Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 09:00 am GMT

PDB ID	:	5ANY
EMDB ID	:	EMD-3144
Title	:	Electron cryo-microscopy of chikungunya virus in complex with neutralizing antibody Fab CHK265
Authors	:	Fox, J.M.; Long, F.; Edeling, M.A.; Lin, H.; Duijl-Richter, M.; Fong, R.H.; Kahle, K.M.; Smit, J.M.; Jin, J.; Simmons, G.; Doranz, B.J.; Crowe, J.E.; Fremont, D.H.; Rossmann, M.G.; Diamond, M.S.
Deposited on	:	2015-09-08
Resolution	:	16.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

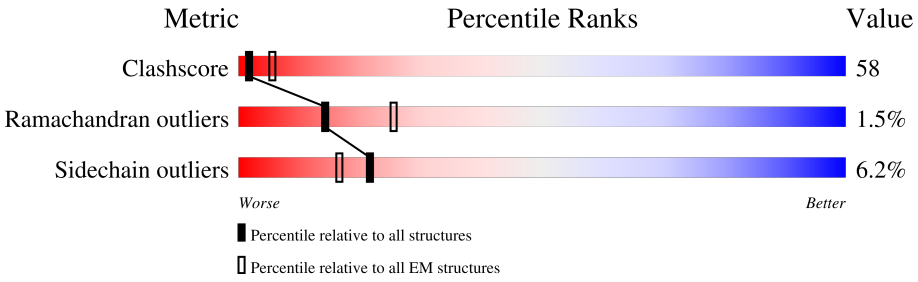
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 16.90 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 >=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 <=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	451	59% 75% 11% • 13%
1	C	451	72% 76% 10% • 13%
1	E	451	24% 76% 10% • 13%
1	G	451	57% 78% 8% • 13%
2	B	354	53% 66% 26% • • 5%
2	D	354	68% 65% 27% • • 5%
2	F	354	43% 65% 27% • • 5%
2	H	354	62% 66% 26% • • 5%

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Mol	Chain	Length	Quality of chain
3	I	218	89% 60% 36%
3	J	218	96% 58% 37%
3	K	218	56% 60% 36%
3	L	218	84% 59% 37%
4	M	214	92% 40% 45% 13%
4	N	214	66% 38% 47% 13%
4	O	214	46% 40% 46% 12%
4	P	214	82% 40% 46% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35620 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 E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	392	Total	C	N	O	S	0	0
			2986	1889	500	573	24		
1	C	392	Total	C	N	O	S	0	0
			2986	1889	500	573	24		
1	E	392	Total	C	N	O	S	0	0
			2986	1889	500	573	24		
1	G	392	Total	C	N	O	S	0	0
			2986	1889	500	573	24		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	GLY	-	expression tag	UNP Q1H8W5
A	414	PRO	-	expression tag	UNP Q1H8W5
A	415	PHE	-	expression tag	UNP Q1H8W5
A	416	GLU	-	expression tag	UNP Q1H8W5
A	417	ASP	-	expression tag	UNP Q1H8W5
A	418	ASP	-	expression tag	UNP Q1H8W5
A	419	ASP	-	expression tag	UNP Q1H8W5
A	420	ASP	-	expression tag	UNP Q1H8W5
A	421	LYS	-	expression tag	UNP Q1H8W5
A	422	ALA	-	expression tag	UNP Q1H8W5
A	423	GLY	-	expression tag	UNP Q1H8W5
A	424	TRP	-	expression tag	UNP Q1H8W5
A	425	SER	-	expression tag	UNP Q1H8W5
A	426	HIS	-	expression tag	UNP Q1H8W5
A	427	PRO	-	expression tag	UNP Q1H8W5
A	428	GLN	-	expression tag	UNP Q1H8W5
A	429	PHE	-	expression tag	UNP Q1H8W5
A	430	GLU	-	expression tag	UNP Q1H8W5
A	431	LYS	-	expression tag	UNP Q1H8W5
A	432	GLY	-	expression tag	UNP Q1H8W5
A	433	GLY	-	expression tag	UNP Q1H8W5
A	434	GLY	-	expression tag	UNP Q1H8W5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	435	SER	-	expression tag	UNP Q1H8W5
A	436	GLY	-	expression tag	UNP Q1H8W5
A	437	GLY	-	expression tag	UNP Q1H8W5
A	438	GLY	-	expression tag	UNP Q1H8W5
A	439	SER	-	expression tag	UNP Q1H8W5
A	440	GLY	-	expression tag	UNP Q1H8W5
A	441	GLY	-	expression tag	UNP Q1H8W5
A	442	GLY	-	expression tag	UNP Q1H8W5
A	443	SER	-	expression tag	UNP Q1H8W5
A	444	TRP	-	expression tag	UNP Q1H8W5
A	445	SER	-	expression tag	UNP Q1H8W5
A	446	HIS	-	expression tag	UNP Q1H8W5
A	447	PRO	-	expression tag	UNP Q1H8W5
A	448	GLN	-	expression tag	UNP Q1H8W5
A	449	PHE	-	expression tag	UNP Q1H8W5
A	450	GLU	-	expression tag	UNP Q1H8W5
A	451	LYS	-	expression tag	UNP Q1H8W5
C	413	GLY	-	expression tag	UNP Q1H8W5
C	414	PRO	-	expression tag	UNP Q1H8W5
C	415	PHE	-	expression tag	UNP Q1H8W5
C	416	GLU	-	expression tag	UNP Q1H8W5
C	417	ASP	-	expression tag	UNP Q1H8W5
C	418	ASP	-	expression tag	UNP Q1H8W5
C	419	ASP	-	expression tag	UNP Q1H8W5
C	420	ASP	-	expression tag	UNP Q1H8W5
C	421	LYS	-	expression tag	UNP Q1H8W5
C	422	ALA	-	expression tag	UNP Q1H8W5
C	423	GLY	-	expression tag	UNP Q1H8W5
C	424	TRP	-	expression tag	UNP Q1H8W5
C	425	SER	-	expression tag	UNP Q1H8W5
C	426	HIS	-	expression tag	UNP Q1H8W5
C	427	PRO	-	expression tag	UNP Q1H8W5
C	428	GLN	-	expression tag	UNP Q1H8W5
C	429	PHE	-	expression tag	UNP Q1H8W5
C	430	GLU	-	expression tag	UNP Q1H8W5
C	431	LYS	-	expression tag	UNP Q1H8W5
C	432	GLY	-	expression tag	UNP Q1H8W5
C	433	GLY	-	expression tag	UNP Q1H8W5
C	434	GLY	-	expression tag	UNP Q1H8W5
C	435	SER	-	expression tag	UNP Q1H8W5
C	436	GLY	-	expression tag	UNP Q1H8W5
C	437	GLY	-	expression tag	UNP Q1H8W5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	438	GLY	-	expression tag	UNP Q1H8W5
C	439	SER	-	expression tag	UNP Q1H8W5
C	440	GLY	-	expression tag	UNP Q1H8W5
C	441	GLY	-	expression tag	UNP Q1H8W5
C	442	GLY	-	expression tag	UNP Q1H8W5
C	443	SER	-	expression tag	UNP Q1H8W5
C	444	TRP	-	expression tag	UNP Q1H8W5
C	445	SER	-	expression tag	UNP Q1H8W5
C	446	HIS	-	expression tag	UNP Q1H8W5
C	447	PRO	-	expression tag	UNP Q1H8W5
C	448	GLN	-	expression tag	UNP Q1H8W5
C	449	PHE	-	expression tag	UNP Q1H8W5
C	450	GLU	-	expression tag	UNP Q1H8W5
C	451	LYS	-	expression tag	UNP Q1H8W5
E	413	GLY	-	expression tag	UNP Q1H8W5
E	414	PRO	-	expression tag	UNP Q1H8W5
E	415	PHE	-	expression tag	UNP Q1H8W5
E	416	GLU	-	expression tag	UNP Q1H8W5
E	417	ASP	-	expression tag	UNP Q1H8W5
E	418	ASP	-	expression tag	UNP Q1H8W5
E	419	ASP	-	expression tag	UNP Q1H8W5
E	420	ASP	-	expression tag	UNP Q1H8W5
E	421	LYS	-	expression tag	UNP Q1H8W5
E	422	ALA	-	expression tag	UNP Q1H8W5
E	423	GLY	-	expression tag	UNP Q1H8W5
E	424	TRP	-	expression tag	UNP Q1H8W5
E	425	SER	-	expression tag	UNP Q1H8W5
E	426	HIS	-	expression tag	UNP Q1H8W5
E	427	PRO	-	expression tag	UNP Q1H8W5
E	428	GLN	-	expression tag	UNP Q1H8W5
E	429	PHE	-	expression tag	UNP Q1H8W5
E	430	GLU	-	expression tag	UNP Q1H8W5
E	431	LYS	-	expression tag	UNP Q1H8W5
E	432	GLY	-	expression tag	UNP Q1H8W5
E	433	GLY	-	expression tag	UNP Q1H8W5
E	434	GLY	-	expression tag	UNP Q1H8W5
E	435	SER	-	expression tag	UNP Q1H8W5
E	436	GLY	-	expression tag	UNP Q1H8W5
E	437	GLY	-	expression tag	UNP Q1H8W5
E	438	GLY	-	expression tag	UNP Q1H8W5
E	439	SER	-	expression tag	UNP Q1H8W5
E	440	GLY	-	expression tag	UNP Q1H8W5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	441	GLY	-	expression tag	UNP Q1H8W5
E	442	GLY	-	expression tag	UNP Q1H8W5
E	443	SER	-	expression tag	UNP Q1H8W5
E	444	TRP	-	expression tag	UNP Q1H8W5
E	445	SER	-	expression tag	UNP Q1H8W5
E	446	HIS	-	expression tag	UNP Q1H8W5
E	447	PRO	-	expression tag	UNP Q1H8W5
E	448	GLN	-	expression tag	UNP Q1H8W5
E	449	PHE	-	expression tag	UNP Q1H8W5
E	450	GLU	-	expression tag	UNP Q1H8W5
E	451	LYS	-	expression tag	UNP Q1H8W5
G	413	GLY	-	expression tag	UNP Q1H8W5
G	414	PRO	-	expression tag	UNP Q1H8W5
G	415	PHE	-	expression tag	UNP Q1H8W5
G	416	GLU	-	expression tag	UNP Q1H8W5
G	417	ASP	-	expression tag	UNP Q1H8W5
G	418	ASP	-	expression tag	UNP Q1H8W5
G	419	ASP	-	expression tag	UNP Q1H8W5
G	420	ASP	-	expression tag	UNP Q1H8W5
G	421	LYS	-	expression tag	UNP Q1H8W5
G	422	ALA	-	expression tag	UNP Q1H8W5
G	423	GLY	-	expression tag	UNP Q1H8W5
G	424	TRP	-	expression tag	UNP Q1H8W5
G	425	SER	-	expression tag	UNP Q1H8W5
G	426	HIS	-	expression tag	UNP Q1H8W5
G	427	PRO	-	expression tag	UNP Q1H8W5
G	428	GLN	-	expression tag	UNP Q1H8W5
G	429	PHE	-	expression tag	UNP Q1H8W5
G	430	GLU	-	expression tag	UNP Q1H8W5
G	431	LYS	-	expression tag	UNP Q1H8W5
G	432	GLY	-	expression tag	UNP Q1H8W5
G	433	GLY	-	expression tag	UNP Q1H8W5
G	434	GLY	-	expression tag	UNP Q1H8W5
G	435	SER	-	expression tag	UNP Q1H8W5
G	436	GLY	-	expression tag	UNP Q1H8W5
G	437	GLY	-	expression tag	UNP Q1H8W5
G	438	GLY	-	expression tag	UNP Q1H8W5
G	439	SER	-	expression tag	UNP Q1H8W5
G	440	GLY	-	expression tag	UNP Q1H8W5
G	441	GLY	-	expression tag	UNP Q1H8W5
G	442	GLY	-	expression tag	UNP Q1H8W5
G	443	SER	-	expression tag	UNP Q1H8W5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	444	TRP	-	expression tag	UNP Q1H8W5
G	445	SER	-	expression tag	UNP Q1H8W5
G	446	HIS	-	expression tag	UNP Q1H8W5
G	447	PRO	-	expression tag	UNP Q1H8W5
G	448	GLN	-	expression tag	UNP Q1H8W5
G	449	PHE	-	expression tag	UNP Q1H8W5
G	450	GLU	-	expression tag	UNP Q1H8W5
G	451	LYS	-	expression tag	UNP Q1H8W5

- Molecule 2 is a protein called E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	336	Total	C	N	O	S	0	0
			2650	1653	480	497	20		
2	D	336	Total	C	N	O	S	0	0
			2650	1653	480	497	20		
2	F	336	Total	C	N	O	S	0	0
			2650	1653	480	497	20		
2	H	336	Total	C	N	O	S	0	0
			2650	1653	480	497	20		

- Molecule 3 is a protein called FAB CHK265.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	J	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	K	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	L	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		

- Molecule 4 is a protein called FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	211	Total	C	N	O	S	0	0
			1598	999	270	322	7		
4	N	211	Total	C	N	O	S	0	0
			1598	999	270	322	7		
4	O	211	Total	C	N	O	S	0	0
			1598	999	270	322	7		

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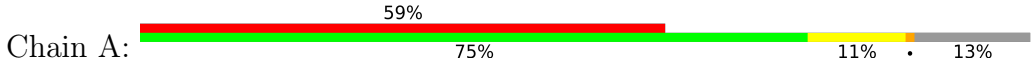
Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	211	Total	C	N	O	S	0	0
			1598	999	270	322	7		

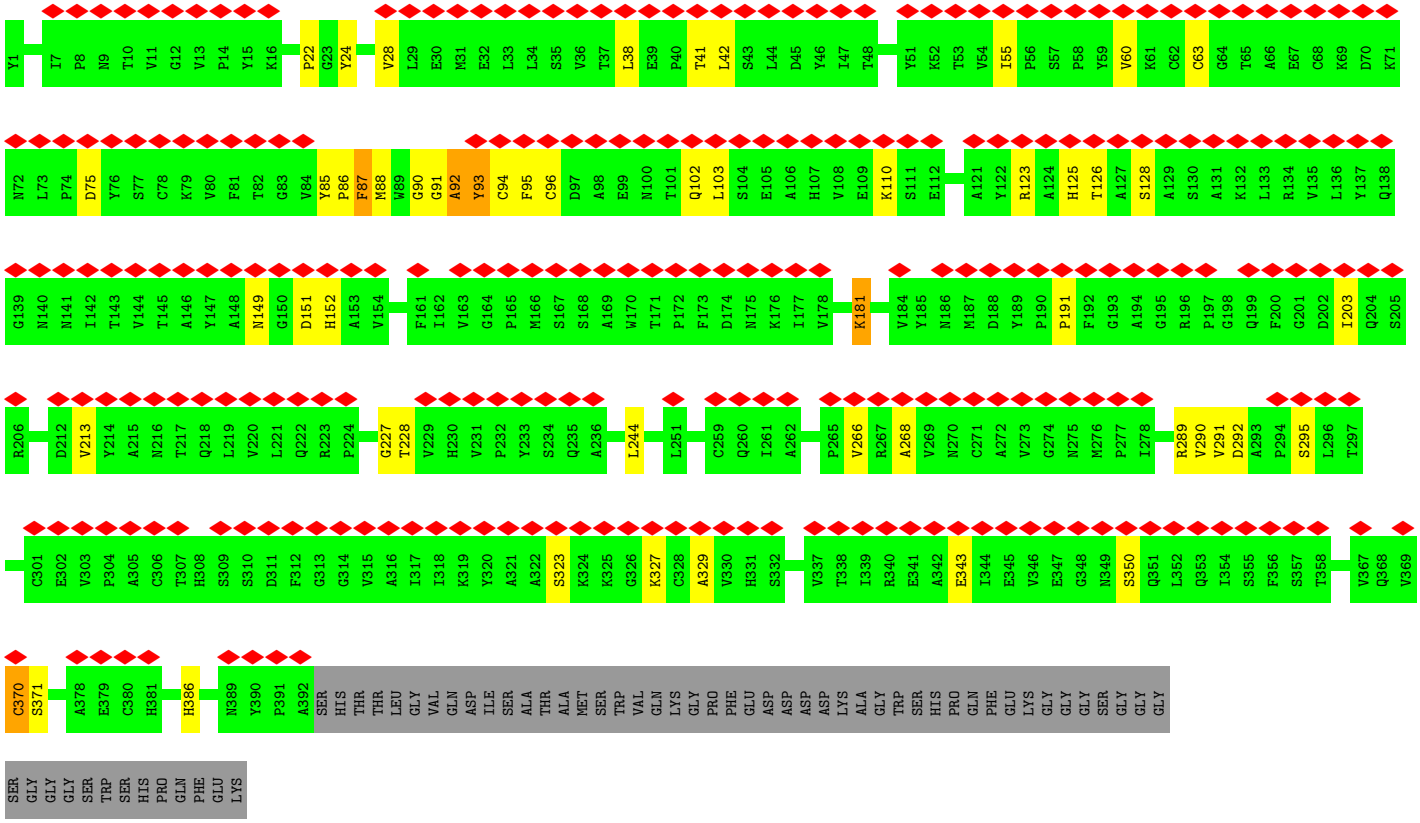
3 Residue-property plots (i)

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: E1

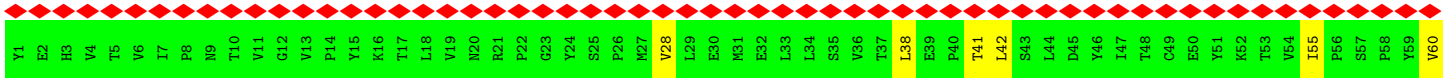
Chain A:

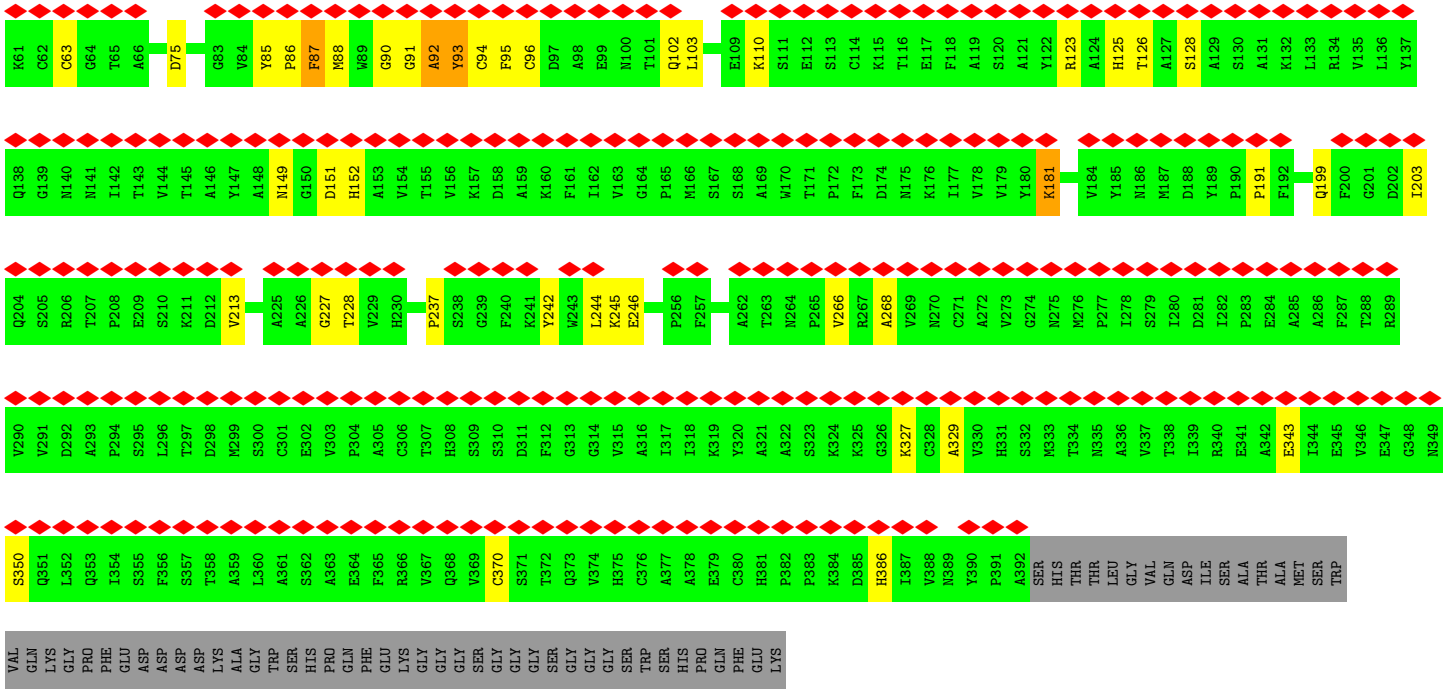




• Molecule 1: E1

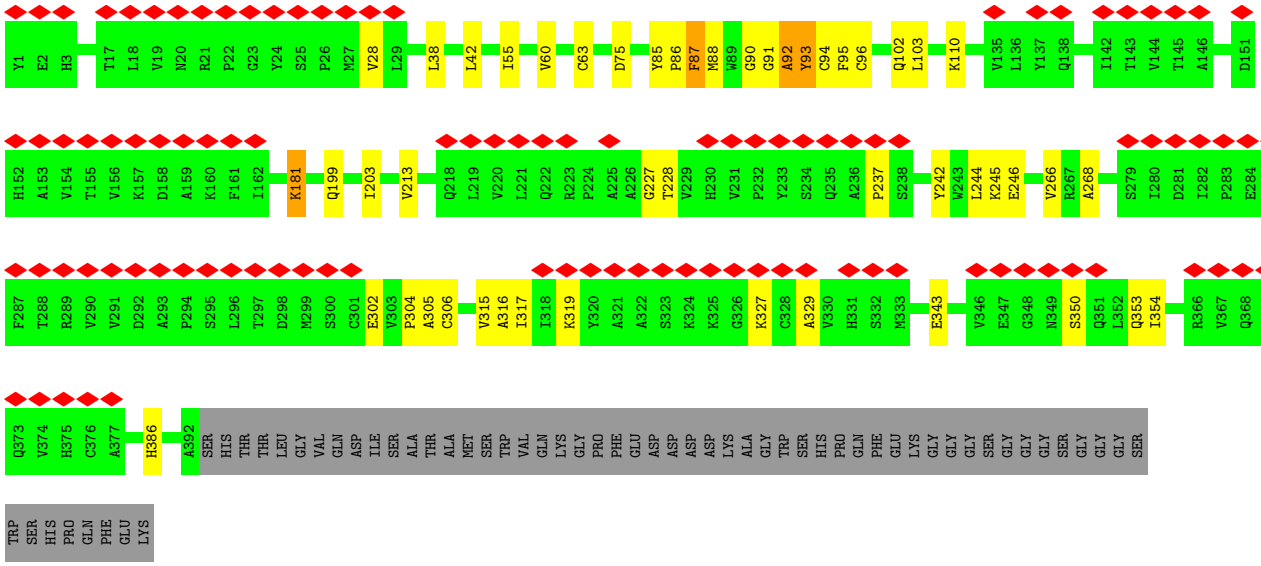
Chain C:





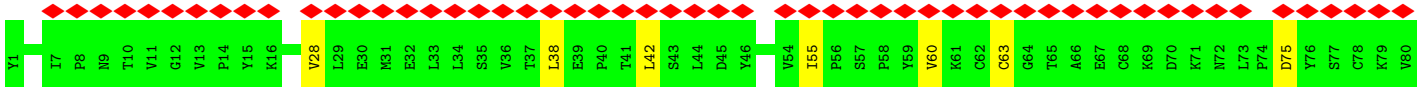
- Molecule 1: E1

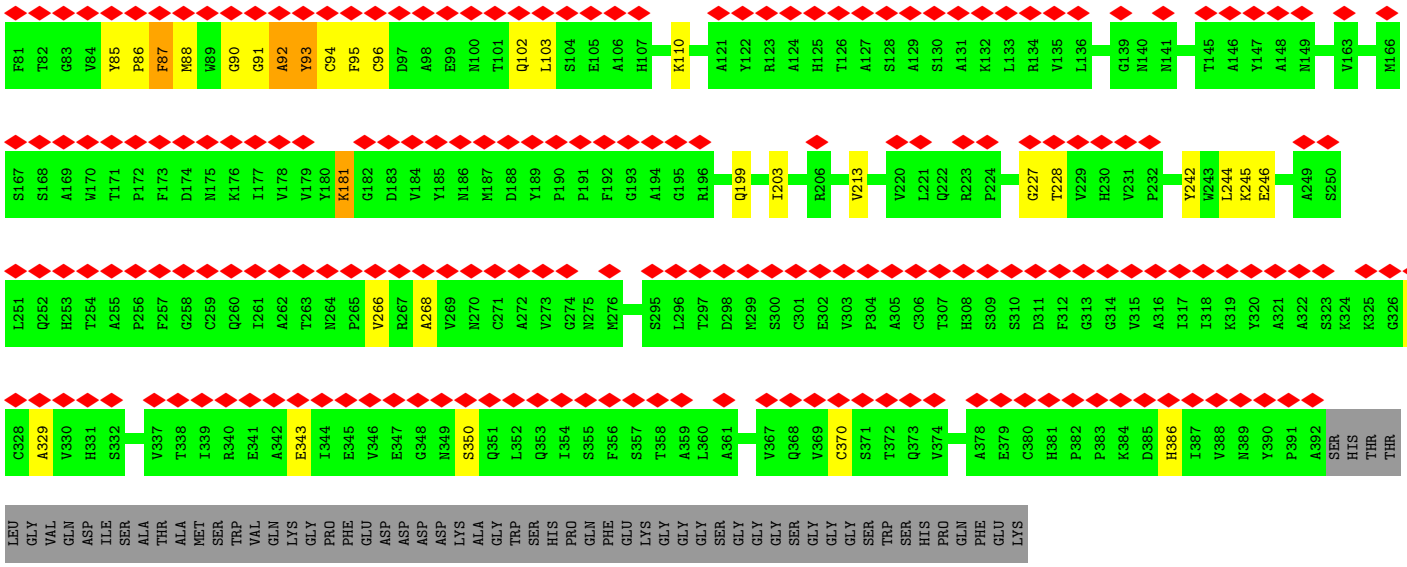
Chain E:



- Molecule 1: E1

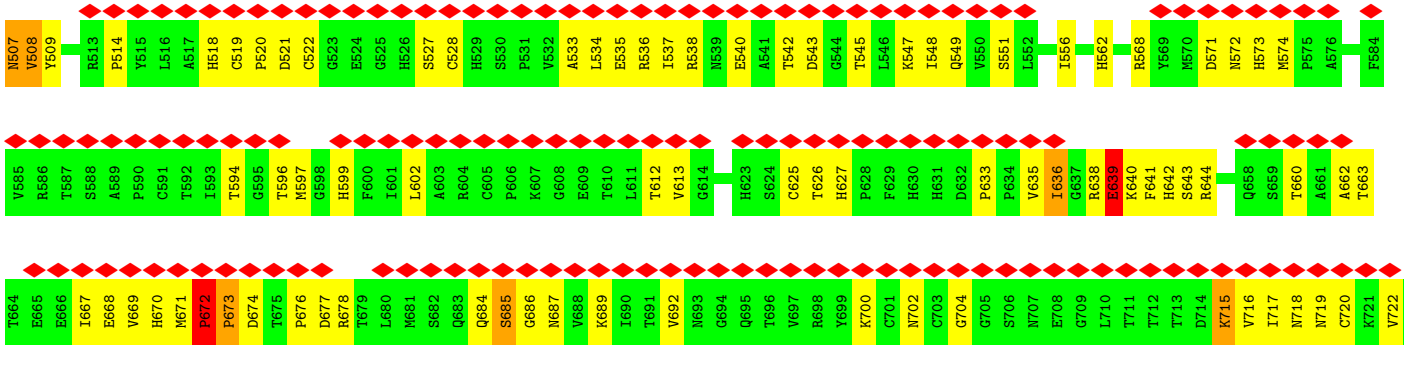
Chain G:





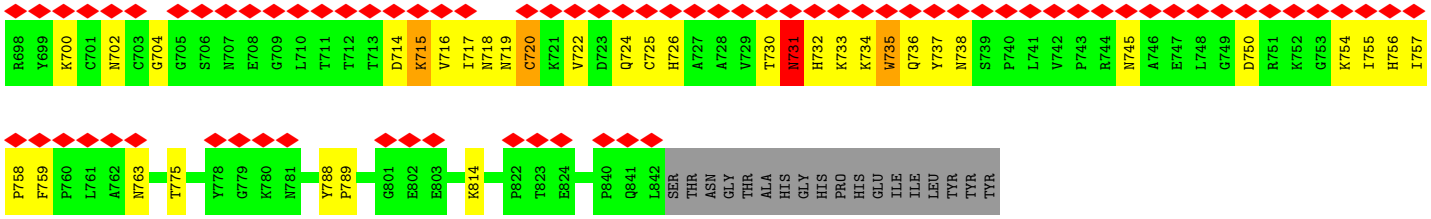
• Molecule 2: E2

Chain B:



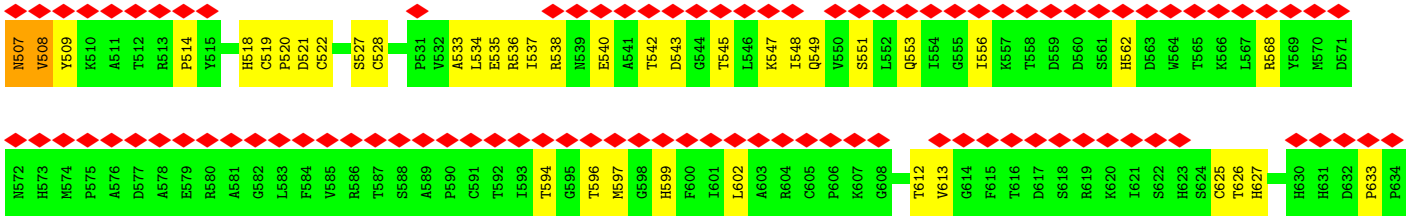
• Molecule 2: E2

Chain D:



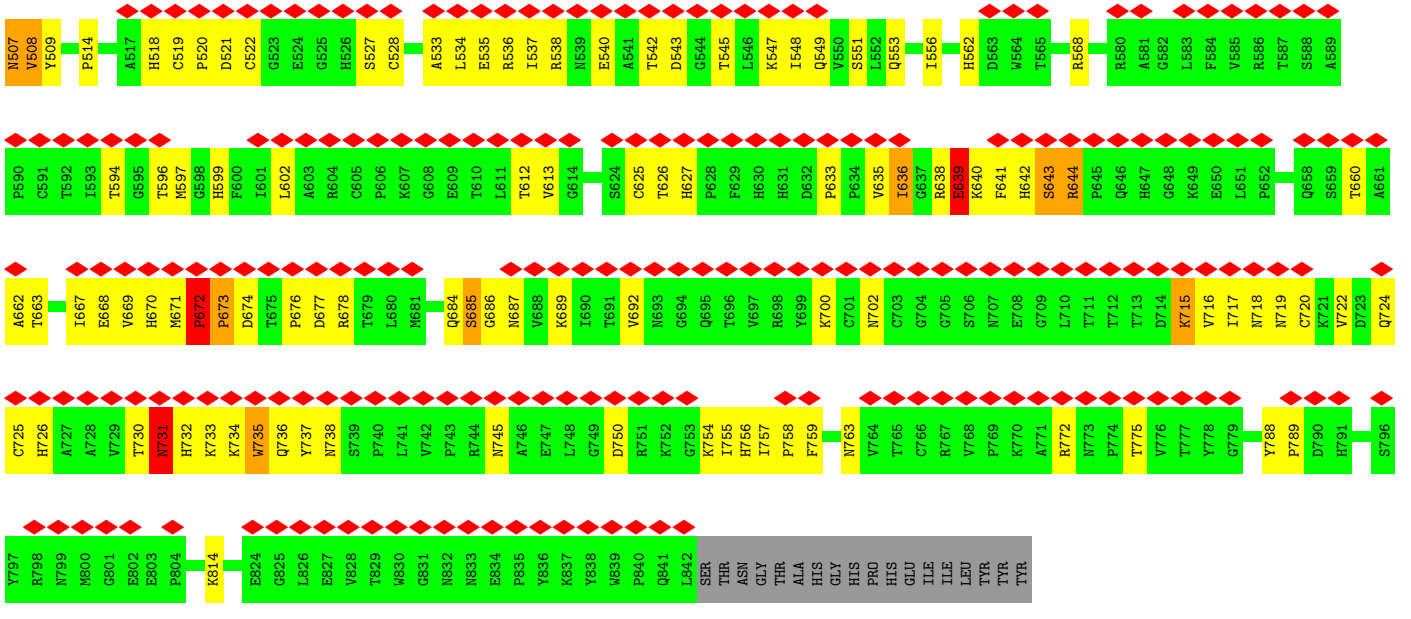
- Molecule 2: E2

Chain F:



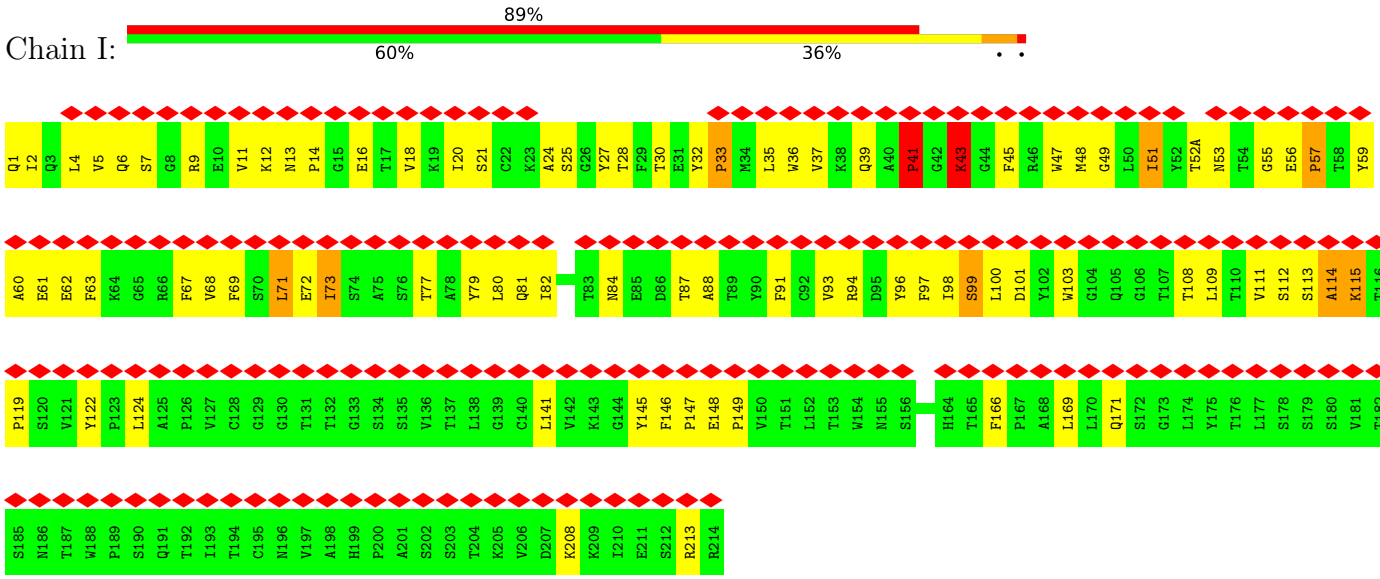
- Molecule 2: E2

Chain H:



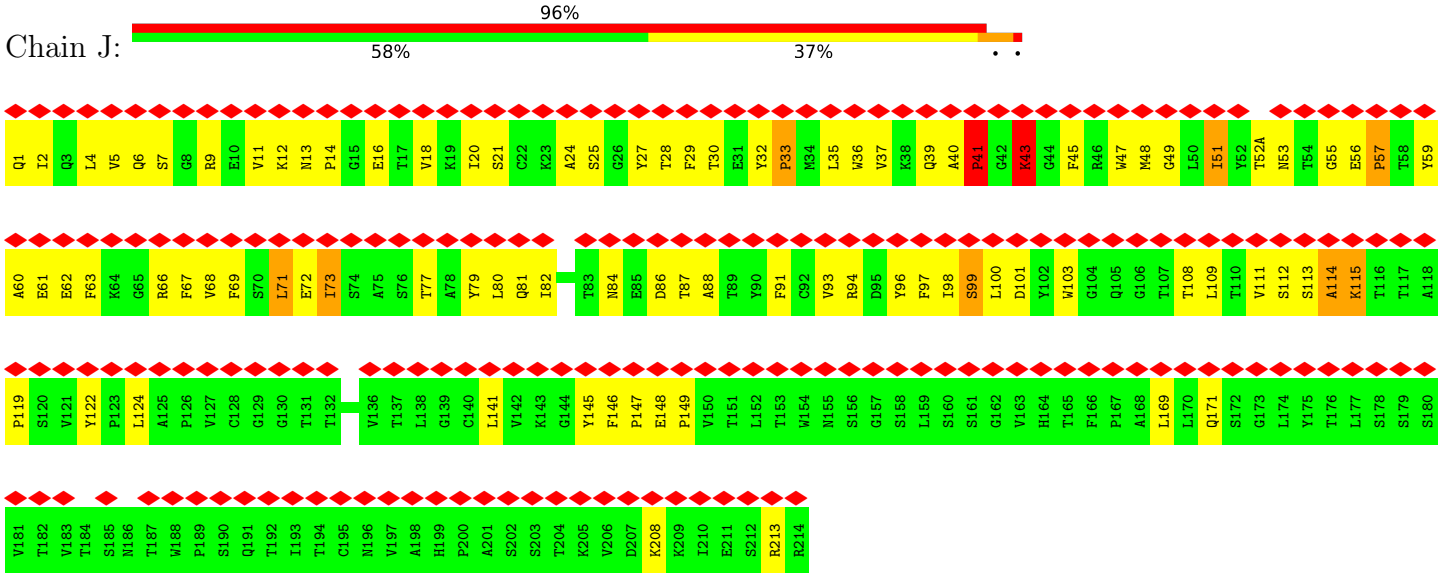
• Molecule 3: FAB CHK265

Chain I:



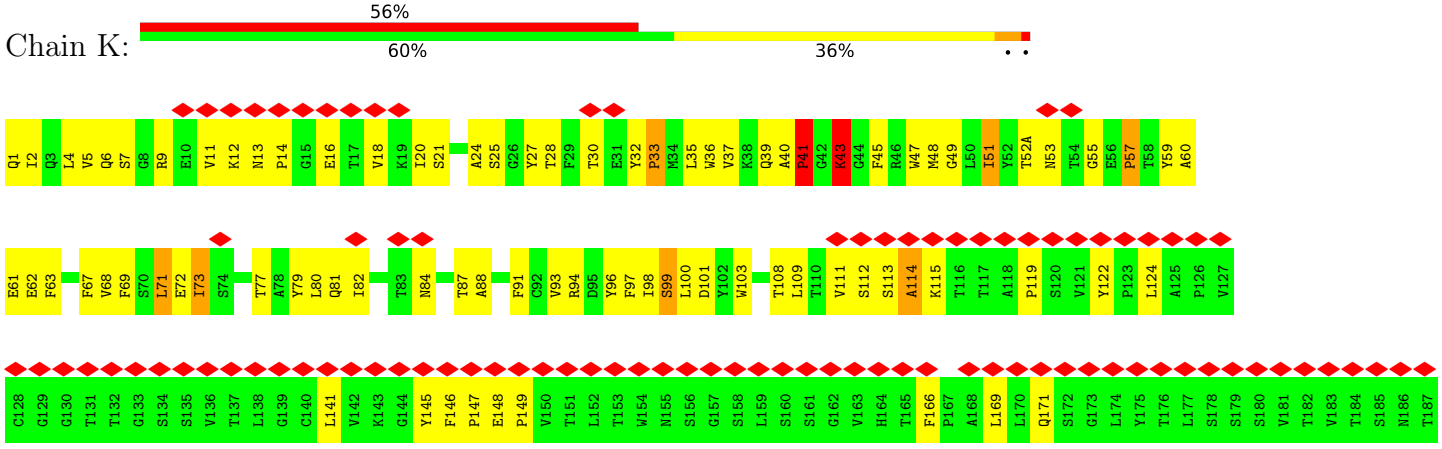
• Molecule 3: FAB CHK265

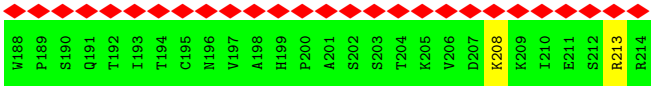
Chain J:



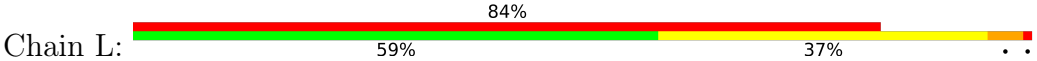
• Molecule 3: FAB CHK265

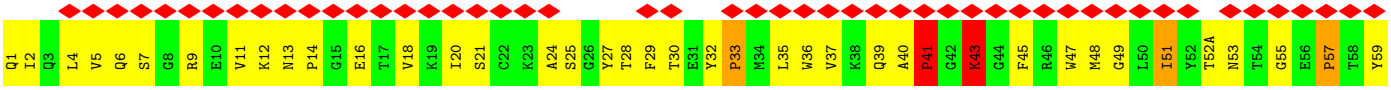
Chain K:

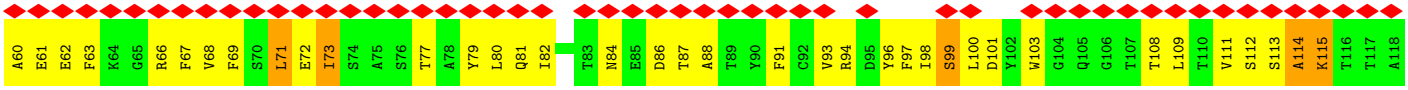


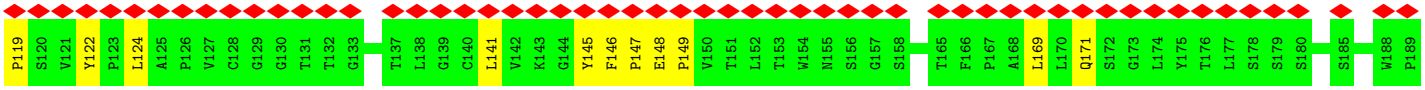


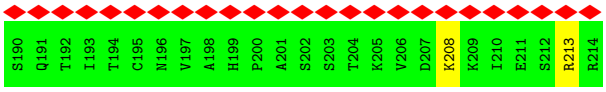
• Molecule 3: FAB CHK265



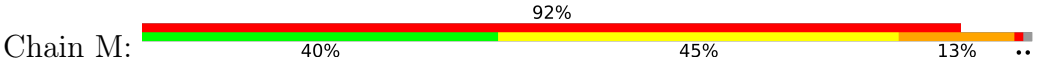


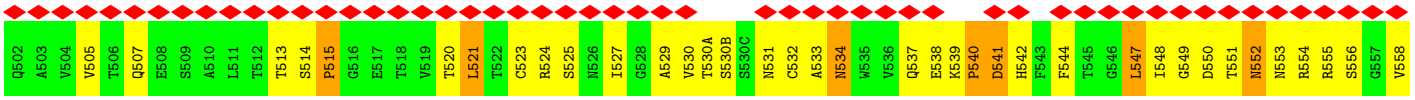


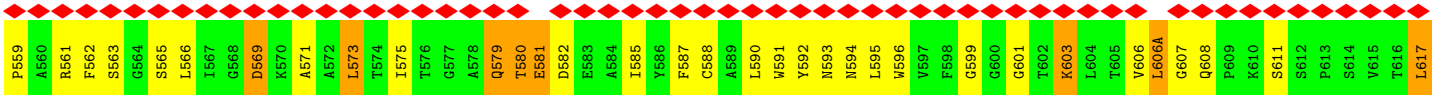


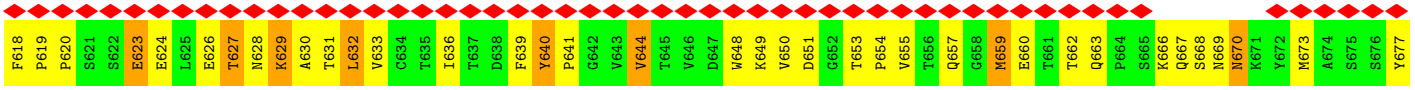


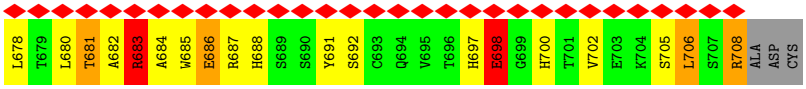
• Molecule 4: FAB



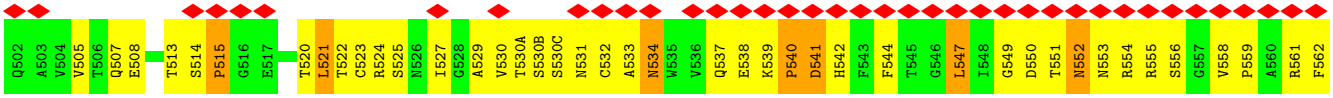


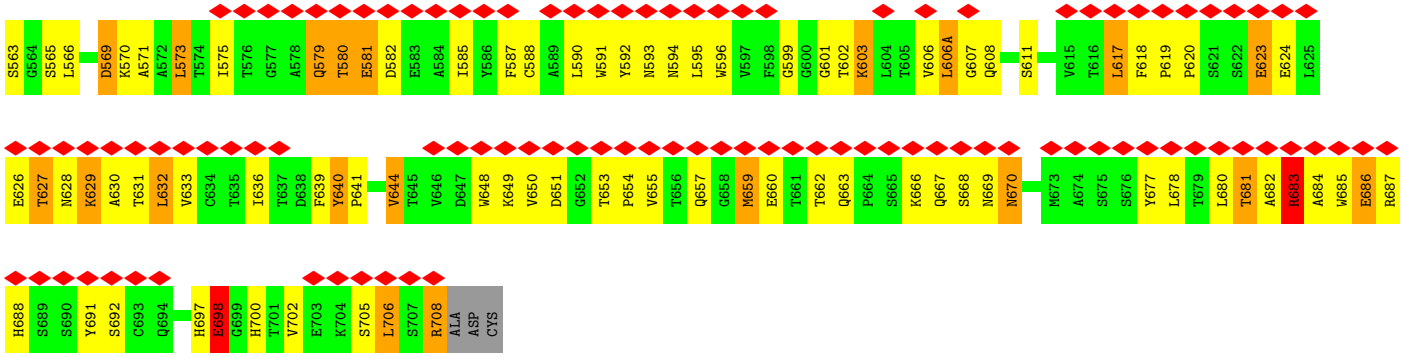






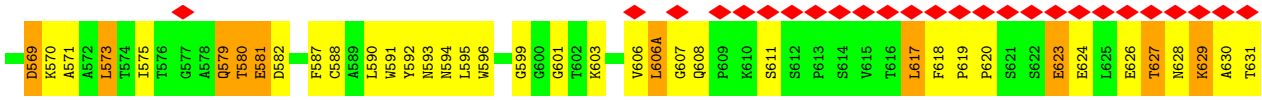
• Molecule 4: FAB

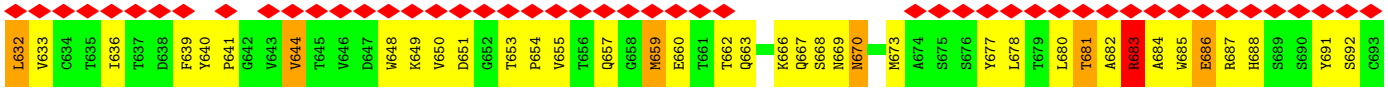


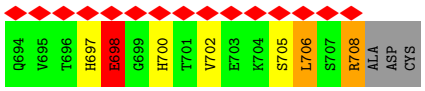


• Molecule 4: FAB

Chain O:

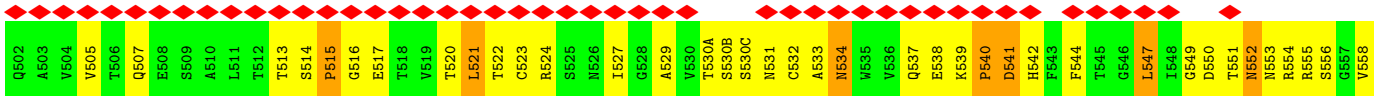


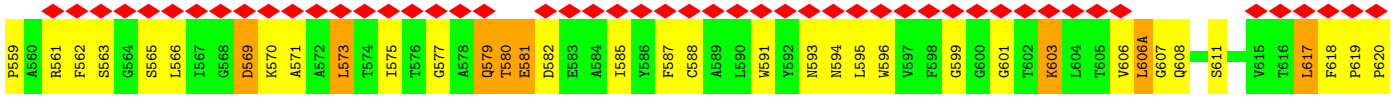


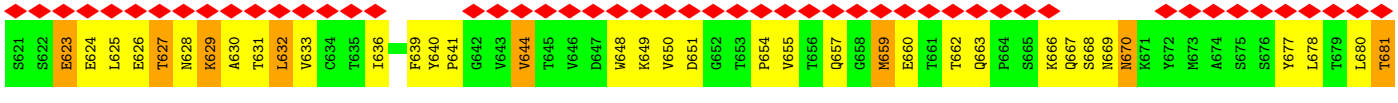


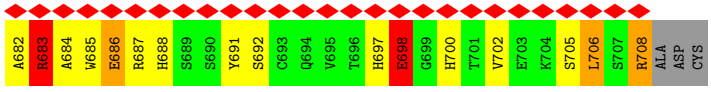
• Molecule 4: FAB

Chain P:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5828	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	22	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	78354	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	16.402	Depositor
Minimum map value	-21.542	Depositor
Average map value	0.052	Depositor
Map value standard deviation	1.789	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	1177.6, 1177.6, 1177.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.6799998, 3.6799998, 3.6799998	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.36	0/3063	0.54	0/4179
1	C	0.36	0/3063	0.54	0/4179
1	E	0.36	0/3063	0.54	0/4179
1	G	0.36	0/3063	0.54	0/4179
2	B	0.67	2/2721 (0.1%)	0.88	8/3704 (0.2%)
2	D	0.67	2/2721 (0.1%)	0.88	8/3704 (0.2%)
2	F	0.67	2/2721 (0.1%)	0.88	8/3704 (0.2%)
2	H	0.67	2/2721 (0.1%)	0.88	8/3704 (0.2%)
3	I	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	J	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	K	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	L	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
4	M	0.91	3/1634 (0.2%)	1.44	12/2232 (0.5%)
4	N	0.91	3/1634 (0.2%)	1.44	12/2232 (0.5%)
4	O	0.91	3/1634 (0.2%)	1.44	11/2232 (0.5%)
4	P	0.91	3/1634 (0.2%)	1.44	11/2232 (0.5%)
All	All	0.65	36/36528 (0.1%)	0.92	90/49820 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	D	0	2
2	F	0	2
2	H	0	2
All	All	0	8

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	731	ASN	C-N	-26.23	0.73	1.34
2	H	731	ASN	C-N	-26.22	0.73	1.34
2	F	731	ASN	C-N	-26.19	0.73	1.34
2	B	731	ASN	C-N	-26.19	0.73	1.34
3	L	57	PRO	N-CD	17.40	1.72	1.47
3	J	57	PRO	N-CD	17.39	1.72	1.47
3	I	57	PRO	N-CD	17.36	1.72	1.47
3	K	57	PRO	N-CD	17.36	1.72	1.47
3	J	41	PRO	N-CD	14.10	1.67	1.47
3	K	41	PRO	N-CD	14.07	1.67	1.47
3	L	41	PRO	N-CD	14.01	1.67	1.47
3	I	41	PRO	N-CD	13.98	1.67	1.47
4	P	515	PRO	N-CD	13.14	1.66	1.47
4	O	515	PRO	N-CD	13.11	1.66	1.47
4	N	515	PRO	N-CD	13.11	1.66	1.47
4	M	515	PRO	N-CD	13.08	1.66	1.47
2	F	672	PRO	C-N	12.07	1.57	1.34
2	B	672	PRO	C-N	12.06	1.57	1.34
2	D	672	PRO	C-N	12.04	1.57	1.34
2	H	672	PRO	C-N	12.04	1.57	1.34
3	K	14	PRO	N-CD	9.54	1.61	1.47
3	I	14	PRO	N-CD	9.51	1.61	1.47
3	J	14	PRO	N-CD	9.49	1.61	1.47
3	L	14	PRO	N-CD	9.45	1.61	1.47
4	P	540	PRO	N-CD	7.08	1.57	1.47
4	N	540	PRO	N-CD	7.06	1.57	1.47
4	O	540	PRO	N-CD	7.03	1.57	1.47
4	M	540	PRO	N-CD	7.01	1.57	1.47
3	K	33	PRO	N-CD	6.25	1.56	1.47
3	J	33	PRO	N-CD	6.24	1.56	1.47
3	L	33	PRO	N-CD	6.24	1.56	1.47
3	I	33	PRO	N-CD	6.21	1.56	1.47
4	M	542	HIS	CG-CD2	6.08	1.46	1.35
4	O	542	HIS	CG-CD2	6.03	1.46	1.35
4	P	542	HIS	CG-CD2	6.02	1.46	1.35
4	N	542	HIS	CG-CD2	6.00	1.46	1.35

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	731	ASN	O-C-N	-23.70	84.77	122.70
2	H	731	ASN	O-C-N	-23.70	84.77	122.70
2	B	731	ASN	O-C-N	-23.67	84.83	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	731	ASN	O-C-N	-23.62	84.90	122.70
2	B	672	PRO	O-C-N	-18.02	86.86	121.10
2	F	672	PRO	O-C-N	-18.02	86.87	121.10
2	H	672	PRO	O-C-N	-18.01	86.89	121.10
2	D	672	PRO	O-C-N	-17.99	86.92	121.10
2	D	672	PRO	CA-C-N	-17.30	68.65	117.10
2	B	672	PRO	CA-C-N	-17.30	68.67	117.10
2	H	672	PRO	CA-C-N	-17.30	68.67	117.10
2	F	672	PRO	CA-C-N	-17.29	68.70	117.10
2	F	731	ASN	CA-C-N	15.48	151.26	117.20
2	B	731	ASN	CA-C-N	15.47	151.23	117.20
2	D	731	ASN	CA-C-N	15.46	151.22	117.20
2	H	731	ASN	CA-C-N	15.46	151.22	117.20
2	D	672	PRO	C-N-CA	-12.32	70.25	122.00
2	F	672	PRO	C-N-CA	-12.32	70.26	122.00
2	H	672	PRO	C-N-CA	-12.32	70.27	122.00
2	B	672	PRO	C-N-CA	-12.31	70.30	122.00
4	O	683	ARG	NE-CZ-NH1	10.19	125.39	120.30
4	M	683	ARG	NE-CZ-NH1	10.17	125.39	120.30
4	N	683	ARG	NE-CZ-NH1	10.14	125.37	120.30
4	P	683	ARG	NE-CZ-NH1	10.10	125.35	120.30
2	B	672	PRO	C-N-CD	-9.96	98.68	120.60
2	F	672	PRO	C-N-CD	-9.96	98.69	120.60
2	H	672	PRO	C-N-CD	-9.93	98.75	120.60
2	D	672	PRO	C-N-CD	-9.93	98.76	120.60
4	M	632	LEU	CA-CB-CG	9.71	137.63	115.30
4	P	632	LEU	CA-CB-CG	9.70	137.61	115.30
4	O	632	LEU	CA-CB-CG	9.69	137.60	115.30
4	N	632	LEU	CA-CB-CG	9.67	137.54	115.30
2	F	731	ASN	C-N-CA	8.68	143.41	121.70
2	H	731	ASN	C-N-CA	8.68	143.41	121.70
2	B	731	ASN	C-N-CA	8.66	143.36	121.70
2	D	731	ASN	C-N-CA	8.66	143.36	121.70
4	O	698	GLU	OE1-CD-OE2	-7.66	114.11	123.30
4	N	698	GLU	OE1-CD-OE2	-7.63	114.14	123.30
4	M	698	GLU	OE1-CD-OE2	-7.62	114.15	123.30
4	P	698	GLU	OE1-CD-OE2	-7.62	114.15	123.30
4	P	708	ARG	NE-CZ-NH1	7.61	124.10	120.30
4	N	708	ARG	NE-CZ-NH1	7.60	124.10	120.30
4	O	708	ARG	NE-CZ-NH1	7.54	124.07	120.30
4	M	708	ARG	NE-CZ-NH1	7.48	124.04	120.30
4	P	698	GLU	CB-CG-CD	7.39	134.16	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	698	GLU	CB-CG-CD	7.38	134.12	114.20
4	O	698	GLU	CB-CG-CD	7.38	134.12	114.20
4	M	698	GLU	CB-CG-CD	7.38	134.12	114.20
4	M	683	ARG	NE-CZ-NH2	-7.27	116.67	120.30
4	O	683	ARG	NE-CZ-NH2	-7.26	116.67	120.30
4	N	683	ARG	NE-CZ-NH2	-7.26	116.67	120.30
4	P	683	ARG	NE-CZ-NH2	-7.25	116.67	120.30
4	O	687	ARG	NE-CZ-NH1	6.80	123.70	120.30
4	M	687	ARG	NE-CZ-NH1	6.71	123.65	120.30
4	P	687	ARG	NE-CZ-NH1	6.71	123.65	120.30
4	N	687	ARG	NE-CZ-NH1	6.68	123.64	120.30
4	N	698	GLU	N-CA-CB	6.40	122.11	110.60
4	O	698	GLU	N-CA-CB	6.38	122.08	110.60
4	M	698	GLU	N-CA-CB	6.38	122.08	110.60
4	P	698	GLU	N-CA-CB	6.38	122.08	110.60
3	I	55	GLY	CA-C-N	5.46	129.21	117.20
3	J	55	GLY	CA-C-N	5.45	129.19	117.20
3	K	55	GLY	CA-C-N	5.45	129.18	117.20
3	L	55	GLY	CA-C-N	5.45	129.18	117.20
4	O	611	SER	N-CA-CB	-5.41	102.38	110.50
4	M	644	VAL	CA-CB-CG1	5.40	119.00	110.90
4	M	611	SER	N-CA-CB	-5.38	102.43	110.50
4	P	644	VAL	CA-CB-CG1	5.38	118.96	110.90
4	M	631	THR	CA-CB-CG2	5.37	119.92	112.40
4	O	631	THR	CA-CB-CG2	5.37	119.91	112.40
4	N	611	SER	N-CA-CB	-5.37	102.45	110.50
4	P	631	THR	CA-CB-CG2	5.36	119.91	112.40
4	N	644	VAL	CA-CB-CG1	5.36	118.94	110.90
4	O	644	VAL	CA-CB-CG1	5.35	118.93	110.90
4	P	611	SER	N-CA-CB	-5.34	102.49	110.50
4	N	631	THR	CA-CB-CG2	5.33	119.86	112.40
3	L	73	ILE	CA-C-N	-5.18	105.80	117.20
3	K	73	ILE	CA-C-N	-5.17	105.83	117.20
3	I	73	ILE	CA-C-N	-5.16	105.85	117.20
3	J	73	ILE	CA-C-N	-5.15	105.87	117.20
2	D	633	PRO	C-N-CD	5.13	139.16	128.40
2	F	633	PRO	C-N-CD	5.11	139.13	128.40
2	H	633	PRO	C-N-CD	5.10	139.11	128.40
2	B	633	PRO	C-N-CD	5.10	139.10	128.40
3	I	43	LYS	N-CA-C	5.08	124.71	111.00
3	L	43	LYS	N-CA-C	5.06	124.67	111.00
3	J	43	LYS	N-CA-C	5.06	124.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	640	TYR	CB-CG-CD2	5.06	124.03	121.00
3	K	43	LYS	N-CA-C	5.05	124.65	111.00
4	M	640	TYR	CB-CG-CD2	5.04	124.02	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	672	PRO	Mainchain
2	B	731	ASN	Mainchain
2	D	672	PRO	Mainchain
2	D	731	ASN	Mainchain
2	F	672	PRO	Mainchain
2	F	731	ASN	Mainchain
2	H	672	PRO	Mainchain
2	H	731	ASN	Mainchain

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	2986	0	2889	188	0
1	C	2986	0	2889	146	0
1	E	2986	0	2885	156	0
1	G	2986	0	2889	102	0
2	B	2650	0	2542	648	0
2	D	2650	0	2537	669	0
2	F	2650	0	2536	638	0
2	H	2650	0	2541	672	0
3	I	1671	0	1641	225	0
3	J	1671	0	1641	216	0
3	K	1671	0	1641	227	0
3	L	1671	0	1640	231	0
4	M	1598	0	1518	312	0
4	N	1598	0	1517	324	0
4	O	1598	0	1517	299	0
4	P	1598	0	1520	342	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35620	0	34343	4086	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 58.

