



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:41 PM UTC

PDB ID : 6DV2 / pdb_00006dv2
Title : Crystal Structure of Human Mitochondrial Trifunctional Protein
Authors : Fu, Z.; Xia, C.; Battaile, K.P.; Kim, J.P.
Deposited on : 2018-06-22
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

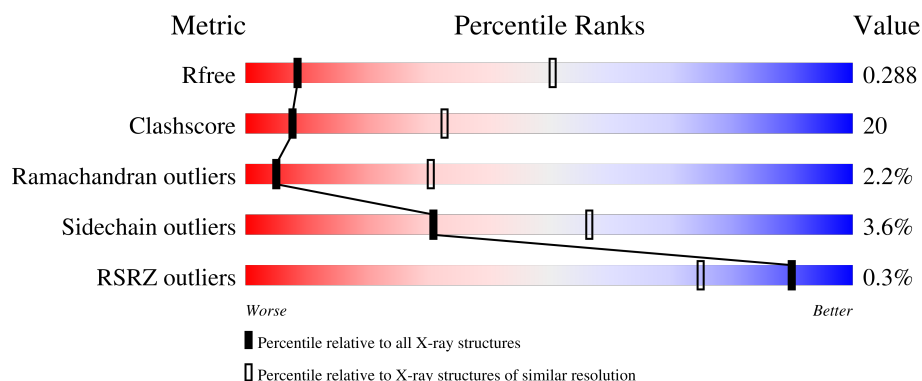
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	457	
1	B	457	
1	C	457	
1	D	457	
1	E	457	

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Mol	Chain	Length	Quality of chain
1	F	457	58% 32% 7%
2	G	727	62% 34%
2	H	727	% 62% 35%
2	I	727	63% 34%
2	J	727	65% 32%
2	K	727	63% 33%
2	L	727	63% 34%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 51375 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Trifunctional enzyme subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3267	2071	566	608	22			
1	B	419	Total	C	N	O	S	0	0	0
			3170	2012	548	589	21			
1	C	421	Total	C	N	O	S	0	0	0
			3073	1938	530	586	19			
1	D	424	Total	C	N	O	S	0	0	0
			3087	1946	533	589	19			
1	E	423	Total	C	N	O	S	0	0	0
			3082	1943	532	588	19			
1	F	425	Total	C	N	O	S	0	0	0
			3092	1949	534	590	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	HIS	-	expression tag	UNP P55084
A	19	HIS	-	expression tag	UNP P55084
A	20	HIS	-	expression tag	UNP P55084
A	21	HIS	-	expression tag	UNP P55084
A	22	HIS	-	expression tag	UNP P55084
A	23	HIS	-	expression tag	UNP P55084
A	24	SER	-	expression tag	UNP P55084
A	25	SER	-	expression tag	UNP P55084
A	26	GLY	-	expression tag	UNP P55084
A	27	LEU	-	expression tag	UNP P55084
A	28	VAL	-	expression tag	UNP P55084
A	29	PRO	-	expression tag	UNP P55084
A	30	ARG	-	expression tag	UNP P55084
A	31	GLY	-	expression tag	UNP P55084
A	32	SER	-	expression tag	UNP P55084
A	33	HIS	-	expression tag	UNP P55084
B	18	HIS	-	expression tag	UNP P55084

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Chain	Residue	Modelled	Actual	Comment	Reference
B	19	HIS	-	expression tag	UNP P55084
B	20	HIS	-	expression tag	UNP P55084
B	21	HIS	-	expression tag	UNP P55084
B	22	HIS	-	expression tag	UNP P55084
B	23	HIS	-	expression tag	UNP P55084
B	24	SER	-	expression tag	UNP P55084
B	25	SER	-	expression tag	UNP P55084
B	26	GLY	-	expression tag	UNP P55084
B	27	LEU	-	expression tag	UNP P55084
B	28	VAL	-	expression tag	UNP P55084
B	29	PRO	-	expression tag	UNP P55084
B	30	ARG	-	expression tag	UNP P55084
B	31	GLY	-	expression tag	UNP P55084
B	32	SER	-	expression tag	UNP P55084
B	33	HIS	-	expression tag	UNP P55084
C	18	HIS	-	expression tag	UNP P55084
C	19	HIS	-	expression tag	UNP P55084
C	20	HIS	-	expression tag	UNP P55084
C	21	HIS	-	expression tag	UNP P55084
C	22	HIS	-	expression tag	UNP P55084
C	23	HIS	-	expression tag	UNP P55084
C	24	SER	-	expression tag	UNP P55084
C	25	SER	-	expression tag	UNP P55084
C	26	GLY	-	expression tag	UNP P55084
C	27	LEU	-	expression tag	UNP P55084
C	28	VAL	-	expression tag	UNP P55084
C	29	PRO	-	expression tag	UNP P55084
C	30	ARG	-	expression tag	UNP P55084
C	31	GLY	-	expression tag	UNP P55084
C	32	SER	-	expression tag	UNP P55084
C	33	HIS	-	expression tag	UNP P55084
D	18	HIS	-	expression tag	UNP P55084
D	19	HIS	-	expression tag	UNP P55084
D	20	HIS	-	expression tag	UNP P55084
D	21	HIS	-	expression tag	UNP P55084
D	22	HIS	-	expression tag	UNP P55084
D	23	HIS	-	expression tag	UNP P55084
D	24	SER	-	expression tag	UNP P55084
D	25	SER	-	expression tag	UNP P55084
D	26	GLY	-	expression tag	UNP P55084
D	27	LEU	-	expression tag	UNP P55084
D	28	VAL	-	expression tag	UNP P55084

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Chain	Residue	Modelled	Actual	Comment	Reference
D	29	PRO	-	expression tag	UNP P55084
D	30	ARG	-	expression tag	UNP P55084
D	31	GLY	-	expression tag	UNP P55084
D	32	SER	-	expression tag	UNP P55084
D	33	HIS	-	expression tag	UNP P55084
E	18	HIS	-	expression tag	UNP P55084
E	19	HIS	-	expression tag	UNP P55084
E	20	HIS	-	expression tag	UNP P55084
E	21	HIS	-	expression tag	UNP P55084
E	22	HIS	-	expression tag	UNP P55084
E	23	HIS	-	expression tag	UNP P55084
E	24	SER	-	expression tag	UNP P55084
E	25	SER	-	expression tag	UNP P55084
E	26	GLY	-	expression tag	UNP P55084
E	27	LEU	-	expression tag	UNP P55084
E	28	VAL	-	expression tag	UNP P55084
E	29	PRO	-	expression tag	UNP P55084
E	30	ARG	-	expression tag	UNP P55084
E	31	GLY	-	expression tag	UNP P55084
E	32	SER	-	expression tag	UNP P55084
E	33	HIS	-	expression tag	UNP P55084
F	18	HIS	-	expression tag	UNP P55084
F	19	HIS	-	expression tag	UNP P55084
F	20	HIS	-	expression tag	UNP P55084
F	21	HIS	-	expression tag	UNP P55084
F	22	HIS	-	expression tag	UNP P55084
F	23	HIS	-	expression tag	UNP P55084
F	24	SER	-	expression tag	UNP P55084
F	25	SER	-	expression tag	UNP P55084
F	26	GLY	-	expression tag	UNP P55084
F	27	LEU	-	expression tag	UNP P55084
F	28	VAL	-	expression tag	UNP P55084
F	29	PRO	-	expression tag	UNP P55084
F	30	ARG	-	expression tag	UNP P55084
F	31	GLY	-	expression tag	UNP P55084
F	32	SER	-	expression tag	UNP P55084
F	33	HIS	-	expression tag	UNP P55084

- Molecule 2 is a protein called Trifunctional enzyme subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	725	Total	C	N	O	S	0	0	0
			5440	3455	929	1027	29			

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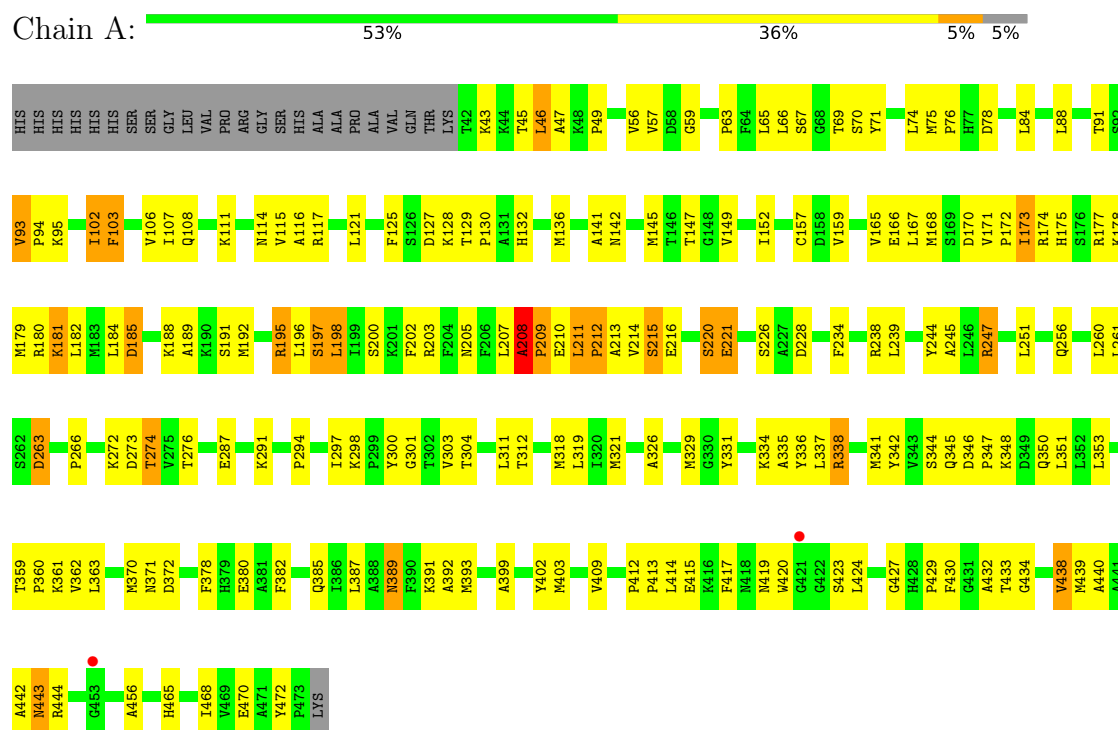
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	725	Total	C	N	O	S	0	0	0
			5440	3455	929	1027	29			
2	I	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	J	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	K	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	L	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			

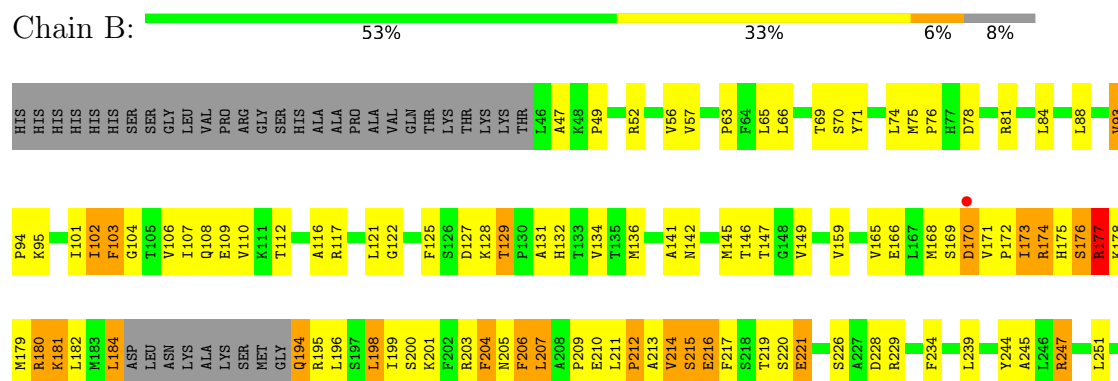
3 Residue-property plots [i](#)

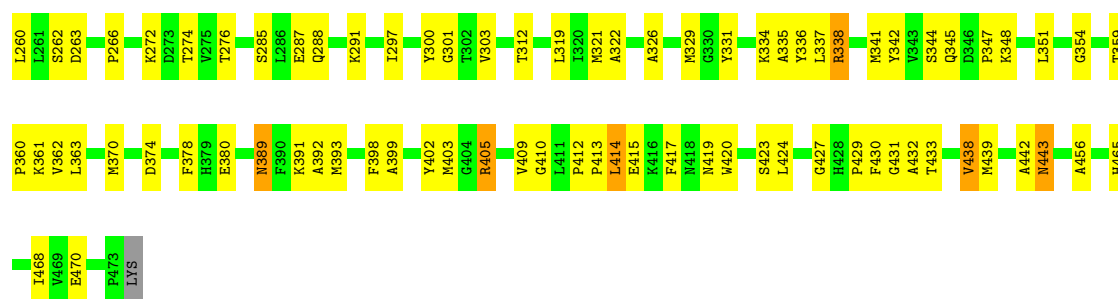
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Trifunctional enzyme subunit beta, mitochondrial



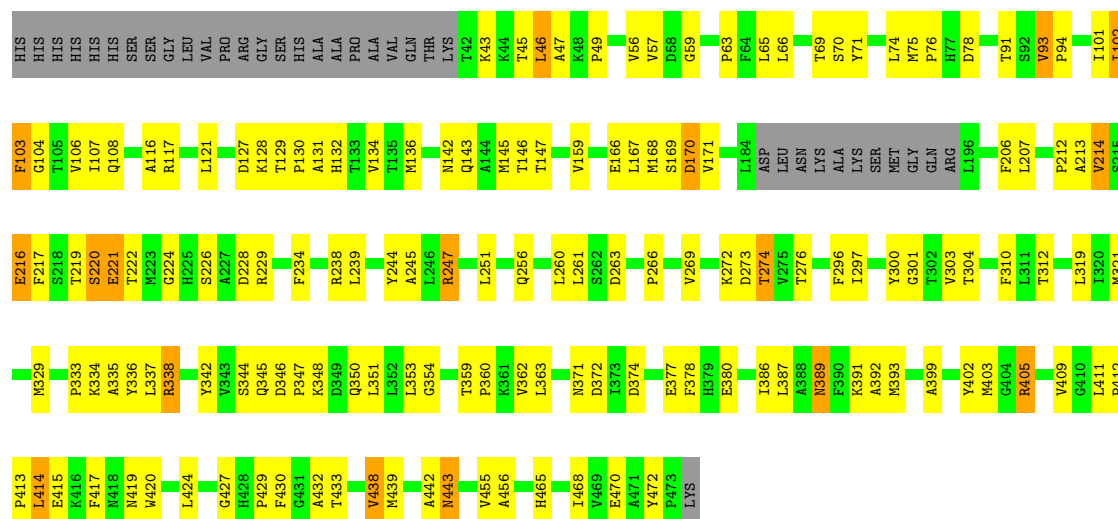
- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial





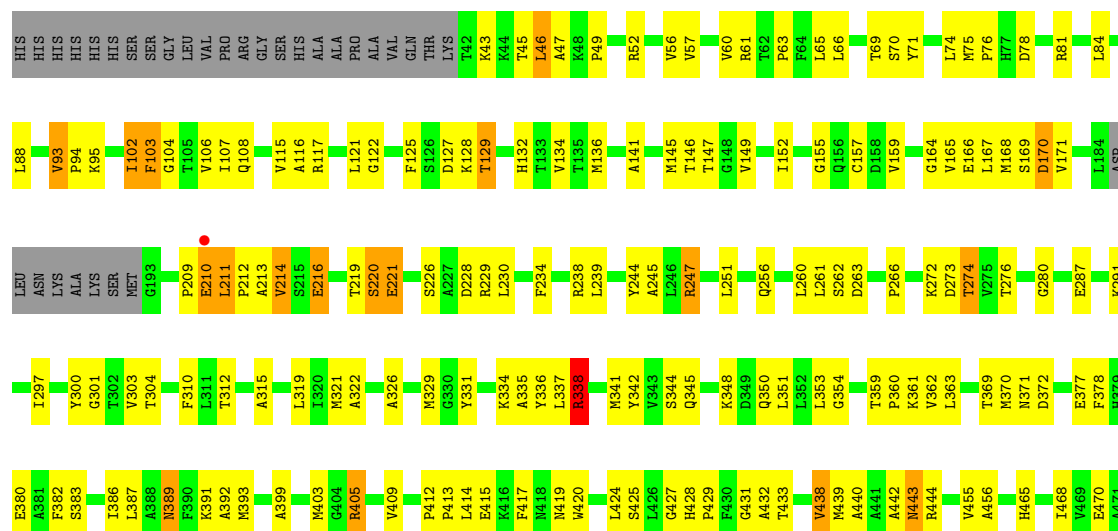
- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain C: 58% 30% 8%



- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

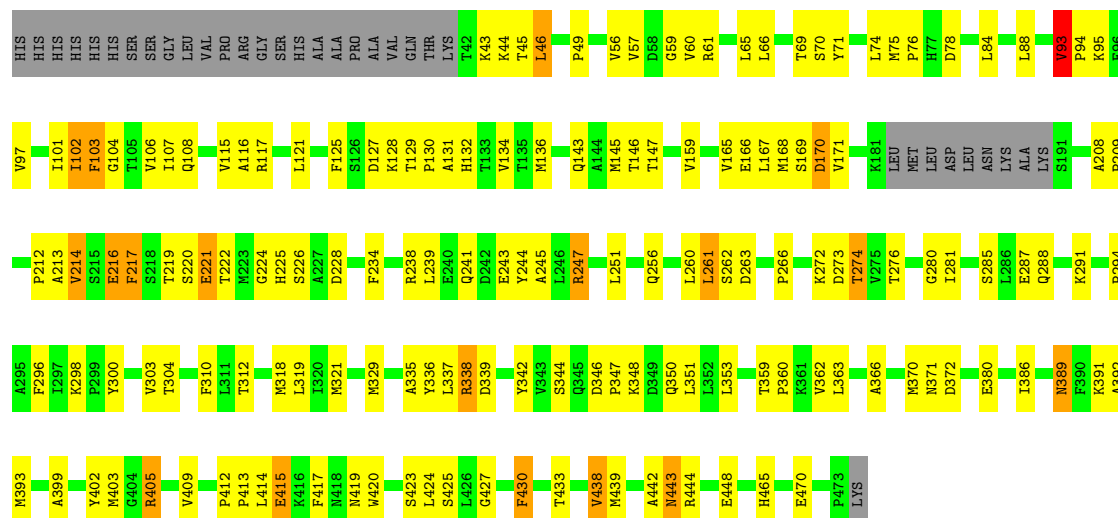
Chain D: 55% 34% 7%



Y472
P473
LYS

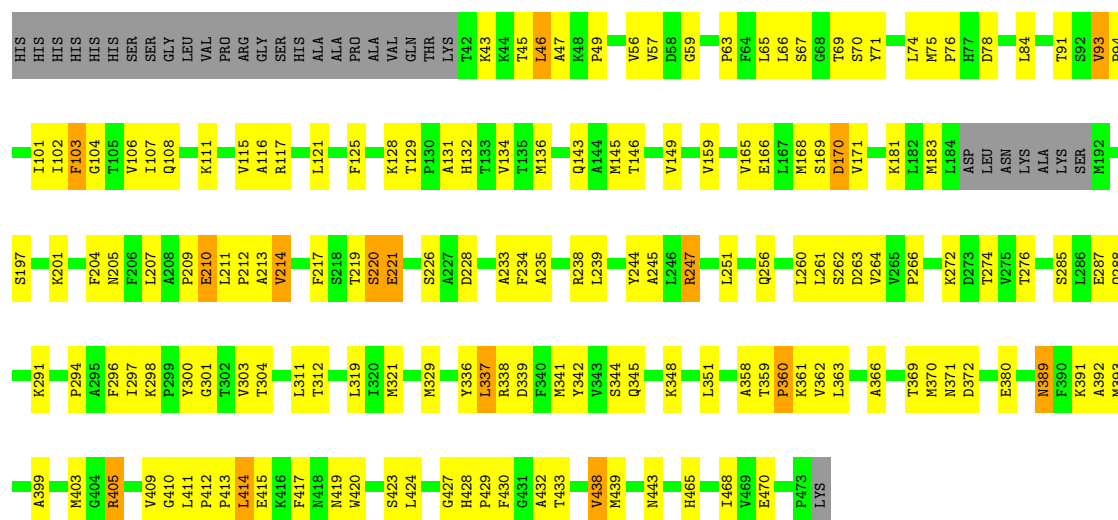
- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain E:  57% 31% 7%



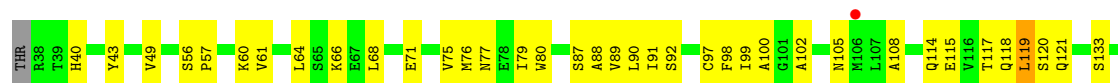
- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

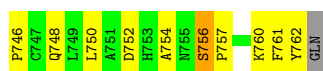
Chain F:  58% 32% 7%



- Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

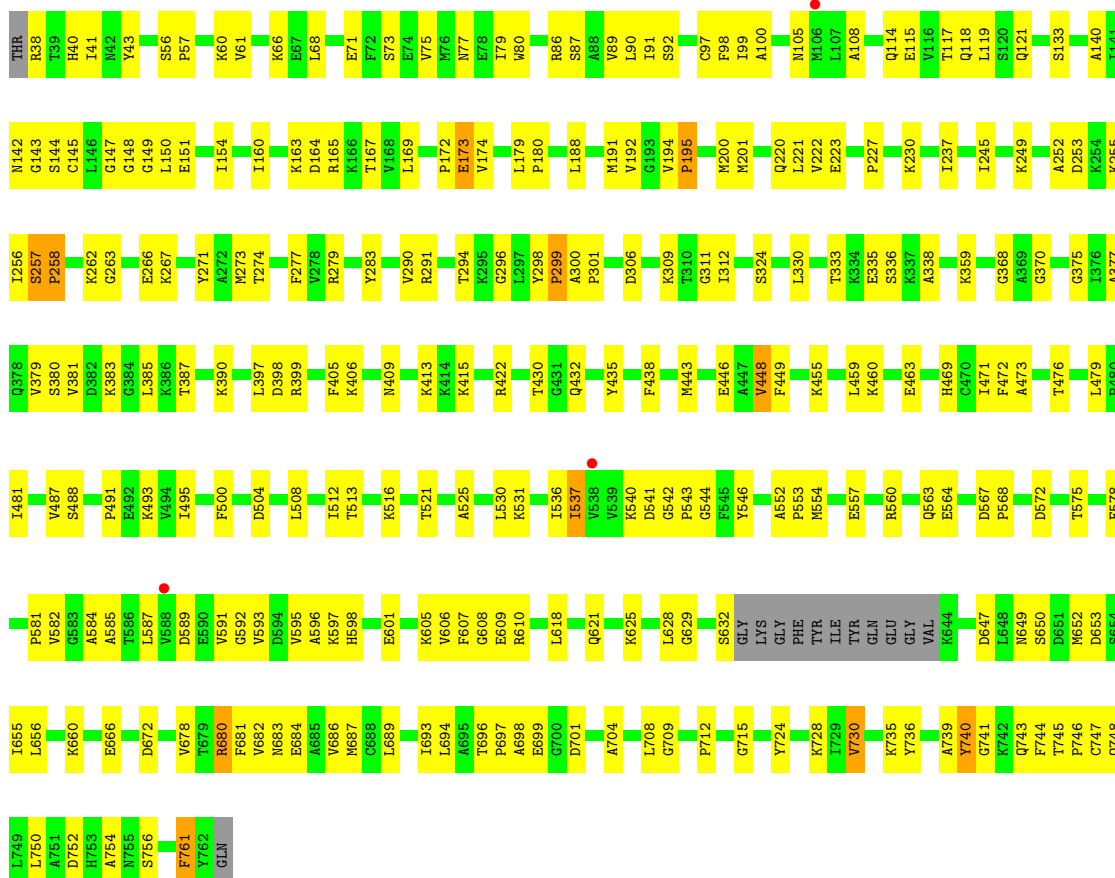
Chain G:  62% 34% 7%





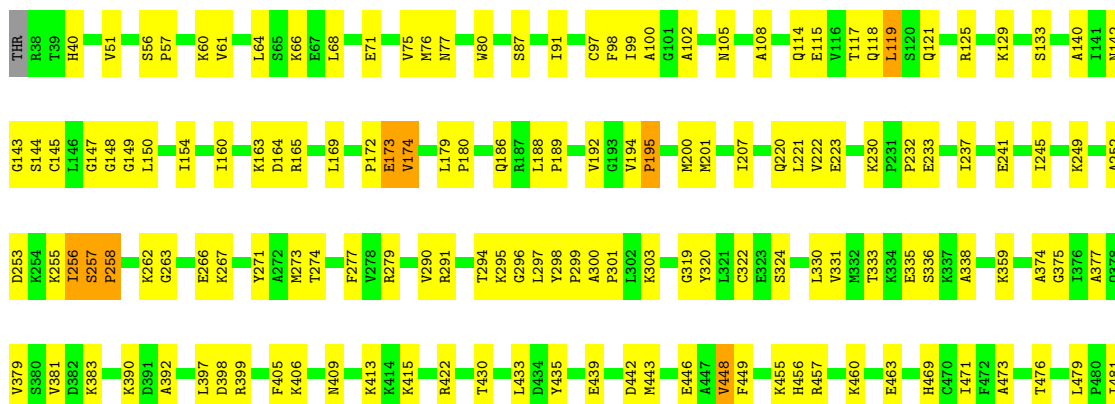
- Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

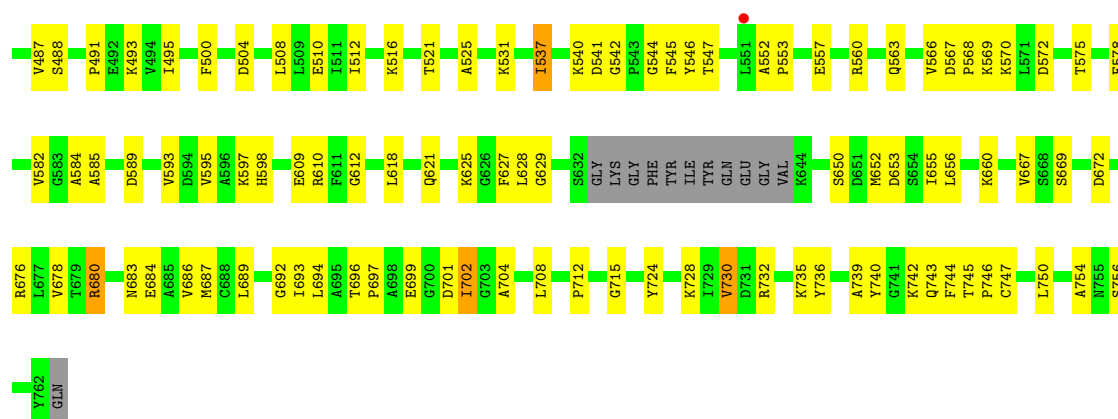
Chain I: 63% 34% ..



- Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

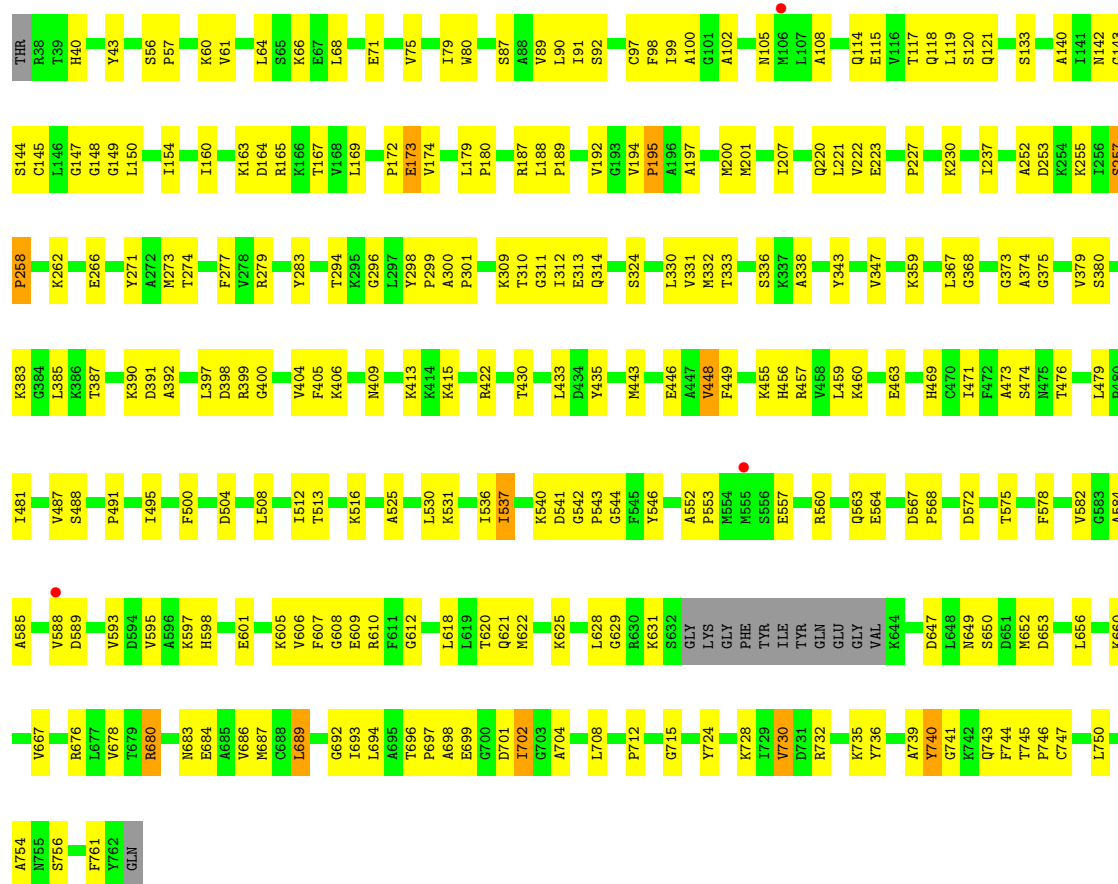
Chain J: 65% 32% ..





• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

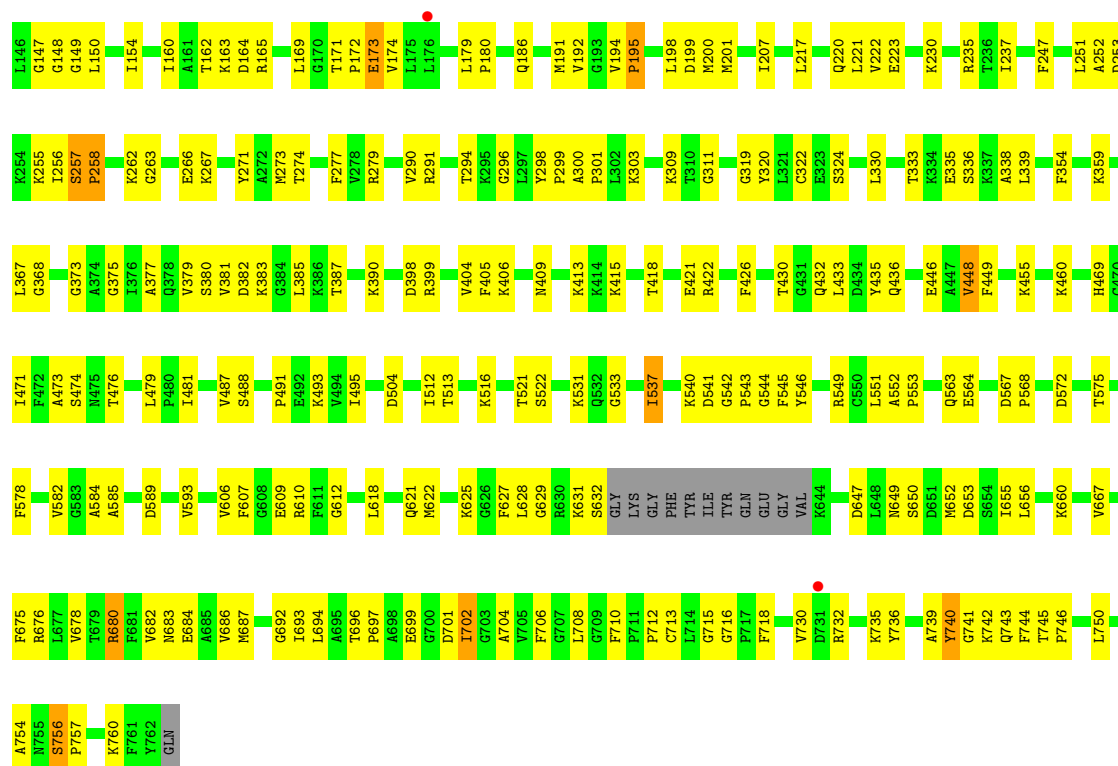
Chain K: 63% 33% ..



• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

Chain L: 63% 34% ..





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.54Å 237.94Å 141.32Å 90.00° 105.61° 90.00°	Depositor
Resolution (Å)	89.56 – 3.60 89.56 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (89.56-3.60) 98.7 (89.56-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.58Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.244 , 0.289 0.244 , 0.288	Depositor DCC
R_{free} test set	4957 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 103.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	51375	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.37	0/3330	0.77	2/4498 (0.0%)
1	B	0.37	0/3232	0.78	2/4368 (0.0%)
1	C	0.34	0/3128	0.74	2/4238 (0.0%)
1	D	0.34	0/3142	0.74	2/4257 (0.0%)
1	E	0.36	0/3137	0.77	4/4250 (0.1%)
1	F	0.37	0/3147	0.77	5/4264 (0.1%)
2	G	0.36	0/5524	0.78	9/7453 (0.1%)
2	H	0.34	0/5524	0.75	2/7453 (0.0%)
2	I	0.31	0/5515	0.73	2/7431 (0.0%)
2	J	0.31	0/5515	0.73	3/7431 (0.0%)
2	K	0.32	0/5515	0.71	0/7431
2	L	0.32	0/5515	0.73	1/7431 (0.0%)
All	All	0.34	0/52224	0.75	34/70505 (0.0%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ARG	N-CA-C	-11.77	98.18	111.71
2	G	631	LYS	N-CA-C	-10.86	100.68	113.38
2	I	761	PHE	N-CA-C	7.87	121.39	111.24
2	H	638	ILE	N-CA-C	7.70	120.52	109.51
2	G	651	ASP	N-CA-C	7.16	119.17	111.36
2	G	646	LYS	N-CA-C	7.05	123.18	112.54
2	J	142	ASN	N-CA-C	6.78	119.99	111.24
1	B	180	ARG	N-CA-C	-6.76	104.90	113.01
2	G	638	ILE	N-CA-C	6.74	123.36	109.34
2	G	636	PHE	N-CA-C	6.62	119.97	109.65
1	A	208	ALA	CA-C-N	-6.45	111.78	119.84
1	A	208	ALA	C-N-CA	-6.45	111.78	119.84
2	H	651	ASP	N-CA-C	6.12	121.64	114.04
1	F	211	LEU	CA-C-N	6.12	127.49	119.84
1	F	211	LEU	C-N-CA	6.12	127.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	392	ALA	N-CA-C	6.11	119.12	111.24
1	D	171	VAL	CA-C-N	6.01	127.36	119.84
1	D	171	VAL	C-N-CA	6.01	127.36	119.84
2	G	627	PHE	N-CA-C	-5.88	101.14	109.96
1	F	171	VAL	CA-C-N	5.86	127.16	119.84
1	F	171	VAL	C-N-CA	5.86	127.16	119.84
1	E	430	PHE	CB-CA-C	-5.74	102.74	109.80
1	C	171	VAL	CA-C-N	5.69	127.00	120.85
1	C	171	VAL	C-N-CA	5.69	127.00	120.85
2	I	761	PHE	CB-CA-C	-5.62	101.58	110.86
1	F	296	PHE	N-CA-C	5.62	120.51	113.43
2	G	633	GLY	N-CA-C	-5.50	108.62	114.67
1	E	171	VAL	CA-C-N	5.46	126.67	119.84
1	E	171	VAL	C-N-CA	5.46	126.67	119.84
2	J	174	VAL	CB-CA-C	-5.32	105.07	112.04
2	L	142	ASN	N-CA-C	5.29	118.07	111.24
2	G	647	ASP	N-CA-C	5.25	117.66	109.52
1	E	93	VAL	CB-CA-C	-5.21	105.77	110.88
2	G	650	SER	N-CA-C	5.10	116.53	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3267	0	3317	208	0
1	B	3170	0	3207	216	0
1	C	3073	0	2988	122	0
1	D	3087	0	2995	130	0
1	E	3082	0	2993	128	0
1	F	3092	0	2997	127	0
2	G	5440	0	5569	228	0
2	H	5440	0	5569	213	0
2	I	5431	0	5632	185	0
2	J	5431	0	5632	192	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	5431	0	5632	193	0
2	L	5431	0	5632	197	0
All	All	51375	0	52163	2072	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 20.

