:MET:HA	1:G:161:ILE:HD12	2.01	0.41
1:G:203:LEU:HG	1:G:204:ASP:N	2.35	0.41
2:H:343:GLU:CD	2:H:375:PRO:HA	2.41	0.41
3:I:109:VAL:HG22	3:I:503:VAL:HG11	2.02	0.41
3:I:194:ILE:CG2	3:I:203:TYR:HD2	2.34	0.41
3:I:230:TRP:CZ3	3:I:231:LEU:HD13	2.56	0.41
3:I:342:GLN:HE22	3:I:690:ALA:HB1	1.84	0.41
3:J:48:LEU:HA	3:J:51:THR:HB	2.01	0.41
3:J:109:VAL:HG11	3:J:488:PHE:HB3	2.01	0.41
3:J:530:MET:HA	3:J:531:PRO:HD3	1.87	0.41
2:B:104:HIS:ND1	2:H:110:CYS:SG	2.85	0.41
2:B:202:VAL:O	2:B:205:VAL:HG12	2.20	0.41
1:E:155:LYS:HE3	1:E:186:VAL:HG23	2.02	0.41
2:F:185:PHE:HA	2:F:188:VAL:HG12	2.02	0.41
2:F:405:ASN:O	2:F:409:ILE:HG13	2.20	0.41
1:G:203:LEU:HG	1:G:204:ASP:H	1.84	0.41
2:H:258:VAL:HG23	2:H:259:MET:HG3	2.02	0.41
2:H:329:THR:O	2:H:333:ILE:HG13	2.20	0.41
3:I:206:HIS:HB2	3:I:209:LYS:HB2	2.02	0.41
3:I:472:VAL:HG23	3:I:491:LEU:HD23	2.03	0.41
3:I:548:GLN:H	3:I:576:VAL:HG22	1.85	0.41
3:J:89:TRP:CE3	3:J:483:SER:HA	2.55	0.41
3:J:141:LEU:HD21	3:J:184:ALA:HB1	2.02	0.41
2:B:166:ARG:HG2	2:B:246:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:THR:HA	1:C:87:GLN:HE21	1.85	0.41
1:C:134:VAL:O	1:C:138:LEU:HG	2.20	0.41
1:C:226:VAL:HG13	2:D:33:ASP:OD1	2.21	0.41
2:H:196:SER:HA	2:H:199:THR:HG22	2.02	0.41
3:I:214:VAL:HG11	3:I:300:LEU:HD23	2.02	0.41
3:I:677:ALA:HB1	3:I:680:PRO:HB3	2.03	0.41
3:J:39:LEU:O	3:J:43:LEU:HG	2.21	0.41
3:J:149:VAL:HG23	3:J:150:TYR:CG	2.55	0.41
3:J:534:GLU:HG2	3:J:535:TYR:N	2.34	0.41
3:J:655:TYR:HD1	3:J:656:LEU:HD23	1.85	0.41
2:B:238:THR:HG22	2:B:267:ILE:HD12	2.02	0.41
1:C:152:TYR:HB3	1:C:200:ILE:HG21	2.03	0.41
2:D:3:ALA:HA	2:D:7:ALA:HA	2.02	0.41
2:D:188:VAL:HG23	3:J:43:LEU:HD23	2.03	0.41
2:F:315:LYS:HA	2:F:315:LYS:HD3	1.89	0.41
1:G:222:LEU:HB3	2:H:31:PRO:HD3	2.02	0.41
2:H:291:VAL:O	2:H:294:VAL:HG22	2.20	0.41
3:I:34:GLY:HA2	3:I:37:ILE:HD12	2.02	0.41
3:I:42:ILE:HA	3:I:45:ILE:HD12	2.01	0.41
3:I:88:LYS:NZ	3:I:481:SER:HB3	2.34	0.41
3:I:446:ASP:OD1	3:I:452:HIS:HB2	2.21	0.41
3:J:69:LYS:HZ1	3:J:71:THR:HG22	1.84	0.41
3:J:283:TYR:CE2	3:J:285:LYS:HE3	2.55	0.41
2:B:314:LEU:HA	2:B:314:LEU:HD23	1.80	0.41
1:C:155:LYS:HE3	1:C:186:VAL:HG23	2.02	0.41
2:D:204:THR:OG1	2:F:354:ILE:HG12	2.20	0.41
2:D:415:ARG:HA	2:D:418:LYS:HB3	2.02	0.41
1:E:129:LEU:HD23	1:E:129:LEU:HA	1.89	0.41
1:E:173:THR:HG21	1:E:177:LEU:HD13	2.02	0.41
2:F:294:VAL:O	2:F:296:ARG:N	2.54	0.41
3:I:104:VAL:HG21	3:I:131:TYR:CZ	2.55	0.41
3:I:244:TRP:CZ3	3:I:295:LEU:HD11	2.55	0.41
3:I:386:PHE:CE1	3:I:458:THR:HB	2.55	0.41
3:I:630:ALA:O	3:I:634:MET:HG2	2.20	0.41
3:I:648:PHE:HD2	3:I:782:PHE:CE2	2.36	0.41
3:J:69:LYS:NZ	3:J:71:THR:HG22	2.36	0.41
3:J:109:VAL:HG11	3:J:488:PHE:CG	2.55	0.41
3:J:173:PRO:HD2	3:J:179:ALA:HB3	2.02	0.41
3:J:321:TYR:HD2	3:J:338:LEU:O	2.04	0.41
3:J:519:GLU:O	3:J:523:LYS:N	2.33	0.41
1:A:195:LYS:HE2	1:A:209:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:LEU:HB2	2:B:398:PRO:HD3	2.03	0.41
1:C:68:TYR:HD1	1:C:119:PHE:CE2	2.39	0.41
1:C:88:ILE:O	1:C:91:GLN:HG2	2.20	0.41
2:F:169:MET:HE2	2:F:247:ALA:HB2	2.03	0.41
2:F:470:SER:O	2:F:471:LEU:HG	2.21	0.41
2:H:270:TYR:OH	2:H:274:LEU:HD11	2.21	0.41
3:I:109:VAL:O	3:I:513:PHE:HE1	2.04	0.41
3:I:227:LEU:HD22	3:I:240:HIS:CD2	2.56	0.41
3:I:275:TYR:CE2	3:J:285:LYS:HG3	2.56	0.41
3:I:388:VAL:HA	3:I:401:HIS:O	2.21	0.41
3:I:426:VAL:HG13	3:I:441:PHE:HD2	1.85	0.41
3:J:85:PRO:HD2	3:J:492:LYS:NZ	2.35	0.41
3:J:235:GLU:OE2	3:J:691:PHE:HB2	2.21	0.41
3:J:424:TRP:CE2	3:J:445:GLU:HA	2.56	0.41
3:J:758:TYR:HA	3:J:759:PRO:HD3	1.98	0.41
1:A:214:ASP:OD1	1:A:215:ASN:N	2.53	0.41
1:A:226:VAL:HG11	2:B:13:ARG:NH1	2.36	0.41
2:B:41:LEU:HD22	2:H:83:PHE:CZ	2.56	0.41
2:B:56:THR:O	2:B:60:ARG:HG3	2.21	0.41
2:B:341:TYR:CD2	2:H:291:VAL:HG22	2.55	0.41
2:B:397:LEU:O	2:B:400:PRO:HD2	2.21	0.41
1:C:63:GLU:HG2	2:D:1:MET:N	2.36	0.41
2:D:35:ASN:O	2:D:37:ARG:NH1	2.53	0.41
1:E:159:MET:HG2	1:E:163:LYS:HE2	2.03	0.41
2:H:75:PHE:CE2	2:H:77:GLU:HA	2.56	0.41
2:H:87:ASP:OD1	2:H:89:GLU:N	2.40	0.41
2:H:100:THR:HB	2:H:102:LYS:NZ	2.36	0.41
2:H:383:PHE:HA	2:H:386:ILE:HG22	2.03	0.41
3:I:192:GLN:HE22	3:I:249:GLY:HA3	1.85	0.41
3:I:229:ASP:OD1	3:I:232:TYR:HD2	2.04	0.41
3:I:298:ILE:HG22	3:I:306:ASP:HA	2.03	0.41
3:I:404:VAL:O	3:I:416:ILE:HA	2.20	0.41
3:I:456:ALA:HA	3:I:463:ASN:O	2.21	0.41
3:J:199:ASN:ND2	3:J:223:ILE:O	2.54	0.41
3:J:337:TRP:O	3:J:345:SER:HA	2.20	0.41
3:J:348:THR:CB	3:J:357:CYS:HB3	2.50	0.41
3:J:378:PHE:HB3	3:J:382:GLY:HA2	2.02	0.41
3:J:385:PHE:CD2	3:J:387:PHE:HB3	2.56	0.41
3:J:622:LEU:H	3:J:622:LEU:HD12	1.85	0.41
3:J:641:ASP:OD2	3:J:643:THR:OG1	2.38	0.41