All (4086) 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:93:TYR:CD1	2:D:676:PRO:HG3	1.19	1.71
1:E:93:TYR:CD1	2:F:676:PRO:HG3	1.19	1.69
3:K:114:ALA:HB3	3:K:146:PHE:CE2	1.17	1.69
3:L:114:ALA:HB3	3:L:146:PHE:CE2	1.17	1.68
3:L:32:TYR:HE1	3:L:96:TYR:CD1	1.00	1.67
2:H:716:VAL:HG12	4:P:591:TRP:CD1	1.25	1.66
3:I:32:TYR:HE1	3:I:96:TYR:CD1	1.00	1.66
3:J:32:TYR:HE1	3:J:96:TYR:CD1	1.00	1.66
2:F:602:LEU:HD13	2:F:758:PRO:CD	1.24	1.65
2:H:547:LYS:CD	2:H:757:ILE:CG2	1.75	1.65
2:H:547:LYS:HD2	2:H:757:ILE:CG2	1.23	1.65
2:B:534:LEU:CD1	2:B:734:LYS:HB3	1.20	1.64
2:B:716:VAL:CG1	4:M:591:TRP:HB3	1.28	1.64
2:F:716:VAL:CG1	4:O:591:TRP:CD1	1.76	1.63
3:L:32:TYR:CE1	3:L:96:TYR:CD1	1.86	1.63
2:D:602:LEU:HD13	2:D:758:PRO:CD	1.24	1.63
1:G:93:TYR:CD1	2:H:676:PRO:HG3	1.19	1.63
2:B:602:LEU:CD1	2:B:758:PRO:CD	1.77	1.63
3:K:32:TYR:HE1	3:K:96:TYR:CD1	1.00	1.63
2:B:547:LYS:CD	2:B:757:ILE:CG2	1.75	1.62
2:H:602:LEU:CD1	2:H:758:PRO:CD	1.77	1.62
3:J:32:TYR:CE1	3:J:96:TYR:CD1	1.86	1.62
1:A:93:TYR:CD1	2:B:676:PRO:HG3	1.19	1.61
2:F:716:VAL:CG1	4:O:591:TRP:HB3	1.30	1.61
2:F:547:LYS:CD	2:F:757:ILE:CG2	1.75	1.61
3:K:32:TYR:CE1	3:K:96:TYR:CD1	1.86	1.61
2:F:602:LEU:CD1	2:F:758:PRO:CD	1.77	1.61
2:B:716:VAL:HG21	4:M:532:CYS:CB	1.24	1.60
2:D:689:LYS:CB	3:J:98:ILE:HD12	1.22	1.60
2:H:602:LEU:HD13	2:H:758:PRO:CD	1.24	1.60
3:I:114:ALA:HB3	3:I:146:PHE:CE2	1.17	1.59
2:B:716:VAL:HG12	4:M:591:TRP:CD1	1.17	1.59
2:F:547:LYS:HD2	2:F:757:ILE:CG2	1.23	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:114:ALA:HB3	3:J:146:PHE:CE2	1.17	1.59
2:D:716:VAL:CG1	4:N:591:TRP:CB	1.79	1.58
2:B:547:LYS:HD3	2:B:667:ILE:CG1	1.33	1.58
2:F:547:LYS:HD3	2:F:667:ILE:CG1	1.33	1.58
2:F:716:VAL:HG12	4:O:591:TRP:CG	1.34	1.58
2:B:602:LEU:HD13	2:B:758:PRO:CD	1.24	1.58
2:H:534:LEU:CD1	2:H:734:LYS:HB3	1.20	1.57
2:B:602:LEU:CD1	2:B:758:PRO:HD3	1.31	1.57
2:F:534:LEU:CD1	2:F:734:LYS:HB3	1.20	1.57
2:F:716:VAL:HG11	4:O:591:TRP:CB	1.29	1.57
3:I:32:TYR:CE1	3:I:96:TYR:CD1	1.86	1.57
1:A:93:TYR:CD1	2:B:676:PRO:CG	1.86	1.57
2:D:547:LYS:HD2	2:D:757:ILE:CG2	1.23	1.57
1:C:93:TYR:CD1	2:D:676:PRO:CG	1.85	1.56
2:H:534:LEU:HD12	2:H:734:LYS:CB	1.33	1.56
1:A:24:TYR:CD1	1:E:305:ALA:HB1	1.35	1.56
1:E:93:TYR:CD1	2:F:676:PRO:CG	1.85	1.56
2:H:686:GLY:CA	4:P:552:ASN:H	1.00	1.56
2:D:602:LEU:CD1	2:D:758:PRO:CD	1.77	1.56
2:H:602:LEU:CD1	2:H:758:PRO:HD3	1.31	1.56
2:D:547:LYS:CD	2:D:757:ILE:CG2	1.75	1.55
2:F:547:LYS:CD	2:F:667:ILE:CG1	1.83	1.55
2:D:547:LYS:CD	2:D:667:ILE:CG1	1.83	1.54
3:I:35:LEU:CD1	3:I:100:LEU:HD21	1.36	1.54
2:D:689:LYS:HB2	3:J:98:ILE:CD1	1.30	1.54
3:L:45:PHE:CZ	4:P:544:PHE:HZ	1.25	1.54
3:L:35:LEU:CD1	3:L:100:LEU:HD21	1.36	1.54
2:B:547:LYS:HD2	2:B:757:ILE:CG2	1.23	1.54
2:B:535:GLU:C	2:B:736:GLN:H	1.07	1.54
2:D:534:LEU:CD1	2:D:734:LYS:HB3	1.20	1.54
3:I:35:LEU:HD13	3:I:100:LEU:CD2	1.36	1.53
3:K:45:PHE:CZ	4:O:544:PHE:CZ	1.96	1.53
2:B:534:LEU:HD12	2:B:734:LYS:CB	1.32	1.53
2:B:716:VAL:HG12	4:M:591:TRP:CG	1.37	1.53
3:L:45:PHE:CZ	4:P:544:PHE:CZ	1.96	1.53
2:F:602:LEU:CD1	2:F:758:PRO:HD3	1.31	1.53
2:F:547:LYS:CD	2:F:757:ILE:HG21	1.33	1.53
2:D:534:LEU:HD12	2:D:734:LYS:CB	1.32	1.53
2:F:627:HIS:CD2	2:F:734:LYS:HB2	1.00	1.53
3:K:35:LEU:CD1	3:K:100:LEU:HD21	1.36	1.53
3:J:35:LEU:CD1	3:J:100:LEU:HD21	1.36	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:35:LEU:HD13	3:J:100:LEU:CD2	1.36	1.52
2:H:627:HIS:CD2	2:H:734:LYS:HB2	1.00	1.52
3:I:114:ALA:CB	3:I:146:PHE:CE2	1.92	1.52
2:D:689:LYS:CB	3:J:98:ILE:CD1	1.80	1.52
1:G:93:TYR:CD1	2:H:676:PRO:CG	1.85	1.52
2:D:547:LYS:HD3	2:D:667:ILE:CG1	1.33	1.52
2:D:627:HIS:CD2	2:D:734:LYS:HB2	1.00	1.52
2:F:687:ASN:CB	4:O:532:CYS:HA	1.18	1.52
2:H:547:LYS:CD	2:H:667:ILE:CG1	1.83	1.52
3:K:45:PHE:CZ	4:O:544:PHE:HZ	1.25	1.52
2:B:716:VAL:CG1	4:M:591:TRP:CB	1.86	1.51
2:F:535:GLU:C	2:F:736:GLN:H	1.07	1.51
3:K:35:LEU:HD13	3:K:100:LEU:CD2	1.36	1.51
3:J:114:ALA:CB	3:J:146:PHE:CE2	1.93	1.50
2:F:534:LEU:CD1	2:F:734:LYS:CD	1.89	1.50
2:F:716:VAL:CG1	4:O:591:TRP:CG	1.88	1.50
3:L:114:ALA:CB	3:L:146:PHE:CE2	1.93	1.50
3:K:114:ALA:CB	3:K:146:PHE:CE2	1.93	1.50
2:B:627:HIS:CD2	2:B:734:LYS:HB2	1.00	1.50
2:F:716:VAL:CG1	4:O:591:TRP:CB	1.84	1.50
2:H:535:GLU:C	2:H:736:GLN:H	1.07	1.50
3:I:45:PHE:CZ	4:M:544:PHE:CZ	1.96	1.50
1:C:63:CYS:HB2	2:D:700:LYS:CE	1.40	1.50
2:B:597:MET:CB	2:B:756:HIS:HD2	1.24	1.49
2:F:534:LEU:CD1	2:F:734:LYS:CB	1.85	1.49
2:H:597:MET:CB	2:H:756:HIS:HD2	1.25	1.49
3:L:35:LEU:HD13	3:L:100:LEU:CD2	1.36	1.49
3:J:45:PHE:CZ	4:N:544:PHE:CZ	1.96	1.49
2:D:597:MET:CB	2:D:756:HIS:HD2	1.25	1.49
2:H:627:HIS:CD2	2:H:734:LYS:CB	1.95	1.49
3:J:45:PHE:CZ	4:N:544:PHE:HZ	1.25	1.49
2:D:535:GLU:C	2:D:736:GLN:H	1.08	1.49
2:D:547:LYS:CD	2:D:757:ILE:HG21	1.33	1.49
2:F:534:LEU:HD12	2:F:734:LYS:CB	1.32	1.49
2:F:597:MET:CB	2:F:756:HIS:HD2	1.25	1.49
2:D:534:LEU:CD1	2:D:734:LYS:CD	1.89	1.49
2:H:547:LYS:CD	2:H:757:ILE:HG21	1.33	1.48
1:A:63:CYS:HB2	2:B:700:LYS:CE	1.40	1.48
2:D:627:HIS:CD2	2:D:734:LYS:CB	1.95	1.48
3:I:45:PHE:CZ	4:M:544:PHE:HZ	1.25	1.48
2:D:716:VAL:CG1	4:N:591:TRP:HB3	1.03	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:627:HIS:CD2	2:F:734:LYS:CB	1.95	1.47
2:H:534:LEU:CD1	2:H:734:LYS:CD	1.89	1.47
2:D:704:GLY:C	4:N:530(A):THR:CG2	1.76	1.47
2:F:684:GLN:HB3	3:K:98:ILE:CG2	1.00	1.47
2:H:602:LEU:CG	2:H:758:PRO:HD3	1.43	1.47
2:B:534:LEU:CD1	2:B:734:LYS:CD	1.89	1.47
2:H:689:LYS:HB2	3:L:98:ILE:CD1	1.43	1.47
1:G:63:CYS:HB2	2:H:700:LYS:CE	1.40	1.47
1:E:63:CYS:HB2	2:F:700:LYS:CE	1.40	1.47
3:J:41:PRO:CD	3:J:41:PRO:N	1.67	1.47
2:B:522:CYS:H	2:B:733:LYS:NZ	1.05	1.46
2:F:685:SER:HB2	4:O:549:GLY:C	1.10	1.46
2:B:602:LEU:CG	2:B:758:PRO:HD3	1.43	1.46
2:D:534:LEU:CD1	2:D:734:LYS:CB	1.85	1.46
2:B:547:LYS:CD	2:B:667:ILE:CG1	1.83	1.46
2:D:547:LYS:CD	2:D:667:ILE:HG12	0.98	1.46
2:D:602:LEU:CG	2:D:758:PRO:HD3	1.43	1.45
2:B:534:LEU:HD12	2:B:734:LYS:CG	1.46	1.45
2:F:602:LEU:CG	2:F:758:PRO:HD3	1.43	1.45
2:B:547:LYS:CD	2:B:667:ILE:HG12	0.98	1.45
2:D:613:VAL:H	2:D:734:LYS:NZ	1.10	1.45
2:H:547:LYS:HD3	2:H:667:ILE:CG1	1.33	1.45
3:L:57:PRO:CD	3:L:57:PRO:N	1.72	1.45
2:H:547:LYS:CD	2:H:667:ILE:HG12	0.98	1.45
2:F:547:LYS:CD	2:F:667:ILE:HG12	0.98	1.44
2:B:627:HIS:CD2	2:B:734:LYS:CB	1.95	1.44
2:H:549:GLN:O	2:H:735:TRP:CB	1.64	1.44
1:A:289:ARG:NH2	1:E:353:GLN:HG2	1.30	1.44
2:F:534:LEU:HD12	2:F:734:LYS:CG	1.46	1.44
2:D:522:CYS:H	2:D:733:LYS:NZ	1.05	1.43
2:D:602:LEU:CD1	2:D:758:PRO:HD3	1.31	1.43
2:H:534:LEU:HD12	2:H:734:LYS:CG	1.46	1.43
2:H:534:LEU:CD1	2:H:734:LYS:CB	1.85	1.43
2:F:686:GLY:HA3	4:O:552:ASN:N	1.33	1.43
2:B:549:GLN:O	2:B:735:TRP:CB	1.65	1.42
2:F:549:GLN:O	2:F:735:TRP:CB	1.64	1.42
2:D:549:GLN:O	2:D:735:TRP:CB	1.64	1.42
1:G:93:TYR:HD1	2:H:676:PRO:CB	1.32	1.42
2:B:522:CYS:N	2:B:733:LYS:CD	1.83	1.42
2:D:522:CYS:N	2:D:733:LYS:CD	1.83	1.42
2:F:522:CYS:H	2:F:733:LYS:NZ	1.05	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:613:VAL:H	2:H:734:LYS:NZ	1.10	1.42
3:J:57:PRO:CD	3:J:57:PRO:N	1.72	1.42
2:B:613:VAL:H	2:B:734:LYS:NZ	1.10	1.41
1:A:93:TYR:HD1	2:B:676:PRO:CB	1.32	1.41
2:D:534:LEU:HD12	2:D:734:LYS:CG	1.46	1.41
2:F:686:GLY:CA	4:O:552:ASN:H	1.30	1.41
2:F:686:GLY:N	4:O:552:ASN:H	1.08	1.41
1:E:93:TYR:HD1	2:F:676:PRO:CB	1.32	1.41
3:K:98:ILE:CB	4:O:550:ASP:HB2	1.49	1.41
1:A:24:TYR:CD1	1:E:305:ALA:CB	2.04	1.40
2:B:549:GLN:O	2:B:735:TRP:CG	1.75	1.40
2:H:522:CYS:N	2:H:733:LYS:CD	1.83	1.40
2:D:602:LEU:HD13	2:D:758:PRO:CG	1.50	1.40
2:D:687:ASN:ND2	4:N:533:ALA:N	1.68	1.40
2:H:716:VAL:CG2	4:P:532:CYS:CB	1.96	1.40
2:B:602:LEU:HD13	2:B:758:PRO:CG	1.50	1.40
2:B:716:VAL:CG2	4:M:532:CYS:CB	1.80	1.40
2:D:547:LYS:CE	2:D:757:ILE:HG23	1.50	1.40
3:I:57:PRO:CD	3:I:57:PRO:N	1.72	1.40
2:F:597:MET:HB3	2:F:756:HIS:CD2	1.57	1.40
2:H:718:ASN:H	4:P:531:ASN:N	1.13	1.40
2:B:547:LYS:CD	2:B:757:ILE:HG21	1.33	1.40
2:B:597:MET:HB3	2:B:756:HIS:CD2	1.57	1.40
2:D:547:LYS:CE	2:D:667:ILE:HG12	1.50	1.40
2:D:716:VAL:HG12	4:N:591:TRP:CG	1.55	1.40
2:F:547:LYS:CE	2:F:757:ILE:HG23	1.50	1.40
2:H:602:LEU:HD13	2:H:758:PRO:CG	1.50	1.40
2:H:687:ASN:ND2	4:P:532:CYS:C	1.74	1.40
2:B:547:LYS:CE	2:B:757:ILE:HG23	1.50	1.39
2:F:613:VAL:H	2:F:734:LYS:NZ	1.10	1.39
1:C:93:TYR:HD1	2:D:676:PRO:CB	1.32	1.39
2:F:522:CYS:N	2:F:733:LYS:CD	1.83	1.39
2:F:715:LYS:HE2	4:O:593:ASN:CG	1.41	1.39
2:H:522:CYS:H	2:H:733:LYS:NZ	1.05	1.39
2:H:716:VAL:HG12	4:P:591:TRP:CG	1.55	1.39
2:D:597:MET:HB3	2:D:756:HIS:CD2	1.57	1.39
2:F:549:GLN:O	2:F:735:TRP:CG	1.75	1.38
2:F:704:GLY:O	4:O:530(A):THR:CG2	1.69	1.38
2:B:535:GLU:HB3	2:B:670:HIS:CA	1.50	1.38
2:B:602:LEU:CD2	2:B:758:PRO:HD3	1.52	1.38
2:D:549:GLN:O	2:D:735:TRP:CG	1.75	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:718:ASN:N	4:P:531:ASN:H	0.95	1.38
1:A:93:TYR:CE1	2:B:676:PRO:HG3	1.59	1.38
2:F:602:LEU:HD13	2:F:758:PRO:CG	1.50	1.38
1:G:93:TYR:CE1	2:H:676:PRO:HG3	1.59	1.38
2:B:687:ASN:CB	4:M:532:CYS:HA	1.39	1.38
2:H:547:LYS:CE	2:H:667:ILE:HG12	1.50	1.38
2:B:534:LEU:CD1	2:B:734:LYS:CB	1.85	1.38
2:H:549:GLN:O	2:H:735:TRP:CG	1.75	1.38
2:D:535:GLU:HB3	2:D:670:HIS:CA	1.50	1.37
2:H:547:LYS:CE	2:H:757:ILE:HG23	1.50	1.37
3:I:77:THR:HG21	3:I:79:TYR:CZ	1.59	1.37
2:D:520:PRO:HD3	2:D:731:ASN:C	1.21	1.37
2:D:602:LEU:CD2	2:D:758:PRO:HD3	1.52	1.37
2:F:547:LYS:CE	2:F:667:ILE:HG12	1.50	1.37
2:F:602:LEU:HD11	2:F:758:PRO:N	1.40	1.37
2:F:671:MET:O	2:F:673:PRO:CD	1.72	1.37
2:H:597:MET:HB3	2:H:756:HIS:CD2	1.57	1.37
3:K:77:THR:HG21	3:K:79:TYR:CZ	1.60	1.37
2:B:715:LYS:HE2	4:M:593:ASN:CB	1.55	1.37
2:H:520:PRO:HD3	2:H:731:ASN:C	1.21	1.37
2:H:602:LEU:CD2	2:H:758:PRO:HD3	1.52	1.36
2:D:671:MET:O	2:D:673:PRO:N	1.57	1.36
3:J:45:PHE:CE2	4:N:544:PHE:CZ	2.14	1.36
2:B:547:LYS:CE	2:B:667:ILE:HG12	1.50	1.36
1:C:93:TYR:CE1	2:D:676:PRO:HG3	1.59	1.36
2:F:602:LEU:CD2	2:F:758:PRO:HD3	1.52	1.36
2:B:520:PRO:HD3	2:B:731:ASN:C	1.22	1.36
2:D:671:MET:O	2:D:673:PRO:CD	1.72	1.36
2:H:671:MET:O	2:H:673:PRO:N	1.57	1.36
3:J:77:THR:HG21	3:J:79:TYR:CZ	1.60	1.36
2:D:602:LEU:HD11	2:D:758:PRO:N	1.40	1.35
2:D:717:ILE:HG22	4:N:530(B):SER:N	1.40	1.35
1:E:93:TYR:CE1	2:F:676:PRO:HG3	1.59	1.35
2:B:689:LYS:HB2	3:I:98:ILE:CD1	1.56	1.35
2:H:671:MET:O	2:H:673:PRO:CD	1.72	1.35
3:K:45:PHE:CE2	4:O:544:PHE:CZ	2.14	1.35
3:L:41:PRO:N	3:L:41:PRO:CD	1.67	1.35
3:L:77:THR:HG21	3:L:79:TYR:CZ	1.60	1.35
2:B:538:ARG:HD3	2:B:667:ILE:CD1	1.56	1.35
2:D:687:ASN:O	4:N:550:ASP:CG	1.64	1.35
2:F:686:GLY:CA	4:O:552:ASN:N	1.85	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:602:LEU:HD11	2:H:758:PRO:N	1.40	1.35
2:F:685:SER:O	4:O:552:ASN:ND2	1.59	1.34
3:K:57:PRO:CD	3:K:57:PRO:N	1.72	1.34
2:B:671:MET:O	2:B:673:PRO:CD	1.72	1.34
2:F:716:VAL:HG12	4:O:591:TRP:CD1	0.83	1.34
2:B:602:LEU:HD11	2:B:758:PRO:N	1.40	1.34
2:D:538:ARG:HD3	2:D:667:ILE:CD1	1.56	1.34
2:D:718:ASN:ND2	4:N:533:ALA:HB2	1.42	1.34
3:L:45:PHE:CE2	4:P:544:PHE:CZ	2.14	1.34
3:I:45:PHE:CE2	4:M:544:PHE:CZ	2.13	1.34
3:K:32:TYR:OH	3:K:96:TYR:CZ	1.69	1.33
2:F:535:GLU:HB3	2:F:670:HIS:CA	1.50	1.33
2:D:520:PRO:CD	2:D:731:ASN:C	1.89	1.33
2:F:538:ARG:HD3	2:F:667:ILE:CD1	1.56	1.33
1:A:63:CYS:CB	2:B:700:LYS:HE2	1.59	1.32
1:G:63:CYS:CB	2:H:700:LYS:HE2	1.59	1.32
2:H:538:ARG:HD3	2:H:667:ILE:CD1	1.56	1.32
2:B:715:LYS:CD	4:M:593:ASN:OD1	1.75	1.32
2:D:522:CYS:N	2:D:733:LYS:NZ	1.78	1.32
2:F:671:MET:O	2:F:673:PRO:N	1.57	1.32
2:B:535:GLU:HB3	2:B:670:HIS:N	1.44	1.32
2:D:718:ASN:OD1	4:N:531:ASN:CB	1.75	1.32
2:F:520:PRO:HD3	2:F:731:ASN:C	1.21	1.32
2:F:715:LYS:HE2	4:O:593:ASN:CB	1.58	1.32
2:H:535:GLU:HB3	2:H:670:HIS:N	1.44	1.32
3:J:32:TYR:OH	3:J:96:TYR:CZ	1.69	1.32
1:C:63:CYS:CB	2:D:700:LYS:HE2	1.59	1.31
1:E:63:CYS:CB	2:F:700:LYS:HE2	1.59	1.31
2:F:520:PRO:CD	2:F:731:ASN:C	1.89	1.31
3:L:32:TYR:OH	3:L:96:TYR:CZ	1.69	1.31
2:B:671:MET:O	2:B:673:PRO:N	1.57	1.31
2:D:535:GLU:HB3	2:D:670:HIS:N	1.44	1.31
2:D:613:VAL:N	2:D:734:LYS:NZ	1.79	1.31
2:D:719:ASN:OD1	4:N:565:SER:C	1.66	1.31
2:F:715:LYS:CD	4:O:593:ASN:OD1	1.78	1.31
2:H:535:GLU:HB3	2:H:670:HIS:CA	1.50	1.31
2:H:718:ASN:N	4:P:531:ASN:N	1.67	1.30
2:B:520:PRO:CD	2:B:731:ASN:C	1.89	1.30
2:F:715:LYS:CG	4:O:593:ASN:OD1	1.80	1.30
3:J:32:TYR:OH	3:J:96:TYR:CE1	1.84	1.30
3:K:41:PRO:CD	3:K:41:PRO:N	1.67	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:715:LYS:HE2	4:M:593:ASN:CG	1.49	1.30
2:H:716:VAL:HG21	4:P:532:CYS:CB	1.54	1.30
3:I:32:TYR:OH	3:I:96:TYR:CE1	1.84	1.30
3:K:32:TYR:OH	3:K:96:TYR:CE1	1.84	1.30
2:B:522:CYS:N	2:B:733:LYS:NZ	1.77	1.30
2:B:716:VAL:CG1	4:M:591:TRP:CD1	2.13	1.30
2:H:684:GLN:N	4:P:550:ASP:OD2	1.63	1.30
3:I:2:ILE:CD1	3:I:94:ARG:NH1	1.95	1.30
3:K:2:ILE:CD1	3:K:94:ARG:NH1	1.95	1.30
2:D:716:VAL:HG12	4:N:591:TRP:CB	1.49	1.29
2:F:613:VAL:N	2:F:734:LYS:NZ	1.79	1.29
3:L:32:TYR:OH	3:L:96:TYR:CE1	1.84	1.29
2:D:719:ASN:O	4:N:566:LEU:CD1	1.77	1.29
1:C:95:PHE:CD1	2:D:725:CYS:HA	1.57	1.29
2:D:687:ASN:CB	4:N:532:CYS:HA	1.62	1.29
3:J:2:ILE:CD1	3:J:94:ARG:NH1	1.95	1.29
3:L:2:ILE:CD1	3:L:94:ARG:NH1	1.95	1.29
2:H:520:PRO:CD	2:H:731:ASN:C	1.89	1.29
2:H:522:CYS:N	2:H:733:LYS:NZ	1.78	1.29
2:F:535:GLU:HB3	2:F:670:HIS:N	1.44	1.28
2:F:522:CYS:N	2:F:733:LYS:NZ	1.77	1.28
2:H:613:VAL:N	2:H:734:LYS:NZ	1.79	1.28
1:A:95:PHE:CD1	2:B:725:CYS:HA	1.56	1.28
2:B:613:VAL:N	2:B:734:LYS:NZ	1.79	1.28
2:B:671:MET:C	2:B:673:PRO:N	1.84	1.28
2:F:547:LYS:CG	2:F:667:ILE:HG12	1.62	1.28
2:F:687:ASN:CB	4:O:532:CYS:CA	2.12	1.28
2:H:686:GLY:C	4:P:551:THR:HB	1.54	1.28
2:H:718:ASN:CB	4:P:531:ASN:HB2	1.47	1.27
2:D:547:LYS:CG	2:D:667:ILE:HG12	1.62	1.27
2:B:547:LYS:CG	2:B:667:ILE:HG12	1.62	1.27
2:D:718:ASN:HD22	4:N:533:ALA:CB	1.46	1.27
2:F:685:SER:CA	4:O:549:GLY:O	1.82	1.27
2:H:547:LYS:CG	2:H:667:ILE:HG12	1.62	1.27
2:D:534:LEU:HD12	2:D:734:LYS:CD	1.54	1.27
1:E:93:TYR:CD1	2:F:676:PRO:CB	2.13	1.26
2:D:547:LYS:HB3	2:D:667:ILE:CD1	1.65	1.26
2:F:522:CYS:CA	2:F:733:LYS:HD3	1.62	1.26
2:D:718:ASN:N	4:N:531:ASN:H	1.34	1.26
2:F:547:LYS:HB3	2:F:667:ILE:CD1	1.65	1.26
2:H:547:LYS:HB3	2:H:667:ILE:CD1	1.65	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:45:PHE:HZ	4:M:544:PHE:CZ	1.43	1.26
2:D:716:VAL:HG12	4:N:591:TRP:CD1	1.70	1.26
3:I:32:TYR:OH	3:I:96:TYR:CZ	1.69	1.26
2:B:534:LEU:HD12	2:B:734:LYS:CD	1.54	1.25
2:H:536:ARG:HD3	2:H:668:GLU:O	1.36	1.25
2:H:716:VAL:CG1	4:P:591:TRP:CD1	2.16	1.25
1:E:95:PHE:CD1	2:F:725:CYS:HA	1.57	1.25
2:H:687:ASN:CB	4:P:550:ASP:HA	1.66	1.25
2:H:522:CYS:CA	2:H:733:LYS:HD3	1.62	1.25
3:K:32:TYR:CE1	3:K:96:TYR:CG	2.24	1.25
2:D:533:ALA:HA	2:D:733:LYS:O	1.34	1.25
2:F:536:ARG:HD3	2:F:668:GLU:O	1.36	1.25
1:G:95:PHE:CD1	2:H:725:CYS:HA	1.57	1.25
3:I:32:TYR:CE1	3:I:96:TYR:CG	2.24	1.25
2:F:535:GLU:C	2:F:736:GLN:N	1.90	1.25
1:A:93:TYR:CD1	2:B:676:PRO:CB	2.13	1.24
2:B:547:LYS:HB3	2:B:667:ILE:CD1	1.65	1.24
2:H:535:GLU:C	2:H:736:GLN:N	1.90	1.24
3:L:32:TYR:CE1	3:L:96:TYR:CG	2.24	1.24
3:L:98:ILE:HB	4:P:550:ASP:CB	1.66	1.24
2:D:718:ASN:ND2	4:N:533:ALA:CB	1.99	1.24
2:B:536:ARG:HD3	2:B:668:GLU:O	1.36	1.24
2:H:687:ASN:CB	4:P:532:CYS:HA	1.66	1.24
2:H:687:ASN:CG	4:P:532:CYS:HA	1.58	1.24
3:J:32:TYR:CE1	3:J:96:TYR:CG	2.24	1.24
2:D:686:GLY:HA2	4:N:552:ASN:CG	1.49	1.23
2:D:687:ASN:CG	4:N:551:THR:N	1.91	1.23
2:D:718:ASN:ND2	4:N:533:ALA:CA	2.01	1.23
3:L:21:SER:OG	3:L:79:TYR:CE2	1.92	1.23
2:B:536:ARG:CB	2:B:669:VAL:HA	1.68	1.23
2:B:718:ASN:ND2	4:M:533:ALA:N	1.85	1.23
1:C:93:TYR:CD1	2:D:676:PRO:CB	2.13	1.23
2:D:671:MET:C	2:D:673:PRO:N	1.84	1.23
2:D:718:ASN:HD21	4:N:533:ALA:CA	1.50	1.23
2:H:534:LEU:HD12	2:H:734:LYS:CD	1.54	1.23
2:H:686:GLY:HA3	4:P:552:ASN:N	0.92	1.23
2:B:522:CYS:CA	2:B:733:LYS:HD3	1.62	1.23
2:D:535:GLU:C	2:D:736:GLN:N	1.90	1.23
2:D:536:ARG:CB	2:D:669:VAL:HA	1.68	1.23
2:F:533:ALA:HA	2:F:733:LYS:O	1.34	1.23
2:H:536:ARG:CB	2:H:669:VAL:HA	1.68	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:21:SER:OG	3:J:79:TYR:HE2	1.21	1.23
2:D:602:LEU:CD1	2:D:758:PRO:N	1.94	1.22
2:F:671:MET:C	2:F:673:PRO:N	1.84	1.22
2:B:533:ALA:HA	2:B:733:LYS:O	1.34	1.22
2:B:535:GLU:C	2:B:736:GLN:N	1.90	1.22
2:F:536:ARG:CB	2:F:669:VAL:HA	1.68	1.22
2:F:613:VAL:N	2:F:734:LYS:HZ2	1.32	1.22
2:H:597:MET:CB	2:H:756:HIS:CD2	2.17	1.22
2:H:716:VAL:CG1	4:P:591:TRP:CG	2.20	1.22
2:F:549:GLN:O	2:F:735:TRP:HB3	1.22	1.22
2:H:533:ALA:HA	2:H:733:LYS:O	1.34	1.22
2:H:599:HIS:O	2:H:755:ILE:CG2	1.81	1.22
2:H:686:GLY:O	4:P:551:THR:CB	1.88	1.22
2:D:687:ASN:C	4:N:550:ASP:OD1	1.78	1.22
2:B:549:GLN:O	2:B:735:TRP:HB3	1.22	1.21
2:B:602:LEU:CD1	2:B:758:PRO:N	1.94	1.21
2:F:597:MET:CB	2:F:756:HIS:CD2	2.17	1.21
2:H:716:VAL:CB	4:P:532:CYS:SG	2.29	1.21
3:I:213:ARG:NH2	4:M:619:PRO:HD2	1.55	1.21
2:D:522:CYS:CA	2:D:733:LYS:HD3	1.62	1.21
2:F:534:LEU:HD12	2:F:734:LYS:CD	1.54	1.21
2:F:602:LEU:CD1	2:F:758:PRO:N	1.94	1.21
2:D:536:ARG:HD3	2:D:668:GLU:O	1.35	1.21
2:D:597:MET:CB	2:D:756:HIS:CD2	2.17	1.21
1:G:93:TYR:CD1	2:H:676:PRO:CB	2.13	1.21
2:H:521:ASP:C	2:H:733:LYS:HD2	1.61	1.21
2:H:673:PRO:HA	2:H:745:ASN:ND2	1.56	1.21
3:L:213:ARG:NH2	4:P:619:PRO:HD2	1.55	1.21
2:D:521:ASP:C	2:D:733:LYS:HD2	1.61	1.20
2:B:521:ASP:C	2:B:733:LYS:HD2	1.61	1.20
2:F:599:HIS:O	2:F:755:ILE:CG2	1.81	1.20
3:J:45:PHE:HZ	4:N:544:PHE:CZ	1.43	1.20
3:K:21:SER:OG	3:K:79:TYR:HE2	1.21	1.20
3:K:213:ARG:NH2	4:O:619:PRO:HD2	1.55	1.20
2:B:673:PRO:HA	2:B:745:ASN:ND2	1.56	1.20
1:G:93:TYR:CD1	2:H:676:PRO:HB3	1.76	1.20
3:J:213:ARG:NH2	4:N:619:PRO:HD2	1.55	1.20
1:A:86:PRO:CA	1:A:227:GLY:HA2	1.72	1.19
1:C:86:PRO:CA	1:C:227:GLY:HA2	1.72	1.19
2:H:671:MET:O	2:H:673:PRO:HD3	1.38	1.19
2:H:716:VAL:CG1	4:P:591:TRP:CB	2.19	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:687:ASN:ND2	4:N:532:CYS:C	1.93	1.19
2:H:612:THR:HA	2:H:734:LYS:NZ	1.58	1.19
2:B:597:MET:CB	2:B:756:HIS:CD2	2.17	1.19
2:D:673:PRO:HA	2:D:745:ASN:ND2	1.56	1.19
2:D:719:ASN:OD1	4:N:565:SER:O	1.59	1.19
2:H:602:LEU:CD1	2:H:758:PRO:N	1.94	1.19
2:F:673:PRO:HA	2:F:745:ASN:ND2	1.56	1.19
1:A:24:TYR:CG	1:E:305:ALA:CB	2.25	1.18
2:D:612:THR:HA	2:D:734:LYS:NZ	1.58	1.18
2:D:627:HIS:CG	2:D:734:LYS:HB2	1.78	1.18
1:E:93:TYR:CA	2:F:726:HIS:NE2	1.69	1.18
2:H:549:GLN:N	2:H:669:VAL:HG11	1.58	1.18
3:J:77:THR:CG2	3:J:79:TYR:CZ	2.26	1.18
3:L:21:SER:OG	3:L:79:TYR:HE2	1.21	1.18
2:B:719:ASN:HA	4:M:551:THR:HG21	1.23	1.18
2:F:538:ARG:HD3	2:F:667:ILE:HD12	1.24	1.18
1:C:93:TYR:CD1	2:D:676:PRO:HB3	1.76	1.18
3:I:77:THR:CG2	3:I:79:TYR:CZ	2.26	1.18
2:F:612:THR:HA	2:F:734:LYS:NZ	1.58	1.18
3:K:77:THR:CG2	3:K:79:TYR:CZ	2.26	1.18
2:B:612:THR:HA	2:B:734:LYS:NZ	1.58	1.18
2:D:534:LEU:HD11	2:D:734:LYS:CD	1.63	1.18
1:A:24:TYR:CG	1:E:305:ALA:HB2	1.79	1.17
2:F:687:ASN:H	4:O:550:ASP:C	1.46	1.17
3:K:21:SER:OG	3:K:79:TYR:CE2	1.91	1.17
3:L:77:THR:CG2	3:L:79:TYR:CZ	2.26	1.17
2:D:549:GLN:O	2:D:735:TRP:HB3	1.22	1.17
1:E:86:PRO:CA	1:E:227:GLY:HA2	1.72	1.17
2:F:602:LEU:CD2	2:F:758:PRO:CD	2.22	1.17
1:G:86:PRO:CA	1:G:227:GLY:HA2	1.72	1.17
2:H:627:HIS:CG	2:H:734:LYS:HB2	1.78	1.17
2:H:602:LEU:CD2	2:H:758:PRO:CD	2.23	1.17
2:H:718:ASN:CA	4:P:530(A):THR:O	1.76	1.17
2:H:719:ASN:HA	4:P:551:THR:HG21	1.20	1.17
2:B:538:ARG:HD3	2:B:667:ILE:HD12	1.24	1.17
2:B:627:HIS:CG	2:B:734:LYS:HB2	1.78	1.17
2:B:718:ASN:N	4:M:531:ASN:H	0.89	1.17
2:D:547:LYS:HB3	2:D:667:ILE:HD13	1.23	1.17
2:H:686:GLY:O	4:P:551:THR:HB	1.02	1.17
4:P:515:PRO:CG	4:P:606(A):LEU:O	1.93	1.17
1:A:93:TYR:CD1	2:B:676:PRO:HB3	1.76	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:O	1:C:191:PRO:HG3	1.45	1.16
2:B:685:SER:CB	4:M:553:ASN:H	1.49	1.16
2:B:687:ASN:HB3	4:M:532:CYS:HA	1.19	1.16
1:E:93:TYR:CD1	2:F:676:PRO:HB3	1.76	1.16
2:F:521:ASP:C	2:F:733:LYS:HD2	1.61	1.16
3:J:32:TYR:HE1	3:J:96:TYR:CG	1.61	1.16
3:L:98:ILE:HG22	4:P:532:CYS:HB3	1.25	1.16
1:A:191:PRO:HG3	1:C:151:ASP:O	1.45	1.16
2:B:536:ARG:NE	2:B:738:ASN:C	1.99	1.16
2:B:602:LEU:CD2	2:B:758:PRO:CD	2.23	1.16
2:D:704:GLY:C	4:N:530(A):THR:HG21	1.50	1.16
4:O:515:PRO:CG	4:O:606(A):LEU:O	1.93	1.16
2:B:534:LEU:HD11	2:B:734:LYS:CD	1.63	1.16
2:D:602:LEU:CD2	2:D:758:PRO:CD	2.23	1.16
2:F:627:HIS:CG	2:F:734:LYS:HB2	1.77	1.16
2:F:687:ASN:N	4:O:550:ASP:C	1.98	1.16
1:G:91:GLY:HA3	2:H:678:ARG:CB	1.74	1.16
4:M:515:PRO:CG	4:M:606(A):LEU:O	1.93	1.16
1:G:91:GLY:CA	2:H:678:ARG:HB2	1.76	1.16
2:D:547:LYS:CG	2:D:757:ILE:CG2	2.24	1.16
2:H:671:MET:C	2:H:673:PRO:N	1.84	1.16
2:H:719:ASN:OD1	4:P:551:THR:HG23	1.46	1.16
4:O:515:PRO:HG3	4:O:606(A):LEU:O	1.45	1.16
2:D:719:ASN:HA	4:N:551:THR:CG2	1.76	1.15
2:F:536:ARG:CZ	2:F:738:ASN:O	1.95	1.15
2:F:536:ARG:NE	2:F:738:ASN:C	1.99	1.15
2:H:547:LYS:CG	2:H:757:ILE:CG2	2.24	1.15
2:H:536:ARG:CZ	2:H:738:ASN:O	1.95	1.15
2:H:716:VAL:CG1	4:P:591:TRP:HB3	1.76	1.15
1:A:289:ARG:HH11	1:E:315:VAL:CA	1.59	1.15
2:B:536:ARG:CZ	2:B:738:ASN:O	1.94	1.15
1:C:95:PHE:HA	2:D:725:CYS:C	1.67	1.15
2:F:547:LYS:CG	2:F:757:ILE:CG2	2.24	1.15
2:F:594:THR:O	2:F:660:THR:CG2	1.84	1.15
1:G:95:PHE:HA	2:H:725:CYS:C	1.67	1.15
2:H:536:ARG:NE	2:H:738:ASN:C	1.99	1.15
2:H:547:LYS:HB3	2:H:667:ILE:HD13	1.23	1.15
4:N:515:PRO:CG	4:N:606(A):LEU:O	1.93	1.15
2:D:594:THR:O	2:D:660:THR:CG2	1.84	1.15
2:F:534:LEU:HD11	2:F:734:LYS:HD2	1.15	1.15
4:P:515:PRO:HG3	4:P:606(A):LEU:O	1.45	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:613:VAL:N	2:B:734:LYS:HZ2	1.39	1.14
2:D:536:ARG:NE	2:D:738:ASN:C	1.99	1.14
2:H:549:GLN:O	2:H:735:TRP:HB3	1.22	1.14
3:I:21:SER:OG	3:I:79:TYR:CE2	1.92	1.14
3:J:98:ILE:HG22	4:N:532:CYS:HB3	1.25	1.14
1:C:91:GLY:CA	2:D:678:ARG:HB2	1.76	1.14
2:D:602:LEU:HD21	2:D:757:ILE:HA	1.16	1.14
3:I:21:SER:OG	3:I:79:TYR:HE2	1.21	1.14
3:I:32:TYR:HE1	3:I:96:TYR:CG	1.61	1.14
2:B:716:VAL:HG11	4:M:591:TRP:CB	1.59	1.14
2:D:599:HIS:O	2:D:755:ILE:CG2	1.81	1.14
1:E:91:GLY:HA3	2:F:678:ARG:CB	1.75	1.14
3:J:2:ILE:HD11	3:J:94:ARG:NH1	1.62	1.14
3:L:45:PHE:HZ	4:P:544:PHE:CZ	1.43	1.14
2:B:716:VAL:CB	4:M:532:CYS:SG	2.36	1.14
2:H:534:LEU:CD1	2:H:734:LYS:HD3	1.78	1.14
2:H:718:ASN:HB2	4:P:531:ASN:CB	1.70	1.14
2:B:689:LYS:CB	3:I:98:ILE:HD12	1.78	1.14
2:F:686:GLY:N	4:O:552:ASN:N	1.89	1.14
2:B:534:LEU:CD1	2:B:734:LYS:HD2	1.66	1.13
2:B:547:LYS:CG	2:B:757:ILE:CG2	2.24	1.13
2:F:612:THR:CA	2:F:734:LYS:HZ1	1.61	1.13
1:G:93:TYR:CA	2:H:726:HIS:NE2	1.69	1.13
2:H:534:LEU:CD1	2:H:734:LYS:HD2	1.66	1.13
2:H:716:VAL:HG22	4:P:532:CYS:CB	1.71	1.13
1:A:91:GLY:HA3	2:B:678:ARG:CB	1.74	1.13
2:B:685:SER:HB3	4:M:553:ASN:N	1.50	1.13
2:B:715:LYS:CE	4:M:593:ASN:OD1	1.95	1.13
1:E:91:GLY:CA	2:F:678:ARG:HB2	1.76	1.13
2:F:687:ASN:N	4:O:550:ASP:O	1.63	1.13
1:A:95:PHE:HA	2:B:725:CYS:C	1.67	1.13
2:D:687:ASN:HB3	4:N:532:CYS:HA	1.16	1.13
2:D:718:ASN:CB	4:N:531:ASN:HB2	1.78	1.13
3:K:45:PHE:HZ	4:O:544:PHE:CZ	1.43	1.13
1:A:91:GLY:CA	2:B:678:ARG:HB2	1.76	1.13
1:A:291:VAL:O	1:E:317:ILE:HG21	1.33	1.13
1:C:91:GLY:HA3	2:D:678:ARG:CB	1.75	1.13
2:D:536:ARG:CZ	2:D:738:ASN:O	1.95	1.13
2:D:687:ASN:HB2	4:N:550:ASP:HA	1.13	1.13
2:D:718:ASN:OD1	4:N:531:ASN:HB3	1.40	1.13
2:F:685:SER:CB	4:O:549:GLY:C	1.83	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:687:ASN:HB2	3:L:98:ILE:HG21	1.26	1.13
2:B:689:LYS:CB	3:I:98:ILE:CD1	2.25	1.13
2:D:534:LEU:HD11	2:D:734:LYS:HD2	1.15	1.12
2:D:718:ASN:ND2	4:N:533:ALA:N	1.97	1.13
2:F:685:SER:CB	4:O:553:ASN:H	1.62	1.12
3:J:2:ILE:HD11	3:J:94:ARG:HH12	1.12	1.12
2:B:599:HIS:O	2:B:755:ILE:CG2	1.81	1.12
2:D:549:GLN:N	2:D:669:VAL:HG11	1.58	1.12
1:E:63:CYS:CB	2:F:700:LYS:CE	2.19	1.12
2:F:534:LEU:CD1	2:F:734:LYS:HD3	1.78	1.12
1:A:291:VAL:O	1:E:317:ILE:CG2	1.83	1.12
2:D:547:LYS:HD3	2:D:667:ILE:CB	1.80	1.12
2:D:685:SER:OG	4:N:553:ASN:O	1.65	1.12
1:E:95:PHE:HA	2:F:725:CYS:C	1.67	1.12
2:F:549:GLN:N	2:F:669:VAL:HG11	1.58	1.12
1:G:63:CYS:CB	2:H:700:LYS:CE	2.19	1.12
2:H:689:LYS:CB	3:L:98:ILE:CD1	2.27	1.12
2:H:719:ASN:CG	4:P:551:THR:HG23	1.70	1.12
2:B:594:THR:O	2:B:660:THR:CG2	1.84	1.12
2:D:689:LYS:HB3	3:J:98:ILE:CD1	1.61	1.12
3:L:32:TYR:HE1	3:L:96:TYR:CG	1.61	1.12
2:B:572:ASN:CB	4:P:516:GLY:CA	2.26	1.12
1:C:63:CYS:CB	2:D:700:LYS:CE	2.19	1.12
2:F:715:LYS:HG3	4:O:593:ASN:OD1	1.48	1.12
2:H:687:ASN:HB2	4:P:550:ASP:CA	1.80	1.12
3:K:32:TYR:HE1	3:K:96:TYR:CG	1.61	1.12
1:A:126:THR:CG2	1:C:126:THR:N	2.06	1.11
3:L:35:LEU:CD2	3:L:37:VAL:HG23	1.81	1.11
2:B:687:ASN:HB2	4:M:550:ASP:HA	1.18	1.11
2:H:538:ARG:HD3	2:H:667:ILE:HD12	1.24	1.11
3:J:21:SER:OG	3:J:79:TYR:CE2	1.91	1.11
2:B:547:LYS:HD3	2:B:667:ILE:CB	1.80	1.11
2:B:671:MET:O	2:B:673:PRO:HD3	1.38	1.11
2:D:542:THR:HG22	2:D:636:ILE:CD1	1.81	1.11
2:F:547:LYS:HD3	2:F:667:ILE:CB	1.80	1.11
1:G:91:GLY:HA3	2:H:678:ARG:HB2	1.11	1.11
2:H:719:ASN:OD1	4:P:551:THR:CG2	1.99	1.11
2:B:542:THR:HG22	2:B:636:ILE:CD1	1.81	1.11
2:B:547:LYS:HB3	2:B:667:ILE:HD13	1.23	1.11
2:D:671:MET:O	2:D:673:PRO:HD3	1.38	1.11
2:H:542:THR:HG22	2:H:636:ILE:CD1	1.81	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:547:LYS:HD3	2:H:667:ILE:CB	1.80	1.11
3:I:35:LEU:CD2	3:I:37:VAL:HG23	1.80	1.11
4:N:515:PRO:HG3	4:N:606(A):LEU:O	1.45	1.11
1:A:123:ARG:NH1	1:C:149:ASN:ND2	1.98	1.10
2:D:534:LEU:CD1	2:D:734:LYS:HD3	1.78	1.10
2:F:547:LYS:HB3	2:F:667:ILE:HD13	1.23	1.10
2:H:534:LEU:HD11	2:H:734:LYS:CD	1.63	1.10
3:I:98:ILE:HB	4:M:550:ASP:CB	1.66	1.10
3:K:98:ILE:HG22	4:O:532:CYS:HB3	1.25	1.10
3:L:35:LEU:CD2	3:L:37:VAL:CG2	2.29	1.10
1:A:149:ASN:ND2	1:C:123:ARG:NH1	1.98	1.10
1:A:289:ARG:NH1	1:E:315:VAL:HA	1.65	1.10
2:B:522:CYS:N	2:B:733:LYS:CE	2.14	1.10
2:D:538:ARG:HD3	2:D:667:ILE:HD12	1.24	1.10
2:F:685:SER:HB3	4:O:549:GLY:O	1.44	1.10
3:K:35:LEU:CD2	3:K:37:VAL:HG23	1.81	1.10
2:B:597:MET:CG	2:B:756:HIS:CD2	2.35	1.10
2:B:686:GLY:N	4:M:550:ASP:O	1.67	1.10
2:D:716:VAL:HG11	4:N:591:TRP:CB	1.67	1.10
2:F:536:ARG:N	2:F:736:GLN:N	1.99	1.10
2:F:671:MET:O	2:F:673:PRO:HD3	1.38	1.10
3:I:35:LEU:CD2	3:I:37:VAL:CG2	2.29	1.10
3:J:35:LEU:CD2	3:J:37:VAL:CG2	2.29	1.10
1:A:22:PRO:O	1:E:306:CYS:N	1.83	1.10
2:B:571:ASP:O	4:P:516:GLY:CA	2.00	1.10
2:F:542:THR:HG22	2:F:636:ILE:CD1	1.81	1.10
3:J:35:LEU:CD2	3:J:37:VAL:HG23	1.81	1.10
3:K:35:LEU:CD2	3:K:37:VAL:CG2	2.29	1.10
2:B:571:ASP:O	4:P:516:GLY:HA2	1.50	1.10
1:C:93:TYR:CA	2:D:726:HIS:NE2	1.69	1.10
2:D:718:ASN:O	4:N:566:LEU:HD11	1.48	1.10
2:F:522:CYS:N	2:F:733:LYS:CE	2.14	1.10
2:F:686:GLY:HA3	4:O:551:THR:C	1.66	1.10
2:F:687:ASN:HB2	4:O:532:CYS:HA	1.18	1.10
2:H:613:VAL:N	2:H:734:LYS:HZ2	1.39	1.10
1:A:93:TYR:CA	2:B:726:HIS:NE2	1.69	1.09
2:B:549:GLN:N	2:B:669:VAL:HG11	1.58	1.09
2:H:522:CYS:N	2:H:733:LYS:CE	2.14	1.09
2:H:686:GLY:HA2	4:P:552:ASN:ND2	1.66	1.09
1:A:91:GLY:HA3	2:B:678:ARG:HB2	1.11	1.09
2:F:716:VAL:HG13	4:O:591:TRP:HB3	1.23	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:594:THR:O	2:H:660:THR:CG2	1.84	1.09
2:B:520:PRO:HD3	2:B:732:HIS:N	1.66	1.09
2:B:536:ARG:N	2:B:736:GLN:N	1.99	1.09
1:C:91:GLY:HA3	2:D:678:ARG:HB2	1.11	1.09
2:D:613:VAL:N	2:D:734:LYS:HZ2	1.35	1.09
2:H:547:LYS:HG3	2:H:757:ILE:HG22	1.34	1.09
2:H:716:VAL:HG13	4:P:591:TRP:HB3	1.22	1.09
3:K:2:ILE:HD11	3:K:94:ARG:NH1	1.62	1.09
4:M:515:PRO:HG3	4:M:606(A):LEU:O	1.45	1.09
2:B:718:ASN:N	4:M:531:ASN:N	1.74	1.09
2:D:522:CYS:N	2:D:733:LYS:CE	2.14	1.09
2:D:536:ARG:N	2:D:736:GLN:N	1.99	1.09
2:F:547:LYS:CB	2:F:667:ILE:CD1	2.31	1.09
2:H:536:ARG:N	2:H:736:GLN:N	1.99	1.09
2:H:547:LYS:CB	2:H:667:ILE:CD1	2.31	1.09
1:A:289:ARG:NH1	1:E:354:ILE:O	1.84	1.09
2:B:673:PRO:HA	2:B:745:ASN:HD22	0.93	1.09
2:D:538:ARG:CD	2:D:667:ILE:HB	1.83	1.09
2:H:548:ILE:O	2:H:755:ILE:HG21	1.53	1.09
1:A:63:CYS:CB	2:B:700:LYS:CE	2.19	1.08
2:B:534:LEU:CD1	2:B:734:LYS:HD3	1.78	1.08
2:D:597:MET:CG	2:D:756:HIS:CD2	2.35	1.08
2:H:597:MET:CG	2:H:756:HIS:CD2	2.35	1.08
2:H:602:LEU:HD21	2:H:757:ILE:HA	1.16	1.08
2:B:535:GLU:HB3	2:B:670:HIS:HA	1.31	1.08
3:I:98:ILE:HG22	4:M:532:CYS:HB3	1.25	1.08
3:K:114:ALA:HB3	3:K:146:PHE:CZ	1.88	1.08
2:B:547:LYS:CB	2:B:667:ILE:CD1	2.31	1.08
2:D:535:GLU:HB3	2:D:670:HIS:HA	1.31	1.08
2:D:547:LYS:HG3	2:D:757:ILE:HG22	1.34	1.08
2:D:689:LYS:HB3	3:J:98:ILE:HD11	1.31	1.08
2:F:547:LYS:HE3	2:F:757:ILE:HG23	1.10	1.08
2:F:547:LYS:HG3	2:F:757:ILE:HG22	1.34	1.08
2:F:548:ILE:O	2:F:755:ILE:HG21	1.53	1.08
2:F:715:LYS:HE2	4:O:593:ASN:HB3	1.35	1.08
2:H:534:LEU:HD11	2:H:734:LYS:HD2	1.15	1.08
2:D:548:ILE:O	2:D:755:ILE:HG21	1.53	1.08
2:F:536:ARG:HB3	2:F:669:VAL:HA	1.08	1.08
2:F:602:LEU:HD21	2:F:757:ILE:HA	1.16	1.08
2:H:602:LEU:HD22	2:H:758:PRO:CD	1.83	1.08
2:B:715:LYS:HD3	4:M:593:ASN:OD1	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:547:LYS:CG	2:D:757:ILE:HG22	1.83	1.08
2:F:535:GLU:HB3	2:F:670:HIS:HA	1.31	1.08
2:F:547:LYS:CG	2:F:757:ILE:HG22	1.83	1.08
2:H:673:PRO:HA	2:H:745:ASN:HD22	0.93	1.08
2:H:687:ASN:CG	4:P:551:THR:N	2.07	1.08
3:L:114:ALA:HB3	3:L:146:PHE:CZ	1.88	1.08
2:B:602:LEU:HD13	2:B:758:PRO:CB	1.84	1.07
2:B:716:VAL:HG21	4:M:532:CYS:HB2	1.11	1.07
2:D:536:ARG:O	2:D:669:VAL:HG12	1.54	1.07
1:E:91:GLY:HA3	2:F:678:ARG:HB2	1.11	1.07
2:F:534:LEU:HD11	2:F:734:LYS:CD	1.63	1.07
2:F:685:SER:HB3	4:O:553:ASN:N	1.68	1.07
2:F:704:GLY:O	4:O:530(A):THR:HG21	0.90	1.07
2:H:689:LYS:HB2	3:L:98:ILE:HD12	1.15	1.07
1:A:126:THR:HG22	1:C:126:THR:N	1.53	1.07
2:D:602:LEU:HD13	2:D:758:PRO:CB	1.84	1.07
2:F:522:CYS:HA	2:F:733:LYS:HD3	1.36	1.07
2:F:536:ARG:O	2:F:669:VAL:HG12	1.54	1.07
2:F:597:MET:CG	2:F:756:HIS:CD2	2.35	1.07
2:H:547:LYS:CG	2:H:757:ILE:HG22	1.83	1.07
2:H:626:THR:C	2:H:734:LYS:HG3	1.75	1.07
3:I:114:ALA:HB3	3:I:146:PHE:CZ	1.88	1.07
3:J:114:ALA:HB3	3:J:146:PHE:CZ	1.88	1.07
2:B:602:LEU:HD21	2:B:757:ILE:HA	1.16	1.07
2:D:687:ASN:ND2	4:N:533:ALA:O	1.87	1.07
2:D:704:GLY:O	4:N:530(A):THR:HG22	1.52	1.07
2:F:520:PRO:HD3	2:F:732:HIS:N	1.66	1.07
2:F:535:GLU:CB	2:F:670:HIS:CA	2.31	1.07
2:F:602:LEU:HD22	2:F:758:PRO:CD	1.83	1.07
2:F:715:LYS:CE	4:O:593:ASN:CG	2.23	1.07
2:H:535:GLU:CB	2:H:670:HIS:CA	2.31	1.07
2:B:602:LEU:HD22	2:B:758:PRO:CD	1.83	1.07
2:B:716:VAL:CG1	4:M:591:TRP:CG	2.09	1.07
2:D:602:LEU:HD11	2:D:757:ILE:C	1.75	1.07
2:D:704:GLY:O	4:N:530(A):THR:CG2	0.78	1.07
2:D:718:ASN:HB2	4:N:531:ASN:HB2	1.33	1.07
2:F:597:MET:CG	2:F:756:HIS:HD2	1.68	1.07
2:F:704:GLY:C	4:O:530(A):THR:HG21	1.74	1.07
2:B:536:ARG:N	2:B:736:GLN:H	1.52	1.07
2:B:536:ARG:O	2:B:669:VAL:HG12	1.54	1.07
2:B:547:LYS:HE3	2:B:757:ILE:HG23	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:535:GLU:CB	2:D:670:HIS:CA	2.31	1.07
2:F:689:LYS:HB2	3:K:98:ILE:HD12	1.36	1.07
3:I:2:ILE:HD11	3:I:94:ARG:HH12	1.12	1.07
3:L:2:ILE:HD11	3:L:94:ARG:NH1	1.62	1.07
2:D:522:CYS:HA	2:D:733:LYS:HD3	1.36	1.06
2:F:685:SER:HB3	4:O:553:ASN:H	0.94	1.06
2:H:520:PRO:HD3	2:H:732:HIS:N	1.66	1.06
3:I:2:ILE:HD11	3:I:94:ARG:NH1	1.62	1.06
2:B:548:ILE:O	2:B:755:ILE:HG21	1.53	1.06
2:B:626:THR:C	2:B:734:LYS:HG3	1.75	1.06
2:D:547:LYS:CB	2:D:667:ILE:CD1	2.31	1.06
2:D:626:THR:C	2:D:734:LYS:HG3	1.75	1.06
2:F:534:LEU:CD1	2:F:734:LYS:HD2	1.66	1.06
2:F:538:ARG:CD	2:F:667:ILE:HB	1.83	1.06
2:F:602:LEU:HD13	2:F:758:PRO:CB	1.84	1.06
2:H:547:LYS:HE3	2:H:757:ILE:HG23	1.10	1.06
1:A:95:PHE:CD1	2:B:725:CYS:CA	2.35	1.06
2:H:602:LEU:HD13	2:H:758:PRO:CB	1.84	1.06
3:K:98:ILE:HG21	4:O:550:ASP:OD1	1.55	1.06
1:C:95:PHE:CD1	2:D:725:CYS:CA	2.35	1.06
1:E:86:PRO:HA	1:E:227:GLY:CA	1.86	1.06
2:H:536:ARG:N	2:H:736:GLN:H	1.52	1.06
2:H:536:ARG:O	2:H:669:VAL:HG12	1.54	1.06
2:H:602:LEU:HD11	2:H:757:ILE:C	1.75	1.06
2:H:685:SER:O	4:P:552:ASN:ND2	1.89	1.06
3:J:39:GLN:NE2	3:J:45:PHE:CE1	2.24	1.06
2:B:536:ARG:HB3	2:B:669:VAL:HA	1.08	1.06
2:B:602:LEU:HD11	2:B:757:ILE:C	1.75	1.06
2:D:520:PRO:HD3	2:D:732:HIS:N	1.66	1.06
2:D:687:ASN:O	4:N:550:ASP:OD1	1.71	1.06
2:D:718:ASN:OD1	4:N:531:ASN:C	1.93	1.06
2:F:626:THR:C	2:F:734:LYS:HG3	1.75	1.06
2:F:673:PRO:HA	2:F:745:ASN:HD22	0.93	1.06
3:K:2:ILE:HD11	3:K:94:ARG:HH12	1.12	1.06
3:K:39:GLN:NE2	3:K:45:PHE:CE1	2.24	1.06
3:L:98:ILE:HG21	4:P:550:ASP:OD1	1.55	1.06
2:B:547:LYS:HD3	2:B:667:ILE:CG2	1.87	1.05
1:C:86:PRO:HA	1:C:227:GLY:CA	1.86	1.05
2:D:535:GLU:OE1	2:D:670:HIS:HA	1.56	1.05
2:D:547:LYS:HE3	2:D:757:ILE:HG23	1.10	1.05
2:D:602:LEU:HD22	2:D:758:PRO:CD	1.83	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:535:GLU:OE1	2:F:670:HIS:HA	1.56	1.05
3:L:39:GLN:NE2	3:L:45:PHE:CE1	2.24	1.05
2:B:538:ARG:CD	2:B:667:ILE:HB	1.83	1.05
2:B:597:MET:CG	2:B:756:HIS:HD2	1.68	1.05
2:D:594:THR:O	2:D:660:THR:O	1.74	1.05
2:F:536:ARG:N	2:F:736:GLN:H	1.52	1.05
2:H:535:GLU:OE1	2:H:670:HIS:HA	1.56	1.05
2:H:547:LYS:HD3	2:H:667:ILE:CG2	1.87	1.05
2:H:547:LYS:CG	2:H:667:ILE:CG1	2.28	1.05
2:H:594:THR:O	2:H:660:THR:O	1.74	1.05
3:L:98:ILE:HG13	4:P:550:ASP:CG	1.75	1.05
2:D:536:ARG:HB3	2:D:669:VAL:HA	1.08	1.05
2:D:547:LYS:CG	2:D:667:ILE:CD1	2.35	1.05
2:D:673:PRO:HA	2:D:745:ASN:HD22	0.93	1.05
1:G:86:PRO:HA	1:G:227:GLY:CA	1.86	1.05
3:I:98:ILE:HG13	4:M:550:ASP:CG	1.75	1.05
2:B:538:ARG:N	2:B:737:TYR:HB2	1.72	1.05
2:D:547:LYS:HD3	2:D:667:ILE:CG2	1.87	1.05
2:B:547:LYS:CG	2:B:757:ILE:HG22	1.83	1.05
2:D:685:SER:CB	4:N:553:ASN:O	2.03	1.05
2:D:687:ASN:ND2	4:N:551:THR:H	1.52	1.05
2:F:594:THR:O	2:F:660:THR:O	1.74	1.05
2:F:687:ASN:HB3	4:O:532:CYS:HA	1.38	1.05
2:D:534:LEU:CD1	2:D:734:LYS:HD2	1.66	1.04
2:F:547:LYS:HD3	2:F:667:ILE:CG2	1.87	1.04
2:F:602:LEU:HD11	2:F:757:ILE:C	1.75	1.04
2:H:535:GLU:HB3	2:H:670:HIS:HA	1.31	1.04
2:H:687:ASN:CB	4:P:550:ASP:CA	2.35	1.04
3:I:39:GLN:NE2	3:I:45:PHE:CE1	2.24	1.04
3:I:98:ILE:HG21	4:M:550:ASP:OD1	1.55	1.04
3:L:98:ILE:CB	4:P:550:ASP:HB2	1.49	1.04
2:B:547:LYS:CG	2:B:667:ILE:CD1	2.35	1.04
2:B:594:THR:O	2:B:660:THR:O	1.74	1.04
2:B:715:LYS:HE2	4:M:593:ASN:OD1	1.56	1.04
2:F:538:ARG:N	2:F:737:TYR:HB2	1.72	1.04
2:F:685:SER:OG	4:O:549:GLY:O	1.75	1.04
2:H:538:ARG:N	2:H:737:TYR:HB2	1.72	1.04
3:K:45:PHE:CE2	4:O:544:PHE:CE1	2.46	1.04
4:N:515:PRO:HD3	4:N:606(A):LEU:CB	1.87	1.04
1:A:126:THR:N	1:C:126:THR:HG22	1.53	1.04
2:D:536:ARG:N	2:D:736:GLN:H	1.52	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:538:ARG:CD	2:H:667:ILE:HB	1.83	1.04
3:J:98:ILE:HG21	4:N:550:ASP:OD1	1.55	1.04
3:L:45:PHE:CE2	4:P:544:PHE:CE1	2.46	1.04
4:M:515:PRO:HD3	4:M:606(A):LEU:CB	1.87	1.04
1:A:86:PRO:HA	1:A:227:GLY:CA	1.86	1.04
2:B:685:SER:HB3	4:M:553:ASN:H	1.00	1.04
2:D:718:ASN:HD21	4:N:533:ALA:HA	1.23	1.04
2:H:547:LYS:CG	2:H:667:ILE:CD1	2.35	1.04
2:H:597:MET:CG	2:H:756:HIS:HD2	1.68	1.04
3:J:45:PHE:CE2	4:N:544:PHE:CE1	2.46	1.04
4:P:515:PRO:HD3	4:P:606(A):LEU:CB	1.87	1.04
2:B:547:LYS:CG	2:B:667:ILE:CG1	2.28	1.03
2:D:704:GLY:O	4:N:530(A):THR:CB	2.06	1.03
2:D:716:VAL:HG13	4:N:591:TRP:HB3	1.08	1.03
4:O:515:PRO:HD3	4:O:606(A):LEU:CB	1.87	1.03
2:B:535:GLU:CB	2:B:670:HIS:CA	2.31	1.03
2:B:547:LYS:HG3	2:B:757:ILE:HG22	1.34	1.03
2:B:687:ASN:CB	4:M:532:CYS:CA	2.36	1.03
2:F:547:LYS:CG	2:F:667:ILE:CD1	2.35	1.03
2:H:536:ARG:HB3	2:H:669:VAL:HA	1.08	1.03
2:H:686:GLY:HA3	4:P:552:ASN:CA	1.87	1.03
3:I:45:PHE:CE2	4:M:544:PHE:CE1	2.46	1.03
1:A:291:VAL:HG22	1:E:302:GLU:O	1.58	1.03
1:A:126:THR:HG22	1:C:126:THR:H	1.10	1.03
2:D:521:ASP:C	2:D:733:LYS:CD	2.24	1.03
2:D:597:MET:CG	2:D:756:HIS:HD2	1.68	1.03
2:H:687:ASN:ND2	4:P:532:CYS:CA	2.21	1.03
2:B:536:ARG:NH1	2:B:737:TYR:CE1	2.22	1.03
2:D:538:ARG:N	2:D:737:TYR:HB2	1.72	1.03
1:G:95:PHE:CD1	2:H:725:CYS:CA	2.35	1.02
2:B:522:CYS:HA	2:B:733:LYS:HD3	1.36	1.02
2:B:534:LEU:HD11	2:B:734:LYS:HD2	1.15	1.02
2:B:572:ASN:HB2	4:P:516:GLY:CA	1.71	1.02
2:F:521:ASP:C	2:F:733:LYS:CD	2.23	1.02
2:H:599:HIS:HB2	2:H:754:LYS:O	1.59	1.02
2:B:535:GLU:OE1	2:B:670:HIS:HA	1.56	1.02
2:B:685:SER:C	4:M:553:ASN:N	2.03	1.02
2:B:718:ASN:ND2	4:M:533:ALA:CA	2.21	1.02
2:B:719:ASN:O	4:M:566:LEU:CD1	2.01	1.02
2:F:599:HIS:HB2	2:F:754:LYS:O	1.59	1.02
2:H:686:GLY:N	4:P:552:ASN:H	1.57	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:547:LYS:CB	2:B:667:ILE:HD11	1.89	1.02
2:D:612:THR:CA	2:D:734:LYS:HZ1	1.72	1.02
2:D:687:ASN:HB2	4:N:550:ASP:CA	1.81	1.02
3:L:45:PHE:CZ	4:P:544:PHE:CE1	2.48	1.02
2:B:599:HIS:HB2	2:B:754:LYS:O	1.59	1.01
2:D:687:ASN:HD21	4:N:533:ALA:CA	1.72	1.01
2:H:715:LYS:HE2	4:P:593:ASN:CB	1.89	1.01
3:I:45:PHE:CZ	4:M:544:PHE:CE1	2.48	1.01
2:B:521:ASP:C	2:B:733:LYS:CD	2.24	1.01
2:D:599:HIS:HB2	2:D:754:LYS:O	1.59	1.01
2:D:719:ASN:CA	4:N:551:THR:HG21	1.90	1.01
2:D:612:THR:HA	2:D:734:LYS:HZ1	1.18	1.01
2:F:547:LYS:CB	2:F:667:ILE:HD11	1.89	1.01
2:F:685:SER:CB	4:O:549:GLY:O	0.71	1.01
2:H:719:ASN:HA	4:P:551:THR:CG2	1.91	1.01
1:A:22:PRO:C	1:E:306:CYS:H	1.47	1.01
1:A:152:HIS:HA	1:C:191:PRO:CB	1.90	1.01
1:A:191:PRO:CB	1:C:152:HIS:HA	1.90	1.01
2:F:612:THR:HA	2:F:734:LYS:HZ1	1.06	1.01
2:F:684:GLN:HB3	3:K:98:ILE:HG21	1.04	1.01
2:H:522:CYS:HA	2:H:733:LYS:HD3	1.36	1.01
2:H:602:LEU:HD22	2:H:758:PRO:HD3	1.42	1.01
2:H:687:ASN:HB3	4:P:532:CYS:HA	1.38	1.01
3:J:45:PHE:CZ	4:N:544:PHE:CE1	2.48	1.01
2:D:687:ASN:HD22	4:N:532:CYS:C	1.62	1.00
2:D:547:LYS:CG	2:D:667:ILE:CG1	2.28	1.00
2:D:788:TYR:CE2	1:G:246:GLU:HB2	1.96	1.00
2:F:685:SER:OG	4:O:553:ASN:HB2	1.57	1.00
3:I:35:LEU:HD21	3:I:37:VAL:HG22	1.43	1.00
3:K:35:LEU:HD21	3:K:37:VAL:HG22	1.43	1.00
2:B:535:GLU:CB	2:B:670:HIS:N	2.24	1.00
2:B:716:VAL:HG13	4:M:591:TRP:HB3	1.04	1.00
2:D:547:LYS:CB	2:D:667:ILE:HD11	1.89	1.00
1:E:246:GLU:HB2	2:H:788:TYR:CE2	1.96	1.00
2:F:536:ARG:NH1	2:F:737:TYR:CE1	2.22	1.00
2:H:719:ASN:N	4:P:551:THR:OG1	1.95	1.00
3:K:45:PHE:CZ	4:O:544:PHE:CE1	2.48	1.00
3:L:98:ILE:CB	4:P:550:ASP:CB	2.30	1.00
1:C:246:GLU:HB2	2:F:788:TYR:CE2	1.96	1.00
2:H:547:LYS:CB	2:H:667:ILE:HD11	1.89	1.00
2:D:718:ASN:HB3	4:N:530:VAL:CG1	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:718:ASN:HB3	4:O:530:VAL:HG13	1.43	0.99
1:A:289:ARG:NH2	1:E:353:GLN:CG	2.23	0.99
3:L:32:TYR:CZ	3:L:96:TYR:CE1	2.50	0.99
2:F:535:GLU:N	2:F:735:TRP:CD1	1.83	0.99
2:H:542:THR:HG22	2:H:636:ILE:HD12	1.45	0.99
1:A:95:PHE:CG	2:B:725:CYS:HA	1.98	0.99
2:F:715:LYS:CE	4:O:593:ASN:OD1	2.10	0.99
2:B:715:LYS:CE	4:M:593:ASN:CG	2.26	0.99
1:C:93:TYR:HD1	2:D:676:PRO:HB3	1.12	0.99
1:C:95:PHE:CG	2:D:725:CYS:HA	1.98	0.99
1:E:93:TYR:HD1	2:F:676:PRO:HB3	1.12	0.99
1:E:95:PHE:CD1	2:F:725:CYS:CA	2.35	0.99
2:D:535:GLU:CB	2:D:670:HIS:N	2.24	0.99
1:E:95:PHE:CG	2:F:725:CYS:HA	1.97	0.99
2:F:535:GLU:CB	2:F:670:HIS:N	2.24	0.99
3:J:11:VAL:HG11	3:J:147:PRO:CB	1.93	0.99
2:H:535:GLU:CB	2:H:670:HIS:N	2.24	0.99
3:K:11:VAL:HG11	3:K:147:PRO:CB	1.93	0.99
2:B:685:SER:CB	4:M:553:ASN:N	2.10	0.99
2:D:547:LYS:CE	2:D:757:ILE:CG2	2.23	0.99
2:H:549:GLN:O	2:H:735:TRP:CD2	2.02	0.99
2:H:718:ASN:CB	4:P:531:ASN:CB	2.32	0.99
3:K:32:TYR:CZ	3:K:96:TYR:CE1	2.50	0.99
1:A:126:THR:N	1:C:126:THR:CG2	2.06	0.98
2:B:547:LYS:CE	2:B:757:ILE:CG2	2.23	0.98
2:F:537:ILE:HG13	2:F:736:GLN:HA	1.45	0.98
3:L:93:VAL:HG11	3:L:100:LEU:HD23	1.45	0.98
1:A:93:TYR:HD1	2:B:676:PRO:HB3	1.12	0.98
2:B:718:ASN:C	4:M:530(B):SER:HA	1.83	0.98
2:B:719:ASN:O	4:M:566:LEU:HD12	1.21	0.98
1:G:95:PHE:CG	2:H:725:CYS:HA	1.98	0.98
3:I:11:VAL:HG11	3:I:147:PRO:CB	1.93	0.98
3:J:35:LEU:HD21	3:J:37:VAL:HG22	1.43	0.98
3:K:93:VAL:HG11	3:K:100:LEU:HD23	1.45	0.98
3:J:32:TYR:CZ	3:J:96:TYR:CE1	2.50	0.98
3:L:2:ILE:HD11	3:L:94:ARG:HH12	1.12	0.98
2:F:613:VAL:H	2:F:734:LYS:HZ3	1.10	0.98
4:P:561:ARG:NH2	4:P:582:ASP:OD1	1.96	0.98
2:B:612:THR:CA	2:B:734:LYS:NZ	2.25	0.98
2:D:718:ASN:CB	4:N:530:VAL:HG13	1.94	0.98
2:F:538:ARG:CD	2:F:667:ILE:HD12	1.94	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:612:THR:CA	2:H:734:LYS:NZ	2.26	0.98
2:H:718:ASN:CB	4:P:530(A):THR:O	2.10	0.98
2:B:715:LYS:HE2	4:M:593:ASN:HB3	1.45	0.98
2:B:716:VAL:CG2	4:M:532:CYS:SG	0.99	0.98
2:H:535:GLU:N	2:H:735:TRP:CD1	1.83	0.98
2:H:594:THR:O	2:H:660:THR:HG22	0.99	0.98
3:I:32:TYR:CZ	3:I:96:TYR:CE1	2.50	0.98
2:B:686:GLY:HA2	4:M:552:ASN:CG	1.83	0.98
3:L:35:LEU:HD21	3:L:37:VAL:HG22	1.43	0.98
2:B:716:VAL:HG23	4:M:532:CYS:SG	0.48	0.98
2:B:549:GLN:O	2:B:735:TRP:CD2	2.02	0.98
2:F:547:LYS:CG	2:F:667:ILE:CG1	2.28	0.98
3:I:93:VAL:HG11	3:I:100:LEU:HD23	1.45	0.98
2:D:538:ARG:CD	2:D:667:ILE:HD12	1.94	0.98
3:I:45:PHE:HE2	4:M:544:PHE:CZ	1.80	0.98
4:O:561:ARG:NH2	4:O:582:ASP:OD1	1.96	0.98
2:B:538:ARG:CD	2:B:667:ILE:HD12	1.94	0.97
2:B:597:MET:HB3	2:B:756:HIS:HD2	0.85	0.97
2:F:594:THR:O	2:F:660:THR:HG22	0.99	0.97
3:L:11:VAL:HG11	3:L:147:PRO:CB	1.93	0.97
4:N:561:ARG:NH2	4:N:582:ASP:OD1	1.96	0.97
4:P:514:SER:OG	4:P:606(A):LEU:HD22	1.65	0.97
2:D:716:VAL:HG11	4:N:591:TRP:HB2	1.45	0.97
2:D:612:THR:CA	2:D:734:LYS:NZ	2.25	0.97
4:M:514:SER:OG	4:M:606(A):LEU:HD22	1.65	0.97
2:D:545:THR:HG21	2:D:758:PRO:CG	1.95	0.97
2:H:537:ILE:HG13	2:H:736:GLN:HA	1.45	0.97
2:H:545:THR:HG21	2:H:758:PRO:CG	1.95	0.97
3:J:98:ILE:CG2	4:N:532:CYS:HB3	1.94	0.97
2:B:536:ARG:NE	2:B:737:TYR:CG	2.33	0.97
2:F:534:LEU:HD13	2:F:734:LYS:HB3	0.98	0.97
2:D:536:ARG:NE	2:D:737:TYR:CG	2.33	0.97
2:H:536:ARG:NE	2:H:737:TYR:CG	2.33	0.97
3:I:213:ARG:HH21	4:M:619:PRO:HD2	1.18	0.97
3:K:32:TYR:CE1	3:K:96:TYR:CE1	2.53	0.97
2:H:538:ARG:CD	2:H:667:ILE:HD12	1.94	0.97
3:L:32:TYR:CE1	3:L:96:TYR:CE1	2.52	0.97
4:O:628:ASN:HA	4:O:682:ALA:HB2	1.47	0.97
2:F:597:MET:HB3	2:F:756:HIS:HD2	0.85	0.97
2:H:547:LYS:HE2	2:H:667:ILE:CG1	1.93	0.97
3:L:11:VAL:HG21	3:L:148:GLU:H	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:561:ARG:NH2	4:M:582:ASP:OD1	1.96	0.97
2:D:542:THR:HG22	2:D:636:ILE:HD12	1.44	0.96
4:O:514:SER:OG	4:O:606(A):LEU:HD22	1.65	0.96
1:A:289:ARG:HH21	1:E:353:GLN:HG2	1.14	0.96
2:B:572:ASN:HB2	4:P:516:GLY:HA3	1.40	0.96
2:B:718:ASN:ND2	4:M:533:ALA:H	1.58	0.96
1:C:246:GLU:HB2	2:F:788:TYR:CZ	2.00	0.96
3:I:98:ILE:CG2	4:M:532:CYS:HB3	1.94	0.96
3:J:32:TYR:CE1	3:J:96:TYR:CE1	2.53	0.96
2:B:542:THR:HG22	2:B:636:ILE:HD12	1.45	0.96
2:D:522:CYS:N	2:D:733:LYS:HD3	1.63	0.96
2:F:597:MET:HG2	2:F:756:HIS:CD2	1.99	0.96
2:B:534:LEU:HD13	2:B:734:LYS:HB3	0.98	0.96
2:B:547:LYS:HE2	2:B:667:ILE:CG1	1.93	0.96
2:D:685:SER:CB	4:N:549:GLY:H	1.78	0.96
2:D:788:TYR:CZ	1:G:246:GLU:HB2	2.00	0.96
2:H:687:ASN:HB2	4:P:550:ASP:HA	0.99	0.96
3:K:98:ILE:CG2	4:O:532:CYS:HB3	1.94	0.96
4:P:628:ASN:HA	4:P:682:ALA:HB2	1.47	0.96
2:B:545:THR:HG21	2:B:758:PRO:CG	1.95	0.96
2:F:547:LYS:HE2	2:F:667:ILE:CG1	1.93	0.96
3:I:11:VAL:HG21	3:I:148:GLU:H	1.29	0.96
2:D:536:ARG:NH1	2:D:737:TYR:CE1	2.22	0.96
2:F:545:THR:HG21	2:F:758:PRO:CG	1.94	0.96
3:K:213:ARG:HH21	4:O:619:PRO:HD2	1.18	0.96
4:N:628:ASN:HA	4:N:682:ALA:HB2	1.47	0.96
2:B:537:ILE:HG13	2:B:736:GLN:HA	1.45	0.96
2:H:719:ASN:O	4:P:566:LEU:HD12	1.62	0.96
2:D:535:GLU:N	2:D:735:TRP:CD1	1.83	0.96
2:F:536:ARG:NE	2:F:737:TYR:CG	2.33	0.96
2:F:602:LEU:HD22	2:F:758:PRO:HD3	1.41	0.96
3:L:98:ILE:CG2	4:P:532:CYS:HB3	1.94	0.96
2:F:536:ARG:O	2:F:669:VAL:CG1	2.14	0.96
2:H:597:MET:HG2	2:H:756:HIS:CD2	1.99	0.96
2:H:534:LEU:HD13	2:H:734:LYS:HB3	0.98	0.96
2:D:522:CYS:N	2:D:733:LYS:HD2	1.72	0.95
2:H:536:ARG:NH1	2:H:737:TYR:CE1	2.22	0.95
2:H:597:MET:HB3	2:H:756:HIS:HD2	0.85	0.95
2:D:536:ARG:O	2:D:669:VAL:CG1	2.14	0.95
3:J:11:VAL:HG21	3:J:148:GLU:H	1.29	0.95
4:N:514:SER:OG	4:N:606(A):LEU:HD22	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:VAL:HG12	4:M:591:TRP:HD1	1.15	0.95
2:H:687:ASN:CG	4:P:550:ASP:C	2.25	0.95
3:I:32:TYR:CE1	3:I:96:TYR:CE1	2.53	0.95
1:A:289:ARG:HH11	1:E:315:VAL:HA	0.80	0.95
2:B:718:ASN:HD21	4:M:533:ALA:CA	1.79	0.95
2:D:534:LEU:HD13	2:D:734:LYS:HB3	0.98	0.95
2:F:716:VAL:HG11	4:O:591:TRP:CG	1.75	0.95
2:H:547:LYS:CE	2:H:667:ILE:CG1	2.26	0.95
3:J:93:VAL:HG11	3:J:100:LEU:HD23	1.45	0.95
2:D:537:ILE:HG13	2:D:736:GLN:HA	1.45	0.95
2:D:594:THR:O	2:D:660:THR:HG22	0.99	0.95
1:G:95:PHE:HA	2:H:726:HIS:N	1.81	0.95
2:B:536:ARG:O	2:B:669:VAL:CG1	2.14	0.95
2:F:542:THR:HG22	2:F:636:ILE:HD12	1.45	0.95
3:I:35:LEU:HD22	3:I:37:VAL:HG23	1.48	0.95
2:B:594:THR:O	2:B:660:THR:HG22	0.99	0.95
2:F:507:ASN:OD1	2:F:556:ILE:HG13	1.67	0.95
3:J:45:PHE:HE2	4:N:544:PHE:CZ	1.80	0.95
3:K:11:VAL:HG21	3:K:148:GLU:H	1.29	0.95
3:K:45:PHE:HE2	4:O:544:PHE:CZ	1.80	0.95
2:B:718:ASN:HD22	4:M:533:ALA:HB2	1.29	0.95
2:F:536:ARG:NH2	2:F:738:ASN:O	2.00	0.95
3:K:98:ILE:HG23	4:O:532:CYS:SG	2.07	0.95
4:M:628:ASN:HA	4:M:682:ALA:HB2	1.47	0.95
2:B:536:ARG:NH2	2:B:738:ASN:O	2.00	0.94
2:B:597:MET:HG2	2:B:756:HIS:CD2	1.99	0.94
1:E:246:GLU:HB2	2:H:788:TYR:CZ	2.01	0.94
2:H:536:ARG:O	2:H:669:VAL:CG1	2.14	0.94
2:H:718:ASN:N	4:P:530(A):THR:O	1.97	0.94
2:B:520:PRO:N	2:B:731:ASN:C	2.21	0.94
2:D:534:LEU:HD12	2:D:734:LYS:HD3	1.43	0.94
2:H:521:ASP:C	2:H:733:LYS:CD	2.24	0.94
2:H:522:CYS:N	2:H:733:LYS:HD3	1.63	0.94
1:E:95:PHE:HA	2:F:726:HIS:N	1.81	0.94
2:H:507:ASN:OD1	2:H:556:ILE:HG13	1.67	0.94
2:H:547:LYS:C	2:H:755:ILE:HD11	1.88	0.94
3:I:114:ALA:HB1	3:I:146:PHE:CE2	2.03	0.94
3:L:32:TYR:HE1	3:L:96:TYR:HD1	1.13	0.94
2:B:547:LYS:C	2:B:755:ILE:HD11	1.88	0.94
2:D:520:PRO:N	2:D:731:ASN:C	2.21	0.94
2:D:520:PRO:CA	2:D:731:ASN:HA	1.60	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:547:LYS:C	2:D:755:ILE:HD11	1.88	0.94
2:H:719:ASN:CG	4:P:551:THR:CG2	2.35	0.94
3:I:98:ILE:HG23	4:M:532:CYS:SG	2.07	0.94
2:H:547:LYS:CE	2:H:757:ILE:CG2	2.23	0.94
3:L:213:ARG:HH21	4:P:619:PRO:HD2	1.18	0.94
2:F:547:LYS:C	2:F:755:ILE:HD11	1.88	0.94
2:H:685:SER:C	4:P:553:ASN:N	2.17	0.94