All (2072) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:MET:HE2	1:A:311:LEU:HD22	1.26	1.18
1:A:174:ARG:HB2	1:A:178:LYS:HG2	1.29	1.15
1:A:173:ILE:HG23	1:B:173:ILE:HG22	1.23	1.11
1:B:178:LYS:HD3	1:B:181:LYS:HD3	1.31	1.11
1:B:174:ARG:HB3	1:B:177:ARG:HB3	1.40	1.02
1:E:45:THR:O	1:E:46:LEU:HG	1.63	0.98
1:C:45:THR:O	1:C:46:LEU:HG	1.63	0.98
2:H:390:LYS:HD2	2:H:435:TYR:HE1	1.28	0.98
1:A:45:THR:O	1:A:46:LEU:HG	1.62	0.98
2:K:390:LYS:HD2	2:K:435:TYR:HE1	1.29	0.97
2:G:390:LYS:HD2	2:G:435:TYR:HE1	1.27	0.97
2:H:163:LYS:HE2	2:H:221:LEU:HD23	1.47	0.96
1:F:45:THR:O	1:F:46:LEU:HG	1.64	0.96
2:H:390:LYS:HD2	2:H:435:TYR:CE1	2.00	0.96
2:G:390:LYS:HD2	2:G:435:TYR:CE1	2.01	0.96
1:B:174:ARG:CB	1:B:177:ARG:HB3	1.96	0.95
2:L:390:LYS:HD2	2:L:435:TYR:HE1	1.30	0.95
1:A:178:LYS:HD3	1:A:181:LYS:CD	1.96	0.95
1:A:178:LYS:HD3	1:A:181:LYS:HD3	1.49	0.95
1:A:174:ARG:HG2	1:A:211:LEU:HD13	1.49	0.94
1:A:178:LYS:HD2	1:B:172:PRO:HG2	1.47	0.94
2:L:390:LYS:HD2	2:L:435:TYR:CE1	2.03	0.94
2:J:390:LYS:HD2	2:J:435:TYR:HE1	1.34	0.93
2:K:163:LYS:HE2	2:K:221:LEU:HD23	1.51	0.92
1:B:174:ARG:HD3	1:B:178:LYS:HG2	1.49	0.92
2:K:390:LYS:HD2	2:K:435:TYR:CE1	2.02	0.92
1:A:178:LYS:HA	1:A:181:LYS:HB2	1.48	0.92
2:I:163:LYS:HE2	2:I:221:LEU:HD23	1.53	0.91
1:A:177:ARG:HG3	1:A:209:PRO:CB	2.00	0.91
2:L:163:LYS:HE2	2:L:221:LEU:HD23	1.52	0.90
1:D:45:THR:O	1:D:46:LEU:HG	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:163:LYS:HE2	2:J:221:LEU:HD23	1.54	0.89
2:J:390:LYS:HD2	2:J:435:TYR:CE1	2.07	0.89
1:A:177:ARG:NH1	1:A:209:PRO:HG3	1.88	0.88
1:A:174:ARG:HB2	1:A:178:LYS:CG	2.04	0.88
1:A:173:ILE:CG2	1:B:173:ILE:HG22	2.04	0.87
1:B:211:LEU:HB3	1:B:212:PRO:CD	2.05	0.87
1:A:178:LYS:HA	1:A:181:LYS:CB	2.06	0.85
2:G:163:LYS:HE2	2:G:221:LEU:HD23	1.57	0.85
2:L:330:LEU:O	2:L:333:THR:HG22	1.76	0.84
1:B:180:ARG:HD2	1:B:203:ARG:HB2	1.59	0.83
2:I:330:LEU:O	2:I:333:THR:HG22	1.78	0.83
1:A:168:MET:CE	1:A:311:LEU:HD22	2.08	0.82
1:B:174:ARG:CD	1:B:178:LYS:HG2	2.09	0.82
2:G:330:LEU:O	2:G:333:THR:HG22	1.80	0.81
2:G:629:GLY:C	2:G:631:LYS:H	1.87	0.81
1:A:173:ILE:HG23	1:B:173:ILE:CG2	2.08	0.81
1:B:180:ARG:NE	1:B:207:LEU:HD22	1.96	0.81
1:A:128:LYS:O	1:B:344:SER:HB3	1.81	0.81
2:G:637:TYR:HA	2:G:644:LYS:O	1.80	0.80
1:A:168:MET:HE2	1:A:311:LEU:CD2	2.09	0.80
1:B:200:SER:O	1:B:203:ARG:HG2	1.80	0.80
1:C:69:THR:HG23	1:C:70:SER:H	1.47	0.80
2:H:330:LEU:O	2:H:333:THR:HG22	1.82	0.80
2:I:174:VAL:CG2	2:I:201:MET:O	2.31	0.79
2:I:174:VAL:HG21	2:I:201:MET:O	1.81	0.79
1:A:174:ARG:CB	1:A:178:LYS:HG2	2.11	0.79
1:A:177:ARG:O	1:A:181:LYS:HB2	1.82	0.79
2:J:330:LEU:O	2:J:333:THR:HG22	1.83	0.79
2:H:634:LYS:HA	2:H:648:LEU:O	1.83	0.78
2:H:589:ASP:OD2	2:H:635:GLY:HA3	1.82	0.78
1:E:224:GLY:HA3	1:E:296:PHE:CZ	2.19	0.78
1:A:178:LYS:HE3	1:B:172:PRO:O	1.84	0.77
1:B:159:VAL:HG22	1:B:321:MET:HE3	1.65	0.77
1:B:300:TYR:OH	2:H:222:VAL:HA	1.82	0.77
1:E:69:THR:HG23	1:E:70:SER:H	1.48	0.77
2:G:628:LEU:C	2:G:630:ARG:H	1.91	0.77
2:K:330:LEU:O	2:K:333:THR:HG22	1.85	0.77
2:J:271:TYR:O	2:J:274:THR:HG22	1.84	0.77
1:A:178:LYS:CD	1:A:181:LYS:HD3	2.15	0.77
1:B:205:ASN:O	1:B:206:PHE:CD1	2.37	0.76
1:A:344:SER:HB3	1:B:128:LYS:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:567:ASP:HB2	2:L:568:PRO:HD2	1.68	0.76
1:F:69:THR:HG23	1:F:70:SER:H	1.50	0.76
2:K:375:GLY:O	2:K:379:VAL:HG23	1.85	0.75
2:G:271:TYR:O	2:G:274:THR:HG22	1.87	0.75
2:I:257:SER:N	2:I:258:PRO:HD3	2.02	0.75
2:L:610:ARG:HD3	2:L:743:GLN:O	1.86	0.75
1:D:169:SER:O	1:D:170:ASP:O	2.04	0.75
2:I:375:GLY:O	2:I:379:VAL:HG23	1.87	0.75
1:A:177:ARG:HG3	1:A:209:PRO:HB2	1.69	0.75
2:H:163:LYS:CE	2:H:221:LEU:HD23	2.16	0.75
2:H:257:SER:N	2:H:258:PRO:HD3	2.01	0.74
2:G:610:ARG:HD3	2:G:743:GLN:O	1.87	0.74
1:E:70:SER:HB2	1:E:272:LYS:HD2	1.68	0.74
2:L:121:GLN:HG3	2:L:324:SER:OG	1.86	0.74
2:G:257:SER:N	2:G:258:PRO:HD3	2.03	0.74
2:I:589:ASP:O	2:I:629:GLY:HA3	1.88	0.74
2:J:257:SER:N	2:J:258:PRO:HD3	2.02	0.74
2:K:257:SER:N	2:K:258:PRO:HD3	2.03	0.74
1:A:172:PRO:HB2	1:B:178:LYS:HE3	1.68	0.73
1:C:344:SER:HB3	1:D:128:LYS:O	1.88	0.73
2:L:589:ASP:O	2:L:629:GLY:HA3	1.86	0.73
1:B:178:LYS:HA	1:B:181:LYS:HB3	1.71	0.73
1:C:159:VAL:HG22	1:C:321:MET:HE3	1.70	0.73
1:F:321:MET:HE1	1:F:329:MET:HG3	1.70	0.73
2:L:163:LYS:CE	2:L:221:LEU:HD23	2.19	0.72
1:F:43:LYS:HD3	1:F:372:ASP:HA	1.71	0.72
1:F:69:THR:HG23	1:F:70:SER:N	2.05	0.72
2:G:589:ASP:OD2	2:G:634:LYS:N	2.22	0.72
2:L:257:SER:N	2:L:258:PRO:HD3	2.03	0.72
1:A:177:ARG:HH11	1:A:209:PRO:HG3	1.54	0.72
2:J:589:ASP:O	2:J:629:GLY:HA3	1.90	0.72
1:A:182:LEU:O	1:A:185:ASP:HB2	1.89	0.72
1:F:389:ASN:O	1:F:393:MET:HG3	1.90	0.72
2:H:610:ARG:NH2	2:H:687:MET:HE1	2.04	0.72
1:C:69:THR:HG23	1:C:70:SER:N	2.05	0.72
1:D:70:SER:HB2	1:D:272:LYS:HD2	1.71	0.72
1:A:103:PHE:HB2	1:A:116:ALA:HB2	1.72	0.71
1:B:177:ARG:HB2	1:B:209:PRO:HB2	1.72	0.71
2:G:567:ASP:HB2	2:G:568:PRO:HD2	1.72	0.71
2:G:610:ARG:NH2	2:G:687:MET:HE1	2.04	0.71
2:K:610:ARG:HD3	2:K:743:GLN:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:460:LYS:HG3	2:L:487:VAL:HG11	1.69	0.71
2:I:121:GLN:HG3	2:I:324:SER:OG	1.91	0.71
1:B:200:SER:O	1:B:203:ARG:CG	2.38	0.71
1:E:159:VAL:HG22	1:E:321:MET:HE3	1.73	0.71
2:G:375:GLY:O	2:G:379:VAL:HG23	1.90	0.71
2:L:610:ARG:NH2	2:L:687:MET:HE1	2.06	0.71
1:B:69:THR:HG23	1:B:70:SER:H	1.55	0.71
1:D:159:VAL:HG22	1:D:321:MET:HE3	1.71	0.71
1:F:70:SER:HB2	1:F:272:LYS:HD2	1.73	0.71
2:J:610:ARG:HD3	2:J:743:GLN:O	1.90	0.71
2:I:257:SER:N	2:I:258:PRO:CD	2.54	0.71
2:K:253:ASP:HB2	2:K:255:LYS:HE2	1.73	0.70
1:A:159:VAL:HG22	1:A:321:MET:HE3	1.71	0.70
2:H:257:SER:N	2:H:258:PRO:CD	2.54	0.70
2:G:589:ASP:OD2	2:G:635:GLY:N	2.25	0.70
2:H:610:ARG:HD3	2:H:743:GLN:O	1.91	0.70
2:G:257:SER:N	2:G:258:PRO:CD	2.55	0.70
1:B:209:PRO:O	1:B:210:GLU:HG3	1.91	0.70
2:K:257:SER:N	2:K:258:PRO:CD	2.54	0.70
1:E:389:ASN:O	1:E:393:MET:HG3	1.91	0.70
1:F:159:VAL:HG22	1:F:321:MET:HE3	1.73	0.70
1:D:69:THR:HG23	1:D:70:SER:H	1.56	0.70
2:I:567:ASP:HB2	2:I:568:PRO:HD2	1.73	0.70
1:B:70:SER:HB2	1:B:272:LYS:HD2	1.74	0.70
2:K:163:LYS:CE	2:K:221:LEU:HD23	2.21	0.70
2:K:589:ASP:O	2:K:629:GLY:HA3	1.90	0.70
2:J:253:ASP:HB2	2:J:255:LYS:HE2	1.74	0.69
2:J:460:LYS:HG3	2:J:487:VAL:HG11	1.73	0.69
2:K:460:LYS:HG3	2:K:487:VAL:HG11	1.73	0.69
2:L:552:ALA:HB3	2:L:553:PRO:HD3	1.74	0.69
1:B:69:THR:HG23	1:B:70:SER:N	2.07	0.69
1:B:244:TYR:HD1	1:B:244:TYR:O	1.75	0.69
2:I:610:ARG:NH2	2:I:687:MET:HE1	2.08	0.69
1:C:70:SER:HB2	1:C:272:LYS:HD2	1.75	0.69
2:H:567:ASP:HB2	2:H:568:PRO:HD2	1.72	0.69
2:L:257:SER:N	2:L:258:PRO:CD	2.55	0.69
2:H:375:GLY:O	2:H:379:VAL:HG23	1.93	0.69
1:D:69:THR:HG23	1:D:70:SER:N	2.08	0.69
1:E:69:THR:HG23	1:E:70:SER:N	2.07	0.69
1:E:244:TYR:HD1	1:E:244:TYR:O	1.74	0.69
1:E:321:MET:HE1	1:E:329:MET:HG3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:473:ALA:HA	2:K:495:ILE:O	1.92	0.69
2:L:271:TYR:O	2:L:274:THR:HG22	1.91	0.69
2:G:121:GLN:HG3	2:G:324:SER:OG	1.93	0.69
2:H:460:LYS:HG3	2:H:487:VAL:HG11	1.74	0.69
1:A:208:ALA:HB1	1:A:209:PRO:CD	2.23	0.68
1:B:216:GLU:HG2	1:B:221:GLU:H	1.58	0.68
2:J:567:ASP:HB2	2:J:568:PRO:HD2	1.75	0.68
1:D:43:LYS:HD3	1:D:372:ASP:HA	1.75	0.68
2:G:359:LYS:NZ	2:G:469:HIS:O	2.25	0.68
2:G:552:ALA:HB3	2:G:553:PRO:HD3	1.74	0.68
2:J:257:SER:N	2:J:258:PRO:CD	2.56	0.68
2:G:460:LYS:HG3	2:G:487:VAL:HG11	1.74	0.68
2:I:163:LYS:CE	2:I:221:LEU:HD23	2.21	0.68
2:G:628:LEU:C	2:G:630:ARG:N	2.48	0.68
2:I:593:VAL:HG21	2:I:628:LEU:HA	1.75	0.68
2:I:610:ARG:HD3	2:I:743:GLN:O	1.92	0.68
1:D:321:MET:HE1	1:D:329:MET:HG3	1.75	0.68
2:H:174:VAL:CG2	2:H:201:MET:O	2.42	0.68
2:L:593:VAL:HG21	2:L:628:LEU:HA	1.76	0.68
1:A:70:SER:HB2	1:A:272:LYS:HD2	1.75	0.68
2:J:610:ARG:NH2	2:J:687:MET:HE1	2.08	0.68
2:K:567:ASP:HB2	2:K:568:PRO:HD2	1.76	0.68
1:A:174:ARG:CG	1:A:211:LEU:HD13	2.23	0.68
2:J:593:VAL:HG21	2:J:628:LEU:HA	1.76	0.68
2:K:91:ILE:HB	2:K:140:ALA:HB3	1.75	0.68
2:H:634:LYS:HA	2:H:648:LEU:C	2.18	0.67
1:C:103:PHE:HB2	1:C:116:ALA:HB2	1.76	0.67
1:E:103:PHE:HB2	1:E:116:ALA:HB2	1.74	0.67
2:G:473:ALA:HA	2:G:495:ILE:O	1.93	0.67
1:A:178:LYS:HD3	1:A:181:LYS:HD2	1.73	0.67
2:G:589:ASP:CG	2:G:634:LYS:N	2.53	0.67
1:B:214:VAL:O	1:B:215:SER:HB3	1.94	0.67
1:A:171:VAL:N	1:A:172:PRO:HD3	2.10	0.67
2:H:730:VAL:HG21	2:H:754:ALA:HB2	1.77	0.67
2:J:491:PRO:HB2	2:J:516:LYS:HD3	1.77	0.67
1:A:172:PRO:HB2	1:B:178:LYS:CE	2.25	0.67
1:C:66:LEU:O	1:C:69:THR:HG22	1.94	0.67
2:G:253:ASP:HB2	2:G:255:LYS:HE2	1.77	0.67
1:A:211:LEU:HD21	1:B:174:ARG:NH2	2.10	0.67
2:J:540:LYS:HG2	2:J:693:ILE:HA	1.76	0.67
1:A:359:THR:HB	1:A:360:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:CD	1:B:207:LEU:HD22	2.24	0.66
2:G:61:VAL:HG23	2:G:97:CYS:SG	2.35	0.66
2:G:262:LYS:HB3	2:G:266:GLU:HB3	1.75	0.66
2:K:262:LYS:HB3	2:K:266:GLU:HB3	1.75	0.66
2:L:473:ALA:HA	2:L:495:ILE:O	1.94	0.66
1:E:359:THR:HB	1:E:360:PRO:HD3	1.77	0.66
2:I:460:LYS:HG3	2:I:487:VAL:HG11	1.78	0.66
2:K:150:LEU:O	2:K:154:ILE:HB	1.94	0.66
2:L:192:VAL:O	2:L:192:VAL:HG12	1.95	0.66
2:H:192:VAL:O	2:H:192:VAL:HG12	1.95	0.66
1:C:128:LYS:O	1:D:344:SER:HB3	1.94	0.66
1:B:103:PHE:HB2	1:B:116:ALA:HB2	1.78	0.66
1:D:247:ARG:NH2	1:D:417:PHE:O	2.28	0.66
2:J:192:VAL:O	2:J:192:VAL:HG12	1.94	0.66
1:C:43:LYS:HD3	1:C:372:ASP:HA	1.76	0.66
2:G:192:VAL:O	2:G:192:VAL:HG12	1.95	0.66