2:B:48:GLY:HA3	2:D:52:GLN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:LEU:HG	1:E:207:LEU:HD23	2.03	0.41
2:F:110:CYS:HG	2:F:112:SER:HG	1.68	0.41
1:G:97:ASP:HB3	1:G:167:ASP:OD1	2.21	0.41
1:G:98:ALA:HA	1:G:168:MET:SD	2.60	0.41
2:H:163:LEU:N	2:H:167:GLN:OE1	2.54	0.41
3:I:251:ARG:NH2	3:I:353:THR:HG22	2.36	0.41
3:J:230:TRP:CZ3	3:J:688:ALA:HB2	2.55	0.41
3:J:371:ARG:NH1	3:J:427:THR:HA	2.31	0.41
3:J:387:PHE:CE1	3:J:405:SER:HB2	2.55	0.41
3:J:683:ASP:OD2	3:J:710:LYS:HA	2.21	0.41
1:C:218:ARG:CZ	1:C:222:LEU:HD21	2.52	0.40
2:D:97:PHE:HA	2:D:102:LYS:O	2.20	0.40
2:D:110:CYS:N	2:F:107:ARG:HH12	2.19	0.40
2:D:202:VAL:HA	2:D:205:VAL:CG2	2.49	0.40
2:D:269:PRO:HA	2:D:272:ILE:HG22	2.03	0.40
1:E:98:ALA:HA	1:E:168:MET:CE	2.51	0.40
1:G:126:LEU:HD13	2:H:14:ALA:HB2	2.03	0.40
3:I:96:ILE:HA	3:I:105:ILE:O	2.21	0.40
3:I:203:TYR:CD2	3:I:300:LEU:HB3	2.56	0.40
3:I:711:LEU:HD23	3:I:711:LEU:HA	1.93	0.40
3:J:136:ASP:HB2	3:J:138:GLU:HG3	2.02	0.40
3:J:158:TYR:HE2	3:J:181:LEU:O	2.04	0.40
3:J:567:VAL:HG22	3:J:568:ASP:N	2.36	0.40
3:J:650:LYS:O	3:J:652:TYR:N	2.49	0.40
1:A:103:HIS:O	1:A:103:HIS:ND1	2.54	0.40
2:B:140:LYS:HE2	2:B:140:LYS:HB2	1.85	0.40
1:C:185:HIS:HE1	2:D:22:VAL:O	2.04	0.40
2:D:221:ARG:HG2	2:D:222:TYR:CD1	2.57	0.40
1:E:87:GLN:NE2	1:E:88:ILE:HG13	2.37	0.40
3:I:365:SER:HB3	3:I:369:LEU:HD23	2.03	0.40
3:J:232:TYR:CD2	3:J:291:PRO:HG2	2.56	0.40
3:J:236:ILE:CG2	3:J:323:THR:HG22	2.50	0.40
3:J:480:ALA:HB2	3:J:491:LEU:HG	2.03	0.40
3:J:494:GLU:HG3	3:J:579:ARG:HE	1.85	0.40
3:J:538:ILE:N	3:J:545:LEU:O	2.38	0.40
3:J:736:PHE:O	3:J:739:THR:OG1	2.23	0.40
1:A:82:GLU:HG3	1:A:106:PHE:CD2	2.56	0.40
1:C:86:LYS:HD2	1:C:99:SER:OG	2.21	0.40
2:D:56:THR:HA	2:D:59:GLU:HG2	2.01	0.40
2:D:384:GLY:O	2:D:387:CYS:HB3	2.22	0.40
2:F:40:GLU:CD	2:F:55:ARG:HE	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:CYS:O	1:G:216:ILE:HD11	2.22	0.40
2:H:194:ALA:O	2:H:198:ILE:HG13	2.22	0.40
3:I:89:TRP:CG	3:I:483:SER:HA	2.57	0.40
3:J:97:TYR:CD1	3:J:107:ARG:HB2	2.56	0.40
3:J:436:ARG:HH21	3:J:507:THR:CG2	2.35	0.40
3:J:522:GLN:O	3:J:525:ILE:HG12	2.21	0.40
3:J:561:TYR:CD1	3:J:595:VAL:HG23	2.56	0.40
1:A:171:LYS:HG3	1:A:172:TYR:H	1.86	0.40
2:B:52:GLN:OE1	2:H:48:GLY:HA2	2.21	0.40
2:D:167:GLN:O	2:D:170:TRP:HB3	2.21	0.40
2:D:411:HIS:HB3	2:D:415:ARG:HH22	1.86	0.40
1:E:184:GLN:O	1:E:188:VAL:HG12	2.21	0.40
2:F:5:VAL:HG13	2:F:60:ARG:HA	2.03	0.40
2:F:193:ILE:HG13	2:F:193:ILE:H	1.65	0.40
1:G:159:MET:O	1:G:163:LYS:HG2	2.21	0.40
2:H:74:PHE:O	2:H:83:PHE:N	2.53	0.40
3:I:106:LEU:N	3:I:117:LEU:HG	2.36	0.40
3:I:644:ARG:NH1	3:I:788:VAL:HG13	2.37	0.40
3:J:81:LYS:HE3	3:J:83:HIS:HB2	2.02	0.40
3:J:199:ASN:HA	3:J:227:LEU:HD12	2.02	0.40
3:J:326:LYS:HZ3	3:J:328:ALA:HA	1.86	0.40
3:J:326:LYS:HD3	3:J:327:TRP:C	2.41	0.40
2:B:40:GLU:CD	2:B:55:ARG:HE	2.24	0.40
2:B:146:ARG:NH2	2:D:130:ASP:O	2.54	0.40
2:B:167:GLN:OE1	2:B:167:GLN:N	2.54	0.40
2:B:238:THR:HG21	2:B:271:TYR:OH	2.21	0.40
1:C:223:PHE:HA	1:C:226:VAL:HG23	2.03	0.40
2:D:173:PHE:HB3	2:D:244:ARG:NE	2.36	0.40
2:D:184:VAL:O	2:D:188:VAL:HG12	2.21	0.40
2:D:319:SER:O	2:D:322:GLY:N	2.54	0.40
1:E:171:LYS:HZ3	1:E:172:TYR:HD1	1.69	0.40
1:G:148:ASN:OD1	1:G:148:ASN:N	2.55	0.40
3:I:69:LYS:HD3	3:I:591:SER:HA	2.01	0.40
3:I:378:PHE:HA	3:I:385:PHE:CB	2.51	0.40
3:I:510:ARG:NH1	3:I:512:MET:HA	2.36	0.40
3:I:536:ARG:O	3:I:547:MET:N	2.49	0.40
3:J:218:GLY:N	3:J:225:ASN:ND2	2.70	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	177/228 (78%)	165 (93%)	12 (7%)	0	100	100
1	C	177/228 (78%)	161 (91%)	15 (8%)	1 (1%)	25	62
1	E	177/228 (78%)	160 (90%)	17 (10%)	0	100	100
1	G	177/228 (78%)	164 (93%)	13 (7%)	0	100	100
2	B	424/636 (67%)	380 (90%)	44 (10%)	0	100	100
2	D	424/636 (67%)	383 (90%)	40 (9%)	1 (0%)	47	78
2	F	424/636 (67%)	379 (89%)	45 (11%)	0	100	100
2	H	424/636 (67%)	389 (92%)	35 (8%)	0	100	100
3	I	745/873 (85%)	656 (88%)	89 (12%)	0	100	100
3	J	745/873 (85%)	638 (86%)	107 (14%)	0	100	100
All	All	3894/5202 (75%)	3475 (89%)	417 (11%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	484	GLU
1	C	79	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/208 (78%)	161 (99%)	1 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	162/208 (78%)	162 (100%)	0	100	100
1	E	162/208 (78%)	161 (99%)	1 (1%)	86	91
1	G	162/208 (78%)	162 (100%)	0	100	100
2	B	374/560 (67%)	370 (99%)	4 (1%)	73	84
2	D	374/560 (67%)	371 (99%)	3 (1%)	81	89
2	F	374/560 (67%)	371 (99%)	3 (1%)	81	89
2	H	374/560 (67%)	370 (99%)	4 (1%)	73	84
3	I	667/766 (87%)	662 (99%)	5 (1%)	84	90
3	J	667/766 (87%)	660 (99%)	7 (1%)	76	85
All	All	3478/4604 (76%)	3450 (99%)	28 (1%)	82	89