3:J:114:ALA:HB1	3:J:146:PHE:CE2	2.03	0.94
2:D:536:ARG:NH2	2:D:738:ASN:O	2.00	0.94
2:D:538:ARG:CD	2:D:667:ILE:CD1	2.46	0.94
2:D:547:LYS:HE2	2:D:667:ILE:CG1	1.93	0.94
2:D:704:GLY:O	4:N:530(A):THR:HG23	1.12	0.94
3:K:93:VAL:CG1	3:K:100:LEU:HD23	1.98	0.94
3:L:98:ILE:HG23	4:P:532:CYS:SG	2.07	0.94
4:M:691:TYR:HB2	4:M:706:LEU:HD22	1.50	0.94
2:H:522:CYS:CA	2:H:733:LYS:CD	2.33	0.94
2:H:687:ASN:ND2	4:P:533:ALA:N	2.15	0.94
3:L:93:VAL:CG1	3:L:100:LEU:HD23	1.98	0.94
2:H:538:ARG:CD	2:H:667:ILE:CD1	2.46	0.94
3:L:35:LEU:HD22	3:L:37:VAL:HG23	1.48	0.94
1:C:95:PHE:HA	2:D:726:HIS:N	1.81	0.93
2:D:507:ASN:OD1	2:D:556:ILE:HG13	1.67	0.93
2:D:536:ARG:NE	2:D:738:ASN:CA	2.12	0.93
2:F:549:GLN:O	2:F:735:TRP:CD2	2.02	0.93
2:B:522:CYS:N	2:B:733:LYS:HD2	1.72	0.93
2:B:534:LEU:CD1	2:B:734:LYS:CG	2.20	0.93
2:D:602:LEU:HD22	2:D:758:PRO:HD3	1.42	0.93
3:I:93:VAL:CG1	3:I:100:LEU:HD23	1.98	0.93
3:J:98:ILE:HG23	4:N:532:CYS:SG	2.07	0.93
2:B:687:ASN:CG	4:M:551:THR:N	2.22	0.93
2:D:687:ASN:O	4:N:550:ASP:OD2	1.85	0.93
2:F:534:LEU:CD1	2:F:734:LYS:CG	2.20	0.93
2:F:536:ARG:HB3	2:F:669:VAL:CA	1.97	0.93
2:F:547:LYS:CE	2:F:757:ILE:CG2	2.23	0.93
3:I:32:TYR:CZ	3:I:96:TYR:CD1	2.56	0.93
4:P:691:TYR:HB2	4:P:706:LEU:HD22	1.50	0.93
2:B:536:ARG:HB3	2:B:669:VAL:CA	1.97	0.93
3:J:32:TYR:CZ	3:J:96:TYR:CD1	2.56	0.93
3:L:32:TYR:CZ	3:L:96:TYR:CD1	2.56	0.93
2:B:547:LYS:HD3	2:B:667:ILE:CD1	1.99	0.93
2:D:687:ASN:ND2	4:N:551:THR:N	2.14	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:687:ASN:HD21	4:N:533:ALA:C	1.70	0.93
2:H:520:PRO:N	2:H:731:ASN:C	2.21	0.93
2:H:686:GLY:HA2	4:P:552:ASN:CG	1.87	0.93
4:N:691:TYR:HB2	4:N:706:LEU:HD22	1.50	0.93
2:F:520:PRO:N	2:F:731:ASN:C	2.21	0.93
2:F:716:VAL:CG1	4:O:591:TRP:HD1	1.43	0.93
2:H:687:ASN:CG	4:P:532:CYS:CA	2.36	0.93
2:H:719:ASN:CA	4:P:551:THR:HG21	1.97	0.93
2:B:716:VAL:HG11	4:M:591:TRP:HB2	1.50	0.93
2:D:597:MET:HB3	2:D:756:HIS:HD2	0.85	0.93
2:D:597:MET:HG2	2:D:756:HIS:CD2	1.99	0.93
3:J:93:VAL:CG1	3:J:100:LEU:HD23	1.98	0.93
1:A:95:PHE:HA	2:B:726:HIS:N	1.81	0.93
2:D:522:CYS:H	2:D:733:LYS:CE	1.79	0.93
2:D:775:THR:HG21	1:G:199:GLN:NE2	1.84	0.93
2:H:536:ARG:NH2	2:H:738:ASN:O	2.00	0.93
1:A:128:SER:HB3	1:C:125:HIS:HE1	1.34	0.93
2:B:612:THR:CA	2:B:734:LYS:HZ1	1.82	0.93
2:F:547:LYS:CE	2:F:667:ILE:CG1	2.26	0.93
3:K:32:TYR:CZ	3:K:96:TYR:CD1	2.56	0.93
2:F:688:VAL:N	4:O:530(B):SER:O	2.02	0.93
2:B:686:GLY:H	4:M:550:ASP:C	1.71	0.92
2:F:536:ARG:HD2	2:F:738:ASN:CB	1.72	0.92
2:F:547:LYS:HB3	2:F:667:ILE:HD11	1.47	0.92
2:H:536:ARG:HB3	2:H:669:VAL:CA	1.97	0.92
2:H:716:VAL:CG2	4:P:532:CYS:SG	0.83	0.92
1:A:152:HIS:HA	1:C:191:PRO:HB3	1.51	0.92
3:J:35:LEU:HD22	3:J:37:VAL:HG23	1.48	0.92
2:B:507:ASN:OD1	2:B:556:ILE:HG13	1.67	0.92
2:B:522:CYS:N	2:B:733:LYS:HD3	1.63	0.92
2:B:715:LYS:CG	4:M:593:ASN:OD1	2.18	0.92
2:D:536:ARG:HB3	2:D:669:VAL:CA	1.97	0.92
2:D:547:LYS:HD3	2:D:667:ILE:CD1	1.99	0.92
2:D:547:LYS:HB3	2:D:667:ILE:HD11	1.47	0.92
2:F:520:PRO:HD3	2:F:731:ASN:O	1.69	0.92
2:B:538:ARG:CD	2:B:667:ILE:CD1	2.46	0.92
2:B:673:PRO:CA	2:B:745:ASN:HD22	1.83	0.92
1:E:199:GLN:NE2	2:H:775:THR:HG21	1.84	0.92
2:F:547:LYS:HD3	2:F:667:ILE:CD1	1.99	0.92
2:F:704:GLY:C	4:O:530(A):THR:CG2	2.35	0.92
1:G:93:TYR:HD1	2:H:676:PRO:CG	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TYR:CE1	1:E:305:ALA:HB1	2.04	0.92
2:D:673:PRO:CA	2:D:745:ASN:HD22	1.83	0.92
2:H:716:VAL:HG12	4:P:591:TRP:HD1	1.32	0.92
3:J:213:ARG:HH21	4:N:619:PRO:HD2	1.18	0.92
3:L:45:PHE:HE2	4:P:544:PHE:CZ	1.80	0.92
1:A:126:THR:H	1:C:126:THR:HG22	1.10	0.92
2:D:716:VAL:HG11	4:N:591:TRP:HB3	1.28	0.92
2:H:547:LYS:HD3	2:H:667:ILE:CD1	1.99	0.92
3:J:35:LEU:HD21	3:J:37:VAL:CG2	1.98	0.92
3:K:35:LEU:HD22	3:K:37:VAL:HG23	1.48	0.92
2:D:685:SER:HB3	4:N:553:ASN:O	1.70	0.92
2:F:538:ARG:CD	2:F:667:ILE:CD1	2.46	0.92
2:B:602:LEU:HD22	2:B:758:PRO:HD3	1.41	0.91
1:C:199:GLN:NE2	2:F:775:THR:HG21	1.84	0.91
2:D:547:LYS:HE2	2:D:667:ILE:HG12	1.51	0.91
2:F:612:THR:CA	2:F:734:LYS:NZ	2.25	0.91
2:H:522:CYS:H	2:H:733:LYS:CE	1.79	0.91
2:H:534:LEU:CD1	2:H:734:LYS:CG	2.20	0.91
3:K:77:THR:HG21	3:K:79:TYR:OH	1.69	0.91
3:L:77:THR:HG21	3:L:79:TYR:OH	1.69	0.91
2:B:534:LEU:CG	2:B:734:LYS:HB3	1.93	0.91
2:D:718:ASN:HB2	4:N:530:VAL:HG13	1.50	0.91
2:B:522:CYS:H	2:B:733:LYS:CE	1.79	0.91
2:D:719:ASN:O	4:N:566:LEU:HD12	0.84	0.91
2:D:719:ASN:ND2	4:N:571:ALA:HA	1.85	0.91
2:F:520:PRO:CD	2:F:732:HIS:N	2.29	0.91
3:I:77:THR:HG21	3:I:79:TYR:OH	1.69	0.91
1:A:149:ASN:HD21	1:C:123:ARG:NH1	1.68	0.91
2:D:717:ILE:HG22	4:N:530(B):SER:CA	1.97	0.91
4:O:691:TYR:HB2	4:O:706:LEU:HD22	1.50	0.91
2:B:671:MET:C	2:B:673:PRO:CD	2.35	0.91
2:D:520:PRO:HD3	2:D:731:ASN:O	1.69	0.91
2:F:534:LEU:CG	2:F:734:LYS:HB3	1.93	0.91
2:F:599:HIS:HD1	2:F:735:TRP:HH2	1.18	0.91
2:B:612:THR:HA	2:B:734:LYS:HZ1	1.29	0.91
2:D:718:ASN:N	4:N:531:ASN:N	2.17	0.91
2:H:522:CYS:N	2:H:733:LYS:HD2	1.72	0.91
2:H:613:VAL:H	2:H:734:LYS:HZ3	0.93	0.91
3:J:32:TYR:HE1	3:J:96:TYR:HD1	1.13	0.91
3:L:114:ALA:HB1	3:L:146:PHE:CE2	2.03	0.91
2:B:715:LYS:CE	4:M:593:ASN:CB	2.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:536:ARG:H	2:H:669:VAL:HB	1.36	0.91
3:J:77:THR:HG21	3:J:79:TYR:OH	1.69	0.91
1:A:123:ARG:CZ	1:C:149:ASN:ND2	2.34	0.91
1:A:128:SER:HB3	1:C:125:HIS:CE1	2.06	0.91
2:H:673:PRO:CA	2:H:745:ASN:HD22	1.83	0.91
2:B:536:ARG:NE	2:B:738:ASN:CA	2.12	0.91
2:H:536:ARG:CD	2:H:668:GLU:O	2.20	0.91
2:D:536:ARG:CD	2:D:668:GLU:O	2.19	0.90
2:F:716:VAL:CB	4:O:591:TRP:CD1	2.54	0.90
3:L:35:LEU:HD21	3:L:37:VAL:CG2	1.98	0.90
2:B:545:THR:HG21	2:B:758:PRO:HG2	1.54	0.90
1:G:93:TYR:HD1	2:H:676:PRO:HB3	1.12	0.90
3:J:11:VAL:HG21	3:J:148:GLU:N	1.87	0.90
1:A:149:ASN:ND2	1:C:123:ARG:CZ	2.34	0.90
2:B:520:PRO:HD3	2:B:731:ASN:O	1.69	0.90
2:B:689:LYS:HB2	3:I:98:ILE:HD12	0.92	0.90
2:F:547:LYS:HE2	2:F:667:ILE:HG12	1.50	0.90
2:H:716:VAL:HG21	4:P:532:CYS:HB2	1.54	0.90
2:D:718:ASN:HD22	4:N:533:ALA:HB2	0.75	0.90
2:B:538:ARG:HD3	2:B:667:ILE:CG1	2.01	0.90
2:F:673:PRO:CA	2:F:745:ASN:HD22	1.83	0.90
3:K:11:VAL:HG11	3:K:147:PRO:HB3	1.53	0.90
3:L:11:VAL:HG11	3:L:147:PRO:HB3	1.53	0.90
2:F:538:ARG:HD3	2:F:667:ILE:CG1	2.01	0.90
2:H:520:PRO:HD3	2:H:731:ASN:O	1.69	0.90
3:I:35:LEU:HD21	3:I:37:VAL:CG2	1.98	0.90
1:C:86:PRO:HA	1:C:227:GLY:HA2	0.92	0.90
2:F:718:ASN:HB3	4:O:530:VAL:CG1	2.02	0.90
2:H:547:LYS:HG2	2:H:667:ILE:CG1	2.02	0.90
1:A:125:HIS:CE1	1:C:128:SER:HB3	2.06	0.90
2:B:719:ASN:HA	4:M:551:THR:CG2	2.01	0.90
2:F:715:LYS:HD3	4:O:593:ASN:OD1	1.72	0.90
1:G:96:CYS:HA	2:H:702:ASN:HD21	1.37	0.90
3:K:32:TYR:HE1	3:K:96:TYR:HD1	1.13	0.90
2:B:547:LYS:HB3	2:B:667:ILE:HD11	1.47	0.90
2:F:684:GLN:HB3	3:K:98:ILE:HG23	1.52	0.90
3:I:11:VAL:HG11	3:I:147:PRO:HB3	1.53	0.90
2:D:545:THR:HG21	2:D:758:PRO:HG2	1.54	0.90
2:D:687:ASN:HD21	4:N:533:ALA:N	1.64	0.90
2:D:718:ASN:OD1	4:N:531:ASN:CA	2.19	0.90
2:F:545:THR:HG21	2:F:758:PRO:HG2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PRO:HB3	1:C:152:HIS:HA	1.51	0.89
2:D:538:ARG:HD3	2:D:667:ILE:CG1	2.00	0.89
2:D:613:VAL:H	2:D:734:LYS:HZ3	1.01	0.89
2:D:687:ASN:CG	4:N:551:THR:CA	2.36	0.89
2:F:520:PRO:CA	2:F:731:ASN:HA	1.60	0.89
3:I:11:VAL:HG21	3:I:148:GLU:N	1.87	0.89
3:K:35:LEU:HD21	3:K:37:VAL:CG2	1.98	0.89
1:A:289:ARG:HH21	1:E:353:GLN:CG	1.82	0.89
2:B:685:SER:O	4:M:553:ASN:OD1	1.74	0.89
2:F:522:CYS:N	2:F:733:LYS:HD3	1.63	0.89
2:H:538:ARG:HD3	2:H:667:ILE:CG1	2.01	0.89
3:K:11:VAL:HG21	3:K:148:GLU:N	1.87	0.89
3:K:114:ALA:HB1	3:K:146:PHE:CE2	2.03	0.89
2:B:536:ARG:CD	2:B:668:GLU:O	2.20	0.89
2:D:542:THR:HG22	2:D:636:ILE:CG1	1.81	0.89
2:H:534:LEU:HD12	2:H:734:LYS:CA	2.03	0.89
2:H:686:GLY:CA	4:P:552:ASN:N	1.78	0.89
2:H:520:PRO:CA	2:H:731:ASN:HA	1.60	0.89
2:H:599:HIS:HD1	2:H:735:TRP:HH2	1.18	0.89
3:L:11:VAL:HG21	3:L:148:GLU:N	1.87	0.89
2:B:535:GLU:HB3	2:B:669:VAL:C	1.93	0.89
2:B:547:LYS:HG2	2:B:667:ILE:CG1	2.02	0.89
1:C:96:CYS:HA	2:D:702:ASN:HD21	1.36	0.89
2:D:536:ARG:NE	2:D:737:TYR:CD1	2.41	0.89
2:F:536:ARG:CD	2:F:668:GLU:O	2.20	0.89
2:D:534:LEU:CD1	2:D:734:LYS:CG	2.20	0.89
2:F:522:CYS:H	2:F:733:LYS:CE	1.79	0.89
2:F:547:LYS:HG2	2:F:667:ILE:CG1	2.02	0.89
3:L:169:LEU:HD12	4:P:662:THR:HG22	1.54	0.89
1:C:63:CYS:CB	2:D:700:LYS:HE3	2.03	0.89
2:H:689:LYS:HB2	3:L:98:ILE:HD13	1.50	0.89
3:I:169:LEU:HD12	4:M:662:THR:HG22	1.54	0.89
2:D:522:CYS:CA	2:D:733:LYS:CD	2.33	0.89
2:D:535:GLU:HB3	2:D:669:VAL:C	1.93	0.89
2:D:536:ARG:H	2:D:669:VAL:HB	1.36	0.89
2:D:689:LYS:CB	3:J:98:ILE:HD13	2.03	0.89
2:H:545:THR:HG21	2:H:758:PRO:HG2	1.53	0.89
2:F:534:LEU:HD22	2:F:735:TRP:O	1.73	0.89
2:F:535:GLU:HB3	2:F:669:VAL:C	1.92	0.89
3:K:114:ALA:CB	3:K:146:PHE:CZ	2.51	0.89
3:L:114:ALA:CB	3:L:146:PHE:CZ	2.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:691:TYR:HB2	4:N:706:LEU:CD2	2.03	0.89
2:B:536:ARG:NE	2:B:737:TYR:CD1	2.41	0.88
2:D:534:LEU:HD12	2:D:734:LYS:CA	2.03	0.88
2:D:687:ASN:HA	4:N:551:THR:OG1	1.72	0.88
1:E:96:CYS:HA	2:F:702:ASN:HD21	1.37	0.88
2:H:687:ASN:HB2	3:L:98:ILE:CG2	2.02	0.88
2:B:547:LYS:CE	2:B:667:ILE:CG1	2.26	0.88
2:H:536:ARG:NE	2:H:737:TYR:CD1	2.41	0.88
3:K:169:LEU:HD12	4:O:662:THR:HG22	1.54	0.88
1:A:123:ARG:NH1	1:C:149:ASN:HD21	1.68	0.88
2:B:534:LEU:HD12	2:B:734:LYS:CA	2.03	0.88
2:F:536:ARG:NE	2:F:737:TYR:CD1	2.41	0.88
2:H:534:LEU:HD22	2:H:735:TRP:O	1.73	0.88
4:P:691:TYR:HB2	4:P:706:LEU:CD2	2.03	0.88
2:F:536:ARG:H	2:F:669:VAL:HB	1.36	0.88
2:B:536:ARG:H	2:B:669:VAL:HB	1.36	0.88
1:E:86:PRO:HA	1:E:227:GLY:HA2	0.92	0.88
2:F:599:HIS:O	2:F:755:ILE:HG23	1.73	0.88
2:H:547:LYS:CG	2:H:667:ILE:HD11	2.03	0.88
1:A:96:CYS:HA	2:B:702:ASN:HD21	1.37	0.88
2:B:687:ASN:CB	4:M:550:ASP:HA	2.02	0.88
4:M:691:TYR:HB2	4:M:706:LEU:CD2	2.03	0.88
2:D:599:HIS:O	2:D:755:ILE:HG23	1.73	0.88
2:H:534:LEU:HD12	2:H:734:LYS:HD3	1.42	0.88
2:H:536:ARG:CZ	2:H:737:TYR:CD1	2.46	0.88
3:I:114:ALA:CB	3:I:146:PHE:CZ	2.51	0.88
1:A:86:PRO:HA	1:A:227:GLY:HA2	0.92	0.88
2:B:538:ARG:HD3	2:B:667:ILE:CB	2.03	0.88
2:B:547:LYS:CG	2:B:667:ILE:HD11	2.03	0.88
2:F:538:ARG:HD3	2:F:667:ILE:CB	2.03	0.88
2:H:599:HIS:O	2:H:755:ILE:HG23	1.73	0.88
1:A:22:PRO:C	1:E:306:CYS:N	2.24	0.88
2:B:599:HIS:HD1	2:B:735:TRP:HH2	1.18	0.88
2:B:718:ASN:H	4:M:531:ASN:N	1.45	0.88
2:D:538:ARG:HD3	2:D:667:ILE:CB	2.03	0.88
2:D:717:ILE:C	4:N:531:ASN:H	1.62	0.88
2:F:718:ASN:ND2	4:O:590:LEU:HD22	1.89	0.88
2:H:536:ARG:NE	2:H:738:ASN:CA	2.12	0.88
3:J:11:VAL:HG11	3:J:147:PRO:HB3	1.53	0.88
2:D:534:LEU:HD22	2:D:735:TRP:O	1.73	0.88
2:F:534:LEU:HD12	2:F:734:LYS:CA	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:547:LYS:HB3	2:H:667:ILE:HD11	1.47	0.88
3:J:169:LEU:HD12	4:N:662:THR:HG22	1.54	0.88
1:A:125:HIS:HE1	1:C:128:SER:HB3	1.34	0.87
2:D:719:ASN:HA	4:N:551:THR:HG21	0.94	0.87
2:H:538:ARG:HD3	2:H:667:ILE:CB	2.03	0.87
2:H:612:THR:HA	2:H:734:LYS:HZ1	1.29	0.87
2:H:612:THR:CA	2:H:734:LYS:HZ1	1.82	0.87
3:J:114:ALA:CB	3:J:146:PHE:CZ	2.51	0.87
2:B:534:LEU:HD22	2:B:735:TRP:O	1.73	0.87
2:D:538:ARG:HD3	2:D:667:ILE:HB	1.56	0.87
2:D:719:ASN:HD21	4:N:571:ALA:CB	1.86	0.87
2:H:715:LYS:CD	4:P:593:ASN:OD1	2.21	0.87
4:O:691:TYR:HB2	4:O:706:LEU:CD2	2.03	0.87
2:B:687:ASN:HB2	4:M:550:ASP:CA	2.02	0.87
2:H:716:VAL:HG11	4:P:591:TRP:CB	2.02	0.87
2:D:704:GLY:C	4:N:530(A):THR:HG23	1.60	0.87
2:F:602:LEU:HD22	2:F:758:PRO:HD2	1.56	0.87
1:G:86:PRO:HA	1:G:227:GLY:HA2	0.92	0.87
2:H:535:GLU:HB3	2:H:669:VAL:C	1.93	0.87
3:I:32:TYR:HE1	3:I:96:TYR:HD1	1.13	0.87
2:B:536:ARG:CZ	2:B:737:TYR:CD1	2.46	0.87
2:B:571:ASP:C	4:P:516:GLY:HA3	1.95	0.87
2:F:715:LYS:CE	4:O:593:ASN:CB	2.52	0.87
2:F:716:VAL:HG11	4:O:591:TRP:HB2	1.53	0.87
3:J:11:VAL:CB	3:J:147:PRO:HB2	2.05	0.87
3:L:11:VAL:CB	3:L:147:PRO:HB2	2.05	0.87
1:A:24:TYR:HD1	1:E:305:ALA:HB1	1.35	0.87
2:D:686:GLY:CA	4:N:552:ASN:CG	2.39	0.87
2:D:717:ILE:CG2	4:N:530(B):SER:N	2.34	0.87
1:E:63:CYS:CB	2:F:700:LYS:HE3	2.03	0.87
2:H:715:LYS:HD3	4:P:593:ASN:OD1	1.74	0.87
2:D:716:VAL:N	4:N:591:TRP:HD1	1.72	0.87
2:D:718:ASN:CB	4:N:530:VAL:CG1	2.51	0.87
2:F:715:LYS:HE2	4:O:593:ASN:OD1	1.72	0.87
2:D:684:GLN:O	4:N:549:GLY:O	1.89	0.87
2:B:602:LEU:CD2	2:B:757:ILE:HA	2.04	0.87
2:D:547:LYS:HG2	2:D:667:ILE:CG1	2.02	0.87
2:F:719:ASN:N	4:O:530(B):SER:HA	1.89	0.87
2:B:602:LEU:HD22	2:B:758:PRO:HD2	1.56	0.86
2:D:715:LYS:HA	4:N:591:TRP:HE1	1.39	0.86
2:D:718:ASN:C	4:N:566:LEU:HD11	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:718:ASN:CG	4:N:531:ASN:HB2	1.95	0.86
2:H:520:PRO:CD	2:H:732:HIS:N	2.29	0.86
2:H:602:LEU:CD2	2:H:757:ILE:HA	2.04	0.86
2:H:687:ASN:HD21	4:P:532:CYS:C	1.74	0.86
2:H:717:ILE:HG23	4:P:530(C):SER:OG	1.74	0.86
2:B:519:CYS:C	2:B:733:LYS:HG3	1.95	0.86
2:D:602:LEU:HD22	2:D:758:PRO:HD2	1.56	0.86
2:D:718:ASN:O	4:N:566:LEU:CD1	2.23	0.86
3:J:69:PHE:HE1	3:J:80:LEU:HD13	1.40	0.86
2:B:613:VAL:H	2:B:734:LYS:HZ3	0.93	0.86
2:D:625:CYS:SG	2:D:734:LYS:HG2	2.15	0.86
2:F:625:CYS:SG	2:F:734:LYS:HG2	2.16	0.86
1:A:93:TYR:HD1	2:B:676:PRO:CG	1.52	0.86
2:B:547:LYS:HG3	2:B:757:ILE:CG2	1.99	0.86
2:F:519:CYS:C	2:F:733:LYS:HG3	1.95	0.86
2:H:536:ARG:HD2	2:H:738:ASN:CB	1.71	0.86
2:B:716:VAL:HG22	4:M:532:CYS:SG	1.46	0.86
2:D:596:THR:N	2:D:662:ALA:HB2	1.91	0.86
2:F:547:LYS:CG	2:F:667:ILE:HD11	2.03	0.86
2:F:602:LEU:CD2	2:F:757:ILE:HA	2.04	0.86
2:D:718:ASN:OD1	4:N:531:ASN:HB2	1.74	0.86
2:H:542:THR:HG22	2:H:636:ILE:CG1	1.81	0.86
2:B:571:ASP:O	4:P:516:GLY:HA3	1.75	0.86
2:B:596:THR:N	2:B:662:ALA:HB2	1.91	0.86
2:F:596:THR:N	2:F:662:ALA:HB2	1.91	0.86
1:G:63:CYS:CB	2:H:700:LYS:HE3	2.03	0.86
3:K:11:VAL:CB	3:K:147:PRO:HB2	2.05	0.86
2:D:547:LYS:CG	2:D:667:ILE:HD11	2.03	0.85
2:D:716:VAL:HG12	4:N:591:TRP:HB3	1.12	0.85
2:D:814:LYS:N	1:G:246:GLU:OE2	2.07	0.85
2:H:602:LEU:HD22	2:H:758:PRO:HD2	1.57	0.85
3:I:69:PHE:HE1	3:I:80:LEU:HD13	1.40	0.85
3:L:39:GLN:NE2	3:L:45:PHE:CZ	2.44	0.85
4:P:514:SER:HA	4:P:606(A):LEU:HB2	1.58	0.85
1:A:63:CYS:CB	2:B:700:LYS:HE3	2.03	0.85
2:B:625:CYS:SG	2:B:734:LYS:HG2	2.15	0.85
2:B:718:ASN:HD22	4:M:533:ALA:CB	1.88	0.85
2:F:542:THR:HG22	2:F:636:ILE:CG1	1.81	0.85
2:H:625:CYS:SG	2:H:734:LYS:HG2	2.15	0.85
3:I:11:VAL:CB	3:I:147:PRO:HB2	2.05	0.85
1:C:93:TYR:CB	2:D:726:HIS:NE2	2.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:716:VAL:HG23	4:P:532:CYS:SG	0.84	0.85
3:K:69:PHE:HE1	3:K:80:LEU:HD13	1.40	0.85
2:H:686:GLY:C	4:P:551:THR:CB	2.36	0.85
2:D:519:CYS:C	2:D:733:LYS:HG3	1.95	0.85
2:D:535:GLU:CB	2:D:670:HIS:HA	2.04	0.85
2:D:547:LYS:HG3	2:D:757:ILE:CG2	1.99	0.85
2:H:599:HIS:ND1	2:H:735:TRP:HH2	1.74	0.85
3:L:69:PHE:HE1	3:L:80:LEU:HD13	1.40	0.85
1:A:93:TYR:CB	2:B:726:HIS:NE2	2.39	0.85
2:F:536:ARG:CZ	2:F:737:TYR:CD1	2.46	0.85
2:D:718:ASN:ND2	4:N:533:ALA:H	1.70	0.85
2:D:599:HIS:HD1	2:D:735:TRP:HH2	1.18	0.85
2:F:599:HIS:ND1	2:F:735:TRP:HH2	1.74	0.85
2:D:599:HIS:ND1	2:D:735:TRP:HH2	1.74	0.85
2:H:684:GLN:NE2	3:L:98:ILE:HD13	1.92	0.85
2:B:535:GLU:N	2:B:735:TRP:CD1	1.83	0.85
2:B:599:HIS:ND1	2:B:735:TRP:HH2	1.74	0.85
2:D:686:GLY:HA2	4:N:552:ASN:ND2	1.92	0.85
1:E:93:TYR:CB	2:F:726:HIS:NE2	2.39	0.85
3:K:39:GLN:NE2	3:K:45:PHE:CZ	2.44	0.85
2:B:520:PRO:CD	2:B:732:HIS:N	2.29	0.84
2:H:596:THR:N	2:H:662:ALA:HB2	1.91	0.84
2:F:535:GLU:CA	2:F:736:GLN:H	1.89	0.84
1:G:93:TYR:CB	2:H:726:HIS:NE2	2.39	0.84
3:I:39:GLN:NE2	3:I:45:PHE:CZ	2.45	0.84
2:D:719:ASN:OD1	4:N:566:LEU:N	2.10	0.84
2:D:719:ASN:HD21	4:N:571:ALA:HA	1.42	0.84
2:H:716:VAL:HG22	4:P:532:CYS:SG	0.93	0.84
2:B:536:ARG:HD2	2:B:738:ASN:CB	1.71	0.84
1:C:96:CYS:HA	2:D:702:ASN:ND2	1.93	0.84
2:B:542:THR:HG22	2:B:636:ILE:CG1	1.81	0.84
2:D:547:LYS:CE	2:D:667:ILE:CG1	2.26	0.84
3:I:171:GLN:HG3	4:M:660:GLU:OE2	1.78	0.84
4:N:514:SER:HA	4:N:606(A):LEU:HB2	1.58	0.84
1:A:96:CYS:HA	2:B:702:ASN:ND2	1.93	0.84
2:B:687:ASN:HB3	4:M:532:CYS:CA	2.02	0.84
2:D:716:VAL:H	4:N:591:TRP:HD1	1.23	0.84
2:F:685:SER:CA	4:O:553:ASN:N	2.40	0.84
2:H:687:ASN:HD21	4:P:533:ALA:N	1.74	0.84
3:J:171:GLN:HG3	4:N:660:GLU:OE2	1.78	0.84
3:L:171:GLN:HG3	4:P:660:GLU:OE2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:580:THR:OG1	4:M:607:GLY:HA3	1.78	0.84
2:F:715:LYS:CE	4:O:593:ASN:HB3	2.07	0.84
2:H:538:ARG:HD3	2:H:667:ILE:HB	1.56	0.84
3:J:39:GLN:NE2	3:J:45:PHE:CZ	2.44	0.84
2:B:572:ASN:CB	4:P:516:GLY:HA3	1.76	0.84
2:B:684:GLN:CB	4:M:550:ASP:CG	2.34	0.84
2:H:687:ASN:ND2	4:P:551:THR:H	1.76	0.84
4:O:580:THR:OG1	4:O:607:GLY:HA3	1.78	0.84
1:A:93:TYR:CB	2:B:676:PRO:HB3	2.08	0.84
2:D:717:ILE:HG22	4:N:530(B):SER:H	1.37	0.84
1:E:96:CYS:HA	2:F:702:ASN:ND2	1.93	0.84
3:I:77:THR:CG2	3:I:79:TYR:CE1	2.61	0.84
3:J:37:VAL:HG21	3:J:103:TRP:CH2	2.13	0.84
1:A:24:TYR:CB	1:E:305:ALA:HB2	1.87	0.83
1:A:323:SER:CB	1:E:319:LYS:NZ	2.41	0.83
3:L:37:VAL:HG21	3:L:103:TRP:CH2	2.13	0.83
4:P:650:VAL:HG23	4:P:655:VAL:HG21	1.60	0.83
2:B:599:HIS:O	2:B:755:ILE:HG23	1.73	0.83
2:D:536:ARG:CZ	2:D:737:TYR:CD1	2.46	0.83
2:H:685:SER:HB3	4:P:553:ASN:O	1.73	0.83
3:K:11:VAL:HG11	3:K:147:PRO:HB2	1.60	0.83
3:K:87:THR:HG22	3:K:111:VAL:H	1.43	0.83
2:B:686:GLY:N	4:M:550:ASP:C	2.28	0.83
2:H:519:CYS:C	2:H:733:LYS:HG3	1.95	0.83
2:B:548:ILE:N	2:B:755:ILE:CD1	2.42	0.83
1:E:242:TYR:CD2	2:H:788:TYR:CE2	2.59	0.83
2:F:685:SER:OG	4:O:549:GLY:C	2.09	0.83
2:H:548:ILE:N	2:H:755:ILE:CD1	2.42	0.83
3:K:77:THR:CG2	3:K:79:TYR:CE1	2.61	0.83
3:K:37:VAL:HG21	3:K:103:TRP:CH2	2.13	0.83
3:K:171:GLN:HG3	4:O:660:GLU:OE2	1.78	0.83
2:D:549:GLN:O	2:D:735:TRP:CD2	2.02	0.83
2:D:671:MET:C	2:D:673:PRO:CD	2.35	0.83
2:H:686:GLY:HA3	4:P:551:THR:C	1.98	0.83
3:I:87:THR:HG22	3:I:111:VAL:H	1.43	0.83
2:F:534:LEU:HD12	2:F:734:LYS:HD3	1.43	0.83
2:F:548:ILE:N	2:F:755:ILE:CD1	2.42	0.83
3:L:77:THR:CG2	3:L:79:TYR:CE1	2.61	0.83
4:P:580:THR:OG1	4:P:607:GLY:HA3	1.78	0.83
1:A:289:ARG:CZ	1:E:353:GLN:HG2	2.08	0.83
2:D:547:LYS:CD	2:D:667:ILE:CD1	2.55	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:GLU:OE2	2:H:814:LYS:N	2.07	0.83
3:I:11:VAL:HG11	3:I:147:PRO:HB2	1.60	0.83
3:I:37:VAL:HG21	3:I:103:TRP:CH2	2.13	0.83
4:N:680:LEU:HD11	4:N:691:TYR:HE2	1.44	0.83
4:O:514:SER:HA	4:O:606(A):LEU:HB2	1.58	0.83
2:B:718:ASN:HD21	4:M:533:ALA:N	1.67	0.83
1:E:91:GLY:HA3	2:F:678:ARG:H	1.43	0.83
2:H:535:GLU:CA	2:H:736:GLN:H	1.89	0.83
2:H:687:ASN:OD1	4:P:551:THR:N	2.11	0.83
2:H:689:LYS:CB	3:L:98:ILE:HD12	2.03	0.83
3:I:77:THR:HG21	3:I:79:TYR:CE2	2.14	0.83
1:C:93:TYR:CB	2:D:676:PRO:HB3	2.08	0.82
2:D:548:ILE:N	2:D:755:ILE:CD1	2.42	0.82
2:F:627:HIS:HD2	2:F:734:LYS:CB	1.61	0.82
3:J:77:THR:CG2	3:J:79:TYR:CE1	2.61	0.82
4:M:514:SER:HA	4:M:606(A):LEU:HB2	1.58	0.82
4:M:680:LEU:HD11	4:M:691:TYR:HE2	1.44	0.82
4:P:552:ASN:C	4:P:552:ASN:HD22	1.81	0.82
1:C:91:GLY:HA3	2:D:678:ARG:H	1.43	0.82
2:B:684:GLN:HB3	4:M:550:ASP:CG	1.87	0.82
3:K:98:ILE:CB	4:O:550:ASP:CB	2.30	0.82
4:N:580:THR:OG1	4:N:607:GLY:HA3	1.78	0.82
2:B:684:GLN:N	3:I:98:ILE:HG13	1.56	0.82
2:B:719:ASN:OD1	4:M:565:SER:C	2.18	0.82
2:D:627:HIS:N	2:D:734:LYS:HG3	1.95	0.82
1:E:93:TYR:CB	2:F:676:PRO:HB3	2.08	0.82
2:F:547:LYS:CB	2:F:667:ILE:HD13	2.04	0.82
2:F:718:ASN:CB	4:O:530:VAL:HG13	2.09	0.82
3:I:98:ILE:HG13	4:M:550:ASP:OD2	1.80	0.82
3:J:77:THR:HG21	3:J:79:TYR:CE2	2.14	0.82
3:K:30:THR:HG23	3:K:53:ASN:HD22	1.44	0.82
3:L:30:THR:HG23	3:L:53:ASN:HD22	1.44	0.82
2:D:549:GLN:CD	2:D:669:VAL:O	2.13	0.82
2:D:687:ASN:ND2	4:N:533:ALA:CA	2.35	0.82
3:K:77:THR:HG21	3:K:79:TYR:CE2	2.14	0.82
4:N:650:VAL:HG23	4:N:655:VAL:HG21	1.60	0.82
4:O:650:VAL:HG23	4:O:655:VAL:HG21	1.60	0.82
2:B:507:ASN:OD1	2:B:556:ILE:CG1	2.28	0.82
1:C:246:GLU:OE2	2:F:814:LYS:N	2.07	0.82
1:G:96:CYS:HA	2:H:702:ASN:ND2	1.93	0.82
2:H:627:HIS:N	2:H:734:LYS:HG3	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:684:GLN:H	3:L:98:ILE:HG13	1.43	0.82
2:H:715:LYS:HE2	4:P:593:ASN:HB3	1.62	0.82
3:K:98:ILE:CG2	4:O:532:CYS:SG	2.68	0.82
2:D:547:LYS:CD	2:D:667:ILE:CG2	2.57	0.82
2:D:602:LEU:CD2	2:D:757:ILE:HA	2.04	0.82
2:F:547:LYS:HG3	2:F:757:ILE:CG2	1.99	0.82
3:I:30:THR:HG23	3:I:53:ASN:HD22	1.44	0.82
3:K:94:ARG:NH2	3:K:101:ASP:OD2	2.13	0.82
2:B:687:ASN:HB2	4:M:532:CYS:HA	1.56	0.82
2:D:507:ASN:OD1	2:D:556:ILE:CG1	2.28	0.82
2:F:627:HIS:N	2:F:734:LYS:HG3	1.95	0.82
2:F:549:GLN:CD	2:F:669:VAL:O	2.13	0.82
2:F:549:GLN:H	2:F:669:VAL:HG11	1.42	0.82
3:K:98:ILE:HG22	3:K:98:ILE:O	1.78	0.82
4:O:680:LEU:HD11	4:O:691:TYR:HE2	1.44	0.82
2:D:538:ARG:CD	2:D:667:ILE:CB	2.58	0.82
2:F:689:LYS:HB2	3:K:98:ILE:CD1	2.10	0.82
1:G:93:TYR:CB	2:H:676:PRO:HB3	2.08	0.82
3:J:87:THR:HG22	3:J:111:VAL:H	1.43	0.82
3:J:98:ILE:CG2	4:N:532:CYS:SG	2.68	0.82
2:B:717:ILE:HG22	4:M:530(B):SER:N	1.94	0.81
2:F:716:VAL:CB	4:O:591:TRP:HD1	1.91	0.81
1:A:93:TYR:CG	2:B:726:HIS:NE2	2.48	0.81
1:E:93:TYR:HD1	2:F:676:PRO:CG	1.52	0.81
1:E:93:TYR:CG	2:F:676:PRO:HB3	2.15	0.81
2:F:671:MET:C	2:F:673:PRO:CD	2.35	0.81
2:F:684:GLN:HE21	3:K:98:ILE:HD13	1.46	0.81
2:H:522:CYS:CA	2:H:733:LYS:NZ	2.31	0.81
2:H:547:LYS:HE2	2:H:667:ILE:HG12	1.51	0.81
3:L:77:THR:HG21	3:L:79:TYR:CE2	2.14	0.81
3:L:94:ARG:NH2	3:L:101:ASP:OD2	2.13	0.81
2:B:538:ARG:HB2	2:B:667:ILE:CD1	2.10	0.81
2:B:704:GLY:N	4:M:530(A):THR:HG22	1.95	0.81
1:C:245:LYS:NZ	2:F:789:PRO:O	2.14	0.81
2:D:549:GLN:H	2:D:669:VAL:HG11	1.42	0.81
2:F:536:ARG:HD2	2:F:738:ASN:HB2	1.63	0.81
2:F:547:LYS:CD	2:F:667:ILE:CG2	2.57	0.81
1:G:93:TYR:CG	2:H:676:PRO:HB3	2.15	0.81
2:H:536:ARG:HD2	2:H:738:ASN:HB2	1.62	0.81
2:H:686:GLY:CA	4:P:552:ASN:ND2	2.44	0.81
3:I:35:LEU:HD22	3:I:37:VAL:CG2	2.05	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:98:ILE:CG2	4:M:532:CYS:SG	2.68	0.81
3:J:11:VAL:HG11	3:J:147:PRO:HB2	1.60	0.81
3:J:11:VAL:HG21	3:J:147:PRO:HB2	1.62	0.81
3:J:30:THR:HG23	3:J:53:ASN:HD22	1.44	0.81
3:L:87:THR:HG22	3:L:111:VAL:H	1.43	0.81
2:B:612:THR:C	2:B:734:LYS:NZ	2.34	0.81
2:D:535:GLU:CA	2:D:736:GLN:H	1.89	0.81
1:E:245:LYS:NZ	2:H:789:PRO:O	2.14	0.81
2:F:538:ARG:HB2	2:F:667:ILE:CD1	2.10	0.81
2:F:602:LEU:HD21	2:F:757:ILE:CA	2.07	0.81
2:H:687:ASN:CB	4:P:532:CYS:CA	2.57	0.81
3:L:98:ILE:CG2	4:P:532:CYS:SG	2.68	0.81
2:D:522:CYS:CA	2:D:733:LYS:NZ	2.31	0.81
2:D:538:ARG:HB2	2:D:667:ILE:CD1	2.10	0.81
2:F:536:ARG:CZ	2:F:738:ASN:C	2.45	0.81
2:H:547:LYS:NZ	2:H:667:ILE:HG23	1.96	0.81
3:J:98:ILE:HG22	3:J:98:ILE:O	1.79	0.81
3:L:11:VAL:HG11	3:L:147:PRO:HB2	1.60	0.81
3:L:98:ILE:HG22	3:L:98:ILE:O	1.78	0.81
4:P:515:PRO:HD3	4:P:606(A):LEU:HB2	1.62	0.81
1:A:91:GLY:HA3	2:B:678:ARG:H	1.43	0.81
1:C:93:TYR:CG	2:D:676:PRO:HB3	2.15	0.81
1:E:93:TYR:CG	2:F:726:HIS:NE2	2.48	0.81
2:F:507:ASN:OD1	2:F:556:ILE:CG1	2.28	0.81
2:F:684:GLN:CB	4:O:550:ASP:CB	2.32	0.81
1:G:91:GLY:HA3	2:H:678:ARG:H	1.43	0.81
2:H:612:THR:C	2:H:734:LYS:HZ2	1.84	0.81
3:K:11:VAL:HG21	3:K:147:PRO:HB2	1.62	0.81
3:L:98:ILE:HG13	4:P:550:ASP:OD2	1.80	0.81
4:M:650:VAL:HG23	4:M:655:VAL:HG21	1.60	0.81
4:N:515:PRO:HD3	4:N:606(A):LEU:HB2	1.62	0.81
1:A:93:TYR:CG	2:B:676:PRO:HB3	2.15	0.81
2:B:627:HIS:N	2:B:734:LYS:HG3	1.95	0.81
2:H:671:MET:C	2:H:673:PRO:CD	2.35	0.81
2:H:716:VAL:CG2	4:P:532:CYS:HB2	2.10	0.81
1:A:152:HIS:HA	1:C:191:PRO:HB2	1.62	0.81
2:B:536:ARG:HB2	2:B:669:VAL:HA	1.63	0.81
2:B:549:GLN:CD	2:B:669:VAL:O	2.13	0.81
2:D:536:ARG:HD2	2:D:738:ASN:HB2	1.62	0.81
2:D:538:ARG:N	2:D:737:TYR:CB	2.44	0.81
2:F:536:ARG:HB2	2:F:669:VAL:HA	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:ARG:NH2	3:I:101:ASP:OD2	2.13	0.81
2:B:547:LYS:NZ	2:B:667:ILE:HG23	1.96	0.81
1:C:93:TYR:CG	2:D:726:HIS:NE2	2.48	0.81
2:F:536:ARG:NE	2:F:738:ASN:CA	2.12	0.81
2:F:538:ARG:N	2:F:737:TYR:CB	2.44	0.81
2:F:547:LYS:NZ	2:F:667:ILE:HG23	1.96	0.81
3:I:98:ILE:HG22	3:I:98:ILE:O	1.79	0.81
1:A:191:PRO:HB2	1:C:152:HIS:HA	1.62	0.81
2:D:536:ARG:HD2	2:D:738:ASN:CB	1.72	0.81
2:B:536:ARG:CZ	2:B:738:ASN:C	2.45	0.80
2:D:520:PRO:CD	2:D:732:HIS:N	2.29	0.80
2:D:538:ARG:HB2	2:D:667:ILE:HD13	1.63	0.80
3:L:35:LEU:HD22	3:L:37:VAL:CG2	2.05	0.80
2:B:716:VAL:HG11	4:M:591:TRP:HB3	1.28	0.80
2:D:519:CYS:O	2:D:733:LYS:HG3	1.81	0.80
2:F:522:CYS:CA	2:F:733:LYS:NZ	2.31	0.80
2:F:534:LEU:HB3	2:F:735:TRP:O	1.74	0.80
1:G:93:TYR:CG	2:H:726:HIS:NE2	2.48	0.80
2:H:549:GLN:H	2:H:669:VAL:HG11	1.42	0.80
3:J:94:ARG:NH2	3:J:101:ASP:OD2	2.13	0.80
2:F:522:CYS:CA	2:F:733:LYS:CD	2.33	0.80
2:F:545:THR:HG21	2:F:758:PRO:HG3	1.63	0.80
2:H:534:LEU:HD13	2:H:734:LYS:CB	1.80	0.80
2:H:536:ARG:CZ	2:H:738:ASN:C	2.45	0.80
1:C:242:TYR:CE2	2:F:788:TYR:CE2	2.40	0.80
2:D:599:HIS:HB3	2:D:735:TRP:CH2	2.17	0.80
2:D:612:THR:C	2:D:734:LYS:NZ	2.34	0.80
2:D:718:ASN:CG	4:N:531:ASN:CB	2.49	0.80
2:D:789:PRO:O	1:G:245:LYS:NZ	2.14	0.80
2:F:519:CYS:O	2:F:733:LYS:HG3	1.82	0.80
2:F:538:ARG:HD3	2:F:667:ILE:HB	1.56	0.80
2:H:538:ARG:N	2:H:737:TYR:CB	2.44	0.80
2:H:547:LYS:HG3	2:H:757:ILE:CG2	1.99	0.80
1:A:149:ASN:HD22	1:C:123:ARG:NH1	1.80	0.80
2:B:538:ARG:N	2:B:737:TYR:CB	2.44	0.80
2:D:547:LYS:CB	2:D:667:ILE:HD13	2.04	0.80
2:D:602:LEU:HD21	2:D:757:ILE:CA	2.07	0.80
2:F:599:HIS:HB3	2:F:735:TRP:CH2	2.17	0.80
2:H:507:ASN:OD1	2:H:556:ILE:CG1	2.28	0.80
2:H:545:THR:HG21	2:H:758:PRO:HG3	1.63	0.80
2:H:687:ASN:HD22	4:P:532:CYS:C	1.84	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:98:ILE:CG2	4:M:550:ASP:HA	2.12	0.80
3:L:98:ILE:CG2	4:P:550:ASP:HA	2.12	0.80
4:M:515:PRO:HD3	4:M:606(A):LEU:HB2	1.62	0.80
2:H:538:ARG:HB2	2:H:667:ILE:HD13	1.63	0.80
3:J:98:ILE:CG2	4:N:550:ASP:HA	2.12	0.80
3:K:98:ILE:CG2	4:O:550:ASP:HA	2.11	0.80
2:B:535:GLU:CB	2:B:670:HIS:HA	2.04	0.80
2:D:547:LYS:NZ	2:D:667:ILE:HG23	1.96	0.80
2:D:687:ASN:CG	4:N:533:ALA:N	2.34	0.80
4:O:515:PRO:HD3	4:O:606(A):LEU:HB2	1.62	0.80
2:B:536:ARG:HD2	2:B:738:ASN:HB2	1.62	0.80
2:B:549:GLN:H	2:B:669:VAL:HG11	1.42	0.80
2:H:538:ARG:HB2	2:H:667:ILE:CD1	2.10	0.80
2:H:547:LYS:CD	2:H:667:ILE:CG2	2.57	0.80
2:H:599:HIS:HB3	2:H:735:TRP:CH2	2.17	0.80
2:H:627:HIS:HD2	2:H:734:LYS:CB	1.61	0.80
4:P:680:LEU:HD11	4:P:691:TYR:HE2	1.44	0.80
2:F:687:ASN:HB3	4:O:532:CYS:CA	2.02	0.80
3:I:11:VAL:HG21	3:I:147:PRO:HB2	1.62	0.80
3:J:98:ILE:CG2	4:N:532:CYS:CB	2.60	0.80
3:L:11:VAL:HG21	3:L:147:PRO:HB2	1.62	0.80
2:B:684:GLN:HE21	3:I:98:ILE:HD13	1.46	0.80
2:D:535:GLU:OE1	2:D:670:HIS:CA	2.30	0.80
2:D:549:GLN:NE2	2:D:669:VAL:O	2.15	0.80
2:F:538:ARG:HB2	2:F:667:ILE:HD13	1.63	0.80
2:H:536:ARG:HB2	2:H:669:VAL:HA	1.63	0.80
2:H:687:ASN:ND2	4:P:551:THR:N	2.29	0.80
2:H:535:GLU:OE1	2:H:670:HIS:CA	2.30	0.79
3:J:20:ILE:HD11	3:J:109:LEU:HD11	1.65	0.79
2:B:549:GLN:NE2	2:B:669:VAL:O	2.15	0.79
2:B:599:HIS:HB3	2:B:735:TRP:CH2	2.17	0.79
1:C:95:PHE:O	2:D:724:GLN:C	2.20	0.79
2:H:549:GLN:NE2	2:H:669:VAL:O	2.15	0.79
2:H:687:ASN:CG	4:P:550:ASP:HA	2.02	0.79
2:B:538:ARG:HB2	2:B:667:ILE:HD13	1.63	0.79
2:B:612:THR:C	2:B:734:LYS:HZ2	1.84	0.79
2:H:602:LEU:HD13	2:H:758:PRO:N	1.80	0.79
3:K:35:LEU:HD22	3:K:37:VAL:CG2	2.05	0.79
2:D:547:LYS:HE3	2:D:755:ILE:O	1.83	0.79
2:F:535:GLU:OE1	2:F:670:HIS:CA	2.30	0.79
2:H:547:LYS:CB	2:H:667:ILE:HD13	2.04	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:602:LEU:HD21	2:H:757:ILE:CA	2.07	0.79
2:H:687:ASN:CG	4:P:550:ASP:CA	2.51	0.79
2:B:547:LYS:CD	2:B:667:ILE:CG2	2.57	0.79
2:D:704:GLY:N	4:N:530(A):THR:HG22	1.97	0.79
1:G:95:PHE:O	2:H:724:GLN:C	2.20	0.79
2:H:549:GLN:CD	2:H:669:VAL:O	2.13	0.79
2:F:534:LEU:CD2	2:F:735:TRP:O	2.31	0.79
1:A:291:VAL:H	1:E:304:PRO:CD	1.94	0.79
1:C:242:TYR:CD2	2:F:788:TYR:CE2	2.59	0.79
2:D:536:ARG:CZ	2:D:738:ASN:C	2.45	0.79
2:D:536:ARG:HB2	2:D:669:VAL:HA	1.63	0.79
3:I:98:ILE:HG21	4:M:550:ASP:CG	2.03	0.79
3:K:20:ILE:HD11	3:K:109:LEU:HD11	1.65	0.79
4:M:692:SER:HB2	4:M:705:SER:OG	1.83	0.79
4:O:692:SER:HB2	4:O:705:SER:OG	1.83	0.79
1:A:95:PHE:O	2:B:724:GLN:C	2.20	0.79
2:B:547:LYS:HE3	2:B:755:ILE:O	1.83	0.79
2:F:612:THR:C	2:F:734:LYS:NZ	2.34	0.79
2:H:519:CYS:O	2:H:733:LYS:HG3	1.81	0.79
3:K:98:ILE:CG2	4:O:532:CYS:CB	2.60	0.79
3:K:98:ILE:HG21	4:O:550:ASP:CG	2.03	0.79
4:M:540:PRO:O	4:M:541:ASP:HB2	1.83	0.79
2:F:549:GLN:NE2	2:F:669:VAL:O	2.15	0.79
2:H:687:ASN:ND2	4:P:550:ASP:CA	2.46	0.79
3:L:20:ILE:HD11	3:L:109:LEU:HD11	1.65	0.79
3:L:98:ILE:CG2	4:P:532:CYS:CB	2.60	0.79
4:N:540:PRO:O	4:N:541:ASP:HB2	1.83	0.79
2:B:519:CYS:O	2:B:733:LYS:HG3	1.82	0.78
2:D:687:ASN:CA	4:N:551:THR:OG1	2.15	0.78
1:E:95:PHE:O	2:F:724:GLN:C	2.20	0.78
2:H:536:ARG:HE	2:H:738:ASN:C	1.86	0.78
2:D:534:LEU:CD2	2:D:735:TRP:O	2.31	0.78
2:B:535:GLU:OE1	2:B:670:HIS:CA	2.30	0.78
2:F:520:PRO:N	2:F:732:HIS:N	2.32	0.78
2:F:521:ASP:CA	2:F:733:LYS:HD2	2.14	0.78
2:F:535:GLU:CB	2:F:670:HIS:HA	2.04	0.78
2:H:547:LYS:HE3	2:H:755:ILE:O	1.83	0.78
3:I:2:ILE:HD12	3:I:94:ARG:NH1	1.98	0.78
2:D:545:THR:HG21	2:D:758:PRO:HG3	1.63	0.78
1:E:199:GLN:HE21	2:H:775:THR:HG21	1.46	0.78
2:H:534:LEU:CD2	2:H:735:TRP:O	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:612:THR:C	2:H:734:LYS:NZ	2.34	0.78
2:F:687:ASN:HB2	4:O:532:CYS:CA	1.99	0.78
2:H:534:LEU:HB3	2:H:735:TRP:O	1.75	0.78
2:H:716:VAL:HG21	4:P:532:CYS:SG	1.39	0.78
3:L:69:PHE:CE1	3:L:80:LEU:HD13	2.19	0.78
3:L:98:ILE:CG2	4:P:550:ASP:CB	2.62	0.78
4:P:692:SER:HB2	4:P:705:SER:OG	1.83	0.78
2:B:716:VAL:HG22	4:M:532:CYS:N	1.99	0.78
2:B:521:ASP:CA	2:B:733:LYS:HD2	2.14	0.78
2:B:534:LEU:CD2	2:B:735:TRP:O	2.31	0.78
2:B:545:THR:HG21	2:B:758:PRO:HG3	1.63	0.78
2:D:520:PRO:N	2:D:732:HIS:N	2.31	0.78
2:D:687:ASN:CB	4:N:550:ASP:CA	2.62	0.78
2:F:547:LYS:HE3	2:F:755:ILE:O	1.83	0.78
2:F:547:LYS:HG2	2:F:667:ILE:CD1	2.14	0.78
2:F:684:GLN:HB3	4:O:550:ASP:CB	2.12	0.78
2:H:717:ILE:C	4:P:531:ASN:N	2.36	0.78
3:I:20:ILE:HD11	3:I:109:LEU:HD11	1.65	0.78
3:L:98:ILE:HG21	4:P:550:ASP:CG	2.03	0.78
1:E:93:TYR:HA	2:F:726:HIS:NE2	1.98	0.78
2:H:548:ILE:O	2:H:755:ILE:CG2	2.32	0.78
3:I:98:ILE:CG2	4:M:532:CYS:CB	2.60	0.78
3:K:98:ILE:CG2	4:O:550:ASP:CB	2.62	0.78
4:P:521:LEU:N	4:P:521:LEU:HD23	1.99	0.78
2:B:548:ILE:O	2:B:755:ILE:CG2	2.32	0.78
2:F:685:SER:OG	4:O:549:GLY:CA	2.31	0.78
3:I:11:VAL:CG1	3:I:147:PRO:HB2	2.14	0.78
3:J:48:MET:HG2	3:J:63:PHE:CZ	2.19	0.78
4:P:540:PRO:O	4:P:541:ASP:HB2	1.84	0.78
2:F:548:ILE:N	2:F:755:ILE:HD11	1.99	0.78
2:H:520:PRO:N	2:H:732:HIS:N	2.32	0.78
2:H:715:LYS:HE2	4:P:593:ASN:CG	2.05	0.78
3:K:11:VAL:CG1	3:K:147:PRO:HB2	2.14	0.78
3:K:48:MET:HG2	3:K:63:PHE:CZ	2.19	0.78
3:L:48:MET:HG2	3:L:63:PHE:CZ	2.19	0.78
2:F:718:ASN:ND2	4:O:533:ALA:N	2.32	0.77
2:B:538:ARG:HD3	2:B:667:ILE:HB	1.56	0.77
2:D:687:ASN:HB3	4:N:532:CYS:CA	2.08	0.77
1:E:242:TYR:CE2	2:H:788:TYR:CE2	2.40	0.77
4:N:692:SER:HB2	4:N:705:SER:OG	1.83	0.77
2:B:520:PRO:N	2:B:732:HIS:N	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:718:ASN:ND2	4:M:533:ALA:HB2	1.98	0.77
2:D:716:VAL:CG1	4:N:591:TRP:CG	2.41	0.77
2:H:521:ASP:CA	2:H:733:LYS:HD2	2.14	0.77
3:L:11:VAL:CG1	3:L:147:PRO:HB2	2.14	0.77
4:O:540:PRO:O	4:O:541:ASP:HB2	1.83	0.77
1:A:87:PHE:HD2	2:B:678:ARG:HG3	1.50	0.77
2:B:686:GLY:HA2	4:M:552:ASN:ND2	1.99	0.77
2:F:548:ILE:O	2:F:755:ILE:CG2	2.32	0.77
2:B:547:LYS:CB	2:B:667:ILE:HD13	2.04	0.77
2:H:718:ASN:HB2	4:P:530(A):THR:O	1.84	0.77
3:L:45:PHE:CE1	4:P:587:PHE:CE2	2.73	0.77
4:N:682:ALA:O	4:N:685:TRP:HB3	1.85	0.77
2:B:715:LYS:CE	4:M:593:ASN:HB3	2.12	0.77
2:D:717:ILE:C	4:N:531:ASN:N	2.29	0.77
2:D:719:ASN:HD21	4:N:571:ALA:CA	1.97	0.77
3:J:2:ILE:HD12	3:J:94:ARG:NH1	1.98	0.77
3:J:45:PHE:CE1	4:N:587:PHE:CE2	2.73	0.77
2:D:704:GLY:CA	4:N:530(A):THR:CG2	2.61	0.77
2:F:536:ARG:HE	2:F:738:ASN:C	1.86	0.77
3:I:48:MET:HG2	3:I:63:PHE:CZ	2.19	0.77
4:M:515:PRO:HD3	4:M:606(A):LEU:CA	2.15	0.77
2:F:594:THR:O	2:F:660:THR:C	2.23	0.77
4:N:515:PRO:HD3	4:N:606(A):LEU:CA	2.15	0.77
4:N:521:LEU:HD23	4:N:521:LEU:N	1.99	0.77
2:D:547:LYS:HG2	2:D:667:ILE:HD11	1.66	0.77
3:K:21:SER:OG	3:K:79:TYR:CD2	2.37	0.77
1:A:291:VAL:N	1:E:304:PRO:HD3	2.00	0.77
2:B:534:LEU:HD13	2:B:734:LYS:CB	1.80	0.77
2:B:548:ILE:O	2:B:755:ILE:HD13	1.86	0.77
2:H:687:ASN:CB	4:P:550:ASP:C	2.52	0.77
4:O:515:PRO:HD3	4:O:606(A):LEU:CA	2.15	0.77
2:D:594:THR:O	2:D:660:THR:C	2.23	0.76
2:D:788:TYR:CE2	1:G:242:TYR:CD2	2.59	0.76
2:H:536:ARG:CB	2:H:669:VAL:CA	2.60	0.76
2:H:689:LYS:CB	3:L:98:ILE:HD11	2.13	0.76
3:I:69:PHE:CE1	3:I:80:LEU:HD13	2.19	0.76
3:K:69:PHE:CE1	3:K:80:LEU:HD13	2.19	0.76
3:L:213:ARG:NH2	4:P:619:PRO:CD	2.45	0.76
4:O:521:LEU:N	4:O:521:LEU:HD23	1.99	0.76
1:A:149:ASN:HD21	1:C:123:ARG:CZ	1.96	0.76
2:B:687:ASN:ND2	4:M:551:THR:H	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:775:THR:HG21	1:G:199:GLN:HE21	1.46	0.76
2:F:602:LEU:HD13	2:F:758:PRO:N	1.80	0.76
3:L:21:SER:CB	3:L:79:TYR:CE2	2.69	0.76
2:D:547:LYS:HG2	2:D:667:ILE:CD1	2.14	0.76
2:D:548:ILE:N	2:D:755:ILE:HD11	1.99	0.76
2:D:627:HIS:HD2	2:D:734:LYS:HB2	0.94	0.76
2:H:613:VAL:H	2:H:734:LYS:HZ2	0.96	0.76
4:P:515:PRO:CD	4:P:606(A):LEU:O	2.34	0.76
2:F:627:HIS:HD2	2:F:734:LYS:HB2	0.94	0.76
1:G:91:GLY:CA	2:H:678:ARG:H	1.99	0.76
2:H:548:ILE:O	2:H:755:ILE:HD13	1.86	0.76
3:I:11:VAL:CG2	3:I:147:PRO:HB2	2.16	0.76
3:I:45:PHE:CE1	4:M:587:PHE:CE2	2.73	0.76
3:K:21:SER:CB	3:K:79:TYR:CE2	2.69	0.76
4:P:515:PRO:HD3	4:P:606(A):LEU:CA	2.15	0.76
2:B:602:LEU:CD1	2:B:758:PRO:CB	2.59	0.76
1:C:87:PHE:HD2	2:D:678:ARG:HG3	1.50	0.76
3:J:2:ILE:HD13	3:J:94:ARG:NH1	2.00	0.76
3:J:98:ILE:HG21	4:N:550:ASP:CG	2.03	0.76
3:K:2:ILE:HD13	3:K:94:ARG:NH1	2.00	0.76
4:N:515:PRO:CD	4:N:606(A):LEU:O	2.34	0.76
2:D:686:GLY:N	4:N:550:ASP:O	2.13	0.76
2:H:535:GLU:CB	2:H:670:HIS:HA	2.04	0.76
3:J:11:VAL:CG1	3:J:147:PRO:HB2	2.14	0.76
3:J:69:PHE:CE1	3:J:80:LEU:HD13	2.19	0.76
3:J:77:THR:HG22	3:J:79:TYR:CE1	2.20	0.76
3:K:11:VAL:CG2	3:K:147:PRO:HB2	2.16	0.76
4:P:682:ALA:O	4:P:685:TRP:HB3	1.85	0.76
2:B:547:LYS:HG2	2:B:667:ILE:CD1	2.14	0.76
2:B:689:LYS:HB3	3:I:98:ILE:CD1	2.14	0.76
2:D:673:PRO:HB3	2:D:745:ASN:HB2	1.67	0.76
1:E:87:PHE:HD2	2:F:678:ARG:HG3	1.50	0.76
2:F:535:GLU:C	2:F:670:HIS:H	1.89	0.76
2:H:548:ILE:N	2:H:755:ILE:HD11	1.99	0.76
3:K:77:THR:HG22	3:K:79:TYR:CE1	2.20	0.76
3:K:93:VAL:HG11	3:K:100:LEU:CD2	2.16	0.76
4:M:515:PRO:CD	4:M:606(A):LEU:O	2.34	0.76
1:C:199:GLN:HE21	2:F:775:THR:HG21	1.46	0.76
2:D:534:LEU:HB3	2:D:735:TRP:O	1.75	0.76
2:F:687:ASN:HB2	4:O:550:ASP:HA	1.68	0.76
1:G:87:PHE:HD2	2:H:678:ARG:HG3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:547:LYS:HG2	2:H:667:ILE:HD11	1.65	0.76
3:J:21:SER:OG	3:J:79:TYR:CD2	2.37	0.76
2:D:602:LEU:CD1	2:D:758:PRO:CB	2.59	0.76
1:G:93:TYR:HA	2:H:726:HIS:NE2	1.98	0.76
3:J:35:LEU:HD22	3:J:37:VAL:CG2	2.05	0.76
3:J:93:VAL:HG11	3:J:100:LEU:CD2	2.16	0.76
3:K:45:PHE:CE1	4:O:587:PHE:CE2	2.73	0.76
4:O:682:ALA:O	4:O:685:TRP:HB3	1.85	0.76
2:F:673:PRO:HB3	2:F:745:ASN:HB2	1.67	0.76
2:H:520:PRO:N	2:H:731:ASN:HA	1.93	0.76
3:I:2:ILE:HD13	3:I:94:ARG:NH1	2.00	0.76
3:J:213:ARG:NH2	4:N:619:PRO:CD	2.45	0.76
2:B:612:THR:HA	2:B:734:LYS:HZ2	1.47	0.75
2:H:594:THR:O	2:H:660:THR:C	2.23	0.75
2:H:718:ASN:HB2	4:P:531:ASN:HB2	0.76	0.75
3:I:77:THR:HG22	3:I:79:TYR:CE1	2.20	0.75
3:L:11:VAL:CG2	3:L:147:PRO:HB2	2.16	0.75
3:L:93:VAL:HG11	3:L:100:LEU:CD2	2.16	0.75
1:A:290:VAL:O	1:E:317:ILE:CD1	2.30	0.75
2:B:673:PRO:HB3	2:B:745:ASN:HB2	1.67	0.75
2:D:684:GLN:C	4:N:549:GLY:O	2.21	0.75
2:F:548:ILE:O	2:F:755:ILE:HD13	1.85	0.75
2:H:535:GLU:C	2:H:670:HIS:H	1.89	0.75
4:O:515:PRO:CD	4:O:606(A):LEU:O	2.34	0.75
2:B:520:PRO:CA	2:B:731:ASN:HA	1.60	0.75
2:B:535:GLU:C	2:B:670:HIS:H	1.89	0.75
2:B:535:GLU:CA	2:B:736:GLN:H	1.89	0.75
2:B:547:LYS:HG2	2:B:667:ILE:HD11	1.65	0.75
2:B:594:THR:O	2:B:660:THR:C	2.23	0.75
2:D:521:ASP:CA	2:D:733:LYS:HD2	2.14	0.75
2:D:534:LEU:HD13	2:D:734:LYS:CB	1.80	0.75
2:H:527:SER:HA	2:H:733:LYS:HE3	1.68	0.75
3:I:21:SER:CB	3:I:79:TYR:CE2	2.69	0.75
4:M:521:LEU:N	4:M:521:LEU:HD23	1.99	0.75
4:P:628:ASN:CA	4:P:682:ALA:HB2	2.17	0.75
2:D:716:VAL:N	4:N:591:TRP:CD1	2.54	0.75
1:G:91:GLY:HA3	2:H:678:ARG:N	2.01	0.75
3:I:93:VAL:HG11	3:I:100:LEU:CD2	2.16	0.75
3:J:21:SER:CB	3:J:79:TYR:CE2	2.69	0.75
2:B:548:ILE:N	2:B:755:ILE:HD11	1.99	0.75
3:L:2:ILE:HD12	3:L:94:ARG:NH1	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:77:THR:HG22	3:L:79:TYR:CE1	2.20	0.75
4:M:682:ALA:O	4:M:685:TRP:HB3	1.85	0.75
1:A:93:TYR:HB2	2:B:676:PRO:CB	2.17	0.75
2:H:627:HIS:HD2	2:H:734:LYS:HB2	0.94	0.75
3:J:11:VAL:CG2	3:J:147:PRO:HB2	2.16	0.75
1:C:91:GLY:CA	2:D:678:ARG:H	1.99	0.75
2:D:548:ILE:O	2:D:755:ILE:HD13	1.85	0.75
2:F:537:ILE:HD12	2:F:736:GLN:HG3	1.69	0.75
2:H:537:ILE:HD12	2:H:736:GLN:HG3	1.69	0.75
3:L:98:ILE:HG21	4:P:550:ASP:HA	1.69	0.75
4:M:515:PRO:CD	4:M:606(A):LEU:CB	2.65	0.75
1:A:91:GLY:CA	2:B:678:ARG:H	1.99	0.75
2:B:718:ASN:C	4:M:530(B):SER:CA	2.40	0.75
2:H:547:LYS:CD	2:H:667:ILE:CD1	2.55	0.75
4:P:515:PRO:CD	4:P:606(A):LEU:CB	2.65	0.75
1:C:91:GLY:HA3	2:D:678:ARG:N	2.01	0.75
2:D:535:GLU:C	2:D:670:HIS:H	1.89	0.75
2:D:687:ASN:CB	4:N:551:THR:N	2.46	0.75
3:I:21:SER:OG	3:I:79:TYR:CD2	2.37	0.75
3:K:2:ILE:HD12	3:K:94:ARG:NH1	1.98	0.75
1:C:93:TYR:HB2	2:D:676:PRO:CB	2.17	0.74
2:D:527:SER:HA	2:D:733:LYS:HE3	1.68	0.74
2:D:542:THR:HA	2:D:636:ILE:HG13	1.69	0.74
4:N:628:ASN:CA	4:N:682:ALA:HB2	2.17	0.74
2:D:536:ARG:CB	2:D:669:VAL:CA	2.60	0.74
4:N:515:PRO:CD	4:N:606(A):LEU:CB	2.65	0.74
2:B:547:LYS:HE2	2:B:667:ILE:HG12	1.51	0.74
2:B:718:ASN:H	4:M:531:ASN:H	0.76	0.74
2:D:548:ILE:O	2:D:755:ILE:CG2	2.32	0.74
2:D:687:ASN:ND2	4:N:533:ALA:C	2.36	0.74
3:I:24:ALA:HB1	3:I:27:TYR:CE1	2.22	0.74
3:J:93:VAL:HG21	3:J:103:TRP:CE3	2.22	0.74
3:J:93:VAL:CG2	3:J:103:TRP:CE3	2.70	0.74
3:K:93:VAL:CG2	3:K:103:TRP:CE3	2.70	0.74
3:L:93:VAL:CG2	3:L:103:TRP:CE3	2.70	0.74
4:M:628:ASN:CA	4:M:682:ALA:HB2	2.17	0.74
1:A:123:ARG:NH1	1:C:149:ASN:HD22	1.79	0.74
2:B:534:LEU:CD1	2:B:734:LYS:CA	2.64	0.74
2:B:684:GLN:NE2	3:I:98:ILE:HD13	2.02	0.74
2:F:547:LYS:HG2	2:F:667:ILE:HD11	1.66	0.74
1:G:93:TYR:HB2	2:H:676:PRO:CB	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLY:HA3	2:B:678:ARG:N	2.01	0.74
2:B:507:ASN:HB2	2:B:562:HIS:CD2	1.91	0.74
2:B:602:LEU:HD21	2:B:757:ILE:CA	2.07	0.74
2:D:536:ARG:HE	2:D:738:ASN:C	1.86	0.74
2:F:527:SER:HA	2:F:733:LYS:HE3	1.68	0.74
3:I:98:ILE:HG22	4:M:532:CYS:CB	2.13	0.74
3:J:24:ALA:HB1	3:J:27:TYR:CE1	2.22	0.74
3:L:24:ALA:HB1	3:L:27:TYR:CE1	2.22	0.74
1:A:24:TYR:C	1:E:304:PRO:O	2.26	0.74
2:F:507:ASN:HB2	2:F:562:HIS:CD2	1.91	0.74
2:F:689:LYS:CB	3:K:98:ILE:HD12	2.16	0.74
2:H:687:ASN:ND2	4:P:532:CYS:HA	1.92	0.74
3:I:93:VAL:CG2	3:I:103:TRP:CE3	2.70	0.74
2:B:536:ARG:HE	2:B:738:ASN:C	1.86	0.74
1:E:91:GLY:HA3	2:F:678:ARG:N	2.01	0.74
2:H:673:PRO:HB3	2:H:745:ASN:HB2	1.67	0.74
2:B:685:SER:HB3	4:M:553:ASN:O	1.88	0.74
1:C:93:TYR:HA	2:D:726:HIS:NE2	1.98	0.74
3:I:213:ARG:NH2	4:M:619:PRO:CD	2.45	0.74
2:B:718:ASN:HB3	4:M:530:VAL:CG1	2.18	0.74
1:E:93:TYR:HB2	2:F:676:PRO:CB	2.17	0.74
2:F:538:ARG:HD3	2:F:667:ILE:HD13	1.67	0.74
2:F:602:LEU:CD1	2:F:758:PRO:CB	2.59	0.74
2:H:687:ASN:ND2	4:P:550:ASP:HA	2.00	0.74
1:A:291:VAL:N	1:E:304:PRO:CD	2.50	0.74
2:B:527:SER:HA	2:B:733:LYS:HE3	1.68	0.74
1:E:93:TYR:CG	2:F:676:PRO:CG	2.69	0.74
2:F:716:VAL:HG11	4:O:591:TRP:HB3	0.97	0.74
2:H:538:ARG:HD3	2:H:667:ILE:HD13	1.67	0.74
3:I:122:TYR:CE2	4:M:624:GLU:HG3	2.23	0.74
3:L:93:VAL:HG21	3:L:103:TRP:CE3	2.23	0.74
2:B:627:HIS:HD2	2:B:734:LYS:HB2	0.94	0.73
2:B:718:ASN:ND2	4:M:533:ALA:CB	2.48	0.73
2:B:719:ASN:N	4:M:530(B):SER:HA	2.01	0.73
2:D:507:ASN:HB2	2:D:562:HIS:CD2	1.91	0.73
1:E:91:GLY:CA	2:F:678:ARG:H	1.99	0.73
2:F:520:PRO:N	2:F:731:ASN:CA	2.39	0.73
2:H:536:ARG:N	2:H:670:HIS:H	1.86	0.73
3:I:93:VAL:HG21	3:I:103:TRP:CE3	2.23	0.73
3:K:93:VAL:HG21	3:K:103:TRP:CE3	2.23	0.73
3:L:122:TYR:CE2	4:P:624:GLU:HG3	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:THR:CA	2:B:734:LYS:HZ2	1.97	0.73
2:B:685:SER:CB	4:M:549:GLY:H	2.00	0.73
2:D:602:LEU:CD1	2:D:758:PRO:CA	2.66	0.73
2:H:612:THR:HA	2:H:734:LYS:HZ2	1.47	0.73
3:L:98:ILE:CG1	4:P:550:ASP:CG	2.56	0.73
4:O:628:ASN:CA	4:O:682:ALA:HB2	2.17	0.73
2:B:602:LEU:CD1	2:B:758:PRO:CA	2.66	0.73
2:D:537:ILE:HD12	2:D:736:GLN:HG3	1.69	0.73
2:F:602:LEU:CD1	2:F:758:PRO:CA	2.66	0.73
3:K:24:ALA:HB1	3:K:27:TYR:CE1	2.22	0.73
3:K:122:TYR:CE2	4:O:624:GLU:HG3	2.23	0.73
4:O:515:PRO:CD	4:O:606(A):LEU:CB	2.65	0.73
2:H:542:THR:HA	2:H:636:ILE:HG13	1.69	0.73
2:H:602:LEU:CD1	2:H:758:PRO:CA	2.66	0.73
3:K:98:ILE:HG21	4:O:550:ASP:HA	1.68	0.73
4:M:520:THR:C	4:M:521:LEU:HD23	2.09	0.73
2:D:687:ASN:CB	4:N:532:CYS:CA	2.56	0.73
2:D:547:LYS:CE	2:D:755:ILE:O	2.37	0.73
3:J:98:ILE:HG21	4:N:550:ASP:HA	1.69	0.73
1:A:123:ARG:CZ	1:C:149:ASN:HD21	1.96	0.73
2:B:542:THR:HA	2:B:636:ILE:HG13	1.69	0.73
2:F:542:THR:HA	2:F:636:ILE:HG13	1.69	0.73
1:G:87:PHE:CD2	2:H:678:ARG:HG3	2.24	0.73
3:J:122:TYR:CE2	4:N:624:GLU:HG3	2.23	0.73
2:B:718:ASN:HD21	4:M:533:ALA:HA	1.51	0.73
1:E:87:PHE:CD2	2:F:678:ARG:HG3	2.24	0.73
2:H:719:ASN:O	4:P:566:LEU:CD1	2.35	0.73
2:B:536:ARG:N	2:B:670:HIS:H	1.86	0.73
2:D:536:ARG:N	2:D:670:HIS:H	1.86	0.73
2:D:538:ARG:HD2	2:D:667:ILE:HB	1.71	0.73
2:F:547:LYS:CE	2:F:755:ILE:O	2.37	0.73
2:H:536:ARG:NE	2:H:737:TYR:CD2	2.57	0.73
3:I:11:VAL:CG1	3:I:147:PRO:CB	2.67	0.73
1:A:289:ARG:HH12	1:E:354:ILE:C	1.88	0.73
1:C:87:PHE:CD2	2:D:678:ARG:HG3	2.24	0.73
2:D:536:ARG:NE	2:D:737:TYR:CD2	2.57	0.73
2:D:547:LYS:HG2	2:D:755:ILE:HD11	1.71	0.73
2:D:718:ASN:OD1	4:N:531:ASN:O	2.06	0.73
2:H:684:GLN:CA	4:P:550:ASP:OD2	2.35	0.73
3:I:98:ILE:CG2	4:M:550:ASP:CB	2.62	0.73
3:L:114:ALA:CB	3:L:146:PHE:HE2	1.65	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:520:THR:C	4:N:521:LEU:HD23	2.09	0.73
4:O:520:THR:C	4:O:521:LEU:HD23	2.09	0.73
2:F:536:ARG:N	2:F:670:HIS:H	1.86	0.72
2:H:534:LEU:CG	2:H:734:LYS:HB3	1.94	0.72
2:B:627:HIS:HD2	2:B:734:LYS:CB	1.61	0.72
2:H:627:HIS:CD2	2:H:734:LYS:CA	2.72	0.72
2:B:627:HIS:CD2	2:B:734:LYS:CA	2.72	0.72
2:D:716:VAL:CG1	4:N:591:TRP:CD1	2.65	0.72
2:H:538:ARG:HD2	2:H:667:ILE:HB	1.71	0.72
1:A:91:GLY:HA3	2:B:678:ARG:CA	2.19	0.72
2:B:534:LEU:HB3	2:B:735:TRP:O	1.75	0.72
2:F:536:ARG:NE	2:F:737:TYR:CD2	2.57	0.72
2:H:535:GLU:C	2:H:670:HIS:N	2.43	0.72
2:H:684:GLN:N	3:L:98:ILE:HG13	1.80	0.72
3:J:114:ALA:CB	3:J:146:PHE:HE2	1.65	0.72
4:P:520:THR:C	4:P:521:LEU:HD23	2.09	0.72
2:B:536:ARG:NE	2:B:737:TYR:CD2	2.57	0.72
1:C:93:TYR:CG	2:D:676:PRO:CG	2.69	0.72
2:H:547:LYS:CE	2:H:755:ILE:O	2.37	0.72
2:H:687:ASN:HB3	4:P:532:CYS:CA	2.19	0.72
3:L:2:ILE:HD13	3:L:94:ARG:NH1	2.00	0.72
2:B:535:GLU:C	2:B:670:HIS:N	2.43	0.72
2:B:547:LYS:HG2	2:B:755:ILE:HD11	1.71	0.72
2:F:534:LEU:CD1	2:F:734:LYS:CA	2.65	0.72
2:F:613:VAL:H	2:F:734:LYS:HZ2	0.78	0.72
3:L:11:VAL:CG1	3:L:147:PRO:CB	2.67	0.72
2:B:537:ILE:HD12	2:B:736:GLN:HG3	1.69	0.72
1:C:199:GLN:NE2	2:F:775:THR:CG2	2.53	0.72
3:I:98:ILE:HG21	4:M:550:ASP:HA	1.69	0.72
3:K:11:VAL:CG1	3:K:147:PRO:CB	2.67	0.72
2:F:549:GLN:HA	2:F:755:ILE:HG23	1.72	0.72
2:F:685:SER:HG	4:O:553:ASN:HB2	1.52	0.72
2:F:685:SER:C	4:O:553:ASN:N	2.43	0.72
2:H:599:HIS:CB	2:H:754:LYS:O	2.38	0.72
2:B:549:GLN:HA	2:B:755:ILE:HG23	1.72	0.72
1:C:91:GLY:HA3	2:D:678:ARG:CA	2.19	0.72
2:D:602:LEU:HD13	2:D:758:PRO:N	1.80	0.72
2:D:627:HIS:CD2	2:D:734:LYS:CA	2.72	0.72
2:D:687:ASN:HB2	4:N:532:CYS:HA	1.65	0.72
2:F:536:ARG:CB	2:F:669:VAL:CA	2.60	0.72
2:F:627:HIS:CD2	2:F:734:LYS:CA	2.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:602:LEU:CD1	2:H:758:PRO:CB	2.59	0.72
3:K:98:ILE:HB	4:O:550:ASP:CB	1.66	0.72
2:D:718:ASN:CG	4:N:590:LEU:HD22	2.10	0.72
1:G:93:TYR:CG	2:H:676:PRO:CG	2.69	0.72
1:A:87:PHE:CD2	2:B:678:ARG:HG3	2.24	0.71
2:H:548:ILE:N	2:H:755:ILE:HD13	2.05	0.71
2:D:507:ASN:N	2:D:562:HIS:NE2	2.38	0.71
2:F:538:ARG:HD2	2:F:667:ILE:HB	1.71	0.71
2:F:547:LYS:HG2	2:F:667:ILE:HG12	1.64	0.71
2:D:775:THR:CG2	1:G:199:GLN:NE2	2.53	0.71
1:E:199:GLN:NE2	2:H:775:THR:CG2	2.53	0.71
2:F:534:LEU:HD13	2:F:734:LYS:CB	1.80	0.71
2:F:547:LYS:HG2	2:F:755:ILE:HD11	1.71	0.71
2:F:548:ILE:N	2:F:755:ILE:HD13	2.05	0.71
2:F:685:SER:C	4:O:552:ASN:H	1.91	0.71
2:B:547:LYS:CE	2:B:755:ILE:O	2.37	0.71
2:B:687:ASN:ND2	4:M:551:THR:N	2.38	0.71
2:D:612:THR:C	2:D:734:LYS:HZ2	1.89	0.71
1:A:151:ASP:O	1:C:191:PRO:CG	2.33	0.71
2:B:507:ASN:N	2:B:562:HIS:NE2	2.38	0.71
1:E:91:GLY:HA3	2:F:678:ARG:CA	2.19	0.71
2:B:719:ASN:HD21	4:M:571:ALA:CB	2.03	0.71
2:F:507:ASN:N	2:F:562:HIS:NE2	2.38	0.71
1:G:91:GLY:HA3	2:H:678:ARG:CA	2.19	0.71
3:J:11:VAL:CG1	3:J:147:PRO:CB	2.67	0.71
2:B:599:HIS:CB	2:B:754:LYS:O	2.38	0.71
2:H:547:LYS:HG2	2:H:755:ILE:CD1	2.21	0.71
2:H:686:GLY:N	4:P:553:ASN:N	2.38	0.71
3:K:98:ILE:HB	4:O:550:ASP:HB2	0.75	0.71
2:B:548:ILE:N	2:B:755:ILE:HD13	2.05	0.71
2:H:686:GLY:H	4:P:550:ASP:C	1.93	0.71
2:H:687:ASN:ND2	4:P:532:CYS:O	2.23	0.71
3:I:98:ILE:CG2	4:M:550:ASP:CA	2.69	0.71
1:A:191:PRO:CG	1:C:151:ASP:O	2.33	0.71
2:B:534:LEU:HD12	2:B:734:LYS:HD3	1.43	0.71
2:B:538:ARG:HD2	2:B:667:ILE:HB	1.71	0.71
2:H:547:LYS:CE	2:H:667:ILE:CB	2.69	0.71
3:K:98:ILE:CG2	4:O:550:ASP:CA	2.69	0.71
3:L:98:ILE:CG2	4:P:550:ASP:CA	2.69	0.71
1:A:95:PHE:CA	2:B:726:HIS:N	2.54	0.71
3:J:2:ILE:HD12	3:J:94:ARG:CZ	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:VAL:CG2	4:M:532:CYS:HG	1.36	0.70
2:H:534:LEU:HD11	2:H:734:LYS:HD3	1.51	0.70
2:H:547:LYS:HG2	2:H:755:ILE:HD11	1.71	0.70
2:D:535:GLU:C	2:D:670:HIS:N	2.43	0.70
2:D:548:ILE:N	2:D:755:ILE:HD13	2.05	0.70