2:K:610:ARG:NH2	2:K:687:MET:HE1	2.10	0.66
1:A:69:THR:HG23	1:A:70:SER:N	2.10	0.66
2:I:91:ILE:HB	2:I:140:ALA:HB3	1.78	0.66
2:I:150:LEU:O	2:I:154:ILE:HB	1.96	0.66
1:A:177:ARG:HG3	1:A:209:PRO:HB3	1.75	0.66
2:G:262:LYS:HD3	2:G:266:GLU:HG2	1.78	0.66
2:J:163:LYS:CE	2:J:221:LEU:HD23	2.24	0.66
1:A:67:SER:OG	1:A:168:MET:HB2	1.95	0.65
1:F:169:SER:O	1:F:170:ASP:O	2.14	0.65
2:G:163:LYS:CE	2:G:221:LEU:HD23	2.26	0.65
1:A:200:SER:O	1:A:203:ARG:HB2	1.96	0.65
2:I:257:SER:H	2:I:258:PRO:HD3	1.59	0.65
2:L:253:ASP:HB2	2:L:255:LYS:HE2	1.76	0.65
1:A:173:ILE:O	1:A:211:LEU:HD12	1.96	0.65
1:B:180:ARG:HD3	1:B:207:LEU:HD13	1.77	0.65
1:F:66:LEU:O	1:F:69:THR:HG22	1.96	0.65
2:H:359:LYS:NZ	2:H:469:HIS:O	2.29	0.65
1:B:321:MET:HE1	1:B:329:MET:HG3	1.79	0.65
2:J:552:ALA:HB3	2:J:553:PRO:HD3	1.78	0.65
2:I:473:ALA:HA	2:I:495:ILE:O	1.97	0.65
1:F:201:LYS:O	1:F:205:ASN:N	2.30	0.65
2:G:609:GLU:HG2	2:G:610:ARG:N	2.10	0.65
2:J:262:LYS:HB3	2:J:266:GLU:HB3	1.77	0.65
1:A:43:LYS:HD3	1:A:372:ASP:HA	1.79	0.65
2:L:91:ILE:HB	2:L:140:ALA:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:630:ARG:C	2:G:632:SER:H	2.05	0.65
1:E:43:LYS:HD3	1:E:372:ASP:HA	1.79	0.64
2:H:262:LYS:HB3	2:H:266:GLU:HB3	1.79	0.64
2:H:552:ALA:HB3	2:H:553:PRO:HD3	1.79	0.64
2:I:540:LYS:HG2	2:I:693:ILE:HA	1.79	0.64
2:K:271:TYR:O	2:K:274:THR:HG22	1.97	0.64
2:K:593:VAL:HG21	2:K:628:LEU:HA	1.79	0.64
2:L:730:VAL:HG21	2:L:754:ALA:HB2	1.77	0.64
2:H:174:VAL:HG21	2:H:201:MET:O	1.98	0.64
2:K:192:VAL:O	2:K:192:VAL:HG12	1.97	0.64
2:K:552:ALA:HB3	2:K:553:PRO:HD3	1.79	0.64
2:K:730:VAL:HG21	2:K:754:ALA:HB2	1.79	0.64
1:D:210:GLU:O	1:D:211:LEU:CB	2.46	0.64
2:I:552:ALA:HB3	2:I:553:PRO:HD3	1.78	0.64
2:K:491:PRO:HB2	2:K:516:LYS:HD3	1.78	0.64
1:B:389:ASN:O	1:B:393:MET:HG3	1.98	0.64
2:H:540:LYS:HG2	2:H:693:ILE:HA	1.80	0.64
2:L:540:LYS:HG2	2:L:693:ILE:HA	1.79	0.64
1:B:211:LEU:HD22	1:B:212:PRO:HD3	1.78	0.64
2:I:730:VAL:HG21	2:I:754:ALA:HB2	1.79	0.64
1:B:211:LEU:HB3	1:B:212:PRO:HD3	1.78	0.64
2:H:609:GLU:HG2	2:H:610:ARG:N	2.12	0.64
2:J:375:GLY:O	2:J:379:VAL:HG23	1.98	0.64
2:J:557:GLU:OE2	2:J:560:ARG:HD2	1.98	0.64
2:K:540:LYS:HG2	2:K:693:ILE:HA	1.80	0.64
2:J:473:ALA:HA	2:J:495:ILE:O	1.98	0.64
1:F:266:PRO:HB3	1:F:276:THR:HG22	1.78	0.63
2:G:91:ILE:HB	2:G:140:ALA:HB3	1.80	0.63
2:H:121:GLN:HG3	2:H:324:SER:OG	1.98	0.63
2:L:174:VAL:CG2	2:L:201:MET:O	2.46	0.63
2:J:730:VAL:HG21	2:J:754:ALA:HB2	1.78	0.63
2:K:704:ALA:HA	2:K:708:LEU:HD23	1.80	0.63
1:D:103:PHE:HB2	1:D:116:ALA:HB2	1.81	0.63
2:G:621:GLN:O	2:G:625:LYS:HB2	1.98	0.63
1:B:174:ARG:HB3	1:B:177:ARG:CB	2.24	0.63
1:C:300:TYR:OH	2:I:222:VAL:HA	1.98	0.63
2:G:557:GLU:OE2	2:G:560:ARG:HD2	1.98	0.63
2:J:377:ALA:O	2:J:381:VAL:HG23	1.98	0.63
2:J:563:GLN:HG2	2:J:660:LYS:HA	1.79	0.63
2:G:730:VAL:HG21	2:G:754:ALA:HB2	1.80	0.63
2:J:566:VAL:HG13	2:J:570:LYS:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:192:VAL:O	2:I:192:VAL:HG12	1.99	0.63
2:K:262:LYS:HD3	2:K:266:GLU:HG2	1.79	0.63
1:B:209:PRO:C	1:B:210:GLU:HG3	2.24	0.63
1:E:66:LEU:O	1:E:69:THR:HG22	1.98	0.63
2:G:630:ARG:C	2:G:632:SER:N	2.54	0.62
2:I:448:VAL:HG12	2:I:449:PHE:H	1.64	0.62
1:D:74:LEU:O	1:D:167:LEU:HD21	2.00	0.62
1:E:65:LEU:HB3	1:E:69:THR:HG21	1.81	0.62
1:F:103:PHE:HB2	1:F:116:ALA:HB2	1.80	0.62
2:K:359:LYS:NZ	2:K:469:HIS:O	2.32	0.62
2:L:609:GLU:HG2	2:L:610:ARG:N	2.14	0.62
2:G:257:SER:H	2:G:258:PRO:HD3	1.62	0.62
2:G:491:PRO:HB2	2:G:516:LYS:HD3	1.80	0.62
1:B:174:ARG:NH1	1:B:177:ARG:HG2	2.14	0.62
2:H:150:LEU:O	2:H:154:ILE:HB	1.98	0.62
1:E:266:PRO:HB3	1:E:276:THR:HG22	1.82	0.62
2:H:377:ALA:O	2:H:381:VAL:HG23	1.99	0.62
2:J:91:ILE:HB	2:J:140:ALA:HB3	1.81	0.62
2:J:609:GLU:HG2	2:J:610:ARG:N	2.13	0.62
2:L:262:LYS:HB3	2:L:266:GLU:HB3	1.80	0.62
1:B:195:ARG:HA	1:B:198:LEU:CD1	2.29	0.62
2:I:262:LYS:HB3	2:I:266:GLU:HB3	1.80	0.62
2:G:40:HIS:CE1	2:G:57:PRO:HD3	2.35	0.62
2:G:650:SER:O	2:G:653:ASP:HB2	1.99	0.62
2:I:359:LYS:NZ	2:I:469:HIS:O	2.32	0.62
1:A:208:ALA:CB	1:A:209:PRO:CD	2.78	0.62
2:I:491:PRO:HB2	2:I:516:LYS:HD3	1.82	0.62
1:B:211:LEU:CB	1:B:212:PRO:CD	2.78	0.62
1:D:266:PRO:HB3	1:D:276:THR:HG22	1.82	0.62
2:K:257:SER:H	2:K:258:PRO:HD3	1.63	0.62
1:F:204:PHE:HA	1:F:207:LEU:O	2.00	0.61
2:G:540:LYS:HG2	2:G:693:ILE:HA	1.81	0.61
2:L:491:PRO:HB2	2:L:516:LYS:HD3	1.81	0.61
1:A:66:LEU:O	1:A:69:THR:HG22	2.00	0.61
1:A:321:MET:HE1	1:A:329:MET:HG3	1.80	0.61
1:C:43:LYS:HE2	1:C:371:ASN:O	2.00	0.61
1:B:211:LEU:CB	1:B:212:PRO:HD3	2.29	0.61
2:H:473:ALA:HA	2:H:495:ILE:O	1.99	0.61
1:E:216:GLU:HG2	1:E:221:GLU:H	1.66	0.61
1:B:247:ARG:NH2	1:B:417:PHE:O	2.33	0.61
2:I:409:ASN:HA	2:I:422:ARG:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:174:VAL:HG21	2:L:201:MET:O	2.01	0.61
2:L:338:ALA:HB1	2:L:715:GLY:HA3	1.81	0.61
1:A:45:THR:O	1:A:46:LEU:CG	2.43	0.61
1:D:359:THR:HB	1:D:360:PRO:HD3	1.82	0.61
2:G:563:GLN:HG2	2:G:660:LYS:HA	1.83	0.61
2:G:338:ALA:HB1	2:G:715:GLY:HA3	1.82	0.61
2:H:704:ALA:HA	2:H:708:LEU:HD23	1.82	0.61
1:A:244:TYR:O	1:A:244:TYR:HD1	1.83	0.61
1:A:266:PRO:HB3	1:A:276:THR:HG22	1.83	0.61
2:J:448:VAL:HG12	2:J:449:PHE:H	1.66	0.61
2:J:621:GLN:O	2:J:625:LYS:HB2	2.00	0.61
1:C:169:SER:O	1:C:170:ASP:O	2.19	0.60
1:F:65:LEU:HB3	1:F:69:THR:HG21	1.82	0.60
2:G:150:LEU:O	2:G:154:ILE:HB	2.01	0.60
1:E:344:SER:HB3	1:F:128:LYS:O	2.01	0.60
2:L:262:LYS:HD3	2:L:266:GLU:HG2	1.82	0.60
1:A:172:PRO:HG2	1:B:178:LYS:HD2	1.83	0.60
2:G:628:LEU:CB	2:G:632:SER:CB	2.80	0.60
2:H:541:ASP:OD1	2:H:542:GLY:N	2.33	0.60
1:B:287:GLU:O	1:B:291:LYS:HG3	2.01	0.60
1:E:287:GLU:O	1:E:291:LYS:HG3	2.02	0.60
2:G:390:LYS:CD	2:G:435:TYR:HE1	2.10	0.60
2:J:262:LYS:HD3	2:J:266:GLU:HG2	1.83	0.60
1:A:69:THR:HG23	1:A:70:SER:H	1.66	0.60
1:C:229:ARG:NH1	2:I:223:GLU:OE1	2.34	0.60
2:H:448:VAL:HG12	2:H:449:PHE:H	1.67	0.60
2:J:87:SER:HB2	2:J:252:ALA:HB2	1.83	0.60
1:B:177:ARG:HD2	1:B:209:PRO:CG	2.32	0.60
2:I:609:GLU:HG2	2:I:610:ARG:N	2.14	0.60
1:C:321:MET:HE1	1:C:329:MET:HG3	1.82	0.60
1:C:413:PRO:C	1:C:415:GLU:H	2.09	0.60
2:H:97:CYS:HB2	2:H:144:SER:HB2	1.82	0.60
2:H:563:GLN:HG2	2:H:660:LYS:HA	1.83	0.60
2:J:409:ASN:HA	2:J:422:ARG:HD3	1.82	0.60
1:A:389:ASN:O	1:A:393:MET:HG3	2.01	0.60
2:H:87:SER:HB2	2:H:252:ALA:HB2	1.83	0.60
1:C:266:PRO:HB3	1:C:276:THR:HG22	1.82	0.60
2:G:377:ALA:O	2:G:381:VAL:HG23	2.01	0.60
2:H:621:GLN:O	2:H:625:LYS:HB2	2.01	0.60
2:J:455:LYS:HD3	2:J:476:THR:HG21	1.83	0.60
1:E:213:ALA:O	1:E:214:VAL:CB	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:455:LYS:HD3	2:G:476:THR:HG21	1.83	0.59
2:H:491:PRO:HB2	2:H:516:LYS:HD3	1.84	0.59
2:I:56:SER:HB3	2:I:57:PRO:HD2	1.84	0.59
2:J:121:GLN:HG3	2:J:324:SER:OG	2.02	0.59
2:J:257:SER:H	2:J:258:PRO:HD3	1.67	0.59
2:K:621:GLN:O	2:K:625:LYS:HB2	2.01	0.59
1:B:342:TYR:CE1	1:B:465:HIS:CD2	2.90	0.59
2:H:262:LYS:HD3	2:H:266:GLU:HG2	1.83	0.59
1:F:45:THR:O	1:F:46:LEU:CG	2.47	0.59
2:I:262:LYS:HD3	2:I:266:GLU:HG2	1.84	0.59
2:K:609:GLU:HG2	2:K:610:ARG:N	2.17	0.59
1:D:106:VAL:HG23	1:D:107:ILE:HG13	1.85	0.59
2:G:409:ASN:HA	2:G:422:ARG:HD3	1.84	0.59
2:I:253:ASP:HB2	2:I:255:LYS:HE2	1.83	0.59
2:I:335:GLU:OE1	2:I:335:GLU:N	2.34	0.59
2:J:359:LYS:NZ	2:J:469:HIS:O	2.35	0.59
1:B:171:VAL:O	1:B:171:VAL:HG23	2.02	0.59
1:B:177:ARG:HB2	1:B:209:PRO:CB	2.31	0.59
1:B:300:TYR:HH	2:H:222:VAL:HA	1.67	0.59
2:I:563:GLN:HG2	2:I:660:LYS:HA	1.85	0.59
2:L:40:HIS:CE1	2:L:57:PRO:HD3	2.38	0.59
1:E:169:SER:O	1:E:170:ASP:O	2.20	0.59
2:H:271:TYR:O	2:H:274:THR:HG22	2.02	0.59
2:I:621:GLN:O	2:I:625:LYS:HB2	2.02	0.59
2:K:383:LYS:HG2	2:K:531:LYS:O	2.02	0.59
2:K:409:ASN:HA	2:K:422:ARG:HD3	1.84	0.59
1:A:180:ARG:O	1:A:184:LEU:HD12	2.03	0.59
1:E:403:MET:HE1	1:E:409:VAL:HG23	1.85	0.59
2:K:174:VAL:CG2	2:K:201:MET:O	2.51	0.59
2:K:375:GLY:HA2	2:K:504:ASP:OD1	2.03	0.59
2:K:546:TYR:CE1	2:K:694:LEU:HD11	2.38	0.59
1:C:213:ALA:O	1:C:214:VAL:CB	2.51	0.59
2:H:164:ASP:OD1	2:H:165:ARG:N	2.35	0.59
2:L:257:SER:H	2:L:258:PRO:HD3	1.66	0.59
1:E:216:GLU:CD	1:E:220:SER:HA	2.27	0.58
2:I:735:LYS:O	2:I:739:ALA:HB3	2.02	0.58
2:L:563:GLN:HG2	2:L:660:LYS:HA	1.85	0.58
1:D:65:LEU:HB3	1:D:69:THR:HG21	1.85	0.58
2:H:298:TYR:OH	2:H:712:PRO:HG2	2.04	0.58
1:A:338:ARG:HD2	1:A:470:GLU:OE2	2.03	0.58
1:E:106:VAL:HG22	1:E:166:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ALA:O	1:D:214:VAL:CB	2.51	0.58
1:E:244:TYR:CD1	1:E:244:TYR:C	2.81	0.58
2:H:593:VAL:CG2	2:H:622:MET:CE	2.81	0.58
2:J:537:ILE:HG13	2:J:699:GLU:HB3	1.86	0.58
2:K:121:GLN:HG3	2:K:324:SER:OG	2.03	0.58
2:K:563:GLN:HG2	2:K:660:LYS:HA	1.84	0.58
2:L:621:GLN:O	2:L:625:LYS:HB2	2.02	0.58
1:B:65:LEU:HB3	1:B:69:THR:HG21	1.85	0.58
1:C:45:THR:O	1:C:46:LEU:CG	2.46	0.58
1:A:342:TYR:CE1	1:A:465:HIS:CD2	2.91	0.58
1:B:413:PRO:C	1:B:415:GLU:H	2.12	0.58
1:C:108:GLN:HE22	1:D:108:GLN:H	1.50	0.58
1:F:106:VAL:HG23	1:F:107:ILE:HG13	1.85	0.58
2:I:377:ALA:O	2:I:381:VAL:HG23	2.03	0.58
1:C:359:THR:HB	1:C:360:PRO:HD3	1.85	0.58
2:J:335:GLU:OE1	2:J:335:GLU:N	2.36	0.58
2:H:255:LYS:HB3	2:J:569:LYS:NZ	2.19	0.58
1:A:188:LYS:HE3	1:A:196:LEU:HD11	1.85	0.58
1:C:127:ASP:HB3	1:D:345:GLN:O	2.04	0.58
1:D:387:LEU:O	1:D:391:LYS:HG2	2.04	0.58
2:H:91:ILE:HB	2:H:140:ALA:HB3	1.86	0.58
2:L:409:ASN:HA	2:L:422:ARG:HD3	1.85	0.58
2:H:553:PRO:HG2	2:H:684:GLU:HG3	1.85	0.57