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
2	B	37	ARG
2	B	214	LYS
2	B	309	ILE
2	B	485	LYS
2	D	37	ARG
2	D	166	ARG
2	D	214	LYS
1	E	178	LYS
2	F	37	ARG
2	F	214	LYS
2	F	485	LYS
2	H	37	ARG
2	H	166	ARG
2	H	214	LYS
2	H	485	LYS
3	I	97	TYR
3	I	450	ARG
3	I	650	LYS
3	I	723	PHE
3	I	735	HIS
3	J	84	ASP
3	J	261	ARG
3	J	290	ASN
3	J	532	LYS

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Mol	Chain	Res	Type
3	J	537	LYS
3	J	610	LYS
3	J	764	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	196	ASN
1	A	221	GLN
2	B	177	HIS
2	B	200	ASN
2	B	405	ASN
1	C	58	ASN
1	C	184	GLN
1	C	185	HIS
1	C	221	GLN
2	D	177	HIS
2	D	279	ASN
2	D	481	HIS
1	E	65	GLN
1	E	191	GLN
2	F	96	ASN
2	F	177	HIS
2	F	405	ASN
1	G	58	ASN
1	G	65	GLN
1	G	87	GLN
2	H	177	HIS
2	H	477	HIS
3	I	112	ASN
3	I	151	GLN
3	I	152	HIS
3	I	191	GLN
3	I	192	GLN
3	I	206	HIS
3	I	225	ASN
3	I	370	HIS
3	I	408	GLN
3	I	437	ASN
3	I	474	ASN
3	I	613	GLN