2:D:719:ASN:CA	4:N:551:THR:CG2	2.61	0.70
1:G:95:PHE:CA	2:H:726:HIS:N	2.54	0.70
2:B:547:LYS:HG2	2:B:755:ILE:CD1	2.21	0.70
2:D:547:LYS:CE	2:D:667:ILE:CB	2.69	0.70
3:I:2:ILE:HD12	3:I:94:ARG:CZ	2.21	0.70
1:A:93:TYR:CG	2:B:676:PRO:CG	2.69	0.70
4:M:540:PRO:HB3	4:M:666:LYS:HD3	1.74	0.70
2:B:536:ARG:CB	2:B:669:VAL:CA	2.60	0.70
1:C:95:PHE:CA	2:D:726:HIS:N	2.54	0.70
2:F:547:LYS:HG2	2:F:755:ILE:CD1	2.21	0.70
2:F:685:SER:CA	4:O:553:ASN:H	2.01	0.70
3:L:2:ILE:HD12	3:L:94:ARG:CZ	2.21	0.70
2:B:520:PRO:N	2:B:731:ASN:HA	1.93	0.70
2:D:627:HIS:HD2	2:D:734:LYS:CB	1.61	0.70
2:F:522:CYS:N	2:F:733:LYS:HD2	1.72	0.70
2:H:507:ASN:N	2:H:562:HIS:NE2	2.38	0.70
2:H:549:GLN:HA	2:H:755:ILE:HG23	1.72	0.70
3:J:2:ILE:CD1	3:J:94:ARG:CZ	2.70	0.70
3:K:2:ILE:CD1	3:K:94:ARG:CZ	2.70	0.70
4:O:540:PRO:HB3	4:O:666:LYS:HD3	1.74	0.70
2:F:597:MET:HG2	2:F:756:HIS:NE2	2.06	0.70
3:L:30:THR:HG23	3:L:53:ASN:ND2	2.07	0.70
2:D:537:ILE:C	2:D:737:TYR:CB	2.60	0.70
2:D:626:THR:N	2:D:734:LYS:CG	2.54	0.70
2:F:716:VAL:HG22	4:O:532:CYS:N	2.07	0.70
2:B:537:ILE:C	2:B:737:TYR:CB	2.60	0.70
2:D:547:LYS:HG2	2:D:755:ILE:CD1	2.20	0.70
2:D:549:GLN:HA	2:D:755:ILE:HG23	1.72	0.70
2:D:715:LYS:HA	4:N:591:TRP:NE1	2.06	0.70
2:B:685:SER:C	4:M:552:ASN:C	2.50	0.70
2:B:715:LYS:HA	4:M:591:TRP:HE1	1.57	0.70
2:H:545:THR:HG1	2:H:759:PHE:HE2	1.38	0.69
2:H:718:ASN:N	4:P:532:CYS:H	1.90	0.69
3:K:2:ILE:HD12	3:K:94:ARG:CZ	2.21	0.69
4:P:555:ARG:HD2	4:P:556:SER:O	1.92	0.69
2:F:537:ILE:C	2:F:737:TYR:CB	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:VAL:N	4:M:591:TRP:HD1	1.89	0.69
2:F:535:GLU:C	2:F:670:HIS:N	2.43	0.69
3:J:59:TYR:OH	3:J:68:VAL:HA	1.92	0.69
3:K:59:TYR:OH	3:K:68:VAL:HA	1.92	0.69
3:K:213:ARG:NH2	4:O:619:PRO:CD	2.45	0.69
3:L:98:ILE:HB	4:P:550:ASP:HB2	0.75	0.69
2:D:685:SER:O	4:N:553:ASN:OD1	2.05	0.69
2:F:718:ASN:HB2	4:O:531:ASN:OD1	1.92	0.69
2:H:715:LYS:CE	4:P:593:ASN:OD1	2.40	0.69
4:M:555:ARG:HD2	4:M:556:SER:O	1.92	0.69
4:N:540:PRO:HB3	4:N:666:LYS:HD3	1.74	0.69
2:B:718:ASN:CB	4:M:530:VAL:HG13	2.23	0.69
2:H:537:ILE:C	2:H:737:TYR:CB	2.60	0.69
2:H:597:MET:HG2	2:H:756:HIS:NE2	2.06	0.69
2:H:626:THR:N	2:H:734:LYS:CG	2.54	0.69
4:N:555:ARG:HD2	4:N:556:SER:O	1.92	0.69
1:A:93:TYR:HA	2:B:726:HIS:NE2	1.98	0.69
3:L:59:TYR:OH	3:L:68:VAL:HA	1.92	0.69
1:C:93:TYR:HB2	2:D:676:PRO:HB3	1.75	0.69
2:D:520:PRO:N	2:D:731:ASN:HA	1.93	0.69
2:F:599:HIS:CB	2:F:754:LYS:O	2.38	0.69
2:H:686:GLY:CA	4:P:552:ASN:CA	2.59	0.69
3:I:2:ILE:CD1	3:I:94:ARG:CZ	2.70	0.69
3:I:30:THR:HG23	3:I:53:ASN:ND2	2.07	0.69
3:I:39:GLN:CD	3:I:45:PHE:CZ	2.66	0.69
3:I:59:TYR:OH	3:I:68:VAL:HA	1.92	0.69
3:J:39:GLN:CD	3:J:45:PHE:CZ	2.66	0.69
3:K:30:THR:HG23	3:K:53:ASN:ND2	2.07	0.69
2:B:547:LYS:CD	2:B:667:ILE:HG23	2.23	0.69
2:D:520:PRO:N	2:D:731:ASN:CA	2.39	0.69
2:D:597:MET:HG2	2:D:756:HIS:NE2	2.06	0.69
2:D:688:VAL:N	4:N:550:ASP:OD1	2.24	0.69
2:F:626:THR:N	2:F:734:LYS:CG	2.54	0.69
2:F:626:THR:CA	2:F:734:LYS:HG3	2.23	0.69
1:G:93:TYR:HB2	2:H:676:PRO:HB3	1.75	0.69
2:H:547:LYS:CD	2:H:667:ILE:HG23	2.23	0.69
2:F:612:THR:HA	2:F:734:LYS:CE	2.23	0.69
2:B:547:LYS:CE	2:B:667:ILE:CB	2.69	0.68
2:B:704:GLY:N	4:M:530(A):THR:CG2	2.56	0.68
2:D:543:ASP:OD2	2:D:759:PHE:CE2	2.46	0.68
1:E:95:PHE:CA	2:F:726:HIS:N	2.54	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:98:ILE:HB	4:M:550:ASP:HB2	0.75	0.68
2:D:612:THR:HA	2:D:734:LYS:HZ2	1.58	0.68
2:H:543:ASP:OD2	2:H:759:PHE:CE2	2.46	0.68
2:H:715:LYS:HE2	4:P:593:ASN:OD1	1.93	0.68
3:K:98:ILE:HG21	4:O:550:ASP:CB	2.23	0.68
2:B:543:ASP:OD2	2:B:759:PHE:CE2	2.46	0.68
2:D:547:LYS:CD	2:D:667:ILE:HG23	2.23	0.68
2:F:684:GLN:CB	3:K:98:ILE:HG23	2.12	0.68
2:H:686:GLY:CA	4:P:552:ASN:CG	2.61	0.68
2:H:687:ASN:CB	3:L:98:ILE:HG21	2.15	0.68
2:F:547:LYS:CD	2:F:667:ILE:HG23	2.23	0.68
4:O:555:ARG:HD2	4:O:556:SER:O	1.92	0.68
2:F:602:LEU:CD2	2:F:758:PRO:HD2	2.17	0.68
2:H:507:ASN:HB2	2:H:562:HIS:CD2	1.91	0.68
2:H:626:THR:CA	2:H:734:LYS:HG3	2.23	0.68
3:L:98:ILE:HG21	4:P:550:ASP:CB	2.24	0.68
4:P:540:PRO:HB3	4:P:666:LYS:HD3	1.74	0.68
2:B:534:LEU:HD11	2:B:734:LYS:HD3	1.52	0.68
2:B:597:MET:HG2	2:B:756:HIS:NE2	2.06	0.68
1:C:88:MET:N	1:C:91:GLY:O	2.27	0.68
2:D:704:GLY:CA	4:N:530(A):THR:HG22	2.24	0.68
1:E:88:MET:N	1:E:91:GLY:O	2.27	0.68
3:L:39:GLN:CD	3:L:45:PHE:CZ	2.66	0.68
2:D:612:THR:HA	2:D:734:LYS:CE	2.23	0.68
2:F:534:LEU:C	2:F:735:TRP:CD1	2.55	0.68
2:F:719:ASN:HA	4:O:551:THR:HG21	1.75	0.68
2:H:717:ILE:HG22	4:P:530(B):SER:CA	2.24	0.68
3:J:30:THR:HG23	3:J:53:ASN:ND2	2.07	0.68
2:B:547:LYS:CD	2:B:667:ILE:CD1	2.55	0.68
2:D:538:ARG:HD3	2:D:667:ILE:HD13	1.67	0.68
2:F:545:THR:HG1	2:F:759:PHE:HE2	1.42	0.68
2:B:535:GLU:C	2:B:736:GLN:CA	2.61	0.68
2:B:538:ARG:HD3	2:B:667:ILE:HD13	1.67	0.68
2:B:716:VAL:N	4:M:591:TRP:CD1	2.62	0.68
1:E:85:TYR:OH	2:F:678:ARG:NH1	2.27	0.68
2:F:535:GLU:C	2:F:736:GLN:CA	2.61	0.68
1:G:88:MET:N	1:G:91:GLY:O	2.27	0.68
2:H:612:THR:HA	2:H:734:LYS:CE	2.23	0.68
3:L:77:THR:HG22	3:L:79:TYR:CZ	2.26	0.68
4:M:680:LEU:HD11	4:M:691:TYR:CE2	2.29	0.68
2:B:716:VAL:HG22	4:M:532:CYS:CA	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:719:ASN:ND2	4:N:571:ALA:CA	2.56	0.68
2:F:543:ASP:OD2	2:F:759:PHE:CE2	2.46	0.68
1:G:85:TYR:OH	2:H:678:ARG:NH1	2.27	0.68
1:A:88:MET:N	1:A:91:GLY:O	2.27	0.67
2:B:522:CYS:CA	2:B:733:LYS:NZ	2.31	0.67
2:B:612:THR:HA	2:B:734:LYS:CE	2.23	0.67
2:D:626:THR:CA	2:D:734:LYS:HG3	2.23	0.67
1:E:93:TYR:HB2	2:F:676:PRO:HB3	1.75	0.67
2:F:534:LEU:HD11	2:F:734:LYS:HD3	1.52	0.67
3:J:77:THR:HG22	3:J:79:TYR:CZ	2.25	0.67
1:A:85:TYR:OH	2:B:678:ARG:NH1	2.27	0.67
1:C:85:TYR:OH	2:D:678:ARG:NH1	2.27	0.67
2:D:548:ILE:O	2:D:755:ILE:CG1	2.42	0.67
2:D:599:HIS:CB	2:D:754:LYS:O	2.38	0.67
3:K:39:GLN:CD	3:K:45:PHE:CZ	2.66	0.67
2:H:537:ILE:C	2:H:737:TYR:HB3	2.15	0.67
3:L:124:LEU:HB3	4:P:618:PHE:CD2	2.30	0.67
2:B:626:THR:CA	2:B:734:LYS:HG3	2.23	0.67
2:B:718:ASN:HB3	4:M:530:VAL:HG13	1.74	0.67
2:D:685:SER:OG	4:N:549:GLY:N	2.27	0.67
2:F:537:ILE:C	2:F:737:TYR:HB3	2.15	0.67
3:I:98:ILE:HG21	4:M:550:ASP:CB	2.24	0.67
4:N:669:ASN:O	4:N:670:ASN:HB2	1.95	0.67
4:N:680:LEU:HD11	4:N:691:TYR:CE2	2.29	0.67
2:B:687:ASN:ND2	4:M:533:ALA:O	2.27	0.67
2:D:537:ILE:C	2:D:737:TYR:HB3	2.15	0.67
3:J:124:LEU:HB3	4:N:618:PHE:CD2	2.30	0.67
2:B:548:ILE:O	2:B:755:ILE:CG1	2.42	0.67
2:B:719:ASN:OD1	4:M:565:SER:O	2.13	0.67
1:C:246:GLU:CB	2:F:788:TYR:CZ	2.78	0.67
2:F:548:ILE:O	2:F:755:ILE:CG1	2.42	0.67
2:F:685:SER:CB	4:O:553:ASN:N	2.35	0.67
3:I:124:LEU:HB3	4:M:618:PHE:CD2	2.30	0.67
4:P:680:LEU:HD11	4:P:691:TYR:CE2	2.29	0.67
2:B:715:LYS:HE2	4:M:593:ASN:CA	2.23	0.67
2:H:685:SER:CB	4:P:553:ASN:O	2.41	0.67
2:B:545:THR:HG1	2:B:759:PHE:HE2	1.41	0.67
2:B:626:THR:N	2:B:734:LYS:CG	2.54	0.67
2:H:548:ILE:O	2:H:755:ILE:CG1	2.42	0.67
3:I:41:PRO:HD3	3:I:88:ALA:HA	1.77	0.67
3:K:124:LEU:HB3	4:O:618:PHE:CD2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:719:ASN:CB	4:P:551:THR:HG21	2.25	0.66
2:B:538:ARG:CG	2:B:667:ILE:HD12	2.25	0.66
2:B:685:SER:CB	4:M:553:ASN:O	2.42	0.66
2:B:716:VAL:HG22	4:M:532:CYS:CB	1.80	0.66
2:D:538:ARG:CG	2:D:667:ILE:HD12	2.25	0.66
2:F:684:GLN:NE2	3:K:98:ILE:HD13	2.09	0.66
2:H:684:GLN:HB3	4:P:550:ASP:CG	2.09	0.66
3:J:72:GLU:OE1	3:J:79:TYR:CZ	2.49	0.66
2:B:719:ASN:OD1	4:M:551:THR:HG23	1.96	0.66
2:F:626:THR:N	2:F:734:LYS:HG2	2.11	0.66
3:I:72:GLU:OE1	3:I:79:TYR:CZ	2.49	0.66
3:I:114:ALA:CB	3:I:146:PHE:HE2	1.65	0.66
2:D:719:ASN:ND2	4:N:571:ALA:CB	2.57	0.66
1:A:93:TYR:HB2	2:B:676:PRO:HB3	1.75	0.66
2:F:520:PRO:N	2:F:731:ASN:HA	1.93	0.66
2:F:538:ARG:CG	2:F:667:ILE:HD12	2.25	0.66
2:F:685:SER:CB	4:O:549:GLY:CA	2.71	0.66
2:H:602:LEU:HD13	2:H:758:PRO:CA	2.26	0.66
2:H:719:ASN:CA	4:P:551:THR:CG2	2.66	0.66
3:L:72:GLU:OE1	3:L:79:TYR:CZ	2.49	0.66
2:B:520:PRO:CA	2:B:731:ASN:CA	2.51	0.66
2:D:788:TYR:CE2	1:G:242:TYR:CE2	2.40	0.66
2:F:602:LEU:HD13	2:F:758:PRO:CA	2.26	0.66
3:K:77:THR:HG22	3:K:79:TYR:CZ	2.26	0.66
2:B:537:ILE:C	2:B:737:TYR:HB3	2.15	0.66
2:B:689:LYS:HB3	3:I:98:ILE:HD11	1.78	0.66
2:D:535:GLU:CB	2:D:669:VAL:C	2.63	0.66
3:K:41:PRO:HD3	3:K:88:ALA:HA	1.77	0.66
4:P:669:ASN:O	4:P:670:ASN:HB2	1.95	0.66
3:L:2:ILE:CD1	3:L:94:ARG:CZ	2.70	0.66
3:L:41:PRO:HD3	3:L:88:ALA:HA	1.77	0.66
2:D:545:THR:HG1	2:D:759:PHE:HE2	1.42	0.66
4:M:591:TRP:CH2	4:M:594:ASN:C	2.70	0.66
4:P:591:TRP:CH2	4:P:594:ASN:C	2.70	0.66
2:B:602:LEU:HD11	2:B:758:PRO:CD	1.86	0.65
2:D:602:LEU:HD13	2:D:758:PRO:CA	2.26	0.65
2:H:538:ARG:CG	2:H:667:ILE:HD12	2.25	0.65
4:N:591:TRP:CH2	4:N:594:ASN:C	2.70	0.65
4:O:680:LEU:HD11	4:O:691:TYR:CE2	2.29	0.65
2:B:538:ARG:CD	2:B:667:ILE:CB	2.58	0.65
2:B:612:THR:CG2	2:B:734:LYS:HZ1	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:686:GLY:CA	4:M:552:ASN:CG	2.64	0.65
1:A:149:ASN:ND2	1:C:123:ARG:HH12	1.94	0.65
1:A:323:SER:HB3	1:E:319:LYS:NZ	2.10	0.65
4:P:649:LYS:HG2	4:P:654:PRO:HA	1.78	0.65
2:B:718:ASN:O	4:M:566:LEU:HD11	1.96	0.65
2:D:613:VAL:H	2:D:734:LYS:HZ2	0.87	0.65
2:H:612:THR:CG2	2:H:734:LYS:HZ1	2.09	0.65
2:D:788:TYR:CZ	1:G:246:GLU:CB	2.78	0.65
2:H:612:THR:CA	2:H:734:LYS:HZ2	1.97	0.65
2:H:626:THR:N	2:H:734:LYS:HG2	2.11	0.65
2:H:716:VAL:HG11	4:P:591:TRP:HB2	1.79	0.65
3:K:72:GLU:OE1	3:K:79:TYR:CZ	2.49	0.65
4:M:607:GLY:O	4:M:608:GLN:HG3	1.97	0.65
2:B:534:LEU:C	2:B:735:TRP:CD1	2.55	0.65
3:J:41:PRO:HD3	3:J:88:ALA:HA	1.77	0.65
4:O:591:TRP:CH2	4:O:594:ASN:C	2.70	0.65
4:O:628:ASN:HA	4:O:682:ALA:CB	2.25	0.65
2:F:689:LYS:CB	3:K:98:ILE:CD1	2.74	0.65
2:H:597:MET:HB3	2:H:756:HIS:CG	2.29	0.65
3:K:6:GLN:HE22	3:K:91:PHE:HA	1.61	0.65
4:O:669:ASN:O	4:O:670:ASN:HB2	1.95	0.65
2:B:521:ASP:N	2:B:733:LYS:HD2	2.12	0.65
2:D:521:ASP:N	2:D:733:LYS:HD2	2.12	0.65
2:H:535:GLU:C	2:H:736:GLN:CA	2.61	0.65
2:H:684:GLN:HE21	3:L:98:ILE:HD13	1.60	0.65
2:B:687:ASN:CB	4:M:550:ASP:C	2.66	0.64
3:L:72:GLU:OE1	3:L:79:TYR:CE1	2.51	0.64
2:B:535:GLU:CB	2:B:669:VAL:C	2.63	0.64
2:B:716:VAL:CG2	4:M:532:CYS:HB2	1.87	0.64
4:N:607:GLY:O	4:N:608:GLN:HG3	1.97	0.64
4:N:628:ASN:HA	4:N:682:ALA:CB	2.25	0.64
1:A:85:TYR:HE1	1:A:87:PHE:CZ	2.16	0.64
2:F:521:ASP:N	2:F:733:LYS:HD2	2.12	0.64
2:H:547:LYS:HG2	2:H:667:ILE:CD1	2.14	0.64
4:N:649:LYS:HG2	4:N:654:PRO:HA	1.79	0.64
4:O:607:GLY:O	4:O:608:GLN:HG3	1.97	0.64
1:C:85:TYR:HE1	1:C:87:PHE:CZ	2.16	0.64
2:D:635:VAL:C	2:D:636:ILE:HG12	2.18	0.64
2:H:521:ASP:N	2:H:733:LYS:HD2	2.13	0.64
4:O:562:PHE:CE1	4:O:575:ILE:HG12	2.33	0.64
2:B:626:THR:N	2:B:734:LYS:HG2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:597:MET:HB3	2:D:756:HIS:CG	2.29	0.64
2:F:538:ARG:CD	2:F:667:ILE:CB	2.58	0.64
4:M:669:ASN:O	4:M:670:ASN:HB2	1.95	0.64
2:B:520:PRO:N	2:B:731:ASN:CA	2.39	0.64
2:F:612:THR:C	2:F:734:LYS:HZ2	1.96	0.64
2:F:687:ASN:HB3	4:O:532:CYS:N	2.13	0.64
4:O:515:PRO:HD3	4:O:606(A):LEU:HB3	1.79	0.64
4:P:562:PHE:CE1	4:P:575:ILE:HG12	2.33	0.64
1:A:123:ARG:HH12	1:C:149:ASN:ND2	1.94	0.64
2:B:687:ASN:HB2	3:I:98:ILE:HG21	1.78	0.64
2:B:716:VAL:H	4:M:591:TRP:HD1	1.44	0.64
3:I:6:GLN:HE22	3:I:91:PHE:HA	1.61	0.64
3:I:72:GLU:OE1	3:I:79:TYR:CE1	2.51	0.64
4:M:562:PHE:CE1	4:M:575:ILE:HG12	2.33	0.64
4:P:607:GLY:O	4:P:608:GLN:HG3	1.97	0.64
2:D:627:HIS:HD2	2:D:734:LYS:CG	2.10	0.64
1:G:95:PHE:HA	2:H:725:CYS:CA	2.28	0.64
2:H:627:HIS:HD2	2:H:734:LYS:CG	2.10	0.64
2:H:718:ASN:CA	4:P:532:CYS:H	2.10	0.64
3:J:30:THR:CG2	3:J:30:THR:O	2.46	0.64
3:J:72:GLU:OE1	3:J:79:TYR:CE1	2.51	0.64
3:L:6:GLN:HE22	3:L:91:PHE:HA	1.61	0.64
4:P:566:LEU:HD23	4:P:571:ALA:HA	1.80	0.64
1:A:323:SER:HB3	1:E:319:LYS:HZ1	1.62	0.64
2:D:520:PRO:CA	2:D:731:ASN:CA	2.51	0.64
1:G:93:TYR:CG	2:H:676:PRO:CB	2.78	0.64
3:L:30:THR:CG2	3:L:30:THR:O	2.46	0.64
4:O:649:LYS:HG2	4:O:654:PRO:HA	1.79	0.64
2:B:627:HIS:HD2	2:B:734:LYS:CG	2.10	0.64
4:P:515:PRO:HD3	4:P:606(A):LEU:HB3	1.79	0.64
1:A:149:ASN:HD21	1:C:123:ARG:HH12	1.45	0.63
2:F:627:HIS:HD2	2:F:734:LYS:CG	2.10	0.63
2:H:635:VAL:C	2:H:636:ILE:HG12	2.18	0.63
3:I:30:THR:CG2	3:I:30:THR:O	2.46	0.63
4:P:628:ASN:HA	4:P:682:ALA:CB	2.25	0.63
1:G:86:PRO:HB3	1:G:228:THR:N	2.13	0.63
2:H:718:ASN:CA	4:P:532:CYS:N	2.62	0.63
2:H:719:ASN:N	4:P:530(B):SER:HA	1.76	0.63
3:L:21:SER:HG	3:L:79:TYR:HE2	0.65	0.63
4:M:514:SER:OG	4:M:606(A):LEU:CD2	2.44	0.63
4:N:579:GLN:HB3	4:N:581:GLU:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:519:CYS:C	2:D:732:HIS:N	2.51	0.63
2:D:599:HIS:HB2	2:D:754:LYS:H	1.64	0.63
2:F:519:CYS:C	2:F:732:HIS:N	2.51	0.63
2:F:635:VAL:C	2:F:636:ILE:HG12	2.18	0.63
2:H:599:HIS:ND1	2:H:735:TRP:CH2	2.63	0.63
3:K:71:LEU:HD13	3:K:73:ILE:HG13	1.81	0.63
4:N:515:PRO:HD3	4:N:606(A):LEU:HB3	1.79	0.63
4:O:566:LEU:HD23	4:O:571:ALA:HA	1.80	0.63
4:P:514:SER:OG	4:P:606(A):LEU:CD2	2.44	0.63
1:E:86:PRO:HB3	1:E:228:THR:N	2.13	0.63
1:E:246:GLU:CB	2:H:788:TYR:CZ	2.78	0.63
3:J:6:GLN:HE22	3:J:91:PHE:HA	1.62	0.63
3:K:72:GLU:OE1	3:K:79:TYR:CE1	2.51	0.63
4:P:579:GLN:HB3	4:P:581:GLU:HG2	1.79	0.63
2:B:599:HIS:HB2	2:B:754:LYS:H	1.64	0.63
1:C:95:PHE:HA	2:D:725:CYS:CA	2.28	0.63
1:E:85:TYR:HE1	1:E:87:PHE:CZ	2.16	0.63
2:H:548:ILE:O	2:H:755:ILE:CD1	2.47	0.63
4:M:649:LYS:HG2	4:M:654:PRO:HA	1.79	0.63
4:N:562:PHE:CE1	4:N:575:ILE:HG12	2.33	0.63
2:B:507:ASN:CA	2:B:562:HIS:NE2	2.33	0.63
1:C:86:PRO:HB3	1:C:228:THR:N	2.13	0.63
2:D:718:ASN:C	4:N:530(B):SER:HA	2.19	0.63
2:B:548:ILE:O	2:B:755:ILE:CD1	2.47	0.63
2:B:718:ASN:HD22	4:M:533:ALA:N	1.95	0.63
4:O:579:GLN:HB3	4:O:581:GLU:HG2	1.80	0.63
1:A:95:PHE:HD1	2:B:725:CYS:CA	2.09	0.63
2:D:612:THR:CG2	2:D:734:LYS:HZ1	2.12	0.63
2:F:685:SER:O	4:O:553:ASN:OD1	2.08	0.63
2:H:715:LYS:HE2	4:P:593:ASN:CA	2.28	0.63
2:B:519:CYS:C	2:B:732:HIS:N	2.51	0.63
2:D:626:THR:N	2:D:734:LYS:HG2	2.11	0.63
2:D:718:ASN:HB3	4:N:530:VAL:HG12	1.81	0.63
2:F:547:LYS:CD	2:F:757:ILE:HG23	1.72	0.63
2:F:716:VAL:N	4:O:591:TRP:CD1	2.67	0.63
3:L:71:LEU:HD13	3:L:73:ILE:HG13	1.81	0.63
1:A:95:PHE:HA	2:B:725:CYS:CA	2.28	0.62
2:F:716:VAL:HG12	4:O:591:TRP:HD1	0.81	0.62
1:G:85:TYR:HE1	1:G:87:PHE:CZ	2.16	0.62
2:H:599:HIS:HB2	2:H:754:LYS:H	1.64	0.62
3:I:71:LEU:HD13	3:I:73:ILE:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:579:GLN:HB3	4:M:581:GLU:HG2	1.80	0.62
2:H:534:LEU:C	2:H:735:TRP:CD1	2.55	0.62
3:I:35:LEU:HG	3:I:47:TRP:CD1	2.34	0.62
3:J:40:ALA:C	3:J:41:PRO:CD	2.63	0.62
2:B:574:MET:N	4:P:577:GLY:HA2	2.14	0.62
2:F:597:MET:HB3	2:F:756:HIS:CG	2.29	0.62
2:F:684:GLN:OE1	3:K:98:ILE:CG2	2.45	0.62
2:H:519:CYS:C	2:H:732:HIS:N	2.52	0.62
2:H:719:ASN:HA	4:P:551:THR:CB	2.29	0.62
4:P:515:PRO:HD3	4:P:606(A):LEU:O	2.00	0.62
2:F:535:GLU:CB	2:F:669:VAL:C	2.63	0.62
1:G:93:TYR:CB	2:H:676:PRO:CB	2.77	0.62
3:J:71:LEU:HD13	3:J:73:ILE:HG13	1.81	0.62
3:L:21:SER:OG	3:L:79:TYR:CD2	2.37	0.62
1:E:95:PHE:HA	2:F:725:CYS:CA	2.28	0.62
3:K:30:THR:O	3:K:30:THR:CG2	2.46	0.62
4:M:559:PRO:HG2	4:M:561:ARG:NH1	2.14	0.62
4:M:644:VAL:HG12	4:M:697:HIS:HB2	1.81	0.62
2:B:719:ASN:CA	4:M:551:THR:HG21	2.16	0.62
1:C:95:PHE:HD1	2:D:725:CYS:CA	2.10	0.62
1:E:93:TYR:CG	2:F:676:PRO:CB	2.78	0.62
2:B:518:HIS:CD2	2:B:732:HIS:N	2.67	0.62
2:B:715:LYS:HG3	4:M:593:ASN:OD1	1.98	0.62
2:D:534:LEU:CG	2:D:734:LYS:HB3	1.93	0.62
3:K:114:ALA:CB	3:K:146:PHE:HE2	1.65	0.62
3:L:35:LEU:HG	3:L:47:TRP:CD1	2.34	0.62
4:N:566:LEU:HD23	4:N:571:ALA:HA	1.80	0.62
1:A:86:PRO:HB3	1:A:228:THR:N	2.14	0.62
2:B:602:LEU:HD13	2:B:758:PRO:CA	2.26	0.62
2:B:635:VAL:C	2:B:636:ILE:HG12	2.18	0.62
4:O:514:SER:OG	4:O:606(A):LEU:CD2	2.44	0.62
1:A:63:CYS:HB2	2:B:700:LYS:HE2	0.65	0.62
1:A:123:ARG:HH12	1:C:149:ASN:HD21	1.45	0.62
2:D:548:ILE:O	2:D:755:ILE:CD1	2.47	0.62
2:F:599:HIS:ND1	2:F:735:TRP:CH2	2.63	0.62
4:O:515:PRO:HD3	4:O:606(A):LEU:O	2.00	0.62
4:P:559:PRO:HG2	4:P:561:ARG:NH1	2.14	0.62
2:D:528:CYS:N	2:D:733:LYS:HE3	2.15	0.62
2:F:704:GLY:O	4:O:530(A):THR:HG23	1.89	0.62
2:F:716:VAL:N	4:O:591:TRP:HD1	1.97	0.62
2:H:520:PRO:HB3	2:H:730:THR:C	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:528:CYS:N	2:H:733:LYS:HE3	2.15	0.62
2:H:536:ARG:CD	2:H:737:TYR:CD1	2.83	0.62
4:M:515:PRO:HD3	4:M:606(A):LEU:O	2.00	0.62
2:B:537:ILE:CG1	2:B:736:GLN:HA	2.27	0.61
1:E:63:CYS:HB2	2:F:700:LYS:HE2	0.65	0.61
2:F:718:ASN:HD22	4:O:533:ALA:HB2	1.65	0.61
3:I:98:ILE:CB	4:M:550:ASP:HB2	1.49	0.61
3:L:9:ARG:HG2	3:L:108:THR:H	1.65	0.61
1:E:246:GLU:HB2	2:H:788:TYR:OH	2.00	0.61
2:F:528:CYS:N	2:F:733:LYS:HE3	2.15	0.61
2:F:548:ILE:O	2:F:755:ILE:CD1	2.47	0.61
2:H:536:ARG:C	2:H:669:VAL:HG12	2.21	0.61
3:K:35:LEU:HG	3:K:47:TRP:CD1	2.34	0.61
2:F:547:LYS:CA	2:F:755:ILE:HD11	2.30	0.61
3:J:35:LEU:HG	3:J:47:TRP:CD1	2.35	0.61
4:M:628:ASN:HA	4:M:682:ALA:CB	2.25	0.61
2:D:520:PRO:HB3	2:D:730:THR:C	2.21	0.61
3:I:11:VAL:HG23	3:I:148:GLU:O	2.00	0.61
2:B:536:ARG:N	2:B:669:VAL:HB	2.14	0.61
2:B:536:ARG:CD	2:B:737:TYR:CD1	2.83	0.61
2:B:545:THR:OG1	2:B:759:PHE:HE2	1.84	0.61
1:C:42:LEU:HD11	1:C:266:VAL:HG22	1.83	0.61
2:F:536:ARG:CD	2:F:737:TYR:CD1	2.83	0.61
4:M:552:ASN:ND2	4:M:552:ASN:C	2.54	0.61
4:M:566:LEU:HD23	4:M:571:ALA:HA	1.80	0.61
4:N:515:PRO:CD	4:N:606(A):LEU:HB3	2.30	0.61
4:O:552:ASN:ND2	4:O:552:ASN:C	2.54	0.61
4:O:559:PRO:HG2	4:O:561:ARG:NH1	2.14	0.61
4:O:659:MET:HA	4:O:677:TYR:O	2.01	0.61
4:P:644:VAL:HG12	4:P:697:HIS:HB2	1.81	0.61
1:A:24:TYR:O	1:E:304:PRO:O	2.19	0.61
2:B:520:PRO:HB3	2:B:730:THR:C	2.21	0.61
2:D:547:LYS:CG	2:D:755:ILE:HD11	2.31	0.61
2:H:518:HIS:CD2	2:H:732:HIS:N	2.67	0.61
2:H:535:GLU:CB	2:H:669:VAL:C	2.63	0.61
3:I:32:TYR:CE1	3:I:96:TYR:HD1	1.97	0.61
4:M:515:PRO:CD	4:M:606(A):LEU:HB3	2.30	0.61
4:N:644:VAL:HG12	4:N:697:HIS:HB2	1.81	0.61
4:O:507:GLN:CD	4:O:588:CYS:SG	2.79	0.61
2:D:536:ARG:CD	2:D:737:TYR:CD1	2.83	0.61
2:D:547:LYS:CA	2:D:755:ILE:HD11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:599:HIS:HB2	2:F:754:LYS:H	1.64	0.61
2:H:594:THR:O	2:H:660:THR:CB	2.49	0.61
3:L:11:VAL:HG23	3:L:148:GLU:O	2.00	0.61
4:N:507:GLN:CD	4:N:588:CYS:SG	2.79	0.61
2:B:547:LYS:CA	2:B:755:ILE:HD11	2.30	0.61
2:B:594:THR:O	2:B:660:THR:CB	2.49	0.61
2:D:788:TYR:HE2	1:G:242:TYR:O	1.84	0.61
1:G:42:LEU:HD11	1:G:266:VAL:HG22	1.83	0.61
2:H:687:ASN:CG	4:P:532:CYS:C	2.55	0.61
1:C:246:GLU:HB2	2:F:788:TYR:OH	2.00	0.61
1:G:93:TYR:HD1	2:H:676:PRO:CA	2.11	0.61
2:H:716:VAL:CG2	4:P:532:CYS:HG	1.01	0.61
4:N:515:PRO:HD3	4:N:606(A):LEU:O	2.00	0.61
4:O:644:VAL:HG12	4:O:697:HIS:HB2	1.81	0.61
2:B:528:CYS:N	2:B:733:LYS:HE3	2.15	0.61
2:D:535:GLU:C	2:D:736:GLN:CA	2.61	0.61
3:I:93:VAL:HG21	3:I:103:TRP:CZ3	2.36	0.61
3:K:11:VAL:HG23	3:K:148:GLU:O	2.00	0.61
1:A:42:LEU:HD11	1:A:266:VAL:HG22	1.83	0.60
1:E:242:TYR:O	2:H:788:TYR:HE2	1.84	0.60
2:F:520:PRO:HB3	2:F:730:THR:C	2.21	0.60
2:H:537:ILE:CG1	2:H:736:GLN:HA	2.26	0.60
2:H:547:LYS:CA	2:H:755:ILE:HD11	2.30	0.60
3:J:9:ARG:HG2	3:J:108:THR:H	1.65	0.60
3:L:93:VAL:HG21	3:L:103:TRP:CZ3	2.36	0.60
3:L:98:ILE:HG21	4:P:550:ASP:CA	2.31	0.60
4:N:559:PRO:HG2	4:N:561:ARG:NH1	2.14	0.60
4:P:659:MET:HA	4:P:677:TYR:O	2.01	0.60
2:B:719:ASN:CG	4:M:551:THR:HG23	2.21	0.60
2:F:547:LYS:CG	2:F:755:ILE:HD11	2.31	0.60
1:G:63:CYS:HB2	2:H:700:LYS:HE2	0.65	0.60
1:G:86:PRO:CB	1:G:227:GLY:HA2	2.32	0.60
2:H:533:ALA:HA	2:H:733:LYS:C	2.20	0.60
3:I:141:LEU:HD13	4:M:677:TYR:HE2	1.66	0.60
4:M:659:MET:HA	4:M:677:TYR:O	2.01	0.60
2:D:507:ASN:CA	2:D:562:HIS:NE2	2.33	0.60
2:D:685:SER:CB	4:N:549:GLY:N	2.55	0.60
2:F:536:ARG:N	2:F:669:VAL:HB	2.14	0.60
2:H:547:LYS:CG	2:H:755:ILE:HD11	2.31	0.60
2:H:549:GLN:HA	2:H:755:ILE:CG2	2.31	0.60
3:J:11:VAL:HG23	3:J:148:GLU:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:9:ARG:O	3:K:149:PRO:HD3	2.02	0.60
4:O:515:PRO:CD	4:O:606(A):LEU:HB3	2.30	0.60
2:B:536:ARG:C	2:B:669:VAL:HG12	2.21	0.60
2:B:602:LEU:HD13	2:B:758:PRO:N	1.80	0.60
1:E:86:PRO:CB	1:E:227:GLY:HA2	2.32	0.60
2:F:536:ARG:C	2:F:669:VAL:HG12	2.21	0.60
2:F:537:ILE:C	2:F:737:TYR:HB2	2.22	0.60
3:K:141:LEU:HD13	4:O:677:TYR:HE2	1.67	0.60
4:M:507:GLN:CD	4:M:588:CYS:SG	2.79	0.60
4:N:659:MET:HA	4:N:677:TYR:O	2.01	0.60
2:D:536:ARG:C	2:D:669:VAL:HG12	2.21	0.60
2:F:549:GLN:HA	2:F:755:ILE:CG2	2.31	0.60
3:K:9:ARG:HG2	3:K:108:THR:H	1.66	0.60
2:F:594:THR:O	2:F:660:THR:CB	2.49	0.60
4:N:514:SER:OG	4:N:606(A):LEU:CD2	2.44	0.60
4:O:515:PRO:CD	4:O:606(A):LEU:HB2	2.31	0.60
2:B:687:ASN:CB	4:M:550:ASP:CA	2.70	0.60
2:D:549:GLN:HA	2:D:755:ILE:CG2	2.31	0.60
2:D:638:ARG:O	2:D:639:GLU:HB2	2.02	0.60
2:D:788:TYR:OH	1:G:246:GLU:HB2	2.00	0.60
3:K:98:ILE:HG21	4:O:550:ASP:CA	2.31	0.60
3:K:114:ALA:HB3	3:K:146:PHE:HE2	0.78	0.60
3:K:114:ALA:CB	3:K:146:PHE:CD2	2.77	0.60
4:P:507:GLN:CD	4:P:588:CYS:SG	2.79	0.60
4:P:515:PRO:CD	4:P:606(A):LEU:HB3	2.30	0.60
2:D:545:THR:OG1	2:D:759:PHE:HE2	1.84	0.60
2:D:716:VAL:HG13	4:N:531:ASN:C	2.22	0.60
2:F:685:SER:CB	4:O:549:GLY:H	2.15	0.60
2:H:716:VAL:CB	4:P:532:CYS:HG	1.99	0.60
3:I:9:ARG:O	3:I:149:PRO:HD3	2.02	0.60
3:I:9:ARG:HG2	3:I:108:THR:H	1.65	0.60
4:P:683:ARG:HH11	4:P:683:ARG:HG3	1.67	0.60
2:B:549:GLN:HA	2:B:755:ILE:CG2	2.31	0.60
2:D:508:VAL:HG13	2:D:508:VAL:O	2.02	0.60
3:J:93:VAL:HG21	3:J:103:TRP:CZ3	2.36	0.60
3:L:9:ARG:O	3:L:149:PRO:HD3	2.02	0.60
4:M:539:LYS:HE2	4:M:581:GLU:O	2.02	0.60
4:N:683:ARG:HH11	4:N:683:ARG:HG3	1.67	0.60
1:A:24:TYR:CA	1:E:304:PRO:O	2.27	0.59
2:B:574:MET:N	4:P:516:GLY:O	2.35	0.59
2:F:547:LYS:HD3	2:F:667:ILE:HG21	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:626:THR:CA	2:F:734:LYS:CG	2.80	0.59
2:H:626:THR:CA	2:H:734:LYS:CG	2.81	0.59
3:J:21:SER:HA	3:J:79:TYR:CD2	2.37	0.59
3:J:141:LEU:HD13	4:N:677:TYR:HE2	1.67	0.59
3:K:93:VAL:HG21	3:K:103:TRP:CZ3	2.36	0.59
1:A:91:GLY:CA	2:B:678:ARG:CB	2.46	0.59
2:B:626:THR:CA	2:B:734:LYS:CG	2.81	0.59
2:B:718:ASN:C	4:M:566:LEU:HD11	2.10	0.59
2:D:715:LYS:HZ1	4:N:593:ASN:HB3	1.67	0.59
3:L:40:ALA:C	3:L:41:PRO:CD	2.63	0.59
4:N:515:PRO:CD	4:N:606(A):LEU:HB2	2.31	0.59
2:B:535:GLU:CD	2:B:670:HIS:HA	2.23	0.59
2:D:534:LEU:HD11	2:D:734:LYS:HD3	1.51	0.59
2:D:534:LEU:C	2:D:735:TRP:CD1	2.55	0.59
1:E:42:LEU:HD11	1:E:266:VAL:HG22	1.83	0.59
2:H:718:ASN:HA	4:P:532:CYS:N	2.17	0.59
4:P:515:PRO:CD	4:P:606(A):LEU:HB2	2.31	0.59
2:D:547:LYS:CG	2:D:755:ILE:CD1	2.80	0.59
3:K:21:SER:HA	3:K:79:TYR:CD2	2.37	0.59
4:N:529:ALA:HA	4:N:569:ASP:HB2	1.84	0.59
1:C:242:TYR:O	2:F:788:TYR:HE2	1.84	0.59
2:D:626:THR:CA	2:D:734:LYS:CG	2.80	0.59
2:D:687:ASN:CG	4:N:532:CYS:HA	2.23	0.59
4:N:552:ASN:ND2	4:N:552:ASN:C	2.54	0.59
2:B:602:LEU:CD2	2:B:758:PRO:HD2	2.17	0.59
2:B:718:ASN:ND2	4:M:590:LEU:HD22	2.18	0.59
2:D:714:ASP:O	4:N:591:TRP:NE1	2.35	0.59
2:F:687:ASN:HB3	4:O:532:CYS:H	1.68	0.59
2:H:717:ILE:HG22	4:P:530(B):SER:C	2.04	0.59
3:J:114:ALA:HB1	3:J:146:PHE:CD2	2.36	0.59
3:L:35:LEU:HD23	3:L:37:VAL:HG23	1.83	0.59
2:B:508:VAL:HG13	2:B:508:VAL:O	2.02	0.59
2:B:547:LYS:CG	2:B:755:ILE:CD1	2.80	0.59
2:F:508:VAL:O	2:F:508:VAL:HG13	2.02	0.59
2:F:545:THR:OG1	2:F:759:PHE:HE2	1.84	0.59
2:F:547:LYS:CG	2:F:755:ILE:CD1	2.80	0.59
2:F:685:SER:HB2	4:O:550:ASP:N	2.06	0.59
3:L:114:ALA:HB3	3:L:146:PHE:HE2	0.78	0.59
1:A:93:TYR:CG	2:B:676:PRO:CB	2.78	0.59
2:D:536:ARG:N	2:D:670:HIS:N	2.51	0.59
3:I:98:ILE:CG2	3:I:98:ILE:O	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:98:ILE:CG2	3:L:98:ILE:O	2.51	0.59
4:M:683:ARG:HG3	4:M:683:ARG:HH11	1.67	0.59
4:O:529:ALA:HA	4:O:569:ASP:HB2	1.85	0.59
4:P:529:ALA:HA	4:P:569:ASP:HB2	1.85	0.59
1:A:126:THR:HB	1:C:126:THR:HB	1.85	0.59
2:B:547:LYS:CG	2:B:755:ILE:HD11	2.31	0.59
2:B:547:LYS:HG2	2:B:667:ILE:HG12	1.64	0.59
1:C:60:VAL:HG22	1:C:102:GLN:HG3	1.85	0.59
2:H:536:ARG:HB3	2:H:669:VAL:HG12	1.85	0.59
2:H:545:THR:OG1	2:H:759:PHE:HE2	1.84	0.59
2:D:518:HIS:CD2	2:D:732:HIS:N	2.67	0.59
2:D:602:LEU:HD11	2:D:758:PRO:CD	1.86	0.59
2:H:717:ILE:HG22	4:P:530(B):SER:OG	2.03	0.59
3:I:114:ALA:HB1	3:I:146:PHE:CD2	2.36	0.59
2:D:536:ARG:HB3	2:D:669:VAL:HG12	1.85	0.58
2:D:715:LYS:HE2	4:N:593:ASN:HA	1.82	0.58
2:F:521:ASP:C	2:F:733:LYS:HD3	2.10	0.58
2:F:638:ARG:O	2:F:639:GLU:HB2	2.02	0.58
2:F:718:ASN:ND2	4:O:590:LEU:CD2	2.65	0.58
3:J:9:ARG:O	3:J:149:PRO:HD3	2.02	0.58
3:L:21:SER:HA	3:L:79:TYR:CD2	2.37	0.58
3:L:114:ALA:HB1	3:L:146:PHE:CD2	2.36	0.58
3:L:141:LEU:HD13	4:P:677:TYR:HE2	1.67	0.58
2:D:535:GLU:CD	2:D:670:HIS:HA	2.23	0.58
4:N:539:LYS:HE2	4:N:581:GLU:O	2.02	0.58
1:A:93:TYR:HD1	2:B:676:PRO:CA	2.10	0.58
1:C:90:GLY:HA3	2:D:677:ASP:OD1	2.04	0.58
2:D:718:ASN:ND2	4:N:590:LEU:CD2	2.66	0.58
2:F:536:ARG:HB3	2:F:669:VAL:HG12	1.85	0.58
2:H:508:VAL:HG13	2:H:508:VAL:O	2.02	0.58
2:H:547:LYS:CG	2:H:755:ILE:CD1	2.80	0.58
2:H:638:ARG:O	2:H:639:GLU:HB2	2.02	0.58
3:I:21:SER:HA	3:I:79:TYR:CD2	2.37	0.58
3:I:98:ILE:HG21	4:M:550:ASP:CA	2.31	0.58
4:N:686:GLU:HA	4:N:708:ARG:NH2	2.18	0.58
2:D:689:LYS:CA	3:J:98:ILE:HD12	2.23	0.58
3:I:77:THR:HG22	3:I:79:TYR:CZ	2.25	0.58
3:K:114:ALA:HB1	3:K:146:PHE:CD2	2.36	0.58
4:P:686:GLU:HA	4:P:708:ARG:NH2	2.18	0.58
2:F:684:GLN:HB3	4:O:550:ASP:OD1	2.01	0.58
2:H:520:PRO:N	2:H:731:ASN:CA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:515:PRO:HD3	4:O:606(A):LEU:C	2.23	0.58
2:H:536:ARG:N	2:H:670:HIS:N	2.51	0.58
2:H:687:ASN:N	4:P:550:ASP:CG	2.55	0.58
4:M:515:PRO:CD	4:M:606(A):LEU:HB2	2.31	0.58
4:M:686:GLU:HA	4:M:708:ARG:NH2	2.18	0.58
4:O:686:GLU:HA	4:O:708:ARG:NH2	2.18	0.58
4:P:685:TRP:CZ2	4:P:708:ARG:HG3	2.39	0.58
1:A:90:GLY:HA3	2:B:677:ASP:OD1	2.04	0.58
2:B:685:SER:OG	4:M:553:ASN:O	2.20	0.58
1:C:86:PRO:CB	1:C:227:GLY:HA2	2.32	0.58
1:C:93:TYR:HD1	2:D:676:PRO:CA	2.10	0.58
2:D:718:ASN:ND2	4:N:590:LEU:HD22	2.18	0.58
2:H:547:LYS:HD3	2:H:667:ILE:HG21	1.82	0.58
2:H:686:GLY:N	4:P:549:GLY:O	2.36	0.58
4:N:685:TRP:CZ2	4:N:708:ARG:HG3	2.39	0.58
1:A:60:VAL:HG22	1:A:102:GLN:HG3	1.85	0.58
2:D:594:THR:O	2:D:660:THR:CB	2.49	0.58
1:E:90:GLY:HA3	2:F:677:ASP:OD1	2.04	0.58
2:F:518:HIS:CD2	2:F:732:HIS:N	2.67	0.58
2:F:536:ARG:N	2:F:670:HIS:N	2.51	0.58
2:F:537:ILE:CG1	2:F:736:GLN:HA	2.27	0.58
2:H:670:HIS:CE1	2:H:673:PRO:HD3	2.39	0.58
3:J:98:ILE:CG2	3:J:98:ILE:O	2.51	0.58
4:M:529:ALA:HA	4:M:569:ASP:HB2	1.85	0.58
4:M:685:TRP:CZ2	4:M:708:ARG:HG3	2.39	0.58
4:O:539:LYS:HE2	4:O:581:GLU:O	2.02	0.58
2:D:537:ILE:CG1	2:D:736:GLN:HA	2.27	0.58
1:G:90:GLY:HA3	2:H:677:ASP:OD1	2.04	0.58
2:H:518:HIS:NE2	2:H:732:HIS:N	2.52	0.58
3:I:45:PHE:HE1	4:M:587:PHE:CE2	2.22	0.58
4:N:515:PRO:HD3	4:N:606(A):LEU:C	2.23	0.58
2:D:719:ASN:OD1	4:N:566:LEU:CA	2.51	0.58
1:G:60:VAL:HG22	1:G:102:GLN:HG3	1.85	0.58
4:M:515:PRO:HD3	4:M:606(A):LEU:C	2.23	0.58
4:P:515:PRO:HD3	4:P:606(A):LEU:C	2.23	0.58
1:A:289:ARG:NH1	1:E:316:ALA:H	2.02	0.57
2:D:535:GLU:O	2:D:736:GLN:N	2.36	0.57
2:D:599:HIS:ND1	2:D:735:TRP:CH2	2.63	0.57
2:D:602:LEU:CD2	2:D:758:PRO:HD2	2.17	0.57
2:H:719:ASN:OD1	4:P:565:SER:C	2.43	0.57
4:O:685:TRP:CZ2	4:O:708:ARG:HG3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:539:LYS:HE2	4:P:581:GLU:O	2.02	0.57
2:B:518:HIS:NE2	2:B:732:HIS:N	2.52	0.57
1:E:60:VAL:HG22	1:E:102:GLN:HG3	1.85	0.57
2:F:716:VAL:CA	4:O:591:TRP:HD1	2.17	0.57
2:B:613:VAL:N	2:B:734:LYS:HZ3	1.70	0.57
2:H:547:LYS:CD	2:H:667:ILE:CB	2.56	0.57
3:K:98:ILE:CG2	3:K:98:ILE:O	2.51	0.57
1:A:85:TYR:CZ	2:B:678:ARG:NH2	2.73	0.57
2:B:670:HIS:CE1	2:B:673:PRO:HD3	2.39	0.57
2:D:536:ARG:N	2:D:669:VAL:HB	2.14	0.57
2:H:716:VAL:CG1	4:P:591:TRP:HD1	1.96	0.57
3:I:141:LEU:CD1	4:M:677:TYR:HE2	2.17	0.57
2:B:545:THR:CG2	2:B:758:PRO:HG3	2.33	0.57
2:B:638:ARG:O	2:B:639:GLU:HB2	2.02	0.57
2:D:670:HIS:CE1	2:D:673:PRO:HD3	2.39	0.57
2:F:545:THR:CG2	2:F:758:PRO:HG3	2.33	0.57
3:L:141:LEU:CD1	4:P:677:TYR:HE2	2.18	0.57
4:P:608:GLN:HG3	4:P:608:GLN:O	2.04	0.57
2:B:547:LYS:O	2:B:667:ILE:HD11	2.05	0.57
2:B:719:ASN:HD21	4:M:571:ALA:HB2	1.69	0.57
1:G:85:TYR:CZ	2:H:678:ARG:NH2	2.73	0.57
3:L:11:VAL:HB	3:L:147:PRO:HB2	1.87	0.57
3:L:60:ALA:HB3	3:L:63:PHE:HD2	1.70	0.57
2:B:536:ARG:N	2:B:670:HIS:N	2.51	0.57
2:B:536:ARG:HB3	2:B:669:VAL:HG12	1.85	0.57
1:C:85:TYR:CZ	2:D:678:ARG:NH2	2.73	0.57
2:D:518:HIS:NE2	2:D:732:HIS:N	2.52	0.57
2:D:521:ASP:C	2:D:733:LYS:HD3	2.10	0.57
2:D:683:GLN:C	4:N:553:ASN:ND2	2.57	0.57
2:F:670:HIS:CE1	2:F:673:PRO:HD3	2.39	0.57
2:H:602:LEU:CD2	2:H:758:PRO:HD2	2.17	0.57
3:K:141:LEU:CD1	4:O:677:TYR:HE2	2.18	0.57
4:O:683:ARG:HH11	4:O:683:ARG:HG3	1.67	0.57
2:H:547:LYS:O	2:H:667:ILE:HD11	2.05	0.57
3:K:11:VAL:HB	3:K:147:PRO:HB2	1.87	0.57
4:N:628:ASN:C	4:N:682:ALA:HB2	2.25	0.57
1:A:86:PRO:CB	1:A:227:GLY:HA2	2.32	0.57
1:A:291:VAL:CG2	1:E:302:GLU:O	2.43	0.57
2:F:686:GLY:HA2	4:O:552:ASN:CG	2.25	0.57
2:H:535:GLU:O	2:H:736:GLN:N	2.36	0.57
3:L:45:PHE:HE1	4:P:587:PHE:CE2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:528:CYS:H	2:F:733:LYS:HE3	1.70	0.57
2:F:547:LYS:CE	2:F:667:ILE:CB	2.69	0.57
3:I:60:ALA:HB3	3:I:63:PHE:HD2	1.70	0.57
3:J:141:LEU:CD1	4:N:677:TYR:HE2	2.18	0.57
4:N:608:GLN:HG3	4:N:608:GLN:O	2.05	0.57
2:B:547:LYS:CD	2:B:757:ILE:HG23	1.72	0.56
2:B:718:ASN:HD22	4:M:533:ALA:H	1.49	0.56
1:C:86:PRO:CA	1:C:227:GLY:CA	2.64	0.56
2:D:715:LYS:CE	4:N:593:ASN:HA	2.34	0.56
1:E:85:TYR:CZ	2:F:678:ARG:NH2	2.73	0.56
2:F:547:LYS:O	2:F:667:ILE:HD11	2.05	0.56
3:I:113:SER:O	3:I:114:ALA:HB2	2.05	0.56
4:N:555:ARG:HE	4:N:558:VAL:HG23	1.70	0.56
4:P:650:VAL:HG23	4:P:655:VAL:CG2	2.35	0.56
2:D:547:LYS:CD	2:D:667:ILE:CB	2.56	0.56
2:D:547:LYS:O	2:D:667:ILE:HD11	2.05	0.56
2:F:533:ALA:HA	2:F:733:LYS:C	2.20	0.56
2:F:612:THR:CG2	2:F:734:LYS:HZ1	2.18	0.56
2:H:684:GLN:N	4:P:550:ASP:CG	2.55	0.56
3:J:60:ALA:HB3	3:J:63:PHE:HD2	1.70	0.56
3:K:45:PHE:HE1	4:O:587:PHE:CE2	2.22	0.56
2:B:717:ILE:HG22	4:M:530(B):SER:CA	2.32	0.56
1:C:63:CYS:HB2	2:D:700:LYS:HE2	0.65	0.56
2:F:518:HIS:NE2	2:F:732:HIS:N	2.52	0.56
2:H:673:PRO:CB	2:H:745:ASN:HB2	2.35	0.56
2:H:685:SER:C	4:P:552:ASN:HD22	2.09	0.56
3:I:96:TYR:CE2	3:I:97:PHE:CZ	2.93	0.56
3:K:37:VAL:HG21	3:K:103:TRP:HH2	1.70	0.56
3:K:60:ALA:HB3	3:K:63:PHE:HD2	1.70	0.56
3:K:113:SER:O	3:K:114:ALA:HB2	2.05	0.56
1:A:91:GLY:HA2	2:B:678:ARG:HB2	1.84	0.56
2:B:535:GLU:O	2:B:736:GLN:N	2.36	0.56
2:B:537:ILE:C	2:B:737:TYR:HB2	2.22	0.56
2:D:520:PRO:HB3	2:D:731:ASN:N	1.86	0.56
2:F:704:GLY:CA	4:O:530(A):THR:CG2	2.83	0.56
3:L:77:THR:CG2	3:L:79:TYR:CE2	2.84	0.56
3:L:113:SER:O	3:L:114:ALA:HB2	2.05	0.56
4:P:628:ASN:C	4:P:682:ALA:HB2	2.25	0.56
1:A:289:ARG:NH1	1:E:315:VAL:CA	2.43	0.56
2:B:599:HIS:ND1	2:B:735:TRP:CH2	2.63	0.56
2:H:545:THR:CG2	2:H:758:PRO:HG3	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:96:TYR:CE2	3:L:97:PHE:CZ	2.93	0.56
2:B:716:VAL:CG1	4:M:591:TRP:HD1	1.87	0.56
2:H:535:GLU:N	2:H:735:TRP:HD1	1.44	0.56
2:H:719:ASN:CG	4:P:551:THR:HG21	2.24	0.56
3:J:11:VAL:HB	3:J:147:PRO:HB2	1.87	0.56
2:B:533:ALA:HA	2:B:733:LYS:C	2.20	0.56
2:B:673:PRO:CB	2:B:745:ASN:HB2	2.34	0.56
1:C:93:TYR:CG	2:D:676:PRO:CB	2.78	0.56
2:D:715:LYS:CE	4:N:593:ASN:CA	2.70	0.56
1:E:85:TYR:CE1	1:E:87:PHE:CZ	2.94	0.56
2:F:673:PRO:CB	2:F:745:ASN:HB2	2.35	0.56
1:G:93:TYR:HE1	2:H:674:ASP:O	1.89	0.56
3:J:96:TYR:CE2	3:J:97:PHE:CZ	2.93	0.56
3:J:113:SER:O	3:J:114:ALA:HB2	2.05	0.56
2:H:528:CYS:H	2:H:733:LYS:HE3	1.71	0.56
2:H:535:GLU:CD	2:H:670:HIS:HA	2.23	0.56
2:H:687:ASN:HD22	4:P:550:ASP:HA	1.67	0.56
3:J:122:TYR:CZ	4:N:624:GLU:HG3	2.41	0.56
4:M:555:ARG:HE	4:M:558:VAL:HG23	1.71	0.56
4:O:555:ARG:HE	4:O:558:VAL:HG23	1.70	0.56
2:B:528:CYS:H	2:B:733:LYS:HE3	1.70	0.56
1:E:93:TYR:HE1	2:F:674:ASP:O	1.89	0.56
4:M:608:GLN:HG3	4:M:608:GLN:O	2.05	0.56
2:B:547:LYS:HE2	2:B:667:ILE:HG13	1.84	0.56
1:C:199:GLN:HE21	2:F:775:THR:CG2	2.15	0.56
2:F:685:SER:HB3	4:O:553:ASN:CA	2.35	0.56
2:F:704:GLY:N	4:O:530(A):THR:CG2	2.69	0.56
2:H:719:ASN:CA	4:P:551:THR:OG1	2.54	0.56
3:K:30:THR:CG2	3:K:53:ASN:HD22	2.17	0.56
3:K:122:TYR:CZ	4:O:624:GLU:HG3	2.41	0.56
3:L:45:PHE:CE1	4:P:587:PHE:CZ	2.94	0.56
4:M:628:ASN:C	4:M:682:ALA:HB2	2.25	0.56
2:B:536:ARG:CD	2:B:737:TYR:CG	2.88	0.55
2:B:686:GLY:N	4:M:553:ASN:N	2.54	0.55
1:E:95:PHE:HD1	2:F:725:CYS:CA	2.09	0.55
1:E:246:GLU:CB	2:H:788:TYR:CE2	2.83	0.55
2:F:536:ARG:CD	2:F:737:TYR:CG	2.88	0.55
3:K:96:TYR:CE2	3:K:97:PHE:CZ	2.93	0.55
4:O:617:LEU:HD23	4:O:633:VAL:O	2.06	0.55
4:O:628:ASN:C	4:O:682:ALA:HB2	2.25	0.55
4:O:686:GLU:HA	4:O:708:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:HIS:NE2	2:B:730:THR:C	2.60	0.55
2:B:670:HIS:HE1	2:B:673:PRO:HG3	1.71	0.55
2:B:687:ASN:CG	4:M:550:ASP:C	2.64	0.55
2:D:518:HIS:NE2	2:D:730:THR:C	2.60	0.55
2:D:687:ASN:CG	4:N:533:ALA:H	2.10	0.55
2:F:520:PRO:HB3	2:F:731:ASN:N	1.87	0.55
2:F:535:GLU:CD	2:F:670:HIS:HA	2.23	0.55
2:H:518:HIS:NE2	2:H:730:THR:C	2.60	0.55
2:H:536:ARG:CD	2:H:737:TYR:CG	2.88	0.55
2:H:686:GLY:N	4:P:552:ASN:N	2.31	0.55
3:I:122:TYR:CZ	4:M:624:GLU:HG3	2.41	0.55
3:K:45:PHE:CE1	4:O:587:PHE:CZ	2.94	0.55
4:P:650:VAL:CG2	4:P:655:VAL:HG21	2.35	0.55
1:E:93:TYR:HD1	2:F:676:PRO:CA	2.11	0.55
2:F:547:LYS:HE2	2:F:667:ILE:HG13	1.84	0.55
1:G:85:TYR:CE1	1:G:87:PHE:CZ	2.94	0.55
3:J:45:PHE:CE1	4:N:587:PHE:CZ	2.94	0.55
3:L:122:TYR:CZ	4:P:624:GLU:HG3	2.41	0.55
4:M:514:SER:HG	4:M:606(A):LEU:HD22	1.69	0.55
4:M:686:GLU:HA	4:M:708:ARG:HH21	1.72	0.55
4:P:617:LEU:HD23	4:P:633:VAL:O	2.06	0.55
2:B:597:MET:HB3	2:B:756:HIS:CG	2.29	0.55
2:B:716:VAL:HG21	4:M:532:CYS:SG	1.41	0.55
1:C:85:TYR:CE1	1:C:87:PHE:CZ	2.94	0.55
1:C:93:TYR:CB	2:D:676:PRO:CB	2.77	0.55
2:D:533:ALA:HA	2:D:733:LYS:C	2.20	0.55
1:E:86:PRO:CA	1:E:227:GLY:CA	2.64	0.55
2:H:686:GLY:N	4:P:553:ASN:H	2.02	0.55
2:H:716:VAL:HG11	4:P:591:TRP:CG	2.34	0.55
2:H:718:ASN:CA	4:P:531:ASN:H	2.04	0.55
4:M:686:GLU:HA	4:M:708:ARG:HE	1.72	0.55
4:N:617:LEU:HD23	4:N:633:VAL:O	2.06	0.55
4:N:617:LEU:HD21	4:N:648:TRP:HH2	1.72	0.55
4:O:608:GLN:HG3	4:O:608:GLN:O	2.05	0.55
4:O:650:VAL:HG23	4:O:655:VAL:CG2	2.35	0.55
4:P:555:ARG:HE	4:P:558:VAL:HG23	1.71	0.55
4:P:686:GLU:HA	4:P:708:ARG:HE	1.72	0.55
2:D:547:LYS:HE2	2:D:667:ILE:HG13	1.84	0.55
1:E:199:GLN:HE21	2:H:775:THR:CG2	2.15	0.55
2:H:521:ASP:C	2:H:733:LYS:HD3	2.10	0.55
2:H:670:HIS:HE1	2:H:673:PRO:HG3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:32:TYR:CE1	3:L:96:TYR:CB	2.89	0.55
1:A:93:TYR:HE1	2:B:674:ASP:O	1.89	0.55
2:B:719:ASN:OD1	4:M:551:THR:CG2	2.54	0.55
2:H:687:ASN:HD22	4:P:532:CYS:CA	2.16	0.55
3:J:32:TYR:CE1	3:J:96:TYR:CB	2.89	0.55
2:B:547:LYS:HD3	2:B:667:ILE:HD13	1.87	0.55
2:F:670:HIS:HE1	2:F:673:PRO:HG3	1.71	0.55
2:H:536:ARG:HB2	2:H:670:HIS:H	1.72	0.55
2:H:602:LEU:HD13	2:H:758:PRO:HG3	1.76	0.55
4:N:650:VAL:HG23	4:N:655:VAL:CG2	2.35	0.55
1:A:86:PRO:CA	1:A:227:GLY:CA	2.64	0.55
2:B:520:PRO:HB3	2:B:731:ASN:N	1.87	0.55
1:C:93:TYR:HE1	2:D:674:ASP:O	1.89	0.55
1:G:95:PHE:HD1	2:H:725:CYS:CA	2.09	0.55
3:I:72:GLU:CD	3:I:79:TYR:CE1	2.80	0.55
3:I:98:ILE:CG2	4:M:550:ASP:CG	2.75	0.55
2:B:719:ASN:N	4:M:551:THR:OG1	2.38	0.55
2:D:545:THR:CG2	2:D:758:PRO:HG3	2.33	0.55
2:F:536:ARG:HB2	2:F:670:HIS:H	1.72	0.55
2:F:547:LYS:HD3	2:F:667:ILE:HD13	1.87	0.55
3:J:98:ILE:CG2	4:N:550:ASP:CA	2.69	0.55
3:K:72:GLU:CD	3:K:79:TYR:CE1	2.80	0.55
3:L:98:ILE:HG22	4:P:532:CYS:CB	2.13	0.55
4:M:563:SER:O	4:M:573:LEU:HD23	2.07	0.55
4:M:617:LEU:HD23	4:M:633:VAL:O	2.06	0.55
1:A:63:CYS:SG	2:B:700:LYS:CE	2.95	0.55
2:B:536:ARG:HB2	2:B:670:HIS:H	1.72	0.55
2:B:613:VAL:H	2:B:734:LYS:HZ2	0.96	0.55
2:D:670:HIS:HE1	2:D:673:PRO:HG3	1.71	0.55
2:H:538:ARG:HB2	2:H:547:LYS:HB3	1.89	0.55
3:I:37:VAL:HG21	3:I:103:TRP:HH2	1.70	0.55
3:L:72:GLU:CD	3:L:79:TYR:CE1	2.80	0.55
4:O:563:SER:O	4:O:573:LEU:HD23	2.07	0.55
2:D:716:VAL:HA	4:N:532:CYS:SG	2.45	0.54
2:H:717:ILE:HG22	4:P:530(B):SER:N	2.22	0.54
3:I:45:PHE:CE1	4:M:587:PHE:CZ	2.94	0.54
3:J:45:PHE:HZ	4:N:544:PHE:HZ	0.62	0.54
4:O:650:VAL:CG2	4:O:655:VAL:HG21	2.35	0.54
2:B:673:PRO:HB3	2:B:745:ASN:N	2.23	0.54
1:C:63:CYS:SG	2:D:700:LYS:CE	2.95	0.54
2:F:518:HIS:NE2	2:F:730:THR:C	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:673:PRO:HB3	2:F:745:ASN:N	2.22	0.54
3:I:114:ALA:HB3	3:I:146:PHE:HE2	0.78	0.54
3:K:32:TYR:CE1	3:K:96:TYR:CB	2.89	0.54
4:P:686:GLU:HA	4:P:708:ARG:HH21	1.72	0.54
2:B:521:ASP:C	2:B:733:LYS:HD3	2.10	0.54
2:D:528:CYS:H	2:D:733:LYS:HE3	1.70	0.54
2:D:673:PRO:CB	2:D:745:ASN:HB2	2.34	0.54
2:F:602:LEU:HD13	2:F:758:PRO:HB3	1.85	0.54
3:J:72:GLU:CD	3:J:79:TYR:CE1	2.80	0.54
4:M:617:LEU:HD21	4:M:648:TRP:HH2	1.72	0.54
4:P:563:SER:O	4:P:573:LEU:HD23	2.07	0.54
2:B:689:LYS:HB2	3:I:98:ILE:HD13	1.76	0.54
1:E:93:TYR:CE1	2:F:676:PRO:CG	2.53	0.54
2:H:543:ASP:OD2	2:H:759:PHE:CZ	2.61	0.54
4:P:617:LEU:HD21	4:P:648:TRP:HH2	1.72	0.54
2:D:673:PRO:HB3	2:D:745:ASN:N	2.22	0.54
4:N:563:SER:O	4:N:573:LEU:HD23	2.07	0.54
4:N:686:GLU:HA	4:N:708:ARG:HE	1.72	0.54
4:O:686:GLU:HA	4:O:708:ARG:HE	1.72	0.54
1:A:85:TYR:CE1	1:A:87:PHE:CZ	2.94	0.54
2:D:715:LYS:HE2	4:N:593:ASN:CA	1.95	0.54
2:B:543:ASP:OD2	2:B:759:PHE:CZ	2.61	0.54
2:D:717:ILE:CG2	4:N:530(B):SER:CA	2.74	0.54
2:F:685:SER:OG	4:O:549:GLY:N	2.40	0.54
1:G:63:CYS:SG	2:H:700:LYS:CE	2.95	0.54
2:H:689:LYS:HB3	3:L:98:ILE:HD11	1.86	0.54
2:B:538:ARG:HB2	2:B:547:LYS:HB3	1.89	0.54
2:D:602:LEU:HD13	2:D:758:PRO:HB3	1.85	0.54
2:D:627:HIS:CD2	2:D:734:LYS:CG	2.86	0.54
2:D:686:GLY:CA	4:N:552:ASN:ND2	2.66	0.54
2:F:720:CYS:N	4:O:530(B):SER:CA	2.57	0.54
2:H:686:GLY:HA3	4:P:552:ASN:CB	2.38	0.54
3:L:11:VAL:CG2	3:L:148:GLU:HB2	2.38	0.54
4:M:515:PRO:HG2	4:M:606(A):LEU:O	2.03	0.54
4:M:525:SER:OG	4:M:592:TYR:OH	2.23	0.54
4:M:650:VAL:HG23	4:M:655:VAL:CG2	2.35	0.54
2:D:536:ARG:HB2	2:D:670:HIS:H	1.72	0.54
2:D:775:THR:CG2	1:G:199:GLN:HE21	2.15	0.54
2:H:507:ASN:CA	2:H:562:HIS:NE2	2.33	0.54
4:M:650:VAL:CG2	4:M:655:VAL:HG21	2.35	0.54
4:N:651:ASP:OD2	4:N:688:HIS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:686:GLU:HA	4:N:708:ARG:NE	2.23	0.54
4:O:617:LEU:HD21	4:O:648:TRP:HH2	1.72	0.54
2:B:573:HIS:N	4:P:517:GLU:HA	2.16	0.54
2:D:538:ARG:HB2	2:D:547:LYS:HB3	1.89	0.54
2:D:543:ASP:OD2	2:D:759:PHE:CZ	2.61	0.54
2:D:547:LYS:HD3	2:D:667:ILE:HG21	1.82	0.54
3:K:98:ILE:HG22	4:O:532:CYS:CB	2.13	0.54
4:M:686:GLU:HA	4:M:708:ARG:NE	2.23	0.54
4:O:697:HIS:O	4:O:698:GLU:C	2.46	0.54
2:B:535:GLU:CG	2:B:670:HIS:HA	2.38	0.53
2:H:547:LYS:HE2	2:H:667:ILE:HG13	1.84	0.53
4:N:686:GLU:HA	4:N:708:ARG:HH21	1.72	0.53
2:D:535:GLU:CG	2:D:670:HIS:HA	2.38	0.53
2:D:683:GLN:O	4:N:553:ASN:ND2	2.41	0.53
2:F:704:GLY:N	4:O:530(A):THR:HG22	2.22	0.53
2:H:520:PRO:HB3	2:H:731:ASN:N	1.86	0.53
3:I:11:VAL:CG2	3:I:148:GLU:HB2	2.38	0.53
3:J:11:VAL:CG2	3:J:148:GLU:HB2	2.38	0.53
3:J:32:TYR:CE1	3:J:96:TYR:HD1	1.97	0.53
4:O:515:PRO:HG2	4:O:606(A):LEU:O	2.03	0.53
4:P:686:GLU:HA	4:P:708:ARG:NE	2.23	0.53
1:A:323:SER:CB	1:E:319:LYS:HZ2	2.20	0.53
2:D:788:TYR:CE2	1:G:246:GLU:CB	2.83	0.53
1:E:63:CYS:SG	2:F:700:LYS:CE	2.95	0.53
2:F:538:ARG:HB2	2:F:547:LYS:HB3	1.89	0.53
2:F:543:ASP:OD2	2:F:759:PHE:CZ	2.61	0.53
2:H:673:PRO:HB3	2:H:745:ASN:N	2.22	0.53
3:I:30:THR:CG2	3:I:53:ASN:HD22	2.17	0.53
4:P:515:PRO:HG2	4:P:606(A):LEU:O	2.03	0.53
4:P:697:HIS:O	4:P:698:GLU:C	2.46	0.53
3:L:32:TYR:CE1	3:L:96:TYR:HD1	1.97	0.53
4:N:697:HIS:O	4:N:698:GLU:C	2.46	0.53
4:O:686:GLU:HA	4:O:708:ARG:NE	2.23	0.53
4:P:651:ASP:OD2	4:P:688:HIS:HB3	2.08	0.53
2:H:686:GLY:CA	4:P:551:THR:HB	2.35	0.53
2:H:719:ASN:C	4:P:530(B):SER:HB3	2.01	0.53
3:I:35:LEU:HD23	3:I:37:VAL:HG23	1.82	0.53
3:K:11:VAL:CG2	3:K:148:GLU:HB2	2.38	0.53
3:K:45:PHE:HZ	4:O:544:PHE:HZ	0.62	0.53
4:O:525:SER:OG	4:O:592:TYR:OH	2.23	0.53
2:F:687:ASN:H	4:O:550:ASP:CA	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:98:ILE:HG22	4:M:550:ASP:HA	1.89	0.53
3:J:114:ALA:HB3	3:J:146:PHE:HE2	0.78	0.53
3:J:124:LEU:HB3	4:N:618:PHE:CG	2.44	0.53
3:L:21:SER:CB	3:L:79:TYR:HE2	2.13	0.53
2:D:507:ASN:O	2:D:509:TYR:N	2.42	0.53
2:F:536:ARG:O	2:F:669:VAL:HG11	2.07	0.53
2:H:547:LYS:HG2	2:H:667:ILE:HG12	1.64	0.53
3:J:30:THR:O	3:J:30:THR:HG22	2.09	0.53
4:N:680:LEU:HD22	4:N:684:ALA:HB1	1.91	0.53
2:D:536:ARG:CD	2:D:737:TYR:CG	2.88	0.53
2:D:673:PRO:HB3	2:D:745:ASN:CB	2.38	0.53
1:G:91:GLY:HA2	2:H:678:ARG:HB2	1.83	0.53
2:H:509:TYR:HB3	2:H:568:ARG:HH22	1.74	0.53
2:H:535:GLU:CG	2:H:670:HIS:HA	2.38	0.53
2:H:613:VAL:N	2:H:734:LYS:HZ3	1.70	0.53
3:I:124:LEU:HB3	4:M:618:PHE:CG	2.44	0.53
4:M:680:LEU:HD22	4:M:684:ALA:HB1	1.91	0.53
4:P:505:VAL:CG1	4:P:523:CYS:SG	2.97	0.53
2:F:507:ASN:O	2:F:509:TYR:N	2.42	0.53
2:F:685:SER:CB	4:O:549:GLY:N	2.71	0.53
3:J:30:THR:CG2	3:J:53:ASN:HD22	2.17	0.53
3:J:33:PRO:HB2	3:J:51:ILE:O	2.09	0.53
3:K:33:PRO:HA	3:K:52(A):THR:HG23	1.91	0.53
2:D:625:CYS:SG	2:D:734:LYS:CG	2.94	0.53
2:D:673:PRO:HA	2:D:745:ASN:CG	2.27	0.53
2:F:507:ASN:CA	2:F:562:HIS:NE2	2.33	0.53
2:H:536:ARG:N	2:H:669:VAL:HB	2.14	0.53
1:C:246:GLU:CB	2:F:788:TYR:CE2	2.83	0.52
2:D:613:VAL:N	2:D:734:LYS:HZ3	1.75	0.52
2:H:535:GLU:OE1	2:H:671:MET:N	2.42	0.52
2:H:599:HIS:CB	2:H:735:TRP:CH2	2.91	0.52
3:K:77:THR:CG2	3:K:79:TYR:CE2	2.84	0.52
4:M:651:ASP:OD2	4:M:688:HIS:HB3	2.08	0.52
4:M:697:HIS:O	4:M:698:GLU:C	2.46	0.52
4:O:627:THR:HG22	4:O:629:LYS:HB2	1.91	0.52
4:O:651:ASP:OD2	4:O:688:HIS:HB3	2.08	0.52
4:O:680:LEU:HD22	4:O:684:ALA:HB1	1.91	0.52
2:D:535:GLU:OE1	2:D:671:MET:N	2.42	0.52
2:D:719:ASN:ND2	4:N:571:ALA:HB2	2.25	0.52
2:F:718:ASN:ND2	4:O:533:ALA:CA	2.73	0.52
2:H:715:LYS:HA	4:P:591:TRP:HE1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:PRO:HA	3:L:52(A):THR:HG23	1.91	0.52
2:B:547:LYS:NZ	2:B:757:ILE:HG12	2.25	0.52
2:D:547:LYS:NZ	2:D:757:ILE:HG12	2.25	0.52
2:F:509:TYR:HB3	2:F:568:ARG:HH22	1.74	0.52
2:F:535:GLU:CG	2:F:670:HIS:HA	2.38	0.52
2:F:535:GLU:O	2:F:736:GLN:N	2.36	0.52
2:F:545:THR:CG2	2:F:758:PRO:CG	2.81	0.52
2:F:602:LEU:HD11	2:F:757:ILE:CA	2.39	0.52
2:H:540:GLU:OE2	2:H:737:TYR:CE2	2.63	0.52
1:A:291:VAL:HG23	1:E:304:PRO:HD2	1.90	0.52
2:D:509:TYR:HB3	2:D:568:ARG:HH22	1.74	0.52
2:D:537:ILE:C	2:D:737:TYR:HB2	2.22	0.52
2:D:602:LEU:HD21	2:D:758:PRO:CD	2.31	0.52
2:F:540:GLU:OE2	2:F:737:TYR:CE2	2.62	0.52
2:H:547:LYS:HD3	2:H:667:ILE:HD13	1.87	0.52
3:K:124:LEU:HB3	4:O:618:PHE:CG	2.44	0.52
3:L:124:LEU:HB3	4:P:618:PHE:CG	2.44	0.52
4:M:505:VAL:CG1	4:M:523:CYS:SG	2.97	0.52
4:N:627:THR:HG22	4:N:629:LYS:HB2	1.91	0.52
4:O:505:VAL:CG1	4:O:523:CYS:SG	2.97	0.52
2:B:545:THR:CG2	2:B:758:PRO:CG	2.81	0.52
2:B:687:ASN:CA	4:M:551:THR:OG1	2.58	0.52
3:J:77:THR:CG2	3:J:79:TYR:CE2	2.84	0.52
3:K:21:SER:CB	3:K:79:TYR:HE2	2.13	0.52
4:M:627:THR:HG22	4:M:629:LYS:HB2	1.91	0.52
1:A:86:PRO:CB	1:A:227:GLY:C	2.78	0.52
2:D:540:GLU:OE2	2:D:737:TYR:CE2	2.62	0.52
2:D:685:SER:HG	4:N:549:GLY:H	1.57	0.52
2:F:536:ARG:CD	2:F:738:ASN:CB	2.58	0.52
2:F:538:ARG:CB	2:F:667:ILE:CD1	2.87	0.52
2:F:547:LYS:NZ	2:F:757:ILE:HG12	2.25	0.52
2:F:704:GLY:CA	4:O:530(A):THR:HG21	2.39	0.52
2:H:602:LEU:CD1	2:H:758:PRO:HB3	2.39	0.52
2:H:602:LEU:HD11	2:H:757:ILE:CA	2.39	0.52
3:K:40:ALA:C	3:K:41:PRO:CD	2.63	0.52
1:A:323:SER:CB	1:E:319:LYS:HZ1	2.18	0.52
2:H:547:LYS:NZ	2:H:757:ILE:HG12	2.25	0.52
3:I:30:THR:O	3:I:30:THR:HG22	2.09	0.52
3:I:32:TYR:CE1	3:I:96:TYR:CB	2.89	0.52
3:L:30:THR:O	3:L:30:THR:HG22	2.09	0.52
4:N:505:VAL:CG1	4:N:523:CYS:SG	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:681:THR:O	4:O:682:ALA:C	2.48	0.52
4:P:681:THR:O	4:P:682:ALA:C	2.48	0.52
2:B:507:ASN:O	2:B:509:TYR:N	2.42	0.52
2:B:718:ASN:N	4:M:531:ASN:CA	2.69	0.52
3:J:93:VAL:CG2	3:J:103:TRP:CD2	2.93	0.52
3:J:98:ILE:HG22	4:N:550:ASP:HA	1.89	0.52
2:B:551:SER:HA	2:B:735:TRP:CZ2	2.45	0.52
2:F:685:SER:CB	4:O:553:ASN:CA	2.78	0.52
2:H:718:ASN:HA	4:P:532:CYS:H	1.72	0.52
1:A:292:ASP:OD2	1:E:353:GLN:CB	2.58	0.52
2:B:509:TYR:HB3	2:B:568:ARG:HH22	1.74	0.52
2:B:602:LEU:HD11	2:B:757:ILE:CA	2.39	0.52
2:D:602:LEU:HD11	2:D:757:ILE:CA	2.39	0.52
1:E:86:PRO:CB	1:E:227:GLY:C	2.78	0.52
2:F:612:THR:CB	2:F:734:LYS:HZ1	2.22	0.52
2:F:673:PRO:HA	2:F:745:ASN:CG	2.27	0.52
2:F:673:PRO:HB3	2:F:745:ASN:CB	2.38	0.52
3:I:33:PRO:HB2	3:I:51:ILE:O	2.09	0.52
3:I:35:LEU:HD23	3:I:36:TRP:N	2.25	0.52
3:I:103:TRP:HB2	4:M:544:PHE:CB	2.41	0.52
3:I:208:LYS:CE	4:M:623:GLU:OE1	2.58	0.52
3:J:35:LEU:HD23	3:J:36:TRP:N	2.25	0.52
3:J:35:LEU:HD23	3:J:37:VAL:HG23	1.83	0.52
4:M:681:THR:O	4:M:682:ALA:C	2.48	0.52
4:P:680:LEU:HD22	4:P:684:ALA:HB1	1.91	0.52
2:D:535:GLU:OE2	2:D:671:MET:HG3	2.10	0.51
2:D:551:SER:HA	2:D:735:TRP:CZ2	2.45	0.51
2:F:547:LYS:CD	2:F:667:ILE:CD1	2.55	0.51
3:I:33:PRO:HA	3:I:52(A):THR:HG23	1.91	0.51
3:K:208:LYS:CE	4:O:623:GLU:OE1	2.58	0.51
3:L:33:PRO:HB2	3:L:51:ILE:O	2.09	0.51
4:M:515:PRO:HD3	4:M:606(A):LEU:HB3	1.79	0.51
4:O:540:PRO:HB2	4:O:666:LYS:HB2	1.92	0.51
2:B:548:ILE:O	2:B:755:ILE:HG12	2.10	0.51
2:B:602:LEU:HD13	2:B:758:PRO:HB3	1.84	0.51
2:F:535:GLU:N	2:F:735:TRP:HD1	1.44	0.51
2:F:535:GLU:OE2	2:F:671:MET:HG3	2.10	0.51
2:F:596:THR:H	2:F:662:ALA:HB2	1.72	0.51
2:F:613:VAL:N	2:F:734:LYS:HZ3	1.82	0.51
2:H:537:ILE:C	2:H:737:TYR:HB2	2.22	0.51
2:H:687:ASN:ND2	4:P:533:ALA:O	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:24:ALA:HB1	3:K:27:TYR:HE1	1.75	0.51
2:F:535:GLU:OE1	2:F:671:MET:N	2.42	0.51
1:G:86:PRO:CB	1:G:227:GLY:C	2.78	0.51
2:H:673:PRO:HA	2:H:745:ASN:CG	2.27	0.51
2:H:719:ASN:CB	4:P:551:THR:CG2	2.87	0.51
3:I:114:ALA:CB	3:I:146:PHE:CD2	2.77	0.51
3:K:33:PRO:HB2	3:K:51:ILE:O	2.09	0.51
3:K:103:TRP:HB2	4:O:544:PHE:CB	2.40	0.51
3:L:93:VAL:CG2	3:L:103:TRP:CD2	2.93	0.51