2:I:271:TYR:O	2:I:274:THR:HG22	2.04	0.57
2:L:448:VAL:HG12	2:L:449:PHE:H	1.69	0.57
2:L:704:ALA:HA	2:L:708:LEU:HD23	1.86	0.57
1:C:106:VAL:HG23	1:C:107:ILE:HG13	1.86	0.57
2:J:56:SER:HB3	2:J:57:PRO:HD2	1.86	0.57
2:K:448:VAL:HG12	2:K:449:PHE:H	1.68	0.57
1:B:203:ARG:C	1:B:205:ASN:H	2.13	0.57
1:D:45:THR:O	1:D:46:LEU:CG	2.48	0.57
2:J:150:LEU:O	2:J:154:ILE:HB	2.05	0.57
2:G:589:ASP:OD2	2:G:631:LYS:O	2.22	0.57
2:I:87:SER:HB2	2:I:252:ALA:HB2	1.87	0.57
1:B:178:LYS:CD	1:B:181:LYS:HD3	2.20	0.57
2:L:537:ILE:HG13	2:L:699:GLU:HB3	1.87	0.57
1:C:224:GLY:HA3	1:C:296:PHE:CZ	2.40	0.57
1:C:389:ASN:O	1:C:393:MET:HG3	2.05	0.57
1:F:287:GLU:O	1:F:291:LYS:HG3	2.04	0.57
1:F:413:PRO:C	1:F:415:GLU:H	2.11	0.57
2:G:563:GLN:HG2	2:G:563:GLN:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:338:ALA:HB1	2:H:715:GLY:HA3	1.87	0.57
2:J:40:HIS:CE1	2:J:57:PRO:HD3	2.40	0.57
2:L:553:PRO:HB3	2:L:680:ARG:HD2	1.87	0.57
2:K:385:LEU:O	2:K:387:THR:HG23	2.05	0.57
2:G:454:LEU:HG	2:G:457:ARG:HH21	1.69	0.57
2:K:338:ALA:HB1	2:K:715:GLY:HA3	1.86	0.57
2:K:563:GLN:HG2	2:K:563:GLN:O	2.05	0.57
1:A:65:LEU:HB3	1:A:69:THR:HG21	1.87	0.57
1:B:106:VAL:HG23	1:B:107:ILE:HG13	1.86	0.57
2:G:629:GLY:O	2:G:631:LYS:N	2.35	0.57
1:A:300:TYR:OH	2:G:222:VAL:HA	2.05	0.56
1:B:213:ALA:O	1:B:214:VAL:HB	2.04	0.56
2:H:409:ASN:HA	2:H:422:ARG:HD3	1.87	0.56
2:K:330:LEU:O	2:K:333:THR:N	2.35	0.56
2:L:87:SER:HB2	2:L:252:ALA:HB2	1.87	0.56
1:E:45:THR:O	1:E:46:LEU:CG	2.45	0.56
2:G:628:LEU:O	2:G:630:ARG:N	2.37	0.56
2:H:253:ASP:HB2	2:H:255:LYS:HE2	1.85	0.56
2:H:537:ILE:HG13	2:H:699:GLU:HB3	1.86	0.56
2:K:40:HIS:CE1	2:K:57:PRO:HD3	2.40	0.56
1:A:174:ARG:HD3	1:A:177:ARG:CB	2.35	0.56
1:A:175:HIS:NE2	1:A:212:PRO:HG3	2.20	0.56
1:A:178:LYS:CA	1:A:181:LYS:HB2	2.28	0.56
1:A:403:MET:HE1	1:A:409:VAL:HG23	1.87	0.56
1:D:71:TYR:HA	1:D:74:LEU:HD12	1.86	0.56
1:F:403:MET:HE1	1:F:409:VAL:HG23	1.86	0.56
2:I:455:LYS:HD3	2:I:476:THR:HG21	1.87	0.56
1:E:244:TYR:HD1	1:E:244:TYR:C	2.13	0.56
2:G:179:LEU:C	2:G:179:LEU:HD12	2.30	0.56
2:I:553:PRO:HB3	2:I:680:ARG:HD2	1.87	0.56
2:J:277:PHE:CD1	2:J:277:PHE:C	2.84	0.56
1:A:244:TYR:CD1	1:A:244:TYR:C	2.83	0.56
1:D:342:TYR:CE1	1:D:465:HIS:CD2	2.94	0.56
2:J:338:ALA:HB1	2:J:715:GLY:HA3	1.87	0.56
2:K:455:LYS:HD3	2:K:476:THR:HG21	1.88	0.56
2:L:390:LYS:HE3	2:L:433:LEU:O	2.05	0.56
1:A:202:PHE:HA	1:A:205:ASN:HD21	1.69	0.56
1:C:65:LEU:HB3	1:C:69:THR:HG21	1.87	0.56
2:H:40:HIS:CE1	2:H:57:PRO:HD3	2.41	0.56
1:E:224:GLY:HA3	1:E:296:PHE:CE1	2.41	0.56
1:F:300:TYR:OH	2:L:222:VAL:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:448:VAL:HG12	2:G:449:PHE:H	1.69	0.56
1:B:244:TYR:CD1	1:B:244:TYR:C	2.83	0.56
1:F:247:ARG:NH2	1:F:417:PHE:O	2.39	0.56
2:J:553:PRO:HB3	2:J:680:ARG:HD2	1.88	0.56
1:B:117:ARG:O	1:B:121:LEU:HG	2.05	0.56
1:B:180:ARG:HD2	1:B:203:ARG:CB	2.34	0.56
1:D:244:TYR:C	1:D:244:TYR:CD1	2.84	0.56
1:D:389:ASN:O	1:D:393:MET:HG3	2.06	0.56
1:F:411:LEU:HD23	1:F:412:PRO:O	2.05	0.56
2:G:589:ASP:OD2	2:G:634:LYS:CA	2.53	0.56
2:H:257:SER:H	2:H:258:PRO:HD3	1.68	0.56
1:D:66:LEU:O	1:D:69:THR:HG22	2.05	0.56
2:G:97:CYS:HB2	2:G:144:SER:HB2	1.88	0.56
2:H:593:VAL:CG2	2:H:622:MET:HE2	2.36	0.56
2:J:704:ALA:HA	2:J:708:LEU:HD23	1.88	0.56
2:K:164:ASP:OD1	2:K:165:ARG:N	2.39	0.56
2:L:377:ALA:O	2:L:381:VAL:HG23	2.06	0.56
1:C:247:ARG:NH2	1:C:417:PHE:O	2.38	0.55
2:H:330:LEU:O	2:H:333:THR:N	2.33	0.55
2:I:338:ALA:HB1	2:I:715:GLY:HA3	1.89	0.55
2:K:56:SER:HB3	2:K:57:PRO:HD2	1.87	0.55
2:L:97:CYS:HB2	2:L:144:SER:HB2	1.88	0.55
1:B:178:LYS:HD3	1:B:181:LYS:CD	2.20	0.55
1:F:369:THR:OG1	1:F:372:ASP:OD1	2.23	0.55
2:H:630:ARG:O	2:H:631:LYS:CB	2.54	0.55
2:J:97:CYS:HB2	2:J:144:SER:HB2	1.88	0.55
2:K:87:SER:HB2	2:K:252:ALA:HB2	1.87	0.55
1:B:359:THR:HB	1:B:360:PRO:HD3	1.87	0.55
1:C:244:TYR:CD1	1:C:244:TYR:C	2.84	0.55
1:C:403:MET:HE1	1:C:409:VAL:HG23	1.88	0.55
2:G:164:ASP:HB3	2:G:167:THR:OG1	2.05	0.55
2:H:56:SER:HB3	2:H:57:PRO:HD2	1.88	0.55
2:K:537:ILE:HG13	2:K:699:GLU:HB3	1.88	0.55
2:H:557:GLU:OE2	2:H:560:ARG:HD2	2.06	0.55
2:I:541:ASP:OD1	2:I:542:GLY:N	2.40	0.55
1:A:174:ARG:HD3	1:A:177:ARG:HB2	1.89	0.55
1:A:214:VAL:HG12	1:A:215:SER:N	2.21	0.55
1:A:387:LEU:O	1:A:391:LYS:HG2	2.07	0.55
1:D:93:VAL:HG12	1:D:94:PRO:HD2	1.89	0.55
1:E:117:ARG:O	1:E:121:LEU:HG	2.07	0.55
2:G:333:THR:HG23	2:G:336:SER:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:553:PRO:HB3	2:K:680:ARG:HD2	1.88	0.55
1:F:213:ALA:O	1:F:214:VAL:CB	2.54	0.55
2:L:333:THR:HG23	2:L:336:SER:H	1.71	0.55
1:B:180:ARG:HD3	1:B:207:LEU:HD22	1.86	0.55
2:H:390:LYS:HE3	2:H:433:LEU:O	2.06	0.55
2:H:455:LYS:HD3	2:H:476:THR:HG21	1.87	0.55
2:I:704:ALA:HA	2:I:708:LEU:HD23	1.88	0.55
2:J:390:LYS:HE3	2:J:433:LEU:O	2.06	0.55
2:K:487:VAL:O	2:K:487:VAL:HG12	2.06	0.55
2:K:564:GLU:OE2	2:K:740:TYR:OH	2.24	0.55
2:L:150:LEU:O	2:L:154:ILE:HB	2.07	0.55
1:A:117:ARG:O	1:A:121:LEU:HG	2.06	0.55
2:L:97:CYS:HA	2:L:143:GLY:HA3	1.89	0.55
1:C:387:LEU:O	1:C:391:LYS:HG2	2.07	0.55
1:D:244:TYR:O	1:D:244:TYR:HD1	1.88	0.55
1:A:106:VAL:HG23	1:A:107:ILE:HG13	1.89	0.55
1:A:173:ILE:C	1:A:211:LEU:HD12	2.31	0.55
1:B:178:LYS:CA	1:B:181:LYS:HB3	2.36	0.55
2:G:385:LEU:O	2:G:387:THR:HG23	2.07	0.55
2:G:390:LYS:HE3	2:G:433:LEU:O	2.06	0.55
2:J:696:THR:HB	2:J:697:PRO:HD2	1.87	0.55
2:K:390:LYS:HE3	2:K:433:LEU:O	2.07	0.55
2:K:97:CYS:HB2	2:K:144:SER:HB2	1.89	0.54
1:B:180:ARG:HH12	1:B:204:PHE:HA	1.71	0.54
1:D:413:PRO:C	1:D:415:GLU:H	2.15	0.54
1:E:251:LEU:HG	1:E:419:ASN:O	2.06	0.54
1:F:261:LEU:O	1:F:264:VAL:HG12	2.07	0.54
2:J:80:TRP:CH2	2:J:133:SER:HA	2.42	0.54
2:J:359:LYS:HD2	2:J:469:HIS:HD2	1.72	0.54
2:K:553:PRO:HG2	2:K:684:GLU:HG3	1.89	0.54
1:B:266:PRO:HB3	1:B:276:THR:HG22	1.88	0.54
1:B:429:PRO:HB2	1:B:432:ALA:HB3	1.88	0.54
1:C:244:TYR:O	1:C:244:TYR:HD1	1.90	0.54
1:C:405:ARG:NH1	1:C:409:VAL:HA	2.21	0.54
1:F:244:TYR:O	1:F:244:TYR:HD1	1.90	0.54
2:H:572:ASP:OD1	2:H:585:ALA:HB3	2.07	0.54
1:A:127:ASP:HB3	1:B:345:GLN:O	2.08	0.54
1:B:180:ARG:CD	1:B:203:ARG:NE	2.71	0.54
1:B:198:LEU:HD23	1:B:201:LYS:HE2	1.87	0.54
1:B:229:ARG:NH1	2:H:223:GLU:OE1	2.38	0.54
1:C:66:LEU:O	1:C:69:THR:CG2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:487:VAL:O	2:J:487:VAL:HG12	2.06	0.54
1:A:74:LEU:O	1:A:167:LEU:HD21	2.08	0.54
2:I:333:THR:HG23	2:I:336:SER:H	1.72	0.54
2:J:97:CYS:HA	2:J:143:GLY:HA3	1.89	0.54
2:K:300:ALA:HB3	2:K:301:PRO:HD3	1.89	0.54
1:A:244:TYR:HD1	1:A:244:TYR:C	2.16	0.54
2:G:610:ARG:HH22	2:G:687:MET:HE1	1.73	0.54
2:G:338:ALA:HB1	2:G:715:GLY:CA	2.38	0.54
2:G:589:ASP:OD2	2:G:634:LYS:CB	2.56	0.54
2:J:563:GLN:HG2	2:J:563:GLN:O	2.06	0.54
2:K:557:GLU:OE2	2:K:560:ARG:HD2	2.08	0.54
2:L:732:ARG:O	2:L:736:TYR:CD2	2.61	0.54
1:F:117:ARG:CZ	1:F:121:LEU:HD21	2.37	0.54
2:H:300:ALA:HB3	2:H:301:PRO:HD3	1.90	0.54
2:H:563:GLN:O	2:H:660:LYS:HB2	2.07	0.54
2:J:383:LYS:HG2	2:J:531:LYS:O	2.07	0.54
1:E:413:PRO:C	1:E:415:GLU:H	2.14	0.54
1:F:220:SER:O	1:F:221:GLU:CB	2.55	0.54
1:D:244:TYR:C	1:D:244:TYR:HD1	2.16	0.54
1:E:128:LYS:O	1:F:344:SER:HB3	2.07	0.54
1:E:405:ARG:NH1	1:E:409:VAL:HA	2.22	0.54
1:C:234:PHE:CZ	1:C:392:ALA:HB2	2.42	0.53
1:F:43:LYS:HE2	1:F:371:ASN:O	2.07	0.53
1:F:66:LEU:O	1:F:69:THR:CG2	2.56	0.53
1:F:244:TYR:HD1	1:F:244:TYR:C	2.16	0.53
2:G:87:SER:HB2	2:G:252:ALA:HB2	1.89	0.53
2:H:637:TYR:HA	2:H:644:LYS:O	2.08	0.53
1:B:402:TYR:CE2	2:H:227:PRO:HB3	2.44	0.53
1:B:405:ARG:NH1	1:B:409:VAL:HA	2.23	0.53
1:F:244:TYR:C	1:F:244:TYR:CD1	2.84	0.53
2:I:537:ILE:HG23	2:I:537:ILE:O	2.07	0.53
1:C:251:LEU:HG	1:C:419:ASN:O	2.08	0.53
2:G:330:LEU:O	2:G:333:THR:N	2.33	0.53
2:H:593:VAL:HG22	2:H:622:MET:CE	2.38	0.53
1:A:93:VAL:HG12	1:A:94:PRO:HD2	1.89	0.53
2:G:687:MET:HE3	2:G:747:CYS:HB3	1.89	0.53
2:H:651:ASP:C	2:H:653:ASP:N	2.64	0.53
2:I:383:LYS:HG2	2:I:531:LYS:O	2.08	0.53
2:J:51:VAL:HG11	2:J:241:GLU:OE2	2.08	0.53
2:K:283:TYR:OH	2:K:312:ILE:HD11	2.09	0.53
2:L:56:SER:HB3	2:L:57:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:338:ALA:HB1	2:L:715:GLY:CA	2.38	0.53
1:A:111:LYS:HE2	1:B:213:ALA:CB	2.39	0.53
1:A:127:ASP:O	1:B:344:SER:OG	2.26	0.53
2:K:541:ASP:OD1	2:K:542:GLY:N	2.42	0.53
2:L:487:VAL:O	2:L:487:VAL:HG12	2.07	0.53
1:C:104:GLY:HA2	1:C:134:VAL:O	2.08	0.53
1:D:287:GLU:O	1:D:291:LYS:HG3	2.08	0.53
1:F:166:GLU:HB2	1:F:430:PHE:O	2.09	0.53
2:K:174:VAL:HG21	2:K:201:MET:O	2.08	0.53
1:B:71:TYR:HA	1:B:74:LEU:HD12	1.91	0.53
1:C:71:TYR:HA	1:C:74:LEU:HD12	1.91	0.53
1:F:321:MET:CE	1:F:329:MET:HG3	2.39	0.53
2:G:612:GLY:O	2:G:744:PHE:HZ	1.91	0.53
2:L:60:LYS:HG3	2:L:61:VAL:HG12	1.91	0.53
1:C:93:VAL:HG12	1:C:94:PRO:HD2	1.89	0.53
2:G:56:SER:HB3	2:G:57:PRO:HD2	1.91	0.53
1:A:43:LYS:O	1:A:45:THR:HG23	2.09	0.53
1:B:234:PHE:CZ	1:B:392:ALA:HB2	2.44	0.53
1:C:342:TYR:CE1	1:C:465:HIS:CD2	2.97	0.53
1:F:234:PHE:CZ	1:F:392:ALA:HB2	2.44	0.53
2:G:99:ILE:HB	2:G:149:GLY:HA3	1.91	0.53
2:G:696:THR:HB	2:G:697:PRO:HD2	1.89	0.53
1:A:197:SER:HA	1:A:200:SER:HB3	1.90	0.53
1:B:104:GLY:HA2	1:B:134:VAL:O	2.09	0.53
1:B:180:ARG:HD2	1:B:203:ARG:NE	2.24	0.53
2:H:398:ASP:O	2:H:399:ARG:C	2.52	0.53
2:H:553:PRO:HB3	2:H:680:ARG:HD2	1.90	0.53
2:L:455:LYS:HD3	2:L:476:THR:HG21	1.90	0.53
1:E:71:TYR:HA	1:E:74:LEU:HD12	1.91	0.52
2:I:537:ILE:HG13	2:I:699:GLU:HB3	1.90	0.52
2:J:273:MET:HE2	2:J:279:ARG:HG2	1.92	0.52