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Mol	Chain	Res	Type
3	I	638	GLN
3	I	670	GLN
3	I	738	HIS
3	I	745	GLN
3	I	756	GLN
3	I	773	HIS
3	J	165	HIS
3	J	210	GLN
3	J	282	HIS
3	J	301	ASN
3	J	361	HIS
3	J	372	GLN
3	J	393	GLN
3	J	437	ASN
3	J	522	GLN
3	J	526	ASN
3	J	613	GLN
3	J	763	HIS
3	J	773	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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

There are no chain breaks in this entry.

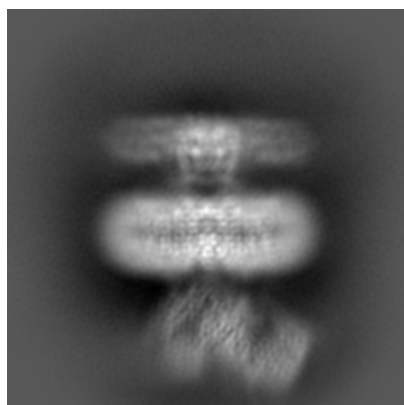
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32335. These allow visual inspection of the internal detail of the map and identification of artifacts.

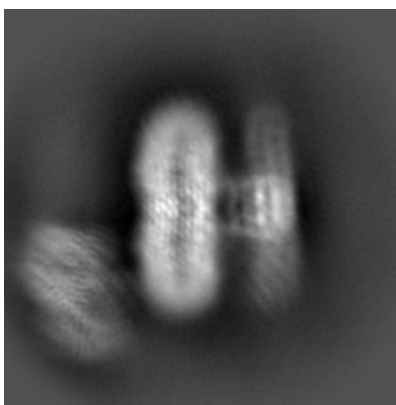
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

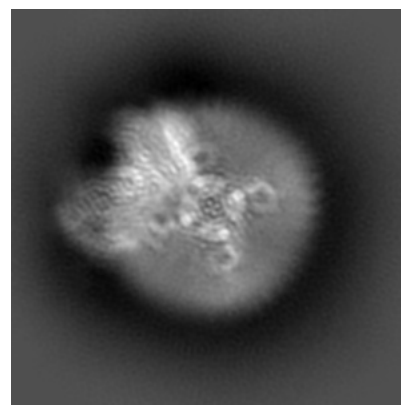
#### 6.1.1 Primary map



X



Y

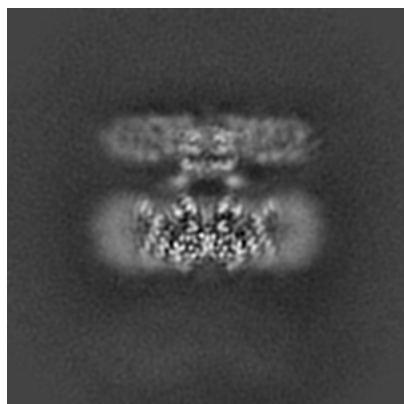


Z

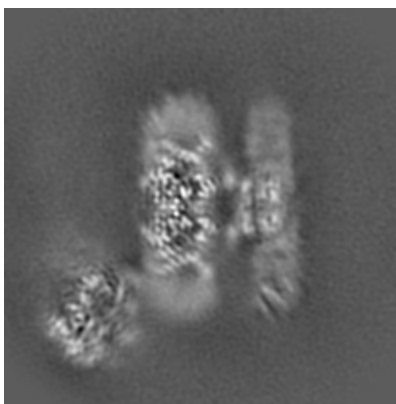
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

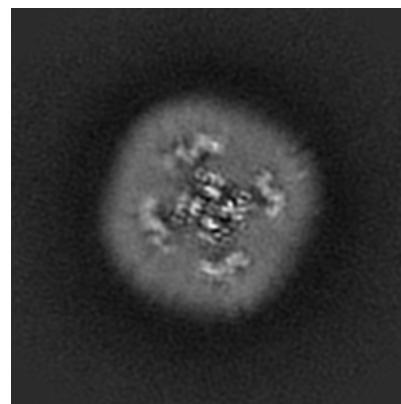
#### 6.2.1 Primary map



X Index: 135



Y Index: 135

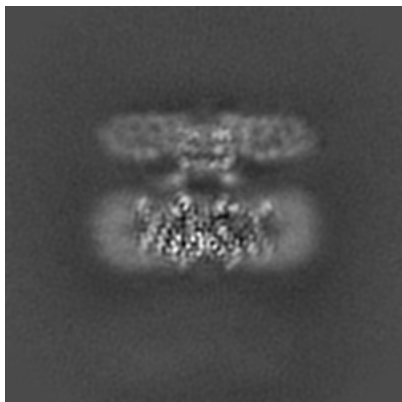


Z Index: 135

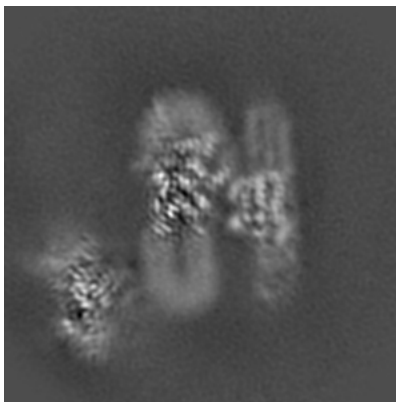
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