4:N:681:THR:O	4:N:682:ALA:C	2.48	0.51
2:B:535:GLU:OE2	2:B:671:MET:HG3	2.10	0.51
2:B:538:ARG:CB	2:B:667:ILE:CD1	2.87	0.51
1:C:86:PRO:CB	1:C:227:GLY:C	2.78	0.51
1:G:63:CYS:SG	2:H:700:LYS:HE3	2.51	0.51
2:H:536:ARG:CD	2:H:738:ASN:CB	2.58	0.51
2:H:551:SER:HA	2:H:735:TRP:CZ2	2.45	0.51
2:H:685:SER:C	4:P:552:ASN:ND2	2.59	0.51
3:J:45:PHE:HE1	4:N:587:PHE:CE2	2.22	0.51
3:J:103:TRP:HB2	4:N:544:PHE:CB	2.40	0.51
3:K:93:VAL:CG2	3:K:103:TRP:CD2	2.93	0.51
1:A:93:TYR:CB	2:B:676:PRO:CB	2.77	0.51
1:A:149:ASN:HD21	1:C:123:ARG:NH2	2.08	0.51
2:B:535:GLU:OE1	2:B:671:MET:N	2.42	0.51
2:F:536:ARG:HB2	2:F:670:HIS:N	2.26	0.51
2:H:548:ILE:O	2:H:755:ILE:HG12	2.10	0.51
3:I:93:VAL:CG2	3:I:103:TRP:CD2	2.93	0.51
3:J:208:LYS:CE	4:N:623:GLU:OE1	2.58	0.51
3:K:30:THR:O	3:K:30:THR:HG22	2.09	0.51
2:B:536:ARG:HB2	2:B:670:HIS:N	2.26	0.51
2:B:612:THR:HG23	2:B:734:LYS:HZ1	1.75	0.51
2:D:687:ASN:ND2	4:N:532:CYS:CA	2.73	0.51
2:D:730:THR:HB	2:D:732:HIS:HE1	1.76	0.51
2:F:514:PRO:HG3	2:F:568:ARG:HG2	1.93	0.51
2:F:687:ASN:CA	4:O:551:THR:OG1	2.58	0.51
2:H:535:GLU:OE2	2:H:671:MET:HG3	2.10	0.51
2:H:687:ASN:HB2	4:P:550:ASP:CB	2.41	0.51
3:K:98:ILE:HG22	4:O:550:ASP:HA	1.89	0.51
3:L:208:LYS:CE	4:P:623:GLU:OE1	2.58	0.51
4:M:540:PRO:HB2	4:M:666:LYS:HB2	1.93	0.51
4:P:627:THR:HG22	4:P:629:LYS:HB2	1.92	0.51
2:B:534:LEU:HD12	2:B:734:LYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:547:LYS:HD3	2:B:667:ILE:HG21	1.82	0.51
1:E:63:CYS:SG	2:F:700:LYS:HE3	2.51	0.51
2:F:548:ILE:O	2:F:755:ILE:HG12	2.10	0.51
2:H:687:ASN:HD21	4:P:533:ALA:C	2.12	0.51
3:L:35:LEU:HD23	3:L:36:TRP:N	2.25	0.51
3:L:37:VAL:HG21	3:L:103:TRP:HH2	1.70	0.51
4:N:547:LEU:HD12	4:N:558:VAL:HG21	1.93	0.51
2:B:540:GLU:OE2	2:B:737:TYR:CE2	2.62	0.51
2:B:602:LEU:CD1	2:B:758:PRO:HB3	2.39	0.51
2:B:689:LYS:CB	3:I:98:ILE:HD11	2.27	0.51
2:D:596:THR:H	2:D:662:ALA:HB2	1.72	0.51
2:H:536:ARG:HB2	2:H:670:HIS:N	2.26	0.51
3:J:33:PRO:HA	3:J:52(A):THR:HG23	1.91	0.51
3:K:32:TYR:CE1	3:K:96:TYR:HD1	1.97	0.51
3:L:98:ILE:HG22	4:P:550:ASP:HA	1.89	0.51
4:N:587:PHE:CE1	4:N:601:GLY:HA3	2.46	0.51
4:N:650:VAL:CG2	4:N:655:VAL:HG21	2.35	0.51
4:P:547:LEU:HD12	4:P:558:VAL:HG21	1.93	0.51
2:B:536:ARG:O	2:B:669:VAL:HG11	2.07	0.51
2:B:542:THR:HA	2:B:636:ILE:CG1	2.37	0.51
2:D:514:PRO:HG3	2:D:568:ARG:HG2	1.93	0.51
2:H:715:LYS:CE	4:P:593:ASN:CG	2.78	0.51
3:K:32:TYR:CD1	3:K:96:TYR:HB2	2.46	0.51
3:K:35:LEU:HD23	3:K:36:TRP:N	2.25	0.51
3:L:30:THR:CG2	3:L:53:ASN:HD22	2.17	0.51
4:N:540:PRO:HB2	4:N:666:LYS:HB2	1.93	0.51
2:D:548:ILE:O	2:D:755:ILE:HG12	2.10	0.51
2:F:551:SER:HA	2:F:735:TRP:CZ2	2.45	0.51
2:F:687:ASN:HB2	4:O:532:CYS:CB	2.41	0.51
2:H:673:PRO:HB3	2:H:745:ASN:CB	2.38	0.51
2:H:716:VAL:CG2	3:L:98:ILE:HG23	2.40	0.51
3:L:45:PHE:HZ	4:P:544:PHE:HZ	0.62	0.51
4:M:587:PHE:CE1	4:M:601:GLY:HA3	2.46	0.51
4:O:587:PHE:CE1	4:O:601:GLY:HA3	2.46	0.51
1:A:63:CYS:SG	2:B:700:LYS:HE3	2.51	0.50
2:B:514:PRO:HG3	2:B:568:ARG:HG2	1.93	0.50
1:C:199:GLN:HE22	2:F:775:THR:HG21	1.74	0.50
2:D:535:GLU:O	2:D:736:GLN:HB3	2.11	0.50
2:D:626:THR:C	2:D:734:LYS:CG	2.65	0.50
2:F:704:GLY:C	4:O:530(A):THR:HG23	2.26	0.50
3:L:32:TYR:CD1	3:L:96:TYR:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:521:LEU:N	4:N:521:LEU:CD2	2.70	0.50
4:P:587:PHE:CE1	4:P:601:GLY:HA3	2.46	0.50
2:H:514:PRO:HG3	2:H:568:ARG:HG2	1.93	0.50
3:I:11:VAL:HB	3:I:147:PRO:HB2	1.87	0.50
4:M:547:LEU:HD12	4:M:558:VAL:HG21	1.93	0.50
4:N:508:GLU:O	4:N:602:THR:OG1	2.27	0.50
1:A:123:ARG:NH2	1:C:149:ASN:HD21	2.08	0.50
2:B:599:HIS:CB	2:B:735:TRP:CH2	2.91	0.50
2:F:599:HIS:CB	2:F:735:TRP:CH2	2.91	0.50
2:H:507:ASN:O	2:H:509:TYR:N	2.42	0.50
3:L:98:ILE:CG2	4:P:550:ASP:CG	2.75	0.50
2:B:535:GLU:O	2:B:736:GLN:HB3	2.11	0.50
2:D:547:LYS:HD3	2:D:667:ILE:HD13	1.87	0.50
1:E:93:TYR:CB	2:F:676:PRO:CB	2.77	0.50
2:F:730:THR:HB	2:F:732:HIS:HE1	1.76	0.50
1:G:86:PRO:CA	1:G:227:GLY:CA	2.64	0.50
1:G:93:TYR:CD2	2:H:726:HIS:NE2	2.80	0.50
2:H:599:HIS:O	2:H:755:ILE:HG22	1.51	0.50
2:H:718:ASN:O	4:P:566:LEU:HD11	2.11	0.50
2:H:730:THR:HB	2:H:732:HIS:HE1	1.76	0.50
3:I:24:ALA:HB1	3:I:27:TYR:HE1	1.75	0.50
3:J:13:ASN:OD1	3:J:112:SER:O	2.30	0.50
1:A:291:VAL:HG23	1:E:304:PRO:CD	2.42	0.50
1:C:237:PRO:O	2:F:772:ARG:NH2	2.38	0.50
2:D:536:ARG:O	2:D:669:VAL:HG11	2.07	0.50
2:D:536:ARG:HB2	2:D:670:HIS:N	2.26	0.50
3:I:32:TYR:CD1	3:I:96:TYR:HB2	2.46	0.50
3:L:13:ASN:OD1	3:L:112:SER:O	2.30	0.50
3:L:103:TRP:HB2	4:P:544:PHE:CB	2.41	0.50
3:L:114:ALA:CB	3:L:146:PHE:CD2	2.77	0.50
2:B:685:SER:HB3	4:M:553:ASN:C	2.19	0.50
2:F:686:GLY:C	4:O:550:ASP:C	2.52	0.50
2:H:612:THR:HG23	2:H:734:LYS:HZ1	1.75	0.50
3:J:32:TYR:CD1	3:J:96:TYR:HB2	2.46	0.50
2:B:719:ASN:OD1	4:M:566:LEU:N	2.44	0.50
4:O:547:LEU:HD12	4:O:558:VAL:CG2	2.42	0.50
4:P:540:PRO:HB2	4:P:666:LYS:HB2	1.92	0.50
1:A:93:TYR:CD2	2:B:726:HIS:NE2	2.80	0.50
2:D:527:SER:CA	2:D:733:LYS:HE3	2.40	0.50
2:F:538:ARG:CA	2:F:737:TYR:CB	2.90	0.50
2:F:684:GLN:OE1	3:K:98:ILE:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:547:LYS:CD	2:H:757:ILE:HG23	1.72	0.50
3:L:32:TYR:CZ	3:L:96:TYR:CZ	2.84	0.50
4:O:547:LEU:HD12	4:O:558:VAL:HG21	1.93	0.50
4:P:552:ASN:ND2	4:P:552:ASN:C	2.54	0.50
1:A:290:VAL:O	1:E:317:ILE:HD12	1.65	0.50
2:B:673:PRO:HB3	2:B:745:ASN:CB	2.38	0.50
1:C:93:TYR:CE1	2:D:676:PRO:CG	2.53	0.50
2:D:521:ASP:HB3	2:D:626:THR:HB	1.94	0.50
2:D:599:HIS:CB	2:D:735:TRP:CH2	2.91	0.50
2:D:730:THR:HB	2:D:732:HIS:CE1	2.47	0.50
2:H:538:ARG:CA	2:H:737:TYR:CB	2.90	0.50
3:J:11:VAL:CB	3:J:147:PRO:CB	2.86	0.50
4:M:547:LEU:HD12	4:M:558:VAL:CG2	2.42	0.50
2:B:518:HIS:NE2	2:B:731:ASN:C	2.66	0.49
2:D:538:ARG:CA	2:D:737:TYR:CB	2.90	0.49
1:E:93:TYR:CD2	2:F:726:HIS:NE2	2.80	0.49
2:F:536:ARG:HB3	2:F:669:VAL:CG1	2.42	0.49
3:J:21:SER:CB	3:J:79:TYR:HE2	2.13	0.49
4:P:547:LEU:HD12	4:P:558:VAL:CG2	2.42	0.49
1:C:63:CYS:HB2	2:D:700:LYS:CD	2.33	0.49
1:C:63:CYS:SG	2:D:700:LYS:HE3	2.51	0.49
2:D:536:ARG:HB3	2:D:669:VAL:CG1	2.42	0.49
2:F:719:ASN:OD1	4:O:566:LEU:CA	2.60	0.49
2:H:538:ARG:CB	2:H:667:ILE:CD1	2.87	0.49
2:H:715:LYS:CE	4:P:593:ASN:HB3	2.38	0.49
3:K:13:ASN:OD1	3:K:112:SER:O	2.30	0.49
2:B:521:ASP:HB3	2:B:626:THR:HB	1.94	0.49
2:B:716:VAL:HG22	4:M:532:CYS:HG	1.14	0.49
2:F:625:CYS:SG	2:F:734:LYS:CG	2.94	0.49
2:H:527:SER:CA	2:H:733:LYS:HE3	2.40	0.49
2:H:536:ARG:HB3	2:H:669:VAL:CG1	2.42	0.49
2:H:599:HIS:CG	2:H:735:TRP:HH2	2.30	0.49
2:D:518:HIS:NE2	2:D:731:ASN:C	2.66	0.49
2:F:521:ASP:HB3	2:F:626:THR:HB	1.94	0.49
3:I:13:ASN:OD1	3:I:112:SER:O	2.29	0.49
2:B:625:CYS:SG	2:B:734:LYS:CG	2.94	0.49
2:B:718:ASN:CA	4:M:530(B):SER:HA	2.42	0.49
2:D:612:THR:CB	2:D:734:LYS:HZ1	2.25	0.49
2:F:518:HIS:NE2	2:F:731:ASN:C	2.66	0.49
2:H:536:ARG:HE	2:H:737:TYR:C	2.14	0.49
3:I:98:ILE:CG1	4:M:550:ASP:CG	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:37:VAL:HG21	3:J:103:TRP:HH2	1.70	0.49
3:K:35:LEU:HD23	3:K:37:VAL:HG23	1.83	0.49
4:O:507:GLN:OE1	4:O:599:GLY:HA3	2.13	0.49
1:A:323:SER:HB2	1:E:319:LYS:HZ2	1.78	0.49
2:B:686:GLY:CA	4:M:552:ASN:ND2	2.74	0.49
2:B:730:THR:HB	2:B:732:HIS:HE1	1.76	0.49
1:C:93:TYR:CD2	2:D:726:HIS:NE2	2.80	0.49
2:D:684:GLN:NE2	3:J:98:ILE:HD13	2.26	0.49
2:F:535:GLU:O	2:F:736:GLN:HB3	2.11	0.49
2:F:536:ARG:CZ	2:F:737:TYR:CG	2.88	0.49
2:H:521:ASP:HB3	2:H:626:THR:HB	1.94	0.49
2:H:535:GLU:O	2:H:736:GLN:HB3	2.11	0.49
3:I:21:SER:CB	3:I:79:TYR:HE2	2.13	0.49
3:J:98:ILE:HG22	4:N:532:CYS:CB	2.13	0.49
4:M:507:GLN:OE1	4:M:599:GLY:HA3	2.13	0.49
4:N:507:GLN:OE1	4:N:599:GLY:HA3	2.13	0.49
2:H:602:LEU:HD13	2:H:758:PRO:HB3	1.85	0.49
2:H:730:THR:HB	2:H:732:HIS:CE1	2.47	0.49
3:I:45:PHE:HZ	4:M:544:PHE:HZ	0.62	0.49
3:J:98:ILE:HG13	4:N:550:ASP:OD2	1.80	0.49
3:K:2:ILE:HA	3:K:25:SER:O	2.13	0.49
3:L:2:ILE:HA	3:L:25:SER:O	2.13	0.49
2:F:527:SER:CA	2:F:733:LYS:HE3	2.40	0.49
2:F:536:ARG:CZ	2:F:737:TYR:CD2	2.92	0.49
2:F:536:ARG:HE	2:F:737:TYR:C	2.14	0.49
2:F:602:LEU:CD1	2:F:758:PRO:HB3	2.39	0.49
3:J:48:MET:HG2	3:J:63:PHE:CE1	2.48	0.49
4:O:525:SER:HG	4:O:592:TYR:HH	1.49	0.49
2:B:538:ARG:CA	2:B:737:TYR:CB	2.90	0.49
2:D:599:HIS:O	2:D:755:ILE:HG21	2.00	0.49
1:E:237:PRO:O	2:H:772:ARG:NH2	2.38	0.49
2:H:716:VAL:N	4:P:591:TRP:CD1	2.80	0.49
4:N:547:LEU:HD12	4:N:558:VAL:CG2	2.42	0.49
2:B:536:ARG:HB3	2:B:669:VAL:CG1	2.42	0.49
2:B:730:THR:HB	2:B:732:HIS:CE1	2.47	0.49
2:D:538:ARG:CB	2:D:667:ILE:CD1	2.87	0.49
2:D:599:HIS:CG	2:D:735:TRP:HH2	2.30	0.49
3:I:2:ILE:HA	3:I:25:SER:O	2.13	0.49
3:L:35:LEU:HB3	3:L:93:VAL:HB	1.95	0.49
4:M:540:PRO:HB3	4:M:666:LYS:CD	2.42	0.49
2:D:686:GLY:N	4:N:550:ASP:C	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:718:ASN:OD1	4:N:590:LEU:HD22	2.12	0.48
2:F:730:THR:HB	2:F:732:HIS:CE1	2.47	0.48
2:H:518:HIS:NE2	2:H:731:ASN:C	2.66	0.48
2:H:536:ARG:O	2:H:669:VAL:HG11	2.07	0.48
3:K:35:LEU:HB3	3:K:93:VAL:HB	1.95	0.48
3:L:48:MET:HG2	3:L:63:PHE:CE1	2.48	0.48
2:B:547:LYS:HE2	2:B:755:ILE:O	2.13	0.48
2:B:547:LYS:C	2:B:667:ILE:HD11	2.34	0.48
2:B:718:ASN:CG	4:M:590:LEU:HD22	2.34	0.48
3:L:18:VAL:O	3:L:81:GLN:HA	2.14	0.48
1:A:289:ARG:HH21	1:E:353:GLN:CD	2.17	0.48
2:D:775:THR:HG21	1:G:199:GLN:HE22	1.73	0.48
1:E:86:PRO:CB	1:E:228:THR:N	2.77	0.48
2:H:716:VAL:H	4:P:591:TRP:HD1	1.60	0.48
3:I:18:VAL:O	3:I:81:GLN:HA	2.14	0.48
3:J:2:ILE:HA	3:J:25:SER:O	2.13	0.48
3:K:98:ILE:HB	4:O:550:ASP:CA	2.40	0.48
4:O:514:SER:HG	4:O:606(A):LEU:HD22	1.76	0.48
2:D:597:MET:HB2	2:D:662:ALA:HB1	1.95	0.48
2:D:689:LYS:HD2	3:J:98:ILE:HD13	1.95	0.48
3:I:35:LEU:HB3	3:I:93:VAL:HB	1.95	0.48
3:I:48:MET:HG2	3:I:63:PHE:CE1	2.48	0.48
4:N:580:THR:HG1	4:N:607:GLY:HA3	1.78	0.48
2:B:684:GLN:HG2	4:M:550:ASP:HB2	1.89	0.48
1:E:86:PRO:CB	1:E:227:GLY:CA	2.92	0.48
3:I:77:THR:CG2	3:I:79:TYR:CE2	2.84	0.48
3:L:77:THR:CG2	3:L:79:TYR:OH	2.48	0.48
4:N:513:THR:HG22	4:N:606:VAL:HG22	1.95	0.48
1:A:123:ARG:CZ	1:C:149:ASN:HD22	2.19	0.48
2:B:635:VAL:O	2:B:636:ILE:HG12	2.14	0.48
2:D:704:GLY:N	4:N:530(A):THR:CG2	2.72	0.48
2:F:597:MET:HB2	2:F:662:ALA:HB1	1.95	0.48
2:F:719:ASN:ND2	4:O:571:ALA:HB2	2.29	0.48
2:H:547:LYS:C	2:H:667:ILE:HD11	2.34	0.48
2:H:596:THR:H	2:H:662:ALA:HB2	1.72	0.48
3:I:11:VAL:CG2	3:I:148:GLU:N	2.70	0.48
3:L:93:VAL:HG22	3:L:103:TRP:CE3	2.49	0.48
1:A:86:PRO:CB	1:A:227:GLY:CA	2.92	0.48
2:B:596:THR:H	2:B:662:ALA:HB2	1.72	0.48
2:B:716:VAL:HG23	4:M:532:CYS:HG	1.16	0.48
1:C:86:PRO:CB	1:C:227:GLY:CA	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:PRO:CB	1:G:228:THR:N	2.76	0.48
2:H:597:MET:HB2	2:H:662:ALA:HB1	1.95	0.48
2:H:716:VAL:HG13	4:P:591:TRP:CB	2.02	0.48
2:H:717:ILE:CG2	4:P:530(B):SER:OG	2.62	0.48
3:I:35:LEU:HG	3:I:47:TRP:NE1	2.29	0.48
3:K:35:LEU:HG	3:K:47:TRP:NE1	2.29	0.48
4:M:513:THR:HG22	4:M:606:VAL:HG22	1.95	0.48
4:P:507:GLN:OE1	4:P:599:GLY:HA3	2.13	0.48
2:B:716:VAL:CB	4:M:591:TRP:CD1	2.92	0.48
2:D:547:LYS:HE2	2:D:755:ILE:O	2.13	0.48
2:D:599:HIS:O	2:D:755:ILE:HG22	1.51	0.48
2:D:602:LEU:CD1	2:D:758:PRO:HB3	2.39	0.48
2:D:719:ASN:N	4:N:551:THR:OG1	2.41	0.48
1:E:87:PHE:N	1:E:87:PHE:CD1	2.82	0.48
2:F:536:ARG:HD3	2:F:737:TYR:CD1	2.48	0.48
3:I:77:THR:CG2	3:I:79:TYR:OH	2.48	0.48
4:P:513:THR:HG22	4:P:606:VAL:HG22	1.95	0.48
2:B:719:ASN:ND2	4:M:571:ALA:HB2	2.29	0.47
2:D:536:ARG:HD3	2:D:737:TYR:CD1	2.48	0.47
1:E:87:PHE:HA	1:E:92:ALA:HA	1.96	0.47
2:H:520:PRO:CA	2:H:731:ASN:CA	2.51	0.47
2:H:547:LYS:HE2	2:H:755:ILE:O	2.13	0.47
2:H:687:ASN:N	4:P:550:ASP:CB	2.76	0.47
2:B:718:ASN:CA	4:M:530(B):SER:CA	2.90	0.47
2:D:670:HIS:CE1	2:D:673:PRO:HG3	2.49	0.47
2:D:687:ASN:CG	4:N:551:THR:HA	2.30	0.47
2:F:599:HIS:CG	2:F:735:TRP:HH2	2.30	0.47
2:F:635:VAL:O	2:F:636:ILE:HG12	2.14	0.47
2:H:635:VAL:O	2:H:636:ILE:HG12	2.14	0.47
2:H:672:PRO:HB2	2:H:731:ASN:OD1	2.14	0.47
3:I:11:VAL:CB	3:I:147:PRO:CB	2.86	0.47
3:J:93:VAL:HG21	3:J:103:TRP:CD2	2.49	0.47
4:M:700:HIS:ND1	4:M:700:HIS:N	2.62	0.47
2:B:597:MET:HB2	2:B:662:ALA:HB1	1.95	0.47
2:B:599:HIS:CG	2:B:735:TRP:HH2	2.30	0.47
1:C:86:PRO:CB	1:C:228:THR:N	2.77	0.47
1:C:87:PHE:HA	1:C:92:ALA:HA	1.97	0.47
2:D:717:ILE:HG22	4:N:530(A):THR:C	2.24	0.47
2:F:626:THR:C	2:F:734:LYS:CG	2.65	0.47
2:F:670:HIS:CE1	2:F:673:PRO:HG3	2.49	0.47
2:F:717:ILE:HG22	4:O:530(B):SER:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:TYR:CE1	2:H:676:PRO:CG	2.53	0.47
3:L:93:VAL:HG21	3:L:103:TRP:CD2	2.49	0.47
4:M:686:GLU:HA	4:M:708:ARG:CZ	2.45	0.47
2:D:612:THR:CA	2:D:734:LYS:HZ2	2.08	0.47
2:D:717:ILE:CG2	4:N:530(A):THR:HB	2.44	0.47
2:F:672:PRO:HB2	2:F:731:ASN:OD1	2.14	0.47
2:F:687:ASN:HB3	4:O:530(B):SER:O	2.14	0.47
1:G:87:PHE:N	1:G:87:PHE:CD1	2.82	0.47
2:H:716:VAL:CA	4:P:532:CYS:SG	3.01	0.47
3:J:18:VAL:O	3:J:81:GLN:HA	2.14	0.47
3:K:39:GLN:CD	3:K:45:PHE:CE1	2.87	0.47
4:N:700:HIS:ND1	4:N:700:HIS:N	2.62	0.47
4:O:513:THR:HG22	4:O:606:VAL:HG22	1.95	0.47
2:B:536:ARG:HD3	2:B:737:TYR:CD1	2.48	0.47
2:D:672:PRO:HB2	2:D:731:ASN:OD1	2.14	0.47
2:F:547:LYS:C	2:F:667:ILE:HD11	2.34	0.47
3:L:35:LEU:HG	3:L:47:TRP:NE1	2.29	0.47
4:P:686:GLU:HA	4:P:708:ARG:CZ	2.45	0.47
2:B:538:ARG:CB	2:B:667:ILE:HD13	2.41	0.47
2:B:640:LYS:C	2:B:641:PHE:CG	2.88	0.47
2:B:684:GLN:HA	3:I:98:ILE:HG12	1.49	0.47
2:D:547:LYS:C	2:D:667:ILE:HD11	2.34	0.47
2:F:538:ARG:CA	2:F:737:TYR:HB2	2.42	0.47
2:H:507:ASN:CB	2:H:562:HIS:CD2	2.61	0.47
2:H:534:LEU:HD12	2:H:734:LYS:HA	1.91	0.47
2:H:538:ARG:CB	2:H:667:ILE:HD13	2.41	0.47
1:A:295:SER:OG	1:E:319:LYS:HE3	2.14	0.47
1:A:323:SER:HB2	1:E:319:LYS:NZ	2.27	0.47
2:B:527:SER:CA	2:B:733:LYS:HE3	2.40	0.47
2:B:670:HIS:CE1	2:B:673:PRO:HG3	2.49	0.47
1:C:91:GLY:HA2	2:D:678:ARG:HB2	1.84	0.47
2:F:534:LEU:HD12	2:F:734:LYS:HA	1.91	0.47
2:F:535:GLU:O	2:F:736:GLN:CA	2.63	0.47
2:F:718:ASN:HD21	4:O:533:ALA:N	2.10	0.47
2:H:537:ILE:HD11	2:H:735:TRP:O	2.15	0.47
3:I:99:SER:HA	4:M:596:TRP:CH2	2.50	0.47
3:J:2:ILE:CD1	3:J:94:ARG:HH12	1.83	0.47
3:K:18:VAL:O	3:K:81:GLN:HA	2.14	0.47
3:L:24:ALA:HB1	3:L:27:TYR:HE1	1.75	0.47
3:L:35:LEU:CD2	3:L:37:VAL:HG22	2.12	0.47
3:L:45:PHE:HE1	4:P:587:PHE:CZ	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:99:SER:HA	4:P:596:TRP:CH2	2.50	0.47
4:N:686:GLU:HA	4:N:708:ARG:CZ	2.45	0.47
4:P:700:HIS:ND1	4:P:700:HIS:N	2.62	0.47
1:A:152:HIS:CA	1:C:191:PRO:HB3	2.35	0.47
2:B:535:GLU:CA	2:B:670:HIS:N	2.78	0.47
2:B:536:ARG:HE	2:B:737:TYR:C	2.14	0.47
2:D:640:LYS:C	2:D:641:PHE:CG	2.88	0.47
2:F:538:ARG:CB	2:F:667:ILE:HD13	2.41	0.47
2:F:719:ASN:OD1	4:O:551:THR:HG23	2.15	0.47
2:H:535:GLU:O	2:H:736:GLN:CA	2.63	0.47
2:H:548:ILE:H	2:H:755:ILE:HD13	1.80	0.47
3:K:48:MET:HG2	3:K:63:PHE:CE1	2.48	0.47
4:N:547:LEU:HA	4:N:558:VAL:HG21	1.97	0.47
2:B:672:PRO:HB2	2:B:731:ASN:OD1	2.14	0.47
1:C:87:PHE:N	1:C:87:PHE:CD1	2.82	0.47
2:D:536:ARG:CD	2:D:738:ASN:CB	2.58	0.47
2:D:635:VAL:O	2:D:636:ILE:HG12	2.14	0.47
3:J:11:VAL:CG2	3:J:148:GLU:N	2.70	0.47
3:J:35:LEU:HG	3:J:47:TRP:NE1	2.29	0.47
3:L:103:TRP:CB	4:P:544:PHE:HB2	2.45	0.47
1:A:87:PHE:HA	1:A:92:ALA:HA	1.97	0.47
2:B:535:GLU:O	2:B:736:GLN:CA	2.63	0.47
2:B:548:ILE:C	2:B:755:ILE:HG12	2.36	0.47
2:D:548:ILE:C	2:D:755:ILE:HG12	2.36	0.47
2:D:627:HIS:CG	2:D:734:LYS:CB	2.64	0.47
2:F:643:SER:HA	2:F:644:ARG:HB3	1.52	0.47
1:G:95:PHE:O	2:H:724:GLN:O	2.33	0.47
2:H:640:LYS:C	2:H:641:PHE:CG	2.88	0.47
2:H:687:ASN:CG	4:P:533:ALA:N	2.69	0.47
3:J:35:LEU:HB3	3:J:93:VAL:HB	1.95	0.47
3:K:32:TYR:CZ	3:K:96:TYR:CG	2.96	0.47
4:O:547:LEU:HA	4:O:558:VAL:HG21	1.97	0.47
4:O:700:HIS:N	4:O:700:HIS:ND1	2.62	0.47
1:A:86:PRO:CB	1:A:228:THR:N	2.77	0.46
1:A:95:PHE:O	2:B:724:GLN:O	2.33	0.46
2:F:719:ASN:OD1	4:O:565:SER:C	2.53	0.46
2:H:536:ARG:HD3	2:H:737:TYR:CD1	2.48	0.46
3:I:93:VAL:HG21	3:I:103:TRP:CD2	2.50	0.46
4:O:686:GLU:HA	4:O:708:ARG:CZ	2.45	0.46
2:B:549:GLN:HG2	2:B:669:VAL:HG23	0.84	0.46
1:C:95:PHE:CD2	2:D:724:GLN:O	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:535:GLU:O	2:D:736:GLN:CA	2.63	0.46
2:D:536:ARG:HE	2:D:737:TYR:C	2.14	0.46
2:F:594:THR:O	2:F:660:THR:CA	2.64	0.46
1:G:87:PHE:HA	1:G:92:ALA:HA	1.97	0.46
3:J:93:VAL:HG22	3:J:103:TRP:CD2	2.51	0.46
3:K:30:THR:CG2	3:K:53:ASN:ND2	2.78	0.46
2:B:599:HIS:CA	2:B:754:LYS:O	2.63	0.46
2:D:612:THR:HG23	2:D:734:LYS:HZ1	1.81	0.46
2:F:627:HIS:CG	2:F:734:LYS:CB	2.63	0.46
2:F:719:ASN:ND2	4:O:530:VAL:HG12	2.31	0.46
1:G:95:PHE:CD2	2:H:724:GLN:O	2.68	0.46
2:H:599:HIS:CA	2:H:754:LYS:O	2.64	0.46
3:I:32:TYR:CZ	3:I:96:TYR:CZ	2.84	0.46
3:J:99:SER:HA	4:N:596:TRP:CH2	2.50	0.46
4:O:540:PRO:HB3	4:O:666:LYS:CD	2.42	0.46
2:B:685:SER:C	4:M:553:ASN:H	1.94	0.46
2:F:627:HIS:CD2	2:F:734:LYS:CG	2.86	0.46
1:G:28:VAL:HG23	1:G:329:ALA:HB1	1.98	0.46
2:H:518:HIS:NE2	2:H:731:ASN:N	2.64	0.46
2:H:594:THR:O	2:H:660:THR:CA	2.64	0.46
3:L:12:LYS:HD2	3:L:16:GLU:OE1	2.16	0.46
3:L:71:LEU:HD13	3:L:73:ILE:CG1	2.46	0.46
3:L:93:VAL:CG1	3:L:100:LEU:HB3	2.46	0.46
4:P:547:LEU:HA	4:P:558:VAL:HG21	1.97	0.46
1:A:87:PHE:N	1:A:87:PHE:CD1	2.82	0.46
2:B:596:THR:C	2:B:662:ALA:CB	2.84	0.46
2:F:599:HIS:CA	2:F:754:LYS:O	2.64	0.46
2:F:640:LYS:C	2:F:641:PHE:CG	2.88	0.46
2:H:548:ILE:C	2:H:755:ILE:HG12	2.36	0.46
2:H:685:SER:CB	4:P:549:GLY:H	2.28	0.46
3:I:93:VAL:HG22	3:I:103:TRP:CE3	2.49	0.46
3:I:103:TRP:CB	4:M:544:PHE:HB2	2.45	0.46
3:J:47:TRP:NE1	3:J:49:GLY:O	2.49	0.46
3:K:11:VAL:CB	3:K:147:PRO:CB	2.86	0.46
3:K:93:VAL:HG21	3:K:103:TRP:CD2	2.49	0.46
3:K:93:VAL:HG22	3:K:103:TRP:CE3	2.49	0.46
3:L:47:TRP:NE1	3:L:49:GLY:O	2.49	0.46
1:A:28:VAL:HG23	1:A:329:ALA:HB1	1.98	0.46
1:A:95:PHE:CD2	2:B:724:GLN:O	2.68	0.46
2:F:596:THR:C	2:F:662:ALA:CB	2.84	0.46
2:F:715:LYS:CD	4:O:593:ASN:CG	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:625:CYS:SG	2:H:734:LYS:CG	2.94	0.46
4:M:640:TYR:HA	4:M:641:PRO:C	2.36	0.46
2:D:535:GLU:CA	2:D:670:HIS:N	2.78	0.46
2:F:537:ILE:HD11	2:F:735:TRP:O	2.15	0.46
2:F:684:GLN:HG2	3:K:98:ILE:HB	1.11	0.46
3:I:71:LEU:HD13	3:I:73:ILE:CG1	2.46	0.46
3:J:103:TRP:CB	4:N:544:PHE:HB2	2.45	0.46
3:K:99:SER:HA	4:O:596:TRP:CH2	2.50	0.46
2:B:536:ARG:NH1	2:B:738:ASN:HB3	2.31	0.46
2:B:594:THR:O	2:B:660:THR:CA	2.64	0.46
1:C:28:VAL:HG23	1:C:329:ALA:HB1	1.98	0.46
1:C:95:PHE:O	2:D:724:GLN:O	2.33	0.46
2:H:519:CYS:C	2:H:733:LYS:CG	2.75	0.46
2:H:627:HIS:CG	2:H:734:LYS:CB	2.63	0.46
3:I:93:VAL:HG22	3:I:103:TRP:CD2	2.51	0.46
3:J:30:THR:CG2	3:J:53:ASN:ND2	2.78	0.46
3:J:100:LEU:N	4:N:534:ASN:OD1	2.43	0.46
3:K:103:TRP:CB	4:O:544:PHE:HB2	2.45	0.46
3:K:213:ARG:HH21	4:O:619:PRO:CD	2.08	0.46
3:L:30:THR:CG2	3:L:53:ASN:ND2	2.78	0.46
3:L:93:VAL:HG22	3:L:103:TRP:CD2	2.51	0.46
4:O:650:VAL:H	4:O:655:VAL:HG23	1.81	0.46
1:A:93:TYR:HB2	2:B:676:PRO:HB2	1.98	0.46
2:D:536:ARG:NH1	2:D:738:ASN:HB3	2.31	0.46
2:D:594:THR:O	2:D:660:THR:CA	2.64	0.46
1:E:28:VAL:HG23	1:E:329:ALA:HB1	1.98	0.46
2:H:687:ASN:ND2	4:P:550:ASP:N	2.63	0.46
3:J:12:LYS:HD2	3:J:16:GLU:OE1	2.16	0.46
3:J:33:PRO:CB	3:J:51:ILE:O	2.64	0.46
3:J:93:VAL:CG1	3:J:100:LEU:HB3	2.46	0.46
3:J:114:ALA:CB	3:J:146:PHE:CD2	2.77	0.46
3:K:93:VAL:HG22	3:K:103:TRP:CD2	2.51	0.46
4:O:666:LYS:HB3	4:O:666:LYS:HE2	1.73	0.46
2:B:507:ASN:OD1	2:B:556:ILE:HG12	2.14	0.46
2:D:545:THR:CG2	2:D:758:PRO:CG	2.81	0.46
1:E:95:PHE:CD2	2:F:724:GLN:O	2.68	0.46
2:F:518:HIS:NE2	2:F:731:ASN:N	2.64	0.46
2:H:538:ARG:CA	2:H:737:TYR:HB2	2.42	0.46
3:I:93:VAL:CG1	3:I:100:LEU:HB3	2.46	0.46
3:J:71:LEU:HD13	3:J:73:ILE:CG1	2.46	0.46
3:K:45:PHE:HE1	4:O:587:PHE:CZ	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:47:TRP:NE1	3:K:49:GLY:O	2.49	0.46
4:N:650:VAL:H	4:N:655:VAL:HG23	1.81	0.46
2:D:599:HIS:CA	2:D:754:LYS:O	2.64	0.45
2:D:717:ILE:HG23	4:N:530(C):SER:OG	2.16	0.45
2:H:545:THR:CG2	2:H:758:PRO:CG	2.81	0.45
3:J:213:ARG:HH21	4:N:619:PRO:CD	2.08	0.45
3:K:33:PRO:CB	3:K:51:ILE:O	2.64	0.45
3:L:100:LEU:N	4:P:534:ASN:OD1	2.43	0.45
4:O:640:TYR:HA	4:O:641:PRO:C	2.36	0.45
2:B:509:TYR:CZ	2:B:556:ILE:HD13	2.52	0.45
2:D:534:LEU:HD12	2:D:734:LYS:HA	1.91	0.45
2:D:596:THR:C	2:D:662:ALA:CB	2.84	0.45
1:E:95:PHE:O	2:F:724:GLN:O	2.33	0.45
1:E:110:LYS:HG3	1:E:213:VAL:HG11	1.99	0.45
3:I:2:ILE:CD1	3:I:94:ARG:HH11	2.15	0.45
3:I:12:LYS:HD2	3:I:16:GLU:OE1	2.16	0.45
3:J:2:ILE:CD1	3:J:94:ARG:HH11	2.15	0.45
3:K:71:LEU:HD13	3:K:73:ILE:CG1	2.46	0.45
3:L:11:VAL:CG2	3:L:148:GLU:N	2.70	0.45
4:M:650:VAL:H	4:M:655:VAL:HG23	1.81	0.45
4:N:666:LYS:HB3	4:N:666:LYS:HE2	1.73	0.45
1:A:85:TYR:HE1	1:A:87:PHE:HZ	1.63	0.45
2:D:537:ILE:HD11	2:D:735:TRP:O	2.15	0.45
2:D:717:ILE:CG2	4:N:530(B):SER:OG	2.64	0.45
2:F:537:ILE:HG13	2:F:735:TRP:O	2.17	0.45
2:F:548:ILE:C	2:F:755:ILE:HG12	2.36	0.45
2:H:536:ARG:NH1	2:H:738:ASN:HB3	2.31	0.45
2:H:596:THR:C	2:H:662:ALA:CB	2.84	0.45
2:H:719:ASN:HA	4:P:551:THR:OG1	2.16	0.45
3:K:12:LYS:HD2	3:K:16:GLU:OE1	2.16	0.45
4:M:561:ARG:CZ	4:M:562:PHE:HE2	2.30	0.45
2:B:684:GLN:NE2	3:I:98:ILE:CD1	2.77	0.45
2:D:518:HIS:N	2:D:671:MET:CE	2.80	0.45
2:F:535:GLU:O	2:F:736:GLN:CB	2.65	0.45
2:F:536:ARG:NH1	2:F:738:ASN:HB3	2.31	0.45
2:F:687:ASN:HB2	3:K:98:ILE:HG21	1.97	0.45
4:M:547:LEU:HA	4:M:558:VAL:HG21	1.97	0.45
4:M:555:ARG:CD	4:M:556:SER:O	2.62	0.45
4:O:561:ARG:CZ	4:O:562:PHE:HE2	2.29	0.45
2:B:537:ILE:HD11	2:B:735:TRP:O	2.15	0.45
2:B:687:ASN:CG	4:M:551:THR:CA	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:535:GLU:CA	2:F:670:HIS:N	2.78	0.45
2:F:536:ARG:HB3	2:F:669:VAL:CB	2.47	0.45
2:H:520:PRO:CD	2:H:733:LYS:N	2.80	0.45
2:H:719:ASN:C	4:P:530(B):SER:CB	2.75	0.45
3:K:11:VAL:CG2	3:K:148:GLU:N	2.70	0.45
4:P:555:ARG:CD	4:P:556:SER:O	2.62	0.45
1:A:24:TYR:CE1	1:E:305:ALA:CB	2.81	0.45
1:A:289:ARG:NH1	1:E:316:ALA:N	2.64	0.45
2:B:537:ILE:HG13	2:B:735:TRP:O	2.17	0.45
2:B:718:ASN:ND2	4:M:590:LEU:CD2	2.80	0.45
1:C:93:TYR:H	2:D:726:HIS:HD2	1.65	0.45
2:D:518:HIS:NE2	2:D:731:ASN:N	2.64	0.45
2:D:520:PRO:CD	2:D:733:LYS:N	2.80	0.45
2:F:549:GLN:HG2	2:F:669:VAL:HG23	0.84	0.45
2:F:685:SER:C	4:O:552:ASN:ND2	2.56	0.45
2:H:509:TYR:CZ	2:H:556:ILE:HD13	2.52	0.45
2:H:670:HIS:CE1	2:H:673:PRO:HG3	2.49	0.45
3:I:47:TRP:NE1	3:I:49:GLY:O	2.49	0.45
3:L:47:TRP:CZ2	3:L:49:GLY:HA2	2.52	0.45
4:N:640:TYR:HA	4:N:641:PRO:C	2.36	0.45
2:B:536:ARG:HB3	2:B:669:VAL:CB	2.47	0.45
2:D:542:THR:HA	2:D:636:ILE:CG1	2.37	0.45
2:D:599:HIS:CB	2:D:754:LYS:H	2.29	0.45
3:J:12:LYS:O	3:J:111:VAL:HA	2.17	0.45
3:K:98:ILE:O	4:O:532:CYS:HB3	2.17	0.45
1:A:110:LYS:HG3	1:A:213:VAL:HG11	1.99	0.45
1:C:110:LYS:HG3	1:C:213:VAL:HG11	1.99	0.45
2:D:509:TYR:CZ	2:D:556:ILE:HD13	2.52	0.45
1:E:93:TYR:H	2:F:726:HIS:HD2	1.65	0.45
2:F:520:PRO:CD	2:F:733:LYS:N	2.80	0.45
2:H:535:GLU:O	2:H:736:GLN:CB	2.65	0.45
2:H:537:ILE:HG13	2:H:735:TRP:O	2.17	0.45
3:I:103:TRP:CB	4:M:544:PHE:CB	2.95	0.45
3:J:98:ILE:O	4:N:532:CYS:HB3	2.17	0.45
3:K:93:VAL:CG1	3:K:100:LEU:HB3	2.46	0.45
3:K:100:LEU:N	4:O:534:ASN:OD1	2.43	0.45
4:N:555:ARG:CD	4:N:556:SER:O	2.62	0.45
2:B:518:HIS:N	2:B:671:MET:CE	2.80	0.45
2:B:535:GLU:O	2:B:736:GLN:CB	2.65	0.45
2:B:673:PRO:HA	2:B:745:ASN:CG	2.27	0.45
1:C:85:TYR:CD1	1:C:85:TYR:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:TYR:HD1	2:D:676:PRO:CG	1.52	0.45
2:D:535:GLU:O	2:D:736:GLN:CB	2.65	0.45
2:D:685:SER:HB2	4:N:549:GLY:N	2.24	0.45
1:E:63:CYS:HB2	2:F:700:LYS:CD	2.33	0.45
3:I:12:LYS:O	3:I:111:VAL:HA	2.17	0.45
3:J:93:VAL:HG22	3:J:103:TRP:CE3	2.49	0.45
3:L:12:LYS:O	3:L:111:VAL:HA	2.17	0.45
4:N:561:ARG:CZ	4:N:562:PHE:HE2	2.30	0.45
4:P:640:TYR:HA	4:P:641:PRO:C	2.36	0.45
2:B:518:HIS:NE2	2:B:731:ASN:N	2.64	0.45
2:B:572:ASN:N	4:P:516:GLY:HA3	1.83	0.45
2:D:641:PHE:O	2:D:642:HIS:CG	2.70	0.45
1:E:91:GLY:CA	2:F:678:ARG:N	2.72	0.45
2:F:509:TYR:CZ	2:F:556:ILE:HD13	2.52	0.45
2:H:535:GLU:CA	2:H:670:HIS:N	2.78	0.45
3:I:33:PRO:CB	3:I:51:ILE:O	2.64	0.45
3:I:47:TRP:CZ2	3:I:49:GLY:HA2	2.52	0.45
3:J:47:TRP:CZ2	3:J:49:GLY:HA2	2.52	0.45
3:L:33:PRO:CB	3:L:51:ILE:O	2.64	0.45
1:A:85:TYR:CD1	1:A:85:TYR:O	2.70	0.44
2:B:599:HIS:CB	2:B:754:LYS:H	2.29	0.44
2:B:640:LYS:O	2:B:641:PHE:CG	2.70	0.44
2:F:684:GLN:CG	3:K:98:ILE:HD13	2.47	0.44
2:H:518:HIS:N	2:H:671:MET:CE	2.80	0.44
2:H:538:ARG:CD	2:H:667:ILE:CB	2.58	0.44
2:H:715:LYS:CG	4:P:593:ASN:OD1	2.65	0.44
3:J:99:SER:OG	4:N:549:GLY:HA3	2.17	0.44
3:K:47:TRP:CZ2	3:K:49:GLY:HA2	2.52	0.44
4:N:524:ARG:HG3	4:N:524:ARG:NH1	2.32	0.44
4:O:537:GLN:NE2	4:O:539:LYS:HE3	2.32	0.44
4:P:650:VAL:H	4:P:655:VAL:HG23	1.81	0.44
2:B:519:CYS:C	2:B:733:LYS:CG	2.75	0.44
2:F:599:HIS:CB	2:F:754:LYS:H	2.29	0.44
1:G:85:TYR:O	1:G:85:TYR:CD1	2.70	0.44
1:G:110:LYS:HG3	1:G:213:VAL:HG11	1.99	0.44
3:I:39:GLN:CD	3:I:45:PHE:CE1	2.87	0.44
3:I:98:ILE:O	4:M:532:CYS:HB3	2.17	0.44
3:J:103:TRP:CB	4:N:544:PHE:CB	2.95	0.44
3:K:2:ILE:CD1	3:K:94:ARG:HH11	2.15	0.44
3:K:103:TRP:CB	4:O:544:PHE:CB	2.95	0.44
4:M:653:THR:HA	4:M:654:PRO:HD2	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:561:ARG:CZ	4:P:562:PHE:HE2	2.30	0.44
2:B:627:HIS:CG	2:B:734:LYS:CB	2.64	0.44
2:D:714:ASP:O	4:N:591:TRP:CZ2	2.71	0.44
2:D:718:ASN:C	4:N:530(B):SER:CA	2.84	0.44
2:F:520:PRO:HB3	2:F:730:THR:O	2.17	0.44
2:F:602:LEU:HD21	2:F:758:PRO:CD	2.31	0.44
1:G:86:PRO:CB	1:G:227:GLY:CA	2.92	0.44
2:H:602:LEU:HD21	2:H:758:PRO:CD	2.31	0.44
2:H:641:PHE:O	2:H:642:HIS:CG	2.70	0.44
3:I:45:PHE:HE1	4:M:587:PHE:CZ	2.33	0.44
3:L:99:SER:OG	4:P:549:GLY:HA3	2.17	0.44
4:M:537:GLN:NE2	4:M:539:LYS:HE3	2.33	0.44
4:M:555:ARG:HD2	4:M:556:SER:N	2.32	0.44
4:O:524:ARG:NH1	4:O:524:ARG:HG3	2.32	0.44
1:A:93:TYR:CE1	2:B:676:PRO:CG	2.53	0.44
2:B:520:PRO:CD	2:B:733:LYS:N	2.80	0.44
2:B:599:HIS:O	2:B:755:ILE:HG21	2.00	0.44
2:B:612:THR:CB	2:B:734:LYS:HZ1	2.30	0.44
2:B:641:PHE:O	2:B:642:HIS:CG	2.70	0.44
2:D:640:LYS:O	2:D:641:PHE:CG	2.70	0.44
2:F:627:HIS:NE2	2:F:734:LYS:O	2.51	0.44
2:F:673:PRO:HB3	2:F:745:ASN:CA	2.48	0.44
2:H:673:PRO:HB3	2:H:745:ASN:CA	2.48	0.44
3:I:99:SER:OG	4:M:549:GLY:HA3	2.17	0.44
2:B:719:ASN:CA	4:M:551:THR:CG2	2.86	0.44
2:D:719:ASN:CG	4:N:551:THR:HG23	2.37	0.44
2:F:518:HIS:N	2:F:671:MET:CE	2.80	0.44
2:F:714:ASP:O	4:O:593:ASN:O	2.36	0.44
2:H:536:ARG:HB3	2:H:669:VAL:CB	2.47	0.44
2:H:640:LYS:O	2:H:641:PHE:CG	2.70	0.44
3:J:96:TYR:CD2	3:J:97:PHE:CE2	3.06	0.44
3:L:103:TRP:CB	4:P:544:PHE:CB	2.95	0.44
4:N:555:ARG:HD2	4:N:556:SER:N	2.32	0.44
4:O:680:LEU:HD22	4:O:684:ALA:CB	2.48	0.44
2:B:627:HIS:NE2	2:B:734:LYS:O	2.51	0.44
2:D:520:PRO:HB3	2:D:730:THR:O	2.17	0.44
2:F:640:LYS:O	2:F:641:PHE:CG	2.70	0.44
2:H:507:ASN:OD1	2:H:556:ILE:HG12	2.14	0.44
3:K:96:TYR:CD2	3:K:97:PHE:CE2	3.06	0.44
4:N:537:GLN:NE2	4:N:539:LYS:HE3	2.32	0.44
4:N:554:ARG:HD3	4:N:558:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:537:GLN:NE2	4:P:539:LYS:HE3	2.33	0.44
1:A:93:TYR:H	2:B:726:HIS:HD2	1.65	0.44
2:D:673:PRO:HB3	2:D:745:ASN:CA	2.48	0.44
2:F:547:LYS:CE	2:F:667:ILE:HG23	2.48	0.44
2:H:635:VAL:O	2:H:636:ILE:HD13	2.18	0.44
2:H:687:ASN:HD22	4:P:550:ASP:CA	2.23	0.44
3:K:12:LYS:O	3:K:111:VAL:HA	2.17	0.44
4:M:554:ARG:HD3	4:M:558:VAL:HG12	2.00	0.44
4:M:686:GLU:O	4:M:686:GLU:HG3	2.18	0.44
4:N:595:LEU:C	4:N:595:LEU:HD12	2.38	0.44
4:N:683:ARG:H	4:N:683:ARG:HG2	1.64	0.44
4:P:554:ARG:HD3	4:P:558:VAL:HG12	2.00	0.44
2:D:507:ASN:OD1	2:D:556:ILE:HG12	2.14	0.44
2:F:534:LEU:O	2:F:671:MET:HA	2.18	0.44
2:H:520:PRO:HB3	2:H:730:THR:O	2.17	0.44
3:I:96:TYR:CD2	3:I:97:PHE:CE2	3.06	0.44
3:L:96:TYR:CD2	3:L:97:PHE:CE2	3.06	0.44
1:A:149:ASN:HD22	1:C:123:ARG:CZ	2.19	0.44
2:B:635:VAL:O	2:B:636:ILE:HD13	2.18	0.44
2:D:534:LEU:O	2:D:671:MET:HA	2.18	0.44
2:D:537:ILE:HG13	2:D:735:TRP:O	2.17	0.44
1:E:85:TYR:O	1:E:85:TYR:CD1	2.70	0.44
2:H:627:HIS:NE2	2:H:734:LYS:O	2.51	0.44
3:K:77:THR:CG2	3:K:79:TYR:OH	2.48	0.44
3:K:99:SER:OG	4:O:549:GLY:HA3	2.17	0.44
3:L:98:ILE:O	4:P:532:CYS:HB3	2.17	0.44
4:O:555:ARG:HD2	4:O:556:SER:N	2.32	0.44
4:O:555:ARG:CD	4:O:556:SER:O	2.62	0.44
4:P:555:ARG:HD2	4:P:556:SER:N	2.32	0.44
4:P:680:LEU:HD22	4:P:684:ALA:CB	2.48	0.44
2:B:534:LEU:O	2:B:671:MET:HA	2.18	0.43
2:B:673:PRO:CA	2:B:745:ASN:HB2	2.48	0.43
2:B:686:GLY:N	4:M:553:ASN:H	2.13	0.43
2:F:547:LYS:HE2	2:F:755:ILE:O	2.13	0.43
2:F:635:VAL:O	2:F:636:ILE:HD13	2.18	0.43
2:F:641:PHE:O	2:F:642:HIS:CG	2.71	0.43
2:H:687:ASN:HD21	4:P:533:ALA:CA	2.31	0.43
3:L:98:ILE:HB	4:P:550:ASP:CA	2.40	0.43
4:O:580:THR:HG1	4:O:607:GLY:HA3	1.79	0.43
1:A:292:ASP:OD2	1:E:353:GLN:HB2	2.18	0.43
2:B:673:PRO:HB3	2:B:745:ASN:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:HIS:NE2	2:D:734:LYS:O	2.51	0.43
2:H:547:LYS:CE	2:H:667:ILE:HG23	2.48	0.43
3:J:45:PHE:HE1	4:N:587:PHE:CZ	2.33	0.43
3:L:213:ARG:HH21	4:P:619:PRO:CD	2.08	0.43
2:B:520:PRO:HB3	2:B:730:THR:O	2.17	0.43
3:J:77:THR:CG2	3:J:79:TYR:OH	2.48	0.43
4:M:595:LEU:HD12	4:M:595:LEU:C	2.38	0.43
4:N:540:PRO:HB3	4:N:666:LYS:CD	2.42	0.43
2:B:718:ASN:HB2	4:M:531:ASN:HB2	0.90	0.43
2:D:596:THR:O	2:D:662:ALA:HB3	2.19	0.43
2:D:635:VAL:O	2:D:636:ILE:HD13	2.18	0.43
2:D:689:LYS:HB2	3:J:98:ILE:HD12	0.48	0.43
2:F:507:ASN:OD1	2:F:556:ILE:HG12	2.14	0.43
1:G:93:TYR:H	2:H:726:HIS:HD2	1.65	0.43
2:H:547:LYS:NZ	2:H:667:ILE:CG2	2.70	0.43
2:H:673:PRO:CA	2:H:745:ASN:HB2	2.49	0.43
3:I:98:ILE:HB	4:M:550:ASP:CA	2.40	0.43
3:L:77:THR:HB	3:L:79:TYR:CE1	2.54	0.43
3:L:119:PRO:HB3	3:L:145:TYR:HB3	2.00	0.43
4:O:653:THR:HA	4:O:654:PRO:HD2	1.62	0.43
4:P:666:LYS:HE2	4:P:666:LYS:HB3	1.73	0.43
4:P:686:GLU:HG3	4:P:686:GLU:O	2.18	0.43
2:D:536:ARG:HB3	2:D:669:VAL:CB	2.47	0.43
2:D:538:ARG:CB	2:D:667:ILE:HD13	2.41	0.43
2:D:547:LYS:NZ	2:D:667:ILE:CG2	2.70	0.43
2:D:548:ILE:C	2:D:755:ILE:HD13	2.39	0.43
2:D:549:GLN:HG2	2:D:669:VAL:HG23	0.84	0.43
2:D:673:PRO:CA	2:D:745:ASN:HB2	2.49	0.43
2:H:686:GLY:C	4:P:551:THR:CA	2.87	0.43
3:J:77:THR:HB	3:J:79:TYR:CE1	2.54	0.43
3:J:119:PRO:HB3	3:J:145:TYR:HB3	2.00	0.43
3:K:171:GLN:CG	4:O:660:GLU:OE2	2.60	0.43
4:M:524:ARG:NH1	4:M:524:ARG:HG3	2.32	0.43
4:N:620:PRO:CG	4:N:630:ALA:HB1	2.49	0.43
2:B:518:HIS:CE1	2:B:732:HIS:N	2.87	0.43
2:B:687:ASN:HA	4:M:551:THR:OG1	2.18	0.43
3:K:40:ALA:CA	3:K:41:PRO:CD	2.96	0.43
3:K:119:PRO:HB3	3:K:145:TYR:HB3	2.00	0.43
4:M:680:LEU:HD22	4:M:684:ALA:CB	2.48	0.43
4:O:595:LEU:C	4:O:595:LEU:HD12	2.38	0.43
4:P:524:ARG:NH1	4:P:524:ARG:HG3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:547:LYS:CE	2:D:667:ILE:HG23	2.48	0.43
1:G:85:TYR:HE1	1:G:87:PHE:HZ	1.64	0.43
1:G:90:GLY:CA	2:H:677:ASP:OD1	2.67	0.43
2:H:599:HIS:CB	2:H:754:LYS:H	2.29	0.43
3:L:40:ALA:CA	3:L:41:PRO:CD	2.96	0.43
4:O:527:ILE:O	4:O:527:ILE:HG22	2.19	0.43
4:O:620:PRO:CG	4:O:630:ALA:HB1	2.49	0.43
2:B:547:LYS:CE	2:B:667:ILE:HG23	2.48	0.43
2:B:673:PRO:HA	2:B:745:ASN:CB	2.49	0.43
2:D:673:PRO:HA	2:D:745:ASN:HB2	2.01	0.43
1:E:90:GLY:CA	2:F:677:ASP:OD1	2.67	0.43
2:F:673:PRO:CA	2:F:745:ASN:HB2	2.49	0.43
2:F:684:GLN:CG	3:K:98:ILE:CD1	2.59	0.43
2:H:534:LEU:O	2:H:671:MET:HA	2.18	0.43
2:H:626:THR:C	2:H:734:LYS:CG	2.65	0.43
4:P:527:ILE:O	4:P:527:ILE:HG22	2.19	0.43
1:A:93:TYR:N	2:B:726:HIS:HD2	2.06	0.43
2:B:685:SER:OG	4:M:549:GLY:CA	2.66	0.43
1:E:63:CYS:SG	2:F:700:LYS:HD3	2.59	0.43
2:F:671:MET:C	2:F:673:PRO:HD3	2.21	0.43
3:J:67:PHE:CD1	3:J:82:ILE:HG12	2.54	0.43
3:L:39:GLN:OE1	3:L:45:PHE:CZ	2.72	0.43
4:M:636:ILE:HG22	4:M:639:PHE:CD2	2.54	0.43
4:N:680:LEU:HD22	4:N:684:ALA:CB	2.48	0.43
4:O:538:GLU:HB2	4:O:544:PHE:CE1	2.54	0.43
4:P:595:LEU:C	4:P:595:LEU:HD12	2.38	0.43
1:A:191:PRO:HB3	1:C:152:HIS:CA	2.35	0.43
2:D:687:ASN:CG	4:N:532:CYS:CA	2.86	0.43
2:F:520:PRO:CA	2:F:731:ASN:CA	2.51	0.43
2:F:673:PRO:HA	2:F:745:ASN:HB2	2.01	0.43
2:H:673:PRO:HA	2:H:745:ASN:HB2	2.01	0.43
3:I:30:THR:CG2	3:I:53:ASN:ND2	2.78	0.43
3:I:32:TYR:CZ	3:I:96:TYR:CG	2.96	0.43
3:L:67:PHE:CD1	3:L:82:ILE:HG12	2.54	0.43
4:N:636:ILE:HG22	4:N:639:PHE:CD2	2.54	0.43
4:N:686:GLU:HG3	4:N:686:GLU:O	2.18	0.43
2:B:626:THR:C	2:B:734:LYS:CG	2.65	0.42
2:D:536:ARG:HB2	2:D:669:VAL:CA	2.42	0.42
2:D:718:ASN:N	4:N:531:ASN:HB2	2.33	0.42
2:H:716:VAL:HG23	3:L:98:ILE:HG23	2.01	0.42
3:J:24:ALA:HB1	3:J:27:TYR:HE1	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:67:PHE:CD1	3:K:82:ILE:HG12	2.54	0.42
4:M:538:GLU:HB2	4:M:544:PHE:CE1	2.54	0.42
4:M:620:PRO:CG	4:M:630:ALA:HB1	2.49	0.42
2:B:518:HIS:N	2:B:671:MET:HE1	2.31	0.42
2:B:596:THR:O	2:B:662:ALA:HB3	2.19	0.42
2:B:599:HIS:HB3	2:B:735:TRP:CZ3	2.54	0.42
1:C:63:CYS:SG	2:D:700:LYS:HD3	2.59	0.42
2:D:689:LYS:CG	3:J:98:ILE:CD1	2.83	0.42
2:F:718:ASN:CG	4:O:590:LEU:HD22	2.36	0.42
3:L:98:ILE:HG23	4:P:532:CYS:HG	1.79	0.42
4:N:538:GLU:HB2	4:N:544:PHE:CE1	2.54	0.42
2:D:718:ASN:CG	4:N:531:ASN:C	2.72	0.42
2:D:788:TYR:OH	1:G:246:GLU:CB	2.67	0.42
2:H:518:HIS:CE1	2:H:732:HIS:N	2.87	0.42
2:H:548:ILE:C	2:H:755:ILE:HD13	2.39	0.42
2:H:596:THR:O	2:H:662:ALA:HB3	2.19	0.42
3:J:39:GLN:OE1	3:J:45:PHE:CZ	2.72	0.42
3:K:4:LEU:HD23	3:K:24:ALA:HA	2.01	0.42
3:K:45:PHE:HE2	4:O:544:PHE:CE1	2.16	0.42
3:K:84:ASN:O	3:K:87:THR:HG23	2.19	0.42
3:L:40:ALA:HA	3:L:41:PRO:CD	2.49	0.42
4:N:606(A):LEU:HD12	4:N:606(A):LEU:HA	1.87	0.42
4:P:636:ILE:HG22	4:P:639:PHE:CD2	2.54	0.42
1:A:63:CYS:SG	2:B:700:LYS:HD3	2.59	0.42
1:A:126:THR:CB	1:C:126:THR:N	2.80	0.42
2:B:685:SER:OG	4:M:549:GLY:N	2.51	0.42
1:C:87:PHE:HB3	1:C:91:GLY:O	2.20	0.42
1:C:93:TYR:HB2	2:D:676:PRO:HB2	1.98	0.42
1:E:38:LEU:HB2	1:E:268:ALA:HB3	2.01	0.42
2:F:673:PRO:HA	2:F:745:ASN:CB	2.49	0.42
1:G:63:CYS:SG	2:H:700:LYS:HD3	2.59	0.42
3:I:77:THR:HB	3:I:79:TYR:CE1	2.54	0.42
3:L:39:GLN:CD	3:L:45:PHE:CE1	2.87	0.42
3:L:84:ASN:O	3:L:87:THR:HG23	2.20	0.42
1:A:90:GLY:CA	2:B:677:ASP:OD1	2.67	0.42
2:B:537:ILE:CG1	2:B:735:TRP:O	2.68	0.42
2:D:518:HIS:CE1	2:D:732:HIS:N	2.87	0.42
2:D:536:ARG:CZ	2:D:738:ASN:CA	2.92	0.42
2:D:673:PRO:HA	2:D:745:ASN:CB	2.49	0.42
2:D:720:CYS:HB2	4:N:530(B):SER:H	1.78	0.42
2:F:719:ASN:N	4:O:530(B):SER:CA	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:518:HIS:N	2:H:671:MET:HE1	2.34	0.42
2:H:673:PRO:HA	2:H:745:ASN:CB	2.49	0.42
3:L:103:TRP:HB2	4:P:544:PHE:HB2	2.01	0.42
4:N:540:PRO:CB	4:N:666:LYS:CD	2.95	0.42
4:N:680:LEU:CD1	4:N:691:TYR:CE2	3.01	0.42
4:O:686:GLU:O	4:O:686:GLU:HG3	2.18	0.42
4:P:680:LEU:CD1	4:P:691:TYR:CE2	3.01	0.42
1:A:38:LEU:HB2	1:A:268:ALA:HB3	2.01	0.42
1:A:370:CYS:HB3	1:A:371:SER:H	1.76	0.42
2:D:717:ILE:HG23	4:N:530(A):THR:CB	2.49	0.42
3:I:35:LEU:HD23	3:I:35:LEU:C	2.40	0.42
3:I:37:VAL:HB	3:I:103:TRP:HZ3	1.84	0.42
3:I:84:ASN:O	3:I:87:THR:HG23	2.20	0.42
3:J:40:ALA:HA	3:J:41:PRO:CD	2.49	0.42
3:J:103:TRP:HB2	4:N:544:PHE:HB2	2.01	0.42
3:K:48:MET:HE1	3:K:80:LEU:HD21	2.00	0.42
3:L:35:LEU:HD23	3:L:35:LEU:C	2.40	0.42
4:M:573:LEU:HD23	4:M:573:LEU:HA	1.87	0.42
4:M:666:LYS:HE2	4:M:666:LYS:HB3	1.73	0.42
4:O:559:PRO:CG	4:O:561:ARG:NH1	2.82	0.42
2:D:626:THR:HA	2:D:734:LYS:HE3	1.01	0.42
2:F:596:THR:O	2:F:662:ALA:HB3	2.19	0.42
3:K:37:VAL:HB	3:K:103:TRP:HZ3	1.85	0.42
3:K:77:THR:HB	3:K:79:TYR:CE1	2.54	0.42
4:N:527:ILE:O	4:N:527:ILE:HG22	2.19	0.42
4:O:554:ARG:HD3	4:O:558:VAL:HG12	2.00	0.42
4:O:581:GLU:HG2	4:O:581:GLU:H	1.59	0.42
1:A:87:PHE:HB3	1:A:91:GLY:O	2.20	0.42
2:D:518:HIS:N	2:D:671:MET:HE1	2.31	0.42
2:D:687:ASN:C	4:N:550:ASP:CG	2.40	0.42
2:F:536:ARG:NE	2:F:737:TYR:C	2.32	0.42
2:F:549:GLN:N	2:F:669:VAL:CG1	2.52	0.42
1:G:87:PHE:HB3	1:G:91:GLY:O	2.20	0.42
2:H:718:ASN:N	4:P:532:CYS:N	2.64	0.42
3:I:39:GLN:OE1	3:I:45:PHE:CZ	2.72	0.42
3:I:103:TRP:HB2	4:M:544:PHE:HB2	2.01	0.42
3:I:119:PRO:HB3	3:I:145:TYR:HB3	2.00	0.42
3:J:40:ALA:CA	3:J:41:PRO:CD	2.96	0.42
3:J:103:TRP:CG	4:N:544:PHE:HB3	2.55	0.42
3:K:40:ALA:HA	3:K:41:PRO:CD	2.49	0.42
3:L:37:VAL:HB	3:L:103:TRP:HZ3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:559:PRO:CG	4:M:561:ARG:NH1	2.82	0.42
4:P:625:LEU:HD23	4:P:625:LEU:HA	1.90	0.42
2:F:551:SER:CA	2:F:735:TRP:CZ2	3.03	0.42
2:F:715:LYS:HA	4:O:591:TRP:HE1	1.84	0.42
1:G:38:LEU:HB2	1:G:268:ALA:HB3	2.01	0.42
2:H:537:ILE:CG1	2:H:735:TRP:O	2.68	0.42
3:J:171:GLN:CG	4:N:660:GLU:OE2	2.60	0.42
3:K:103:TRP:CG	4:O:544:PHE:HB3	2.55	0.42
3:L:11:VAL:CG2	3:L:148:GLU:O	2.68	0.42
1:A:94:CYS:O	2:B:725:CYS:O	2.38	0.42
2:F:684:GLN:CB	3:K:98:ILE:CG2	1.78	0.42
2:F:687:ASN:CB	4:O:550:ASP:HA	2.45	0.42
2:F:720:CYS:HB2	4:O:530(B):SER:H	1.48	0.42
2:H:536:ARG:CZ	2:H:738:ASN:CA	2.92	0.42
2:H:626:THR:HA	2:H:734:LYS:HE3	1.01	0.42
3:I:67:PHE:CD1	3:I:82:ILE:HG12	2.54	0.42
3:I:103:TRP:CG	4:M:544:PHE:HB3	2.55	0.42
3:J:2:ILE:HD13	3:J:94:ARG:HH11	1.81	0.42
3:K:18:VAL:HG11	3:K:109:LEU:HD13	2.02	0.42
4:N:653:THR:HA	4:N:654:PRO:HD2	1.62	0.42
4:P:620:PRO:CG	4:P:630:ALA:HB1	2.49	0.42
2:B:536:ARG:CD	2:B:738:ASN:CB	2.58	0.41
1:G:95:PHE:O	2:H:725:CYS:N	2.53	0.41
3:I:4:LEU:HD23	3:I:24:ALA:HA	2.01	0.41
3:J:18:VAL:HG11	3:J:109:LEU:HD13	2.02	0.41
3:J:84:ASN:O	3:J:87:THR:HG23	2.20	0.41
3:K:39:GLN:OE1	3:K:45:PHE:CZ	2.72	0.41
3:K:103:TRP:HB2	4:O:544:PHE:HB2	2.01	0.41
4:M:585:ILE:HG12	4:M:603:LYS:HG3	2.02	0.41
4:O:636:ILE:HG22	4:O:639:PHE:CD2	2.54	0.41
4:P:505:VAL:HG13	4:P:523:CYS:SG	2.60	0.41
4:P:580:THR:HG1	4:P:607:GLY:HA3	1.81	0.41
1:A:126:THR:N	1:C:126:THR:CB	2.80	0.41
2:B:673:PRO:HA	2:B:745:ASN:HB2	2.01	0.41
1:C:90:GLY:CA	2:D:677:ASP:OD1	2.67	0.41
2:D:599:HIS:HB2	2:D:754:LYS:N	2.34	0.41
2:D:718:ASN:HB2	4:N:530:VAL:CG1	2.28	0.41
2:F:537:ILE:CG1	2:F:735:TRP:O	2.68	0.41
2:F:626:THR:HA	2:F:734:LYS:HE3	1.01	0.41
2:H:596:THR:N	2:H:662:ALA:CB	2.76	0.41
3:I:213:ARG:HH21	4:M:619:PRO:CD	2.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:35:LEU:HD23	3:K:35:LEU:C	2.40	0.41
3:L:4:LEU:HD23	3:L:24:ALA:HA	2.01	0.41
4:M:527:ILE:O	4:M:527:ILE:HG22	2.19	0.41
4:O:540:PRO:CB	4:O:666:LYS:CD	2.95	0.41
4:O:591:TRP:CZ3	4:O:595:LEU:CA	3.03	0.41
4:P:591:TRP:CZ3	4:P:595:LEU:CA	3.03	0.41
2:B:626:THR:HA	2:B:734:LYS:HE3	1.01	0.41
2:B:685:SER:HB3	4:M:549:GLY:H	1.82	0.41
2:D:718:ASN:HD21	4:N:533:ALA:N	1.78	0.41
1:E:87:PHE:HB3	1:E:91:GLY:O	2.20	0.41
2:F:719:ASN:ND2	4:O:530:VAL:CG1	2.84	0.41
2:H:627:HIS:CD2	2:H:734:LYS:CG	2.86	0.41
2:H:671:MET:C	2:H:673:PRO:HD3	2.21	0.41
3:I:18:VAL:HG11	3:I:109:LEU:HD13	2.02	0.41
4:P:538:GLU:HB2	4:P:544:PHE:CE1	2.54	0.41
4:P:554:ARG:HD3	4:P:558:VAL:O	2.21	0.41
2:B:687:ASN:HB2	3:I:98:ILE:CG2	2.46	0.41
2:D:718:ASN:CG	4:N:533:ALA:N	2.68	0.41
1:E:94:CYS:O	2:F:725:CYS:O	2.38	0.41
2:F:518:HIS:CE1	2:F:732:HIS:N	2.87	0.41
2:F:599:HIS:HB2	2:F:754:LYS:N	2.34	0.41
2:F:687:ASN:CB	4:O:532:CYS:N	2.73	0.41
3:J:35:LEU:HD23	3:J:35:LEU:C	2.40	0.41
4:M:505:VAL:HG13	4:M:523:CYS:SG	2.60	0.41
4:M:591:TRP:CZ3	4:M:595:LEU:CA	3.03	0.41
4:O:554:ARG:HD3	4:O:558:VAL:O	2.20	0.41
4:P:686:GLU:CA	4:P:708:ARG:NH2	2.83	0.41
1:A:289:ARG:HB3	1:E:315:VAL:HG12	1.53	0.41
1:A:295:SER:OG	1:E:319:LYS:NZ	2.53	0.41
2:B:548:ILE:H	2:B:755:ILE:HD13	1.80	0.41
2:D:689:LYS:CG	3:J:98:ILE:HD13	2.50	0.41
2:D:717:ILE:HG23	4:N:530(A):THR:HB	2.01	0.41
3:J:115:LYS:O	3:J:146:PHE:HD2	2.04	0.41
3:L:2:ILE:HD13	3:L:94:ARG:HH11	1.81	0.41
3:L:18:VAL:HG11	3:L:109:LEU:HD13	2.02	0.41
4:N:554:ARG:HD3	4:N:558:VAL:O	2.20	0.41
4:N:585:ILE:HG12	4:N:603:LYS:HG3	2.02	0.41
4:O:680:LEU:CD1	4:O:691:TYR:CE2	3.01	0.41
4:P:617:LEU:HD23	4:P:617:LEU:HA	1.89	0.41
4:P:686:GLU:CA	4:P:708:ARG:HH21	2.33	0.41
1:C:38:LEU:HB2	1:C:268:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:718:ASN:HD21	4:O:533:ALA:CA	2.33	0.41
2:H:549:GLN:HG2	2:H:669:VAL:HG23	0.84	0.41
3:I:115:LYS:O	3:I:146:PHE:HD2	2.04	0.41
3:J:66:ARG:HH22	3:J:86:ASP:CG	2.24	0.41
3:L:77:THR:CB	3:L:79:TYR:CE1	3.04	0.41
4:O:505:VAL:HG13	4:O:523:CYS:SG	2.60	0.41
4:O:547:LEU:HD12	4:O:547:LEU:HA	1.85	0.41
1:A:289:ARG:HH22	1:E:354:ILE:N	2.18	0.41
2:B:508:VAL:O	2:B:508:VAL:HG22	2.21	0.41
2:B:534:LEU:CB	2:B:735:TRP:O	2.59	0.41
2:B:686:GLY:H	4:M:551:THR:N	2.17	0.41
2:B:719:ASN:ND2	4:M:571:ALA:HA	2.36	0.41
1:E:93:TYR:CG	2:F:726:HIS:CE1	3.09	0.41
2:F:548:ILE:H	2:F:755:ILE:HD13	1.79	0.41
2:F:687:ASN:N	4:O:551:THR:N	2.64	0.41
2:F:719:ASN:C	4:O:530(B):SER:N	2.74	0.41
2:H:643:SER:HA	2:H:644:ARG:HB3	1.52	0.41
3:L:66:ARG:HH22	3:L:86:ASP:CG	2.24	0.41
3:L:96:TYR:HE2	3:L:97:PHE:CZ	2.39	0.41
3:L:98:ILE:CB	4:P:550:ASP:CG	2.77	0.41
3:L:103:TRP:CG	4:P:544:PHE:HB3	2.55	0.41
4:N:525:SER:OG	4:N:592:TYR:OH	2.23	0.41
1:C:94:CYS:O	2:D:725:CYS:O	2.38	0.41
2:D:537:ILE:CG1	2:D:735:TRP:O	2.68	0.41
1:E:370:CYS:HB3	1:E:371:SER:H	1.76	0.41
2:F:508:VAL:O	2:F:508:VAL:HG22	2.21	0.41
2:F:542:THR:HA	2:F:636:ILE:CG1	2.37	0.41
2:H:686:GLY:CA	4:P:552:ASN:CB	2.97	0.41
3:I:98:ILE:CB	4:M:550:ASP:CB	2.30	0.41
3:I:100:LEU:N	4:M:534:ASN:OD1	2.43	0.41
3:J:32:TYR:CE1	3:J:96:TYR:HB2	2.56	0.41
3:J:37:VAL:HB	3:J:103:TRP:HZ3	1.85	0.41
3:L:48:MET:HE1	3:L:80:LEU:HD21	2.02	0.41
1:A:22:PRO:HB2	1:E:306:CYS:O	2.21	0.41
1:A:93:TYR:CG	2:B:726:HIS:CE1	3.09	0.41
1:A:95:PHE:O	2:B:725:CYS:N	2.53	0.41
2:B:602:LEU:HD13	2:B:758:PRO:HG3	1.76	0.41
2:B:684:GLN:N	3:I:98:ILE:CG1	2.34	0.41
2:D:643:SER:HA	2:D:644:ARG:HB3	1.52	0.41
2:D:716:VAL:HG12	4:N:591:TRP:HD1	1.61	0.41
1:E:91:GLY:N	2:F:678:ARG:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:GLU:CB	2:H:788:TYR:OH	2.67	0.41
2:H:548:ILE:O	2:H:755:ILE:CB	2.69	0.41
3:L:115:LYS:O	3:L:146:PHE:HD2	2.04	0.41
4:N:515:PRO:HG2	4:N:606(A):LEU:O	2.03	0.41
4:N:591:TRP:CZ3	4:N:595:LEU:CA	3.03	0.41
4:O:515:PRO:HD2	4:O:606(A):LEU:HB3	2.03	0.41
4:O:606(A):LEU:HD12	4:O:606(A):LEU:HA	1.87	0.41
4:P:522:THR:HG21	4:P:570:LYS:HE2	2.03	0.41
4:P:559:PRO:CG	4:P:561:ARG:NH1	2.82	0.41
1:A:125:HIS:CD2	1:C:41:THR:OG1	2.74	0.41
2:F:599:HIS:HB3	2:F:735:TRP:CZ3	2.54	0.41
1:G:93:TYR:CG	2:H:726:HIS:CE1	3.09	0.41
1:G:94:CYS:O	2:H:725:CYS:O	2.38	0.41
3:J:4:LEU:HD23	3:J:24:ALA:HA	2.01	0.41
3:J:32:TYR:CZ	3:J:96:TYR:CZ	2.84	0.41
3:J:66:ARG:NH1	3:J:86:ASP:OD2	2.52	0.41
4:M:540:PRO:CB	4:M:666:LYS:CD	2.95	0.41
4:O:559:PRO:HG2	4:O:561:ARG:HH12	1.85	0.41
1:A:295:SER:OG	1:E:319:LYS:CE	2.69	0.40
1:C:93:TYR:CG	2:D:726:HIS:CE1	3.09	0.40
2:D:596:THR:N	2:D:662:ALA:CB	2.76	0.40
2:D:597:MET:CG	2:D:756:HIS:NE2	2.75	0.40
2:D:688:VAL:HG23	4:N:530(B):SER:HB2	2.02	0.40
3:J:77:THR:CB	3:J:79:TYR:CE1	3.04	0.40
3:K:32:TYR:CZ	3:K:96:TYR:CZ	2.84	0.40
3:K:87:THR:O	3:K:88:ALA:HB2	2.21	0.40
4:M:686:GLU:OE2	4:M:708:ARG:NH2	2.54	0.40
4:P:585:ILE:HG12	4:P:603:LYS:HG3	2.02	0.40
2:B:684:GLN:O	4:M:549:GLY:O	2.36	0.40
2:F:548:ILE:C	2:F:755:ILE:HD13	2.39	0.40
1:G:91:GLY:N	2:H:678:ARG:H	2.19	0.40
2:H:508:VAL:O	2:H:508:VAL:HG22	2.21	0.40
2:H:509:TYR:HD2	2:H:553:GLN:NE2	2.19	0.40
3:I:56:GLU:HA	3:I:57:PRO:CD	2.52	0.40
3:I:166:PHE:HE1	4:M:673:MET:HB2	1.87	0.40
3:K:32:TYR:CE1	3:K:96:TYR:HB2	2.56	0.40
4:N:581:GLU:HG2	4:N:581:GLU:H	1.59	0.40
4:P:540:PRO:HB3	4:P:666:LYS:CD	2.42	0.40
1:A:91:GLY:CA	2:B:678:ARG:N	2.72	0.40
2:B:542:THR:HB	2:B:636:ILE:O	2.22	0.40
2:B:718:ASN:HB2	4:M:530:VAL:HG13	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:TYR:HE1	1:C:87:PHE:HZ	1.64	0.40
2:D:509:TYR:HD2	2:D:553:GLN:NE2	2.19	0.40
2:D:548:ILE:H	2:D:755:ILE:HD13	1.80	0.40
1:E:91:GLY:HA2	2:F:678:ARG:HB2	1.84	0.40
3:I:32:TYR:CE1	3:I:96:TYR:HB2	2.56	0.40
3:K:11:VAL:CG2	3:K:148:GLU:O	2.68	0.40
3:K:166:PHE:HE1	4:O:673:MET:HB2	1.87	0.40
4:M:686:GLU:CA	4:M:708:ARG:NH2	2.83	0.40
4:O:522:THR:HG21	4:O:570:LYS:HE2	2.03	0.40
1:A:41:THR:OG1	1:C:125:HIS:CD2	2.74	0.40
2:B:536:ARG:HB2	2:B:669:VAL:CA	2.42	0.40
2:F:687:ASN:CG	4:O:551:THR:N	2.75	0.40
2:F:716:VAL:HB	4:O:591:TRP:CD1	2.51	0.40
1:G:93:TYR:HB2	2:H:676:PRO:HB2	1.98	0.40
3:I:87:THR:O	3:I:88:ALA:HB2	2.21	0.40
3:I:171:GLN:NE2	4:M:660:GLU:HG3	2.37	0.40
3:J:93:VAL:HG11	3:J:100:LEU:HB3	2.03	0.40
3:K:77:THR:CB	3:K:79:TYR:CE1	3.04	0.40
3:L:32:TYR:CE1	3:L:96:TYR:HB2	2.56	0.40
3:L:171:GLN:NE2	4:P:660:GLU:HG3	2.37	0.40
4:N:505:VAL:HG13	4:N:523:CYS:SG	2.60	0.40
4:N:522:THR:HG21	4:N:570:LYS:HE2	2.03	0.40
4:O:659:MET:HE3	4:O:659:MET:HB2	1.96	0.40
2:B:548:ILE:C	2:B:755:ILE:HD13	2.39	0.40
2:F:509:TYR:HD2	2:F:553:GLN:NE2	2.19	0.40
3:I:93:VAL:HG11	3:I:100:LEU:HB3	2.04	0.40
3:I:96:TYR:HE2	3:I:97:PHE:CZ	2.39	0.40
3:J:39:GLN:NE2	3:J:45:PHE:HE1	2.08	0.40
3:J:56:GLU:HA	3:J:57:PRO:CD	2.52	0.40
3:J:146:PHE:HA	3:J:147:PRO:HA	1.84	0.40
3:K:171:GLN:NE2	4:O:660:GLU:HG3	2.37	0.40
4:M:548:ILE:CG2	4:M:549:GLY:N	2.85	0.40
4:M:554:ARG:HD3	4:M:558:VAL:O	2.20	0.40
4:N:547:LEU:HD12	4:N:547:LEU:HA	1.85	0.40
4:P:606(A):LEU:HD12	4:P:606(A):LEU:HA	1.87	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	390/451 (86%)	368 (94%)	19 (5%)	3 (1%)	19	60
1	C	390/451 (86%)	368 (94%)	19 (5%)	3 (1%)	19	60
1	E	390/451 (86%)	368 (94%)	19 (5%)	3 (1%)	19	60
1	G	390/451 (86%)	369 (95%)	18 (5%)	3 (1%)	19	60
2	B	334/354 (94%)	301 (90%)	26 (8%)	7 (2%)	7	36
2	D	334/354 (94%)	301 (90%)	26 (8%)	7 (2%)	7	36
2	F	334/354 (94%)	301 (90%)	26 (8%)	7 (2%)	7	36
2	H	334/354 (94%)	301 (90%)	26 (8%)	7 (2%)	7	36
3	I	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	6	34
3	J	216/218 (99%)	196 (91%)	14 (6%)	6 (3%)	5	30
3	K	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	6	34
3	L	216/218 (99%)	196 (91%)	14 (6%)	6 (3%)	5	30
4	M	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	15	55
4	N	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	15	55
4	O	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	15	55
4	P	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	15	55
All	All	4596/4948 (93%)	4213 (92%)	313 (7%)	70 (2%)	14	46