2:L:105:ASN:HA	2:L:108:ALA:HB3	1.89	0.52
2:L:142:ASN:ND2	2:L:237:ILE:HD11	2.23	0.52
1:A:429:PRO:HB2	1:A:432:ALA:HB3	1.91	0.52
2:G:740:TYR:O	2:G:742:LYS:N	2.42	0.52
2:I:97:CYS:HB2	2:I:144:SER:HB2	1.90	0.52
2:L:359:LYS:CD	2:L:469:HIS:HD2	2.22	0.52
1:E:106:VAL:HG23	1:E:107:ILE:HG13	1.90	0.52
2:H:333:THR:HG23	2:H:336:SER:H	1.74	0.52
2:H:730:VAL:HG22	2:H:750:LEU:CD2	2.40	0.52
2:J:359:LYS:CD	2:J:469:HIS:HD2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:SER:OG	1:C:351:LEU:CD2	2.58	0.52
2:G:300:ALA:HB3	2:G:301:PRO:HD3	1.91	0.52
2:G:589:ASP:CG	2:G:634:LYS:CB	2.83	0.52
2:H:277:PHE:CD1	2:H:277:PHE:C	2.87	0.52
2:H:338:ALA:HB1	2:H:715:GLY:CA	2.39	0.52
2:H:730:VAL:HG22	2:H:750:LEU:HD21	1.91	0.52
2:K:311:GLY:O	2:K:314:GLN:O	2.26	0.52
2:K:333:THR:HG23	2:K:336:SER:H	1.75	0.52
1:A:211:LEU:CD2	1:B:174:ARG:NH2	2.72	0.52
1:B:66:LEU:O	1:B:69:THR:HG22	2.09	0.52
1:C:168:MET:HE1	1:C:429:PRO:HA	1.92	0.52
1:E:59:GLY:HA3	1:E:439:MET:SD	2.49	0.52
2:K:279:ARG:NH1	2:K:313:GLU:OE1	2.43	0.52
1:A:71:TYR:HA	1:A:74:LEU:HD12	1.91	0.52
1:A:174:ARG:HD2	1:A:178:LYS:HE2	1.91	0.52
1:B:117:ARG:CZ	1:B:121:LEU:HD21	2.40	0.52
1:B:178:LYS:HA	1:B:181:LYS:CB	2.38	0.52
1:D:104:GLY:HA2	1:D:134:VAL:O	2.09	0.52
1:D:244:TYR:O	1:D:245:ALA:C	2.52	0.52
2:I:696:THR:HB	2:I:697:PRO:HD2	1.90	0.52
1:A:57:VAL:HG21	1:A:321:MET:SD	2.50	0.52
1:D:117:ARG:O	1:D:121:LEU:HG	2.10	0.52
1:D:405:ARG:NH1	1:D:409:VAL:HA	2.25	0.52
2:G:40:HIS:CE1	2:G:57:PRO:CD	2.93	0.52
2:G:537:ILE:HG13	2:G:699:GLU:HB3	1.92	0.52
2:H:99:ILE:HB	2:H:149:GLY:HA3	1.90	0.52
2:H:179:LEU:C	2:H:179:LEU:HD12	2.35	0.52
2:J:553:PRO:HG2	2:J:684:GLU:HG3	1.92	0.52
1:A:338:ARG:HG3	1:A:470:GLU:HB2	1.91	0.52
1:B:166:GLU:HB2	1:B:430:PHE:O	2.09	0.52
1:C:244:TYR:C	1:C:244:TYR:HD1	2.18	0.52
2:G:66:LYS:HE3	2:G:105:ASN:HB2	1.92	0.52
2:G:493:LYS:HD3	2:G:521:THR:OG1	2.10	0.52
2:H:607:PHE:C	2:H:609:GLU:H	2.18	0.52
2:J:99:ILE:HB	2:J:149:GLY:HA3	1.90	0.52
2:L:735:LYS:O	2:L:739:ALA:HB3	2.08	0.52
1:A:166:GLU:HB2	1:A:430:PHE:O	2.10	0.52
1:A:287:GLU:O	1:A:291:LYS:HG3	2.09	0.52
1:B:57:VAL:O	1:B:334:LYS:HG3	2.09	0.52
1:E:93:VAL:HG12	1:E:94:PRO:HD2	1.91	0.52
2:I:405:PHE:O	2:I:406:LYS:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:71:GLU:O	2:J:75:VAL:HG23	2.10	0.52
2:J:745:THR:CG2	2:J:746:PRO:HD2	2.40	0.52
2:K:179:LEU:C	2:K:179:LEU:HD12	2.35	0.52
2:L:610:ARG:HH22	2:L:687:MET:HE1	1.73	0.52
1:A:439:MET:O	1:A:443:ASN:HB2	2.09	0.52
1:B:244:TYR:HD1	1:B:244:TYR:C	2.17	0.52
1:C:166:GLU:HB2	1:C:430:PHE:O	2.09	0.52
2:H:105:ASN:HA	2:H:108:ALA:HB3	1.92	0.52
2:H:750:LEU:HD23	2:H:750:LEU:C	2.35	0.52
2:I:553:PRO:HG2	2:I:684:GLU:HG3	1.90	0.52
2:J:405:PHE:O	2:J:406:LYS:C	2.53	0.52
2:J:735:LYS:O	2:J:739:ALA:HB3	2.09	0.52
2:K:338:ALA:HB1	2:K:715:GLY:CA	2.40	0.52
2:L:413:LYS:C	2:L:415:LYS:H	2.18	0.52
1:A:208:ALA:HB1	1:A:209:PRO:HD3	1.91	0.51
1:B:195:ARG:HA	1:B:198:LEU:HD12	1.93	0.51
2:G:398:ASP:O	2:G:399:ARG:C	2.53	0.51
2:H:745:THR:CG2	2:H:746:PRO:HD2	2.40	0.51
1:D:403:MET:HE1	1:D:409:VAL:HG23	1.90	0.51
1:E:439:MET:O	1:E:443:ASN:HB2	2.10	0.51
1:F:429:PRO:HB2	1:F:432:ALA:HB3	1.92	0.51
2:G:80:TRP:CH2	2:G:133:SER:HA	2.45	0.51
2:G:279:ARG:NH1	2:G:313:GLU:OE1	2.43	0.51
2:I:60:LYS:HG3	2:I:61:VAL:HG12	1.91	0.51
2:I:338:ALA:HB1	2:I:715:GLY:CA	2.39	0.51
2:L:194:VAL:N	2:L:195:PRO:CD	2.73	0.51
2:L:375:GLY:O	2:L:379:VAL:HG23	2.10	0.51
1:C:439:MET:O	1:C:443:ASN:HB2	2.11	0.51
2:J:398:ASP:O	2:J:399:ARG:C	2.53	0.51
2:L:71:GLU:O	2:L:75:VAL:HG23	2.11	0.51
1:A:207:LEU:O	1:A:208:ALA:O	2.28	0.51
1:D:338:ARG:HB2	1:D:468:ILE:O	2.09	0.51
1:E:260:LEU:HD13	1:E:420:TRP:NE1	2.25	0.51
2:J:750:LEU:HD23	2:J:750:LEU:C	2.35	0.51
2:K:97:CYS:HA	2:K:143:GLY:HA3	1.93	0.51
2:L:359:LYS:NZ	2:L:469:HIS:O	2.42	0.51
1:A:336:TYR:HB2	1:A:470:GLU:HB3	1.93	0.51
1:F:75:MET:O	1:F:78:ASP:HB2	2.10	0.51
1:F:413:PRO:O	1:F:415:GLU:N	2.43	0.51
2:K:64:LEU:O	2:K:102:ALA:HB3	2.10	0.51
1:B:196:LEU:HD23	1:B:199:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:ALA:HA	1:E:403:MET:HE3	1.93	0.51
2:J:333:THR:HG23	2:J:336:SER:H	1.75	0.51
2:K:405:PHE:O	2:K:406:LYS:C	2.54	0.51
2:L:398:ASP:O	2:L:399:ARG:C	2.54	0.51
1:B:174:ARG:HH11	1:B:177:ARG:HG2	1.73	0.51
1:B:178:LYS:C	1:B:181:LYS:HB3	2.35	0.51
1:D:439:MET:O	1:D:443:ASN:HB2	2.10	0.51
1:F:181:LYS:C	1:F:183:MET:H	2.18	0.51
1:F:244:TYR:O	1:F:245:ALA:C	2.54	0.51
2:I:557:GLU:OE2	2:I:560:ARG:HD2	2.10	0.51
2:L:572:ASP:OD1	2:L:585:ALA:HB3	2.11	0.51
1:A:180:ARG:HG2	1:A:203:ARG:HD3	1.93	0.51
1:A:182:LEU:C	1:A:184:LEU:H	2.18	0.51
1:D:216:GLU:HG2	1:D:221:GLU:H	1.74	0.51
1:F:336:TYR:HB2	1:F:470:GLU:HB3	1.93	0.51
2:G:446:GLU:HG2	2:G:448:VAL:HG23	1.92	0.51
2:G:622:MET:O	2:G:627:PHE:N	2.40	0.51
2:H:359:LYS:CD	2:H:469:HIS:HD2	2.24	0.51
2:H:493:LYS:HD3	2:H:521:THR:OG1	2.11	0.51
2:J:413:LYS:C	2:J:415:LYS:H	2.19	0.51
2:K:99:ILE:HB	2:K:149:GLY:HA3	1.92	0.51
2:L:61:VAL:HG23	2:L:97:CYS:SG	2.50	0.51
1:A:210:GLU:O	1:A:211:LEU:HB2	2.11	0.51
2:G:553:PRO:HG2	2:G:684:GLU:HG3	1.92	0.51
1:E:88:LEU:HD21	1:E:95:LYS:HE2	1.93	0.51
2:G:97:CYS:HA	2:G:143:GLY:HA3	1.92	0.51
2:G:701:ASP:O	2:G:702:ILE:C	2.54	0.51
2:H:256:ILE:HG13	2:H:256:ILE:O	2.09	0.51
2:I:40:HIS:CE1	2:I:57:PRO:HD3	2.46	0.51
2:I:563:GLN:HG2	2:I:563:GLN:O	2.11	0.51
2:J:64:LEU:O	2:J:102:ALA:HB3	2.10	0.51
2:K:194:VAL:N	2:K:195:PRO:CD	2.74	0.51
1:C:69:THR:CG2	1:C:70:SER:H	2.21	0.50
1:E:424:LEU:O	1:E:424:LEU:HD23	2.11	0.50
1:F:359:THR:HB	1:F:360:PRO:HD3	1.93	0.50
2:H:66:LYS:HE3	2:H:105:ASN:HB2	1.92	0.50
2:I:359:LYS:CD	2:I:469:HIS:HD2	2.25	0.50
2:L:99:ILE:HB	2:L:149:GLY:HA3	1.93	0.50
2:L:553:PRO:HG2	2:L:684:GLU:HG3	1.92	0.50
1:A:43:LYS:HE2	1:A:371:ASN:O	2.12	0.50
1:A:429:PRO:O	1:A:430:PHE:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:CD2	1:B:212:PRO:HD3	2.41	0.50
1:B:338:ARG:HB2	1:B:468:ILE:O	2.11	0.50
1:C:136:MET:HB2	1:D:132:HIS:HB2	1.93	0.50
1:D:75:MET:HB3	1:D:76:PRO:HD2	1.93	0.50
2:G:405:PHE:O	2:G:406:LYS:C	2.51	0.50
2:K:735:LYS:O	2:K:739:ALA:HB3	2.12	0.50
2:L:68:LEU:C	2:L:68:LEU:HD23	2.36	0.50
2:L:294:THR:C	2:L:296:GLY:H	2.19	0.50
2:L:368:GLY:O	2:L:373:GLY:HA3	2.10	0.50
2:L:488:SER:HB3	2:L:491:PRO:HG3	1.93	0.50
1:A:108:GLN:H	1:B:108:GLN:HE22	1.58	0.50
1:A:312:THR:HG21	1:A:427:GLY:CA	2.42	0.50
1:E:310:PHE:O	1:E:312:THR:HG23	2.11	0.50
1:F:69:THR:CG2	1:F:70:SER:N	2.74	0.50
2:G:724:TYR:CZ	2:G:728:LYS:HE2	2.46	0.50
2:J:186:GLN:HG3	2:J:320:TYR:CD1	2.46	0.50
2:K:200:MET:HG3	2:K:207:ILE:HD11	1.93	0.50
2:L:730:VAL:HG21	2:L:754:ALA:CB	2.41	0.50
1:F:220:SER:O	1:F:221:GLU:HB2	2.11	0.50
2:H:609:GLU:CG	2:H:610:ARG:N	2.73	0.50
1:D:57:VAL:O	1:D:334:LYS:HG3	2.12	0.50
2:G:589:ASP:CG	2:G:634:LYS:H	2.18	0.50
2:G:589:ASP:CB	2:G:634:LYS:CB	2.90	0.50
2:I:194:VAL:N	2:I:195:PRO:CD	2.74	0.50
2:J:174:VAL:CG2	2:J:201:MET:O	2.60	0.50
2:J:744:PHE:CD1	2:J:744:PHE:N	2.78	0.50
1:B:213:ALA:O	1:B:214:VAL:CB	2.59	0.50
1:C:402:TYR:CE2	2:I:227:PRO:HB3	2.47	0.50
1:D:414:LEU:HD12	1:D:414:LEU:H	1.77	0.50
2:I:487:VAL:O	2:I:487:VAL:HG12	2.11	0.50
2:K:98:PHE:CD2	2:K:99:ILE:HG12	2.47	0.50
2:K:105:ASN:HA	2:K:108:ALA:HB3	1.93	0.50
2:K:744:PHE:N	2:K:744:PHE:CD1	2.78	0.50
2:L:750:LEU:HD23	2:L:750:LEU:C	2.36	0.50
1:A:59:GLY:HA3	1:A:439:MET:SD	2.52	0.50
1:B:75:MET:HB3	1:B:76:PRO:HD2	1.93	0.50
1:B:180:ARG:HD3	1:B:207:LEU:CD1	2.41	0.50
2:G:735:LYS:O	2:G:739:ALA:HB3	2.11	0.50
2:I:163:LYS:HG2	2:I:221:LEU:CD2	2.42	0.50
2:I:730:VAL:HG22	2:I:750:LEU:CD2	2.42	0.50
2:K:197:ALA:O	2:K:201:MET:HE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:650:SER:O	2:K:653:ASP:HB2	2.11	0.50
2:L:563:GLN:HG2	2:L:563:GLN:O	2.10	0.50
1:B:93:VAL:HG12	1:B:94:PRO:HD2	1.93	0.50
1:C:336:TYR:HB2	1:C:470:GLU:HB3	1.94	0.50
1:E:43:LYS:HE2	1:E:371:ASN:O	2.11	0.50
2:H:60:LYS:HG3	2:H:61:VAL:HG12	1.94	0.50
2:H:61:VAL:HG23	2:H:97:CYS:SG	2.52	0.50
2:I:277:PHE:C	2:I:277:PHE:CD1	2.89	0.50
2:I:750:LEU:C	2:I:750:LEU:HD23	2.37	0.50
2:K:145:CYS:HB3	2:K:169:LEU:CD2	2.41	0.50
2:L:273:MET:HE2	2:L:279:ARG:HG2	1.94	0.50
1:C:69:THR:CG2	1:C:70:SER:N	2.75	0.50
1:C:312:THR:HG21	1:C:427:GLY:CA	2.42	0.50
1:D:251:LEU:HG	1:D:419:ASN:O	2.11	0.50
1:D:260:LEU:HD13	1:D:420:TRP:NE1	2.27	0.50
1:E:69:THR:CG2	1:E:70:SER:H	2.22	0.50
2:H:628:LEU:O	2:H:631:LYS:O	2.30	0.50
2:I:398:ASP:O	2:I:399:ARG:C	2.55	0.50
2:L:335:GLU:OE1	2:L:335:GLU:N	2.42	0.50
1:A:66:LEU:O	1:A:69:THR:CG2	2.60	0.49
2:G:43:TYR:OH	2:G:79:ILE:HG22	2.12	0.49
2:H:589:ASP:O	2:H:629:GLY:HA3	2.11	0.49
2:I:413:LYS:C	2:I:415:LYS:H	2.19	0.49
2:J:66:LYS:HE3	2:J:105:ASN:HB2	1.94	0.49
2:J:730:VAL:HG22	2:J:750:LEU:HD21	1.92	0.49
1:A:132:HIS:HB2	1:B:136:MET:HB2	1.94	0.49
1:B:200:SER:HA	1:B:203:ARG:HG2	1.95	0.49
1:C:244:TYR:O	1:C:245:ALA:C	2.53	0.49
2:G:553:PRO:HB3	2:G:680:ARG:HD2	1.93	0.49
2:H:610:ARG:HH22	2:H:687:MET:HE1	1.77	0.49
2:I:730:VAL:HG22	2:I:750:LEU:HD21	1.93	0.49
2:J:105:ASN:HA	2:J:108:ALA:HB3	1.93	0.49
2:K:455:LYS:NZ	2:K:479:LEU:HD12	2.27	0.49
2:K:730:VAL:HG22	2:K:750:LEU:HD21	1.93	0.49
1:B:205:ASN:O	1:B:206:PHE:CG	2.64	0.49
1:B:414:LEU:H	1:B:414:LEU:HD12	1.78	0.49
1:D:300:TYR:OH	2:J:222:VAL:HA	2.12	0.49
1:F:71:TYR:HA	1:F:74:LEU:HD12	1.95	0.49
2:G:294:THR:C	2:G:296:GLY:H	2.20	0.49
2:G:745:THR:CG2	2:G:746:PRO:HD2	2.42	0.49