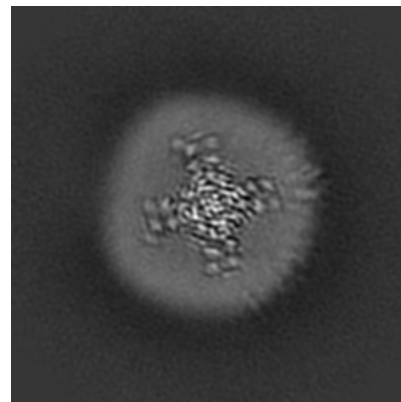
### 6.3.1 Primary map



X Index: 137



Y Index: 144



Z Index: 107

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

## 6.4 Orthogonal surface views [i](#)

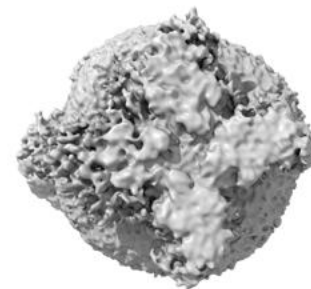
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0956. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

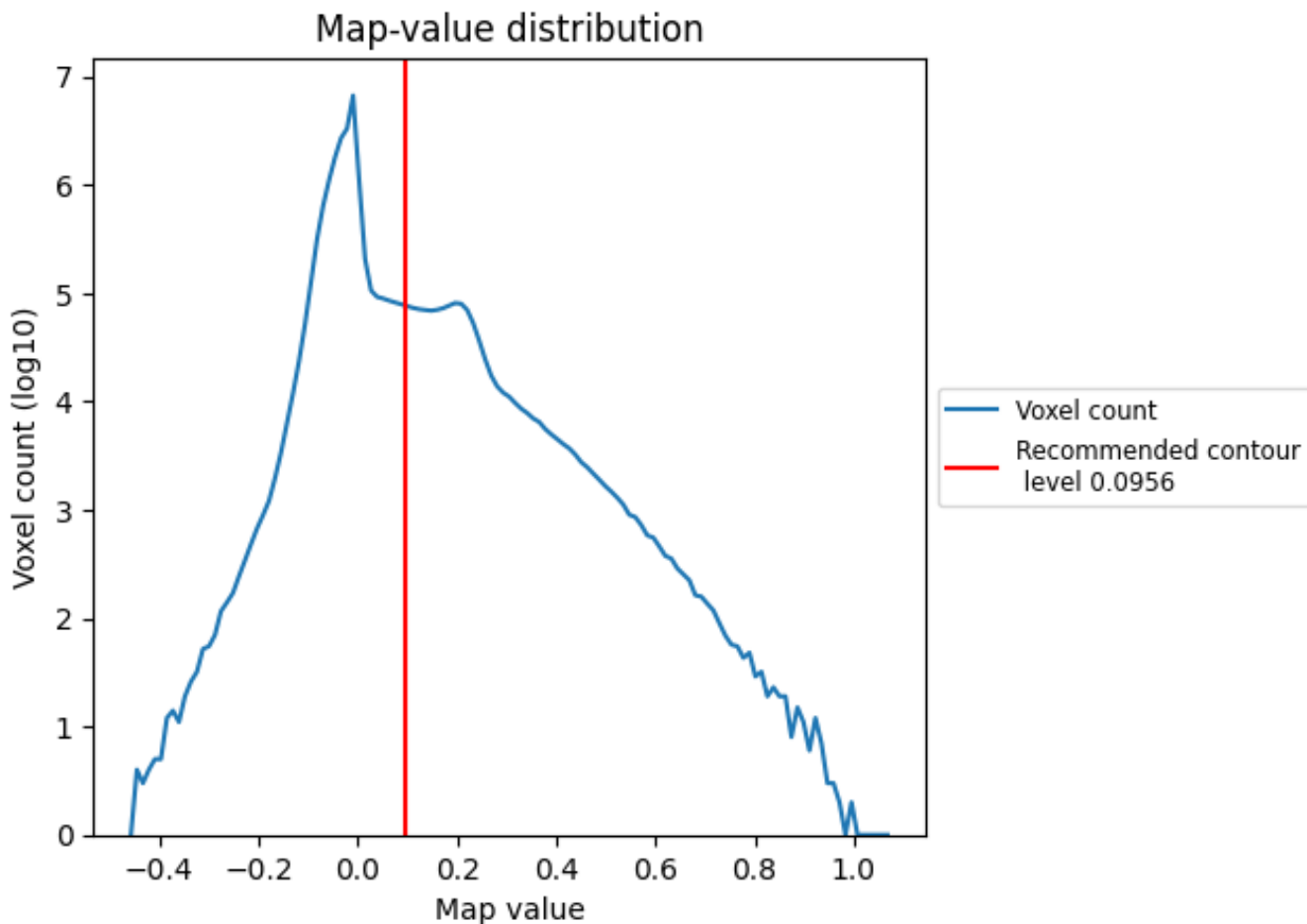
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