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	644	ARG
2	B	673	PRO
2	D	644	ARG
2	D	673	PRO
2	F	644	ARG
2	F	673	PRO

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Mol	Chain	Res	Type
2	H	644	ARG
2	H	673	PRO
3	I	43	LYS
3	J	43	LYS
3	K	43	LYS
3	L	43	LYS
4	M	541	ASP
4	N	541	ASP
4	O	541	ASP
4	P	541	ASP
2	B	508	VAL
2	B	643	SER
2	D	508	VAL
2	D	643	SER
2	F	508	VAL
2	F	643	SER
2	H	508	VAL
2	H	643	SER
3	I	99	SER
3	J	99	SER
3	K	99	SER
3	L	99	SER
1	A	92	ALA
1	A	93	TYR
2	B	639	GLU
2	B	685	SER
1	C	92	ALA
1	C	93	TYR
2	D	639	GLU
2	D	685	SER
1	E	92	ALA
1	E	93	TYR
2	F	639	GLU
2	F	685	SER
1	G	92	ALA
1	G	93	TYR
2	H	639	GLU
2	H	685	SER
3	I	41	PRO
3	J	41	PRO
3	K	41	PRO
3	L	41	PRO

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Mol	Chain	Res	Type
4	M	698	GLU
4	N	698	GLU
4	O	698	GLU
4	P	698	GLU
1	A	181	LYS
1	C	181	LYS
1	E	181	LYS
1	G	181	LYS
3	I	114	ALA
3	J	114	ALA
3	K	114	ALA
3	L	114	ALA
3	I	115	LYS
3	J	115	LYS
3	K	115	LYS
3	L	115	LYS
3	J	29	PHE
3	L	29	PHE
2	B	636	ILE
2	D	636	ILE
2	F	636	ILE
2	H	636	ILE