2:H:563:GLN:HG2	2:H:563:GLN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:696:THR:HB	2:H:697:PRO:HD2	1.95	0.49
2:I:379:VAL:O	2:I:383:LYS:HD3	2.12	0.49
2:I:687:MET:HE3	2:I:747:CYS:HB3	1.94	0.49
2:J:145:CYS:HB3	2:J:169:LEU:CD2	2.42	0.49
2:K:612:GLY:O	2:K:744:PHE:HZ	1.95	0.49
2:K:730:VAL:HG22	2:K:750:LEU:CD2	2.41	0.49
2:L:114:GLN:HA	2:L:117:THR:HB	1.95	0.49
1:A:93:VAL:CG2	1:A:319:LEU:HD22	2.42	0.49
1:E:143:GLN:HA	1:E:342:TYR:OH	2.13	0.49
1:F:93:VAL:CG2	1:F:319:LEU:HD22	2.42	0.49
1:F:101:ILE:HB	1:F:131:ALA:HB2	1.94	0.49
2:G:335:GLU:OE1	2:G:335:GLU:N	2.42	0.49
2:H:194:VAL:N	2:H:195:PRO:CD	2.75	0.49
2:H:460:LYS:CG	2:H:487:VAL:HG11	2.43	0.49
2:I:97:CYS:HA	2:I:143:GLY:HA3	1.95	0.49
2:J:578:PHE:CE2	2:J:678:VAL:HG21	2.47	0.49
2:K:60:LYS:HG3	2:K:61:VAL:HG12	1.94	0.49
2:K:460:LYS:CG	2:K:487:VAL:HG11	2.42	0.49
2:J:68:LEU:HD23	2:J:68:LEU:C	2.37	0.49
2:J:164:ASP:OD1	2:J:165:ARG:N	2.46	0.49
2:J:298:TYR:OH	2:J:712:PRO:HG2	2.13	0.49
2:J:563:GLN:CG	2:J:660:LYS:HA	2.41	0.49
2:L:701:ASP:O	2:L:702:ILE:C	2.56	0.49
1:A:174:ARG:HE	1:B:174:ARG:HH21	1.61	0.49
1:E:93:VAL:CG2	1:E:319:LEU:HD22	2.42	0.49
2:H:390:LYS:CD	2:H:435:TYR:HE1	2.12	0.49
2:H:651:ASP:C	2:H:653:ASP:H	2.21	0.49
2:I:546:TYR:CE1	2:I:694:LEU:HD11	2.48	0.49
2:J:194:VAL:N	2:J:195:PRO:CD	2.75	0.49
1:B:93:VAL:CG2	1:B:319:LEU:HD22	2.43	0.49
2:H:294:THR:C	2:H:296:GLY:H	2.21	0.49
2:I:578:PHE:CE2	2:I:678:VAL:HG21	2.47	0.49
2:L:115:GLU:O	2:L:119:LEU:HD13	2.13	0.49
1:B:69:THR:CG2	1:B:70:SER:H	2.24	0.49
1:B:399:ALA:HA	1:B:403:MET:HE3	1.94	0.49
1:D:69:THR:CG2	1:D:70:SER:H	2.24	0.49
2:I:745:THR:CG2	2:I:746:PRO:HD2	2.42	0.49
2:J:338:ALA:HB1	2:J:715:GLY:CA	2.42	0.49
2:K:701:ASP:O	2:K:702:ILE:C	2.56	0.49
2:L:385:LEU:O	2:L:387:THR:HG23	2.12	0.49
2:L:455:LYS:NZ	2:L:479:LEU:HD12	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ALA:HB2	1:B:338:ARG:NH2	2.28	0.49
1:B:102:ILE:HD13	1:B:147:THR:HB	1.95	0.49
1:F:84:LEU:HB3	1:F:125:PHE:HE2	1.78	0.49
1:F:405:ARG:NH1	1:F:409:VAL:HA	2.28	0.49
2:I:359:LYS:NZ	2:I:471:ILE:HD12	2.27	0.49
2:I:564:GLU:OE2	2:I:740:TYR:OH	2.30	0.49
2:J:200:MET:HG3	2:J:207:ILE:HD11	1.95	0.49
2:J:295:LYS:O	2:J:297:LEU:HD12	2.12	0.49
2:J:330:LEU:O	2:J:333:THR:N	2.36	0.49
2:K:61:VAL:HG23	2:K:97:CYS:SG	2.53	0.49
2:L:298:TYR:OH	2:L:712:PRO:HG2	2.13	0.49
1:A:166:GLU:HG2	1:A:430:PHE:HB2	1.95	0.49
1:A:220:SER:O	1:A:221:GLU:HB2	2.13	0.49
1:B:166:GLU:HG2	1:B:430:PHE:HB2	1.95	0.49
1:C:117:ARG:O	1:C:121:LEU:HG	2.12	0.49
2:G:66:LYS:HE3	2:G:105:ASN:CB	2.43	0.49
2:G:160:ILE:HG12	2:G:220:GLN:HB3	1.95	0.49
2:G:460:LYS:CG	2:G:487:VAL:HG11	2.43	0.49
2:H:546:TYR:CE1	2:H:694:LEU:HD11	2.48	0.49
2:H:593:VAL:HG21	2:H:622:MET:HE2	1.93	0.49
2:I:493:LYS:HD3	2:I:521:THR:OG1	2.13	0.49
2:J:98:PHE:CD2	2:J:99:ILE:HG12	2.47	0.49
2:J:179:LEU:C	2:J:179:LEU:HD12	2.38	0.49
2:L:171:THR:OG1	2:L:200:MET:O	2.30	0.49
1:A:76:PRO:O	1:A:165:VAL:HG21	2.13	0.48
1:A:102:ILE:HD12	1:A:132:HIS:CE1	2.48	0.48
1:B:220:SER:O	1:B:221:GLU:CB	2.61	0.48
1:E:321:MET:CE	1:E:329:MET:HG3	2.43	0.48
1:F:75:MET:HB3	1:F:76:PRO:HD2	1.94	0.48
1:F:339:ASP:OD2	1:F:366:ALA:HA	2.13	0.48
2:G:390:LYS:HA	2:G:432:GLN:O	2.12	0.48
2:H:145:CYS:HB3	2:H:169:LEU:CD2	2.43	0.48
2:H:592:GLY:O	2:H:596:ALA:N	2.46	0.48
2:H:593:VAL:CG2	2:H:622:MET:HE1	2.42	0.48
2:I:744:PHE:N	2:I:744:PHE:CD1	2.78	0.48
2:K:163:LYS:HD2	2:K:223:GLU:HG3	1.95	0.48
2:L:546:TYR:CE1	2:L:694:LEU:HD11	2.48	0.48
1:A:182:LEU:C	1:A:184:LEU:N	2.71	0.48
1:A:234:PHE:CZ	1:A:392:ALA:HB2	2.48	0.48
1:B:179:MET:C	1:B:181:LYS:H	2.20	0.48
1:B:179:MET:C	1:B:181:LYS:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:TYR:CE1	1:B:465:HIS:CG	3.01	0.48
2:G:60:LYS:HG3	2:G:61:VAL:HG12	1.94	0.48
2:G:115:GLU:O	2:G:119:LEU:HD13	2.13	0.48
2:H:359:LYS:NZ	2:H:471:ILE:HD12	2.28	0.48
2:I:172:PRO:O	2:I:173:GLU:C	2.56	0.48
1:A:220:SER:O	1:A:221:GLU:CB	2.61	0.48
1:B:76:PRO:O	1:B:165:VAL:HG21	2.12	0.48
1:B:184:LEU:N	1:B:184:LEU:HD23	2.27	0.48
1:B:439:MET:O	1:B:443:ASN:HB2	2.14	0.48
2:G:60:LYS:HG3	2:G:61:VAL:N	2.28	0.48
2:G:513:THR:O	2:G:513:THR:HG23	2.13	0.48
2:J:541:ASP:OD1	2:J:542:GLY:N	2.46	0.48
2:J:730:VAL:HG22	2:J:750:LEU:CD2	2.44	0.48
2:L:460:LYS:CG	2:L:487:VAL:HG11	2.39	0.48
1:B:69:THR:CG2	1:B:70:SER:N	2.76	0.48
1:E:75:MET:O	1:E:78:ASP:HB2	2.13	0.48
1:E:312:THR:HG21	1:E:427:GLY:CA	2.44	0.48
1:E:414:LEU:H	1:E:414:LEU:HD12	1.78	0.48
2:G:114:GLN:O	2:G:118:GLN:HB2	2.13	0.48
2:H:359:LYS:HD2	2:H:469:HIS:HD2	1.78	0.48
2:K:68:LEU:HD23	2:K:68:LEU:C	2.38	0.48
2:L:578:PHE:CE2	2:L:678:VAL:HG21	2.49	0.48
1:E:405:ARG:HH12	1:E:409:VAL:HA	1.79	0.48
2:H:255:LYS:HB3	2:J:569:LYS:HZ2	1.78	0.48
2:H:273:MET:HE2	2:H:279:ARG:HG2	1.94	0.48
2:H:618:LEU:HD12	2:H:618:LEU:C	2.39	0.48
2:J:300:ALA:HB3	2:J:301:PRO:HD3	1.96	0.48
2:J:745:THR:HG22	2:J:746:PRO:HD2	1.95	0.48
2:L:495:ILE:HG13	2:L:512:ILE:O	2.14	0.48
1:B:180:ARG:HD2	1:B:203:ARG:CD	2.44	0.48
1:B:220:SER:O	1:B:221:GLU:HB2	2.12	0.48
1:D:74:LEU:O	1:D:167:LEU:CD2	2.61	0.48
1:E:300:TYR:OH	2:K:222:VAL:HA	2.13	0.48
1:E:402:TYR:CE2	2:K:227:PRO:HB3	2.48	0.48
1:F:166:GLU:HG3	1:F:168:MET:HE2	1.95	0.48
2:G:359:LYS:CD	2:G:469:HIS:HD2	2.27	0.48
2:G:455:LYS:NZ	2:G:479:LEU:HD12	2.29	0.48
2:G:563:GLN:CG	2:G:660:LYS:HA	2.44	0.48
2:I:105:ASN:HA	2:I:108:ALA:HB3	1.95	0.48
2:K:578:PHE:CE2	2:K:678:VAL:HG21	2.49	0.48
1:A:136:MET:HB2	1:B:132:HIS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HG12	1:B:173:ILE:CG2	2.44	0.48
1:A:413:PRO:C	1:A:415:GLU:H	2.21	0.48
1:B:57:VAL:HG21	1:B:321:MET:SD	2.53	0.48
1:C:74:LEU:O	1:C:167:LEU:HD21	2.14	0.48
1:C:93:VAL:CG2	1:C:319:LEU:HD22	2.44	0.48
1:F:413:PRO:C	1:F:415:GLU:N	2.71	0.48
2:H:563:GLN:CG	2:H:660:LYS:HA	2.43	0.48
2:H:730:VAL:HG21	2:H:754:ALA:CB	2.42	0.48
2:J:114:GLN:HA	2:J:117:THR:HB	1.95	0.48
2:J:495:ILE:HG13	2:J:512:ILE:O	2.14	0.48
2:K:732:ARG:O	2:K:736:TYR:CD2	2.67	0.48
2:L:744:PHE:N	2:L:744:PHE:CD1	2.77	0.48
1:A:75:MET:HB3	1:A:76:PRO:HD2	1.96	0.48
1:B:180:ARG:HB2	1:B:203:ARG:HD2	1.95	0.48
1:C:297:ILE:O	1:C:301:GLY:HA3	2.14	0.48
1:E:216:GLU:OE1	1:E:221:GLU:N	2.47	0.48
1:F:145:MET:SD	1:F:438:VAL:HG11	2.54	0.48
2:G:194:VAL:N	2:G:195:PRO:CD	2.77	0.48
2:G:544:GLY:O	2:G:549:ARG:HB2	2.14	0.48
2:H:488:SER:HB3	2:H:491:PRO:HG3	1.94	0.48
2:J:683:ASN:O	2:J:686:VAL:HG22	2.14	0.48
2:J:701:ASP:O	2:J:702:ILE:C	2.57	0.48
2:K:390:LYS:CD	2:K:435:TYR:HE1	2.14	0.48
2:K:745:THR:CG2	2:K:746:PRO:HD2	2.43	0.48
2:L:650:SER:O	2:L:653:ASP:HB2	2.13	0.48
1:A:370:MET:HE1	1:A:412:PRO:HB3	1.95	0.48
1:B:203:ARG:C	1:B:205:ASN:N	2.69	0.48
1:B:260:LEU:HD13	1:B:420:TRP:NE1	2.29	0.48
1:D:145:MET:SD	1:D:438:VAL:HG11	2.54	0.48
1:D:228:ASP:HA	1:D:303:VAL:HG23	1.94	0.48
1:D:336:TYR:HB2	1:D:470:GLU:HB3	1.96	0.48
1:F:43:LYS:CD	1:F:372:ASP:HA	2.42	0.48
1:F:359:THR:O	1:F:363:LEU:HB2	2.14	0.48
2:G:98:PHE:CD2	2:G:99:ILE:HG12	2.49	0.48
1:A:414:LEU:HD12	1:A:414:LEU:H	1.79	0.48
1:B:75:MET:O	1:B:78:ASP:HB2	2.14	0.48
1:E:75:MET:HB3	1:E:76:PRO:HD2	1.96	0.48
2:G:359:LYS:HD2	2:G:469:HIS:HD2	1.78	0.48
2:G:745:THR:HG22	2:G:746:PRO:HD2	1.95	0.48
2:H:68:LEU:HD23	2:H:68:LEU:C	2.38	0.48
2:K:43:TYR:OH	2:K:79:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:277:PHE:CD1	2:K:277:PHE:C	2.92	0.48
1:A:111:LYS:HE2	1:B:213:ALA:HB2	1.96	0.47
1:A:228:ASP:HA	1:A:303:VAL:HG23	1.96	0.47
2:I:89:VAL:HG12	2:I:90:LEU:N	2.28	0.47
2:I:179:LEU:C	2:I:179:LEU:HD12	2.38	0.47
2:J:375:GLY:HA2	2:J:504:ASP:OD1	2.14	0.47
1:A:145:MET:SD	1:A:438:VAL:HG11	2.54	0.47
1:A:247:ARG:NH2	1:A:417:PHE:O	2.47	0.47
2:H:487:VAL:O	2:H:487:VAL:HG12	2.12	0.47
2:H:612:GLY:O	2:H:744:PHE:HZ	1.97	0.47
2:H:735:LYS:O	2:H:739:ALA:HB3	2.13	0.47
2:L:745:THR:CG2	2:L:746:PRO:HD2	2.44	0.47
1:A:226:SER:OG	1:A:351:LEU:CD2	2.62	0.47
1:A:260:LEU:HD13	1:A:420:TRP:NE1	2.29	0.47
1:A:342:TYR:CE1	1:A:465:HIS:CG	3.02	0.47
1:B:403:MET:HE1	1:B:409:VAL:HG23	1.96	0.47
1:C:57:VAL:O	1:C:334:LYS:HG3	2.15	0.47
1:C:142:ASN:HA	1:C:145:MET:HE3	1.96	0.47
1:D:312:THR:HG21	1:D:427:GLY:CA	2.44	0.47
1:E:285:SER:OG	1:E:288:GLN:HB2	2.14	0.47
1:E:338:ARG:HG3	1:E:470:GLU:HB2	1.96	0.47
2:G:105:ASN:HA	2:G:108:ALA:HB3	1.95	0.47
2:G:413:LYS:C	2:G:415:LYS:H	2.21	0.47
2:G:487:VAL:O	2:G:487:VAL:HG12	2.14	0.47
2:I:174:VAL:HG22	2:I:201:MET:O	2.12	0.47
2:I:298:TYR:OH	2:I:712:PRO:HG2	2.15	0.47
2:I:455:LYS:NZ	2:I:479:LEU:HD12	2.29	0.47
2:J:379:VAL:O	2:J:383:LYS:HD3	2.15	0.47
2:J:390:LYS:CD	2:J:435:TYR:HE1	2.18	0.47
2:K:359:LYS:HD2	2:K:469:HIS:HD2	1.80	0.47
2:L:563:GLN:CG	2:L:660:LYS:HA	2.45	0.47
1:B:359:THR:O	1:B:363:LEU:HB2	2.14	0.47
1:E:117:ARG:CZ	1:E:121:LEU:HD21	2.45	0.47
1:E:136:MET:HB2	1:F:132:HIS:HB2	1.97	0.47
1:F:197:SER:O	1:F:201:LYS:N	2.38	0.47
2:G:744:PHE:N	2:G:744:PHE:CD1	2.78	0.47
2:I:607:PHE:C	2:I:609:GLU:H	2.23	0.47
2:J:487:VAL:O	2:J:487:VAL:CG1	2.62	0.47
1:A:170:ASP:OD2	1:B:178:LYS:O	2.33	0.47
1:B:102:ILE:CD1	1:B:147:THR:HB	2.44	0.47
1:C:75:MET:HB3	1:C:76:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ILE:CD1	1:D:147:THR:HB	2.45	0.47
1:D:226:SER:OG	1:D:351:LEU:CD2	2.62	0.47
1:F:117:ARG:O	1:F:121:LEU:HG	2.15	0.47
2:G:277:PHE:CD1	2:G:277:PHE:C	2.92	0.47
2:H:405:PHE:O	2:H:406:LYS:C	2.58	0.47
2:I:601:GLU:O	2:I:605:LYS:HG3	2.15	0.47
2:K:309:LYS:C	2:K:311:GLY:H	2.22	0.47
2:L:145:CYS:HB3	2:L:169:LEU:CD2	2.44	0.47