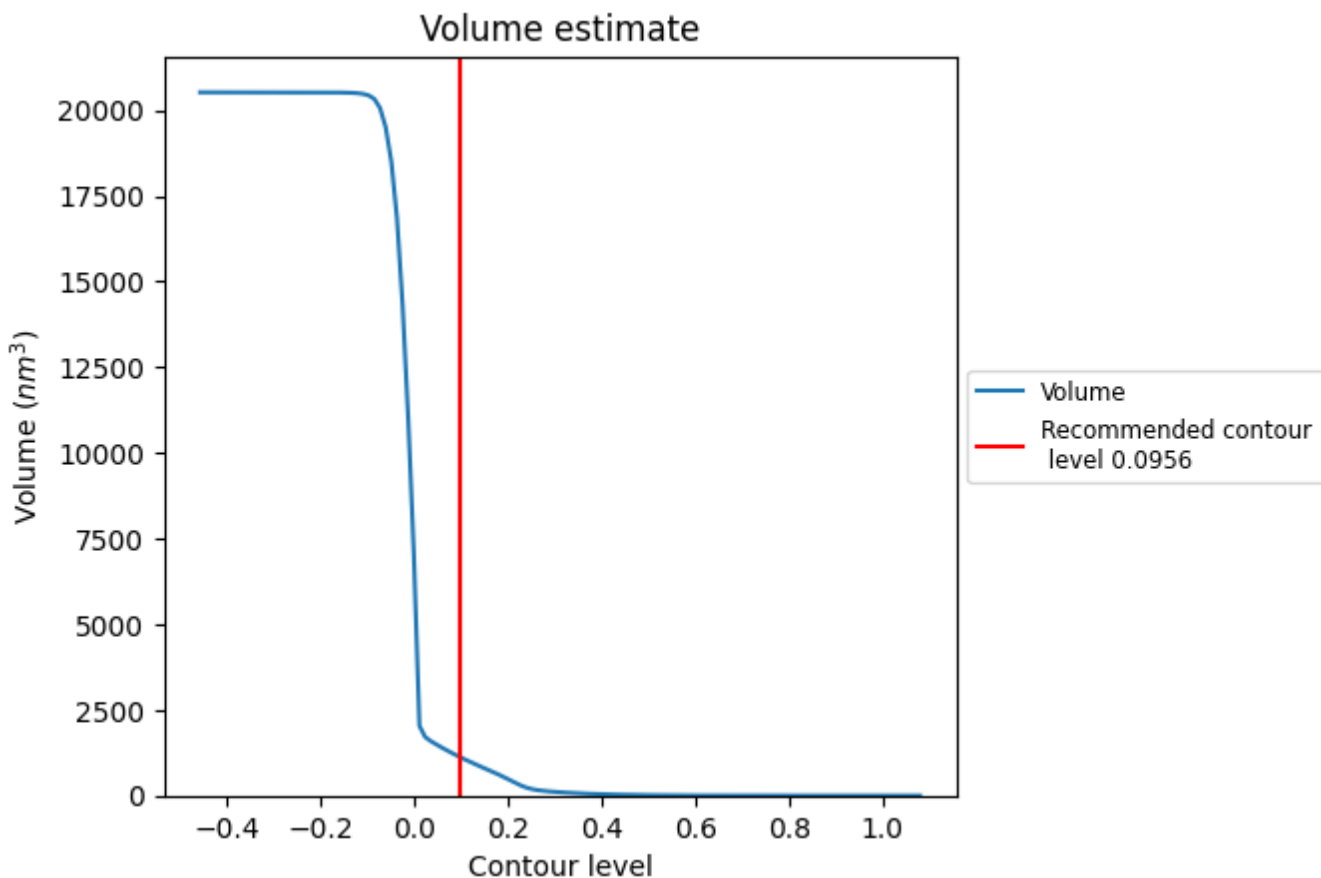
This section contains the results of statistical analysis of the map.

### 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.

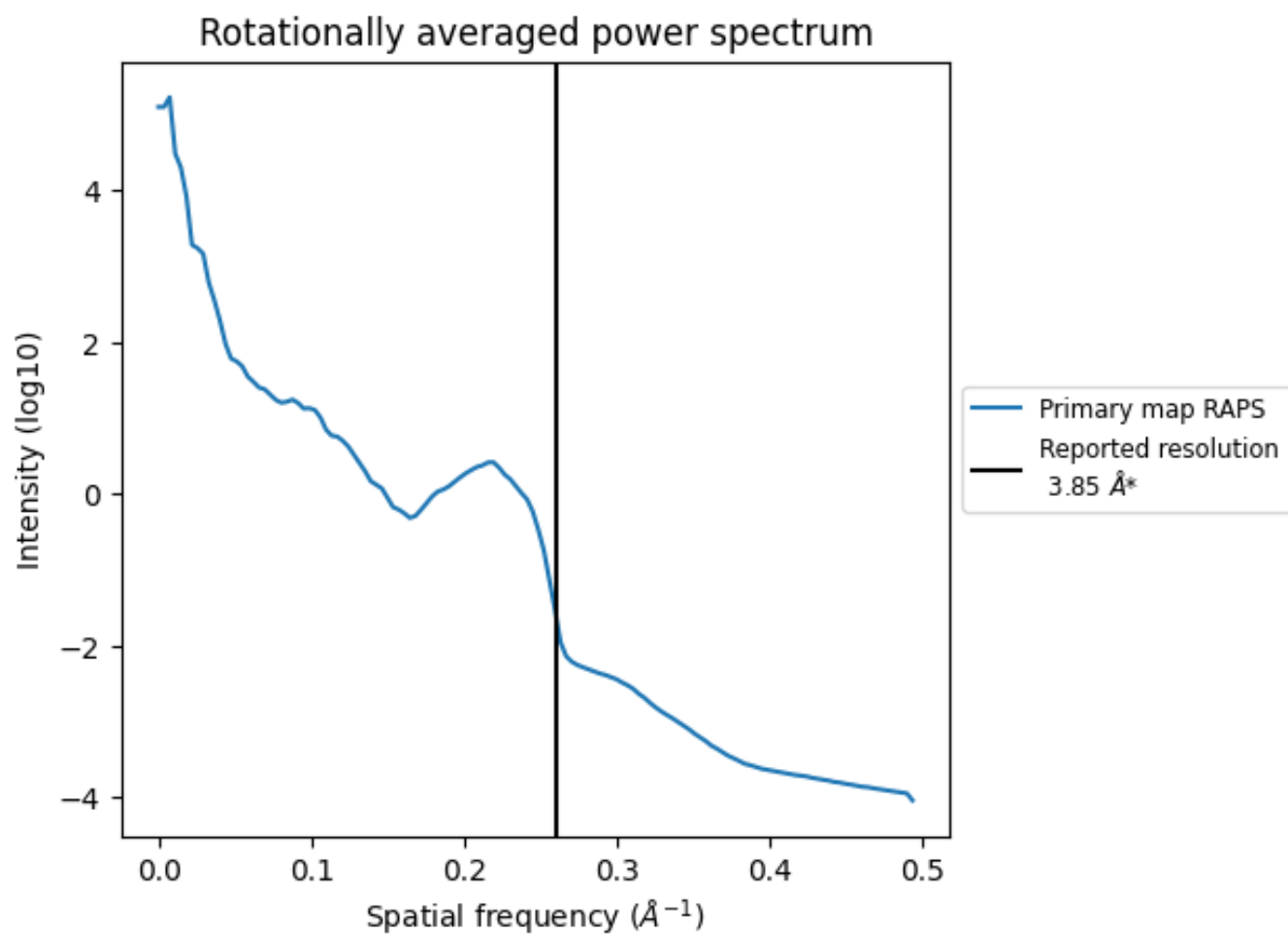
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1137 nm<sup>3</sup>; this corresponds to an approximate mass of 1027 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.260 \text{\AA}^{-1}$