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	328/372 (88%)	316 (96%)	12 (4%)	34	58
1	C	328/372 (88%)	316 (96%)	12 (4%)	34	58
1	E	328/372 (88%)	316 (96%)	12 (4%)	34	58
1	G	328/372 (88%)	316 (96%)	12 (4%)	34	58
2	B	298/313 (95%)	287 (96%)	11 (4%)	34	58
2	D	298/313 (95%)	287 (96%)	11 (4%)	34	58
2	F	298/313 (95%)	287 (96%)	11 (4%)	34	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	298/313 (95%)	287 (96%)	11 (4%)	34 58
3	I	188/188 (100%)	178 (95%)	10 (5%)	22 47
3	J	188/188 (100%)	178 (95%)	10 (5%)	22 47
3	K	188/188 (100%)	178 (95%)	10 (5%)	22 47
3	L	188/188 (100%)	178 (95%)	10 (5%)	22 47
4	M	178/183 (97%)	149 (84%)	29 (16%)	2 13
4	N	178/183 (97%)	149 (84%)	29 (16%)	2 13
4	O	178/183 (97%)	149 (84%)	29 (16%)	2 13
4	P	178/183 (97%)	149 (84%)	29 (16%)	2 13
All	All	3968/4224 (94%)	3720 (94%)	248 (6%)	21 43