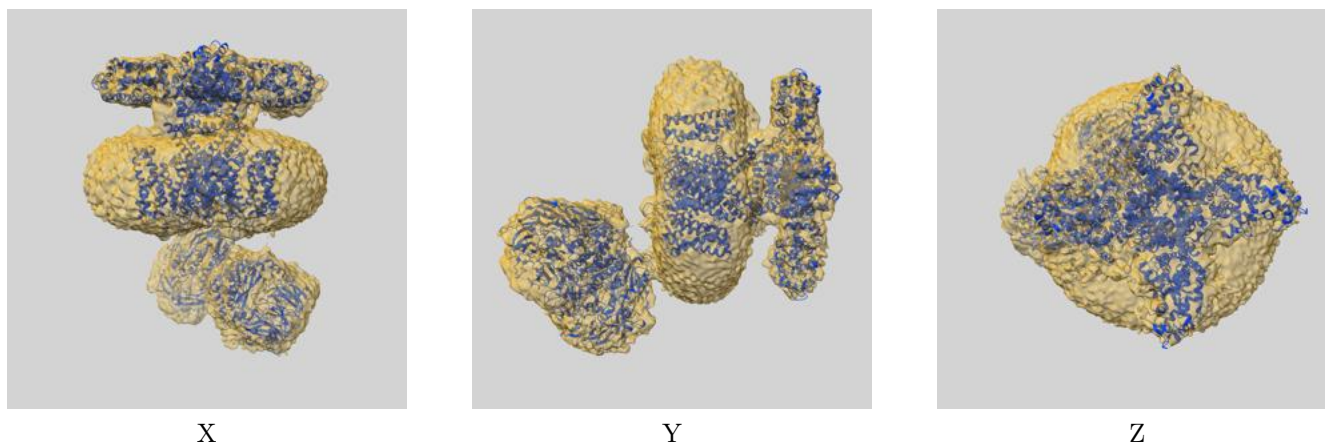
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

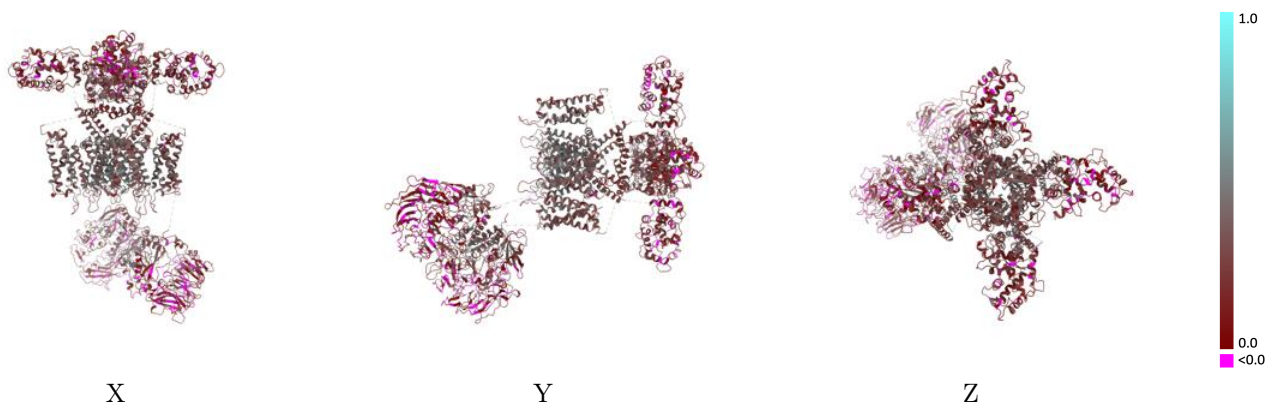
This section contains information regarding the fit between EMDB map EMD-32335 and PDB model 7W6T. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



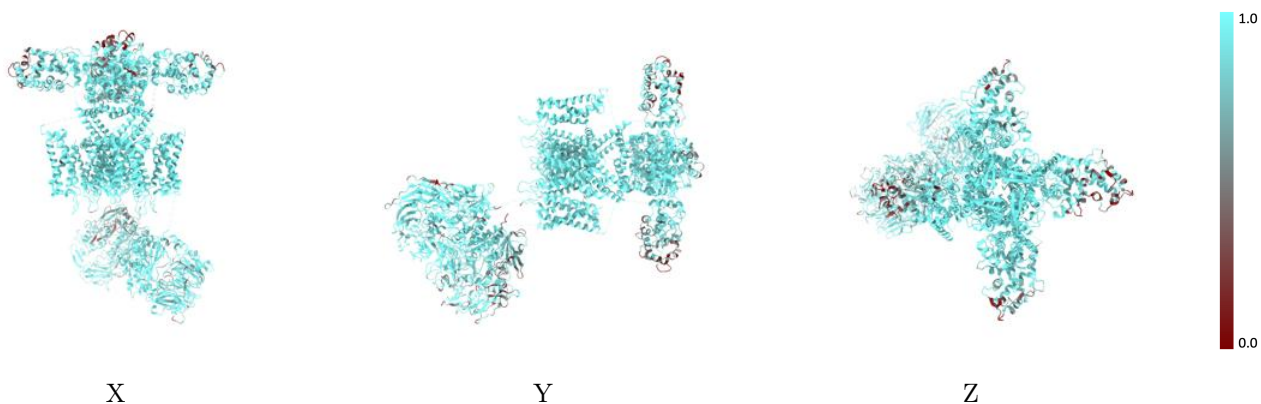
The images above show the 3D surface view of the map at the recommended contour level 0.0956 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



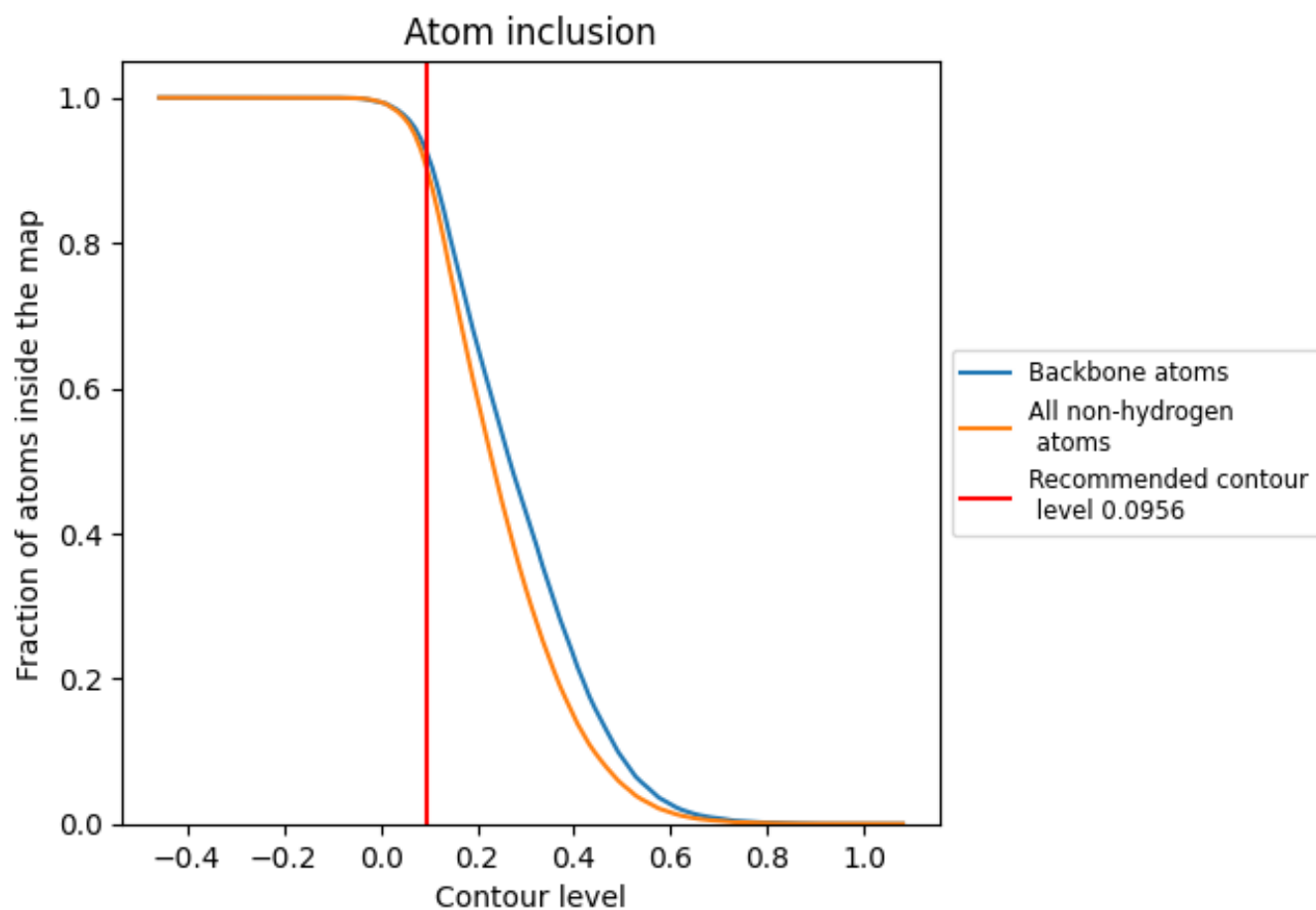
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0956).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (0.0956) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9024	 0.2500
A	 0.6921	 0.1520
B	 0.9769	 0.3270
C	 0.8609	 0.1880
D	 0.9795	 0.3190
E	 0.6777	 0.1440
F	 0.9739	 0.3320
G	 0.8017	 0.1840
H	 0.9772	 0.3340
I	 0.9329	 0.1940
J	 0.8440	 0.2080