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	75	ASP
1	A	87	PHE
1	A	103	LEU
1	A	181	LYS
1	A	203	ILE
1	A	244	LEU
1	A	327	LYS
1	A	343	GLU
1	A	350	SER
1	A	370	CYS
1	A	386	HIS
2	B	507	ASN
2	B	639	GLU
2	B	663	THR
2	B	692	VAL
2	B	715	LYS
2	B	720	CYS
2	B	722	VAL
2	B	731	ASN
2	B	735	TRP
2	B	750	ASP
2	B	763	ASN
1	C	55	ILE
1	C	75	ASP

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Mol	Chain	Res	Type
1	C	87	PHE
1	C	103	LEU
1	C	181	LYS
1	C	203	ILE
1	C	244	LEU
1	C	327	LYS
1	C	343	GLU
1	C	350	SER
1	C	370	CYS
1	C	386	HIS
2	D	507	ASN
2	D	639	GLU
2	D	663	THR
2	D	692	VAL
2	D	715	LYS
2	D	720	CYS
2	D	722	VAL
2	D	731	ASN
2	D	735	TRP
2	D	750	ASP
2	D	763	ASN
1	E	55	ILE
1	E	75	ASP
1	E	87	PHE
1	E	103	LEU
1	E	181	LYS
1	E	203	ILE
1	E	244	LEU
1	E	327	LYS
1	E	343	GLU
1	E	350	SER
1	E	370	CYS
1	E	386	HIS
2	F	507	ASN
2	F	639	GLU
2	F	663	THR
2	F	692	VAL
2	F	715	LYS
2	F	720	CYS
2	F	722	VAL
2	F	731	ASN
2	F	735	TRP

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Mol	Chain	Res	Type
2	F	750	ASP
2	F	763	ASN
1	G	55	ILE
1	G	75	ASP
1	G	87	PHE
1	G	103	LEU
1	G	181	LYS
1	G	203	ILE
1	G	244	LEU
1	G	327	LYS
1	G	343	GLU
1	G	350	SER
1	G	370	CYS
1	G	386	HIS
2	H	507	ASN
2	H	639	GLU
2	H	663	THR
2	H	692	VAL
2	H	715	LYS
2	H	720	CYS
2	H	722	VAL
2	H	731	ASN
2	H	735	TRP
2	H	750	ASP
2	H	763	ASN
3	I	1	GLN
3	I	5	VAL
3	I	7	SER
3	I	28	THR
3	I	41	PRO
3	I	43	LYS
3	I	51	ILE
3	I	61	GLU
3	I	62	GLU
3	I	71	LEU
3	J	1	GLN
3	J	5	VAL
3	J	7	SER
3	J	28	THR
3	J	41	PRO
3	J	43	LYS
3	J	51	ILE

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Mol	Chain	Res	Type
3	J	61	GLU
3	J	62	GLU
3	J	71	LEU
3	K	1	GLN
3	K	5	VAL
3	K	7	SER
3	K	28	THR
3	K	41	PRO
3	K	43	LYS
3	K	51	ILE
3	K	61	GLU
3	K	62	GLU
3	K	71	LEU
3	L	1	GLN
3	L	5	VAL
3	L	7	SER
3	L	28	THR
3	L	41	PRO
3	L	43	LYS
3	L	51	ILE
3	L	61	GLU
3	L	62	GLU
3	L	71	LEU
4	M	521	LEU
4	M	534	ASN
4	M	547	LEU
4	M	552	ASN
4	M	569	ASP
4	M	573	LEU
4	M	579	GLN
4	M	580	THR
4	M	581	GLU
4	M	603	LYS
4	M	606(A)	LEU
4	M	617	LEU
4	M	623	GLU
4	M	626	GLU
4	M	627	THR
4	M	629	LYS
4	M	632	LEU
4	M	657	GLN
4	M	659	MET

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Mol	Chain	Res	Type
4	M	663	GLN
4	M	667	GLN
4	M	668	SER
4	M	670	ASN
4	M	678	LEU
4	M	681	THR
4	M	683	ARG
4	M	686	GLU
4	M	702	VAL
4	M	706	LEU
4	N	521	LEU
4	N	534	ASN
4	N	547	LEU
4	N	552	ASN
4	N	569	ASP
4	N	573	LEU
4	N	579	GLN
4	N	580	THR
4	N	581	GLU
4	N	603	LYS
4	N	606(A)	LEU
4	N	617	LEU
4	N	623	GLU
4	N	626	GLU
4	N	627	THR
4	N	629	LYS
4	N	632	LEU
4	N	657	GLN
4	N	659	MET
4	N	663	GLN
4	N	667	GLN
4	N	668	SER
4	N	670	ASN
4	N	678	LEU
4	N	681	THR
4	N	683	ARG
4	N	686	GLU
4	N	702	VAL
4	N	706	LEU
4	O	521	LEU
4	O	534	ASN
4	O	547	LEU

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Mol	Chain	Res	Type
4	O	552	ASN
4	O	569	ASP
4	O	573	LEU
4	O	579	GLN
4	O	580	THR
4	O	581	GLU
4	O	603	LYS
4	O	606(A)	LEU
4	O	617	LEU
4	O	623	GLU
4	O	626	GLU
4	O	627	THR
4	O	629	LYS
4	O	632	LEU
4	O	657	GLN
4	O	659	MET
4	O	663	GLN
4	O	667	GLN
4	O	668	SER
4	O	670	ASN
4	O	678	LEU
4	O	681	THR
4	O	683	ARG
4	O	686	GLU
4	O	702	VAL
4	O	706	LEU
4	P	521	LEU
4	P	534	ASN
4	P	547	LEU
4	P	552	ASN
4	P	569	ASP
4	P	573	LEU
4	P	579	GLN
4	P	580	THR
4	P	581	GLU
4	P	603	LYS
4	P	606(A)	LEU
4	P	617	LEU
4	P	623	GLU
4	P	626	GLU
4	P	627	THR
4	P	629	LYS

Continued on next page...

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Mol	Chain	Res	Type
4	P	632	LEU
4	P	657	GLN
4	P	659	MET
4	P	663	GLN
4	P	667	GLN
4	P	668	SER
4	P	670	ASN
4	P	678	LEU
4	P	681	THR
4	P	683	ARG
4	P	686	GLU
4	P	702	VAL
4	P	706	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	373	GLN
2	B	572	ASN
2	B	627	HIS
2	B	670	HIS
2	B	684	GLN
2	B	693	ASN
2	B	702	ASN
2	B	718	ASN
2	B	745	ASN
2	B	756	HIS
2	B	782	GLN
1	C	149	ASN
1	C	373	GLN
2	D	627	HIS
2	D	670	HIS
2	D	687	ASN
2	D	693	ASN
2	D	702	ASN
2	D	718	ASN
2	D	745	ASN
2	D	756	HIS
2	D	782	GLN
1	E	373	GLN
2	F	627	HIS

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Mol	Chain	Res	Type
2	F	670	HIS
2	F	684	GLN
2	F	693	ASN
2	F	702	ASN
2	F	718	ASN
2	F	745	ASN
2	F	756	HIS
2	F	782	GLN
1	G	373	GLN
2	H	627	HIS
2	H	670	HIS
2	H	684	GLN
2	H	687	ASN
2	H	693	ASN
2	H	702	ASN
2	H	745	ASN
2	H	756	HIS
2	H	782	GLN
3	I	6	GLN
3	I	39	GLN
3	I	53	ASN
3	I	81	GLN
3	I	82(A)	ASN
3	I	164	HIS
3	J	6	GLN
3	J	39	GLN
3	J	53	ASN
3	J	81	GLN
3	J	82(A)	ASN
3	J	164	HIS
3	K	6	GLN
3	K	39	GLN
3	K	53	ASN
3	K	81	GLN
3	K	82(A)	ASN
3	K	164	HIS
3	L	6	GLN
3	L	39	GLN
3	L	53	ASN
3	L	81	GLN
3	L	82(A)	ASN
3	L	164	HIS

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Mol	Chain	Res	Type
4	M	579	GLN
4	M	670	ASN
4	N	579	GLN
4	N	670	ASN
4	O	579	GLN
4	O	670	ASN
4	P	552	ASN
4	P	579	GLN
4	P	670	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	D	1
2	F	1

Continued on next page...

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Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	731:ASN	C	732:HIS	N	0.73
1	D	731:ASN	C	732:HIS	N	0.73
1	F	731:ASN	C	732:HIS	N	0.73
1	H	731:ASN	C	732:HIS	N	0.73

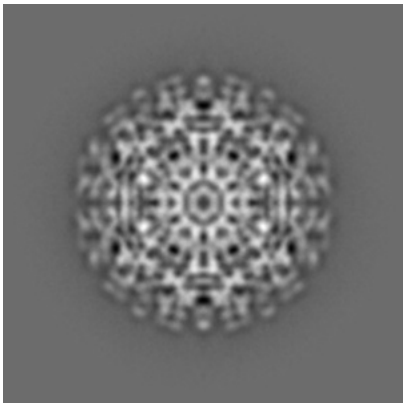
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3144. These allow visual inspection of the internal detail of the map and identification of artifacts.

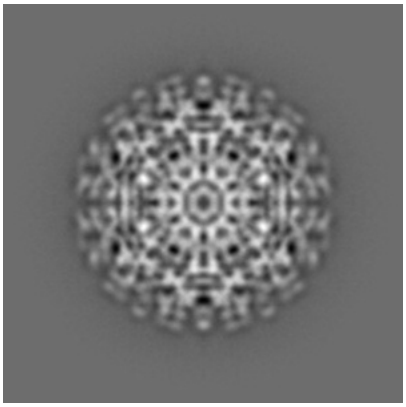
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

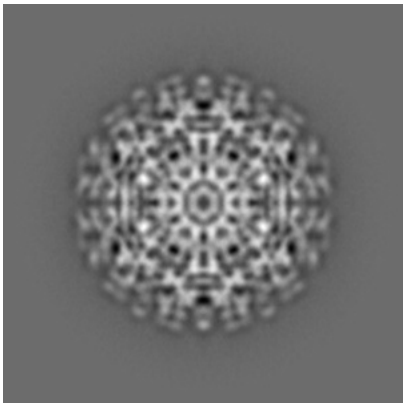
6.1.1 Primary map



X



Y

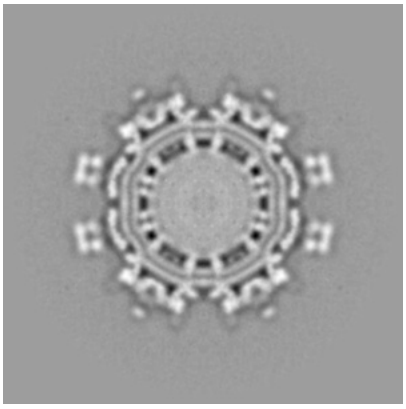


Z

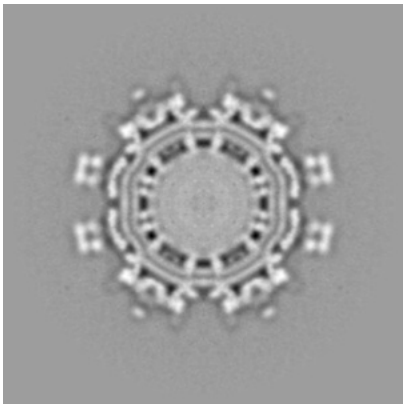
The images above show the map projected in three orthogonal directions.

6.2 Central slices

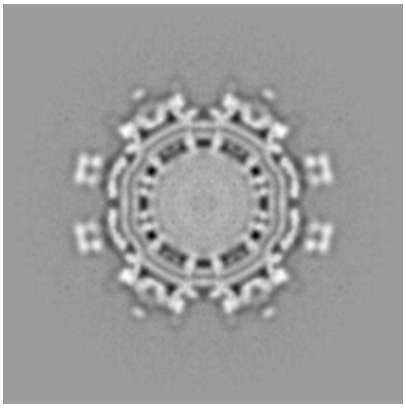
6.2.1 Primary map



X Index: 160



Y Index: 160

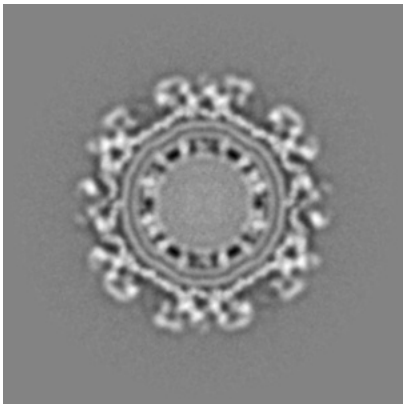


Z Index: 160

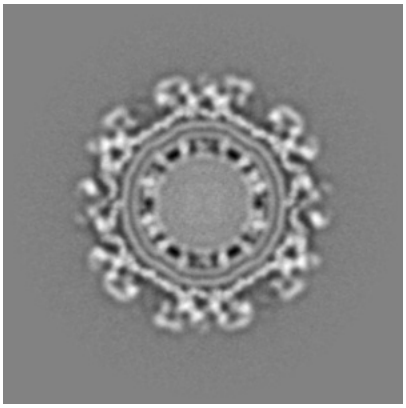
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

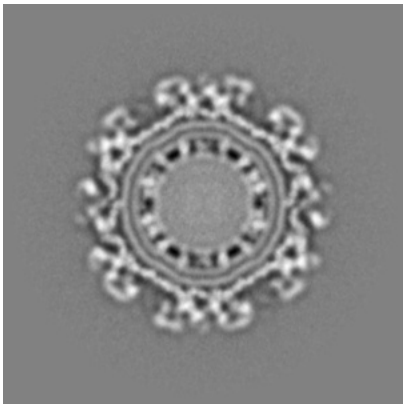
6.3.1 Primary map



X Index: 176



Y Index: 176

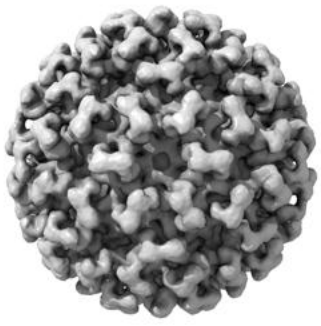


Z Index: 176

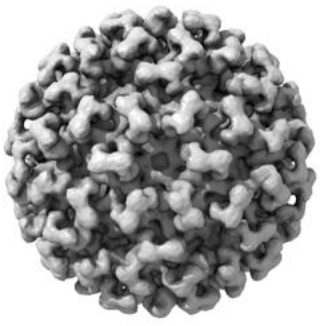
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

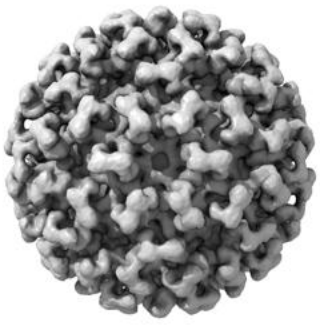
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

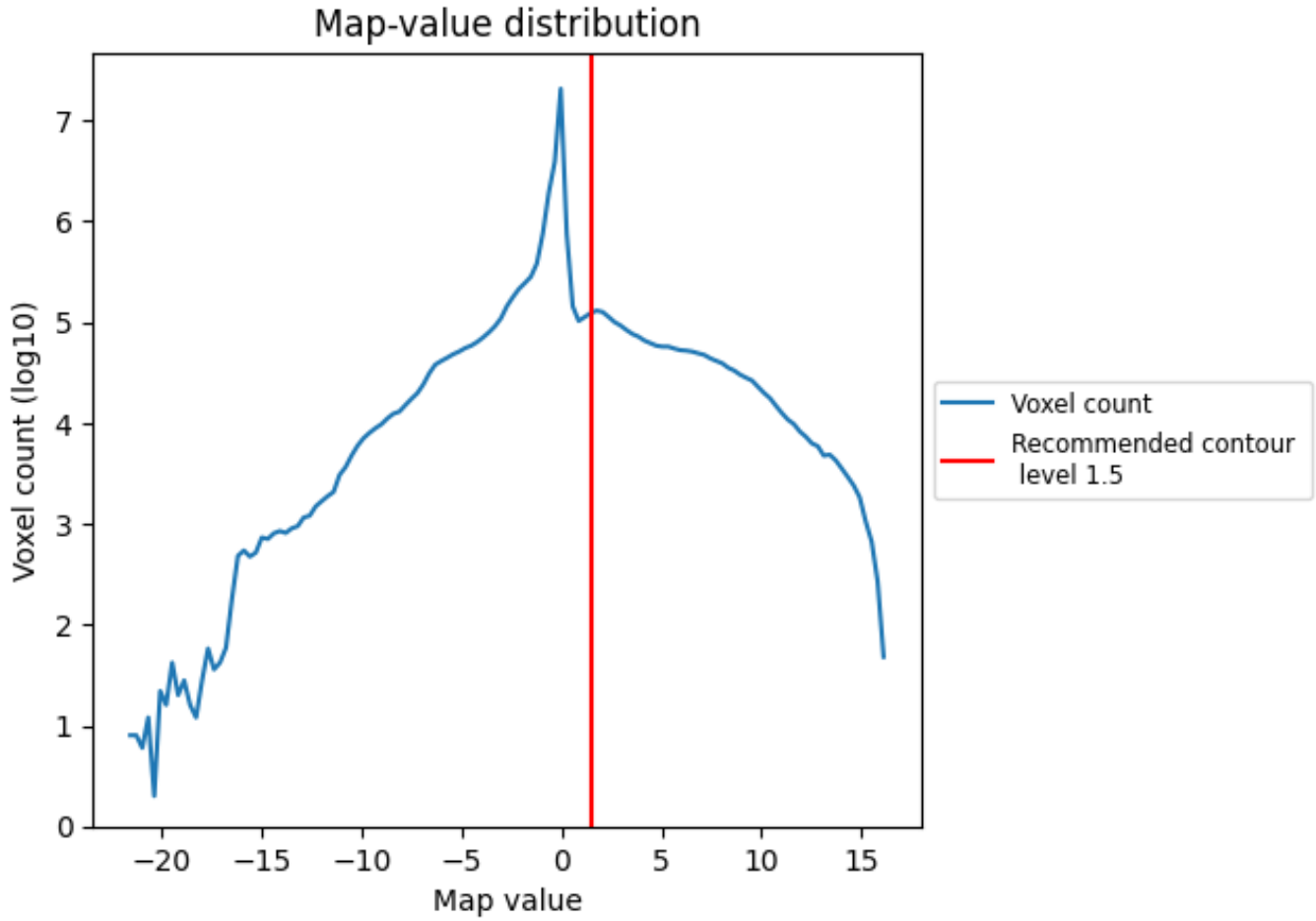
6.5 Mask visualisation (i)

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

7 Map analysis

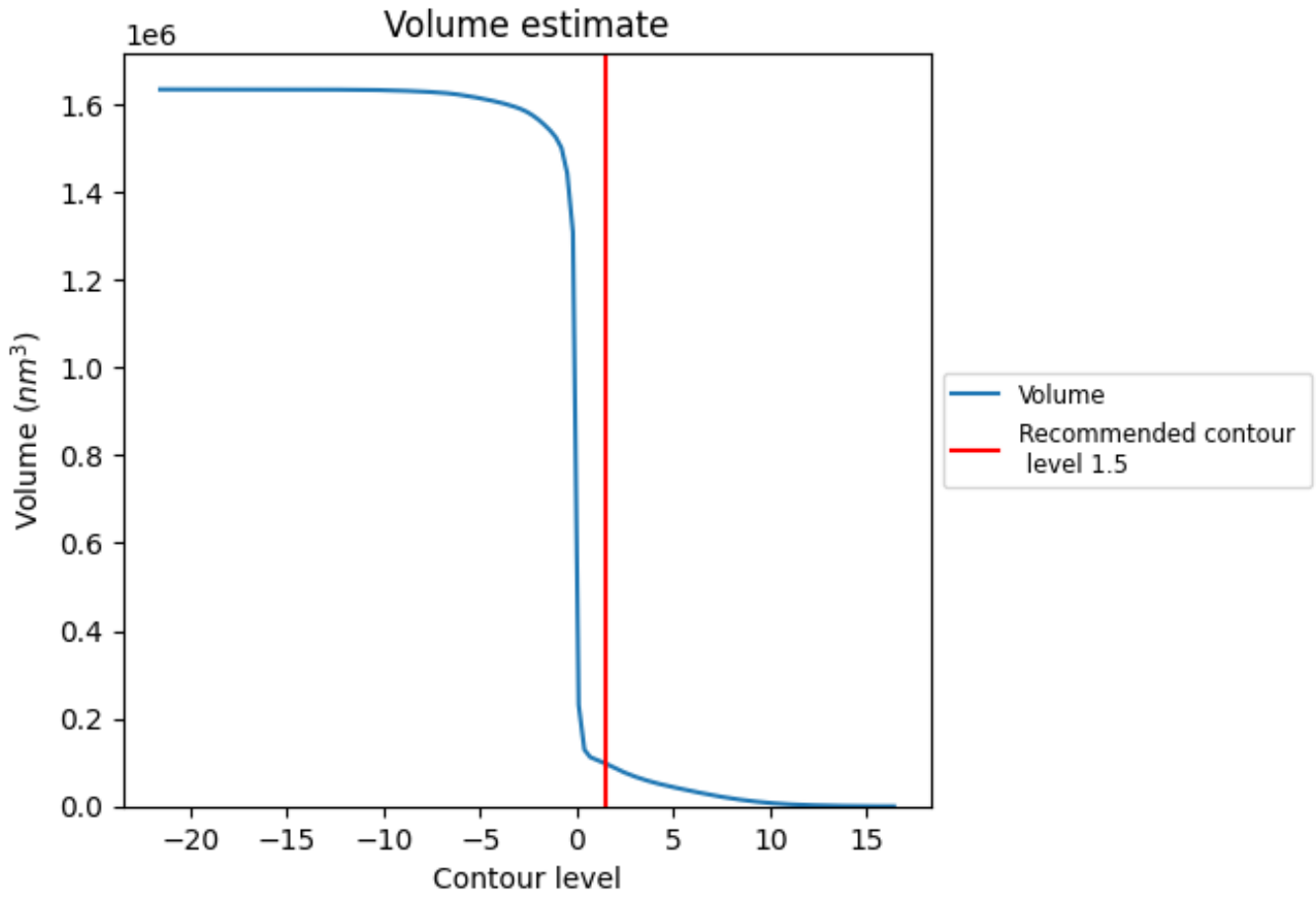
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

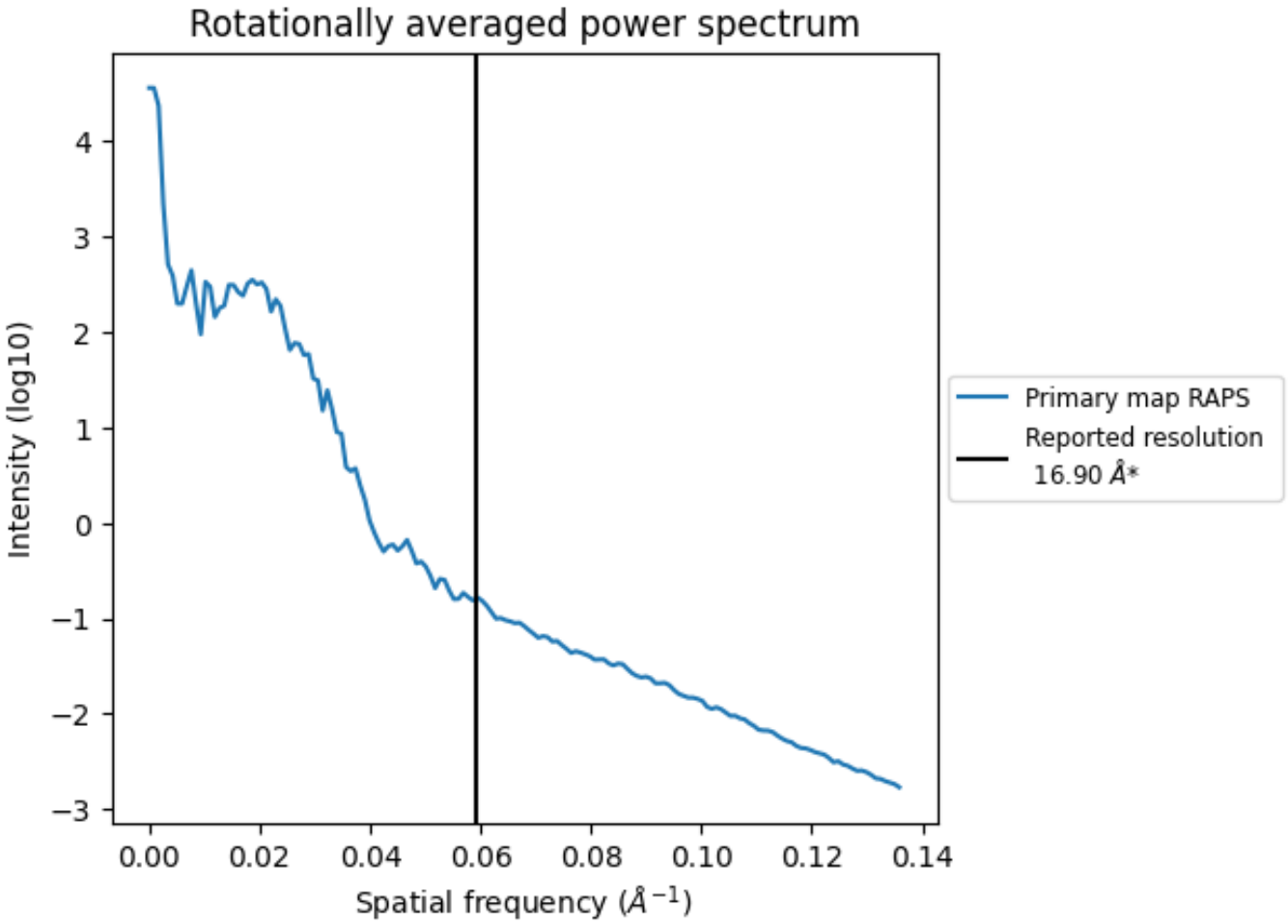
7.2 Volume estimate (i)



The volume at the recommended contour level is 97167 nm^3; this corresponds to an approximate mass of 87774 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 0.059 Å^{-1}

8 Fourier-Shell correlation (i)

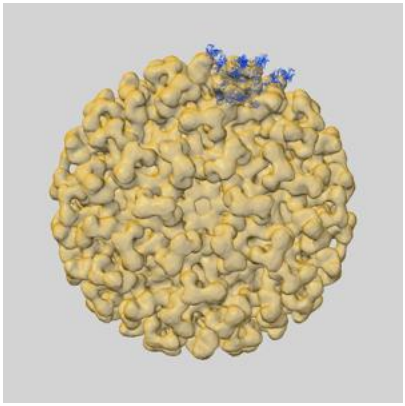
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

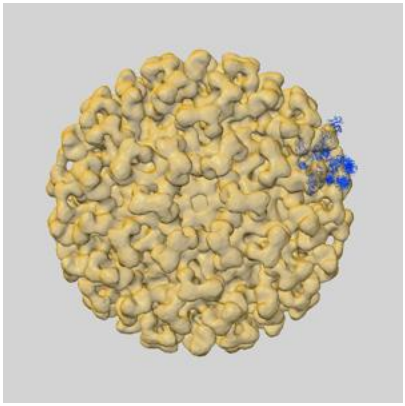
This section contains information regarding the fit between EMDB map EMD-3144 and PDB model 5ANY. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

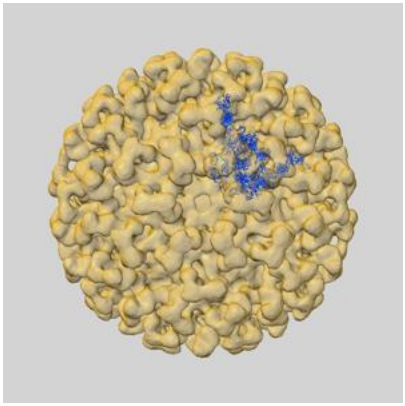
9.1.1 Map-model overlay



X

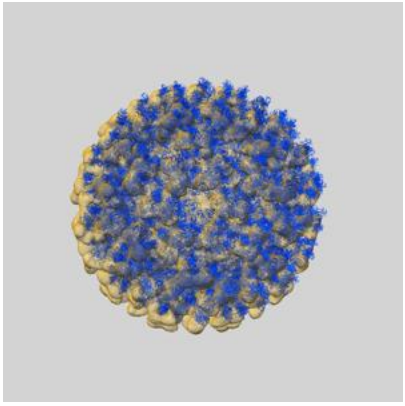


Y

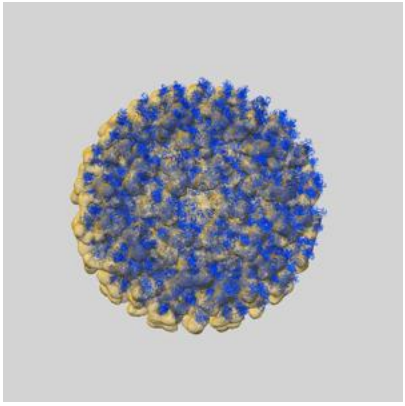


Z

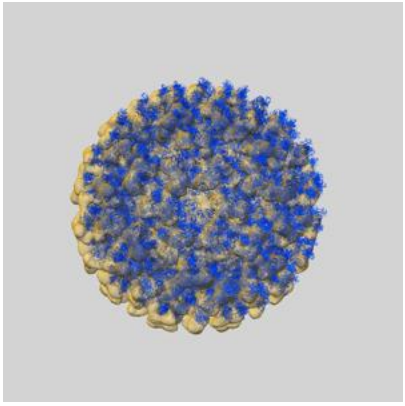
9.1.2 Map-model assembly overlay



X



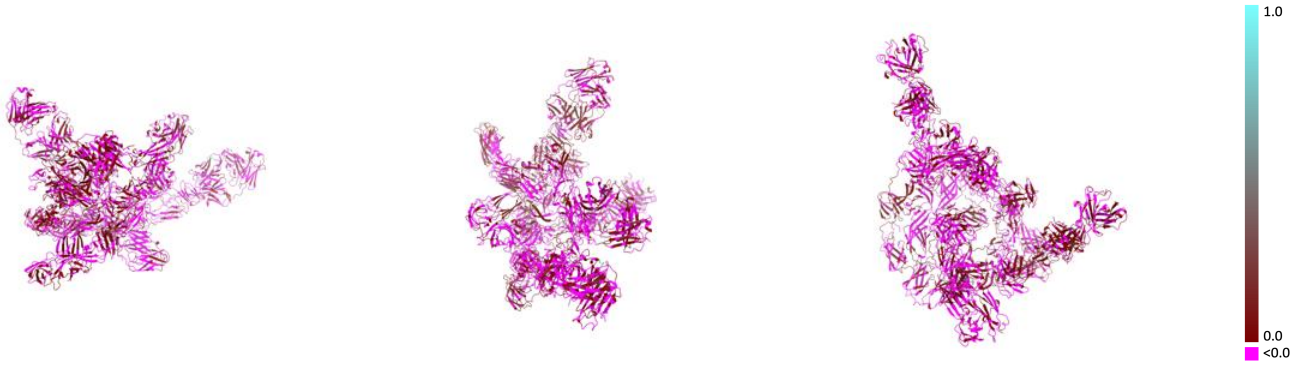
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 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.

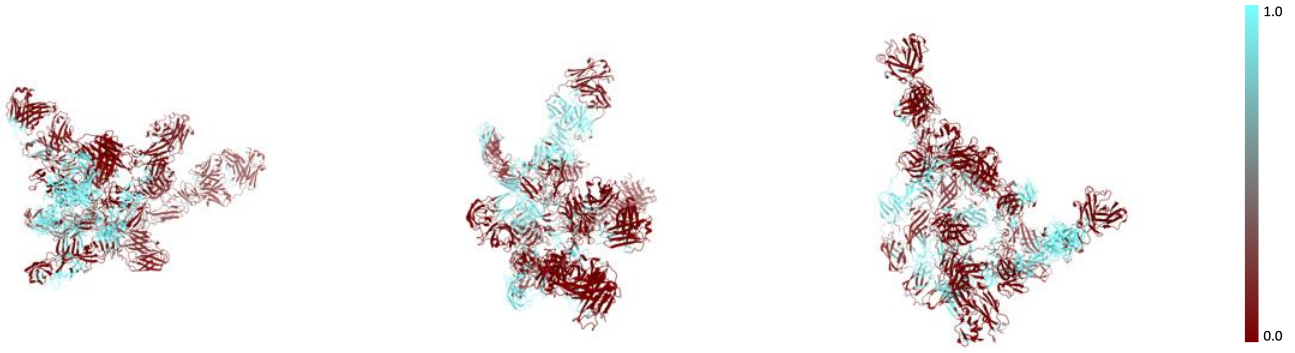
9.2 Q-score mapped to coordinate model



X Y Z

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

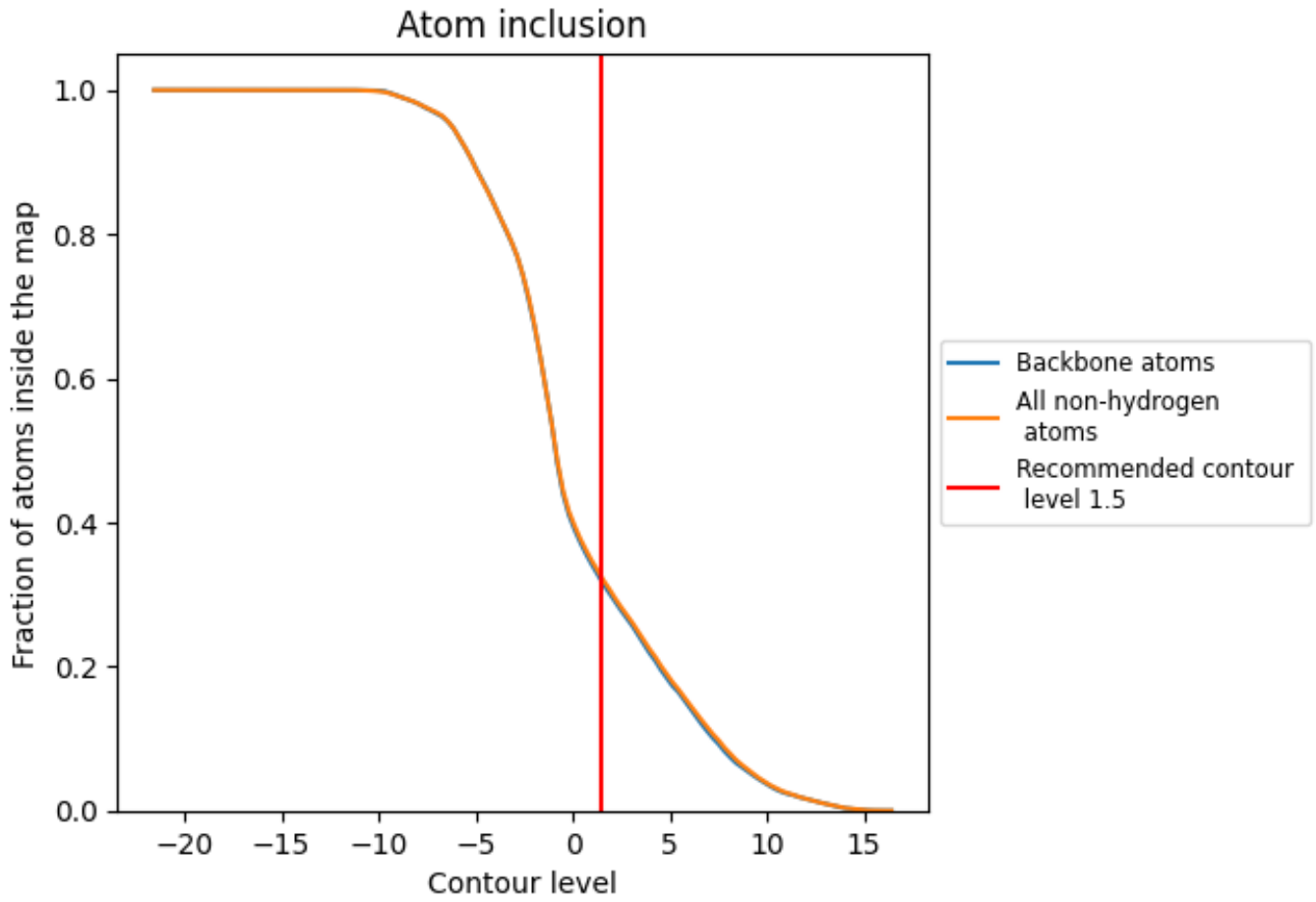
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (1.5).

9.4 Atom inclusion (i)



At the recommended contour level, 32% of all backbone atoms, 32% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3233	-0.0130
A	0.3172	-0.0210
B	0.4521	-0.0120
C	0.1598	-0.0360
D	0.2863	-0.0190
E	0.7021	0.0150
F	0.5306	-0.0060
G	0.3363	-0.0190
H	0.3540	-0.0130
I	0.0828	-0.0150
J	0.0158	-0.0110
K	0.4449	0.0160
L	0.1290	-0.0140
M	0.0420	-0.0260
N	0.2829	-0.0280
O	0.5226	0.0060
P	0.1341	-0.0210