2:L:612:GLY:O	2:L:744:PHE:HZ	1.96	0.47
2:L:730:VAL:HG22	2:L:750:LEU:CD2	2.45	0.47
1:A:402:TYR:CE2	2:G:227:PRO:HB3	2.49	0.47
1:B:47:ALA:CB	1:B:338:ARG:NH2	2.78	0.47
1:E:101:ILE:HB	1:E:131:ALA:HB2	1.97	0.47
2:J:460:LYS:CG	2:J:487:VAL:HG11	2.44	0.47
2:L:179:LEU:C	2:L:179:LEU:HD12	2.39	0.47
2:L:309:LYS:C	2:L:311:GLY:H	2.22	0.47
2:L:359:LYS:HD2	2:L:469:HIS:HD2	1.78	0.47
2:L:487:VAL:O	2:L:487:VAL:CG1	2.63	0.47
1:A:74:LEU:O	1:A:167:LEU:CD2	2.63	0.47
1:A:294:PRO:O	1:A:298:LYS:HE2	2.15	0.47
1:A:378:PHE:HB2	1:A:417:PHE:CZ	2.50	0.47
1:C:47:ALA:HB2	1:C:338:ARG:NH2	2.30	0.47
1:C:128:LYS:CG	1:C:129:THR:N	2.78	0.47
1:C:345:GLN:O	1:D:127:ASP:HB3	2.15	0.47
1:D:342:TYR:CE1	1:D:465:HIS:CG	3.03	0.47
1:E:43:LYS:O	1:E:45:THR:HG23	2.14	0.47
1:E:132:HIS:HB2	1:F:136:MET:HB2	1.96	0.47
1:E:247:ARG:NH2	1:E:417:PHE:O	2.48	0.47
1:F:128:LYS:CG	1:F:129:THR:N	2.77	0.47
1:F:166:GLU:HG2	1:F:430:PHE:HB2	1.96	0.47
1:F:360:PRO:O	1:F:361:LYS:C	2.57	0.47
1:F:399:ALA:HA	1:F:403:MET:HE3	1.97	0.47
2:G:495:ILE:HG13	2:G:512:ILE:O	2.14	0.47
2:H:71:GLU:O	2:H:75:VAL:HG23	2.15	0.47
2:H:379:VAL:O	2:H:383:LYS:HD3	2.14	0.47
2:H:455:LYS:NZ	2:H:479:LEU:HD12	2.30	0.47
2:I:290:VAL:O	2:I:291:ARG:C	2.57	0.47
2:I:572:ASP:OD1	2:I:585:ALA:HB3	2.15	0.47
2:J:612:GLY:O	2:J:744:PHE:HZ	1.97	0.47
2:J:724:TYR:CZ	2:J:728:LYS:HE2	2.50	0.47
2:K:487:VAL:O	2:K:487:VAL:CG1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:495:ILE:HG13	2:K:512:ILE:O	2.14	0.47
2:L:359:LYS:NZ	2:L:471:ILE:HD12	2.30	0.47
1:A:338:ARG:HB2	1:A:468:ILE:O	2.14	0.47
1:C:145:MET:SD	1:C:438:VAL:HG11	2.55	0.47
1:C:146:THR:HG21	1:C:342:TYR:HE2	1.79	0.47
1:C:359:THR:O	1:C:363:LEU:HB2	2.14	0.47
1:C:405:ARG:HH12	1:C:409:VAL:HA	1.80	0.47
1:D:93:VAL:CG2	1:D:319:LEU:HD22	2.45	0.47
1:E:226:SER:OG	1:E:351:LEU:CD2	2.63	0.47
1:F:43:LYS:O	1:F:45:THR:HG23	2.15	0.47
2:G:64:LEU:O	2:G:102:ALA:HB3	2.14	0.47
2:H:99:ILE:HG22	2:H:100:ALA:N	2.30	0.47
2:H:495:ILE:HG13	2:H:512:ILE:O	2.15	0.47
2:I:142:ASN:O	2:I:167:THR:OG1	2.24	0.47
2:I:460:LYS:CG	2:I:487:VAL:HG11	2.44	0.47
2:L:319:GLY:O	2:L:322:CYS:N	2.47	0.47
2:L:609:GLU:CG	2:L:610:ARG:N	2.78	0.47
1:A:399:ALA:HA	1:A:403:MET:HE3	1.96	0.47
1:E:362:VAL:HG13	1:E:363:LEU:N	2.29	0.47
2:H:383:LYS:HG2	2:H:531:LYS:O	2.15	0.47
2:I:115:GLU:O	2:I:119:LEU:HD13	2.15	0.47
2:L:405:PHE:O	2:L:406:LYS:C	2.57	0.47
1:C:429:PRO:HB2	1:C:432:ALA:HB3	1.97	0.47
1:D:63:PRO:HB2	1:D:65:LEU:HD21	1.97	0.47
1:F:233:ALA:O	2:L:235:ARG:HG2	2.14	0.47
2:G:641:GLU:O	2:G:643:VAL:N	2.48	0.47
2:G:651:ASP:C	2:G:653:ASP:N	2.72	0.47
2:G:730:VAL:HG22	2:G:750:LEU:HD21	1.96	0.47
2:H:593:VAL:HG21	2:H:622:MET:CE	2.44	0.47
2:I:99:ILE:HB	2:I:149:GLY:HA3	1.96	0.47
2:I:256:ILE:O	2:I:256:ILE:HG23	2.15	0.47
1:A:88:LEU:HD21	1:A:95:LYS:HE2	1.97	0.46
1:B:101:ILE:O	1:B:131:ALA:HA	2.15	0.46
1:C:414:LEU:H	1:C:414:LEU:HD12	1.80	0.46
2:H:115:GLU:O	2:H:119:LEU:HD13	2.16	0.46
2:I:500:PHE:CE2	2:I:508:LEU:HD23	2.49	0.46
2:I:678:VAL:O	2:I:682:VAL:HG23	2.15	0.46
2:I:745:THR:HG22	2:I:746:PRO:HD2	1.96	0.46
2:K:115:GLU:O	2:K:119:LEU:HD13	2.15	0.46
2:K:391:ASP:OD1	2:K:392:ALA:N	2.44	0.46
2:K:609:GLU:CG	2:K:610:ARG:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:383:LYS:HG2	2:L:531:LYS:O	2.16	0.46
1:A:244:TYR:O	1:A:245:ALA:C	2.58	0.46
1:B:312:THR:HG21	1:B:427:GLY:CA	2.45	0.46
2:G:273:MET:HE2	2:G:279:ARG:HG2	1.97	0.46
2:G:609:GLU:CG	2:G:610:ARG:N	2.76	0.46
2:H:60:LYS:HG3	2:H:61:VAL:N	2.30	0.46
2:J:609:GLU:CG	2:J:610:ARG:N	2.78	0.46
1:D:66:LEU:O	1:D:69:THR:CG2	2.63	0.46
1:E:213:ALA:HB3	1:F:111:LYS:HE2	1.97	0.46
1:E:318:MET:HE1	1:E:438:VAL:HG13	1.97	0.46
1:F:115:VAL:HG11	1:F:165:VAL:HG11	1.98	0.46
2:G:290:VAL:O	2:G:294:THR:N	2.48	0.46
2:G:704:ALA:HA	2:G:708:LEU:HD23	1.95	0.46
2:H:200:MET:HG3	2:H:207:ILE:HD11	1.97	0.46
2:H:560:ARG:O	2:H:564:GLU:HG3	2.14	0.46
2:H:745:THR:HG22	2:H:746:PRO:HD2	1.96	0.46
2:I:68:LEU:HD23	2:I:68:LEU:C	2.41	0.46
2:K:683:ASN:O	2:K:686:VAL:HG22	2.15	0.46
2:L:66:LYS:HE3	2:L:105:ASN:HB2	1.97	0.46
2:L:300:ALA:HB3	2:L:301:PRO:HD3	1.97	0.46
2:L:632:SER:OG	2:L:647:ASP:OD2	2.33	0.46
1:A:128:LYS:CG	1:A:129:THR:N	2.77	0.46
1:B:146:THR:HG21	1:B:342:TYR:HE2	1.79	0.46
1:D:338:ARG:HG3	1:D:470:GLU:HB2	1.97	0.46
1:E:338:ARG:HD2	1:E:470:GLU:OE2	2.16	0.46
1:F:69:THR:CG2	1:F:70:SER:H	2.22	0.46
2:H:163:LYS:HG3	2:H:221:LEU:HG	1.97	0.46
2:H:174:VAL:HG22	2:H:201:MET:O	2.15	0.46
2:H:245:ILE:CG2	2:H:249:LYS:HE3	2.45	0.46
2:H:507:GLN:HA	2:H:534:LYS:HD3	1.98	0.46
2:H:652:MET:O	2:H:656:LEU:HB2	2.16	0.46
2:H:678:VAL:O	2:H:682:VAL:HG23	2.15	0.46
2:H:748:GLN:O	2:H:752:ASP:HB2	2.16	0.46
2:I:99:ILE:HG22	2:I:100:ALA:N	2.29	0.46
2:I:145:CYS:HB3	2:I:169:LEU:CD2	2.45	0.46
2:I:563:GLN:O	2:I:660:LYS:HB2	2.15	0.46
2:J:546:TYR:OH	2:J:704:ALA:HB2	2.16	0.46
2:J:618:LEU:C	2:J:618:LEU:HD12	2.41	0.46
2:K:575:THR:HG21	2:K:584:ALA:HB2	1.98	0.46
2:K:696:THR:HB	2:K:697:PRO:HD2	1.96	0.46
1:A:341:MET:HG2	1:A:361:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:VAL:HG21	1:D:321:MET:SD	2.56	0.46
1:F:93:VAL:HG12	1:F:94:PRO:HD2	1.97	0.46
1:F:338:ARG:HG3	1:F:470:GLU:HB2	1.98	0.46
2:G:68:LEU:C	2:G:68:LEU:HD23	2.41	0.46
2:G:730:VAL:HG22	2:G:750:LEU:CD2	2.45	0.46
2:H:744:PHE:N	2:H:744:PHE:CD1	2.79	0.46
2:I:114:GLN:O	2:I:118:GLN:HB2	2.16	0.46
2:I:593:VAL:CG2	2:I:628:LEU:HD12	2.46	0.46
2:K:359:LYS:CD	2:K:469:HIS:HD2	2.29	0.46
1:A:251:LEU:HG	1:A:419:ASN:O	2.15	0.46
1:B:405:ARG:HH12	1:B:409:VAL:HA	1.79	0.46
1:D:141:ALA:HB2	1:D:431:GLY:C	2.40	0.46
1:F:67:SER:OG	1:F:311:LEU:C	2.59	0.46
2:H:578:PHE:CE2	2:H:678:VAL:HG21	2.50	0.46
2:H:651:ASP:O	2:H:653:ASP:N	2.48	0.46
2:I:632:SER:OG	2:I:647:ASP:OD2	2.33	0.46
2:K:114:GLN:HA	2:K:117:THR:HB	1.97	0.46
1:F:59:GLY:HA3	1:F:439:MET:SD	2.55	0.46
2:G:114:GLN:HA	2:G:117:THR:HB	1.98	0.46
2:H:66:LYS:HE3	2:H:105:ASN:CB	2.45	0.46
2:I:359:LYS:HD2	2:I:469:HIS:HD2	1.81	0.46
2:I:554:MET:SD	2:I:681:PHE:HB2	2.56	0.46
2:K:60:LYS:HG3	2:K:61:VAL:N	2.30	0.46
2:L:40:HIS:CE1	2:L:57:PRO:CD	2.99	0.46
2:L:678:VAL:O	2:L:682:VAL:HG23	2.15	0.46
1:A:177:ARG:CZ	1:A:209:PRO:HG3	2.45	0.46
1:D:234:PHE:CZ	1:D:392:ALA:HB2	2.51	0.46
1:E:66:LEU:O	1:E:69:THR:CG2	2.62	0.46
2:G:119:LEU:O	2:G:120:SER:C	2.59	0.46
2:J:319:GLY:O	2:J:322:CYS:N	2.48	0.46
2:K:66:LYS:HE3	2:K:105:ASN:HB2	1.97	0.46
2:K:481:ILE:O	2:K:481:ILE:HG22	2.16	0.46
2:L:446:GLU:HG2	2:L:448:VAL:HG23	1.98	0.46
2:L:537:ILE:O	2:L:537:ILE:HG23	2.15	0.46
1:B:338:ARG:HG3	1:B:470:GLU:HB2	1.97	0.46
1:C:75:MET:O	1:C:78:ASP:HB2	2.15	0.46
1:D:76:PRO:O	1:D:165:VAL:HG21	2.16	0.46
1:D:88:LEU:HD21	1:D:95:LYS:HE2	1.98	0.46
1:E:165:VAL:HG22	1:E:166:GLU:N	2.31	0.46
1:F:439:MET:O	1:F:443:ASN:HB2	2.15	0.46
2:G:750:LEU:HD23	2:G:750:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:ASN:O	2:H:167:THR:OG1	2.27	0.46
2:J:610:ARG:HH22	2:J:687:MET:HE1	1.81	0.46
2:K:488:SER:HB3	2:K:491:PRO:HG3	1.98	0.46
1:A:177:ARG:CG	1:A:209:PRO:HB3	2.46	0.46
1:B:336:TYR:HB2	1:B:470:GLU:HB3	1.98	0.46
1:F:285:SER:OG	1:F:288:GLN:HB2	2.15	0.46
2:H:49:VAL:HA	2:H:87:SER:O	2.16	0.46
2:I:114:GLN:HA	2:I:117:THR:HB	1.98	0.46
2:I:300:ALA:HB3	2:I:301:PRO:HD3	1.97	0.46
2:I:730:VAL:HG21	2:I:754:ALA:CB	2.44	0.46
2:J:627:PHE:CD1	2:J:652:MET:HE2	2.51	0.46
1:B:106:VAL:HG23	1:B:107:ILE:N	2.30	0.45
1:B:174:ARG:HB2	1:B:177:ARG:HB3	1.92	0.45
1:B:413:PRO:C	1:B:415:GLU:N	2.75	0.45
1:D:219:THR:HG22	1:D:219:THR:O	2.17	0.45
1:F:262:SER:HB3	1:F:443:ASN:HD21	1.80	0.45
1:F:338:ARG:HB2	1:F:468:ILE:O	2.16	0.45
1:F:414:LEU:H	1:F:414:LEU:HD12	1.82	0.45
2:G:618:LEU:C	2:G:618:LEU:HD12	2.41	0.45
2:G:667:VAL:HG12	2:G:676:ARG:HE	1.81	0.45
2:H:179:LEU:HB2	2:H:180:PRO:HD2	1.99	0.45
2:H:413:LYS:C	2:H:415:LYS:H	2.24	0.45
2:I:89:VAL:CG1	2:I:90:LEU:N	2.79	0.45
2:I:575:THR:HG21	2:I:584:ALA:HB2	1.97	0.45
2:J:253:ASP:CB	2:J:255:LYS:HE2	2.46	0.45
2:J:575:THR:HG21	2:J:584:ALA:HB2	1.98	0.45
2:K:40:HIS:CE1	2:K:57:PRO:CD	2.99	0.45
2:K:164:ASP:HB3	2:K:167:THR:OG1	2.16	0.45
2:K:750:LEU:HD23	2:K:750:LEU:C	2.41	0.45
2:L:413:LYS:C	2:L:415:LYS:N	2.74	0.45
1:A:195:ARG:C	1:A:197:SER:N	2.71	0.45
1:A:214:VAL:HG21	1:B:110:VAL:O	2.17	0.45
1:B:228:ASP:HA	1:B:303:VAL:HG23	1.99	0.45
1:B:378:PHE:HB2	1:B:417:PHE:CZ	2.51	0.45
1:C:216:GLU:HG2	1:C:221:GLU:H	1.81	0.45
1:C:413:PRO:C	1:C:415:GLU:N	2.73	0.45
1:D:429:PRO:HB2	1:D:432:ALA:HB3	1.97	0.45
1:F:143:GLN:HA	1:F:342:TYR:OH	2.17	0.45
1:F:362:VAL:HG13	1:F:363:LEU:N	2.31	0.45
2:G:481:ILE:O	2:G:481:ILE:HG22	2.17	0.45
2:H:309:LYS:C	2:H:311:GLY:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:471:ILE:HG22	2:H:472:PHE:N	2.31	0.45
2:I:164:ASP:OD1	2:I:165:ARG:N	2.49	0.45
2:J:60:LYS:HG3	2:J:61:VAL:HG12	1.98	0.45
2:J:563:GLN:O	2:J:660:LYS:HB2	2.17	0.45
2:J:652:MET:O	2:J:656:LEU:HB2	2.15	0.45
2:J:667:VAL:HG12	2:J:676:ARG:HE	1.81	0.45
2:J:732:ARG:O	2:J:736:TYR:CD2	2.70	0.45
2:K:99:ILE:HG22	2:K:100:ALA:N	2.31	0.45
2:L:60:LYS:HG3	2:L:61:VAL:N	2.31	0.45
2:L:179:LEU:HB2	2:L:180:PRO:HD2	1.98	0.45
2:L:335:GLU:O	2:L:339:LEU:HG	2.16	0.45
1:D:84:LEU:HB3	1:D:125:PHE:HE2	1.81	0.45
2:G:91:ILE:CG1	2:G:92:SER:N	2.79	0.45
2:H:98:PHE:CD2	2:H:99:ILE:HG12	2.51	0.45
2:H:390:LYS:HD2	2:H:435:TYR:CD1	2.50	0.45
2:H:732:ARG:O	2:H:736:TYR:CD2	2.70	0.45
2:J:66:LYS:HE3	2:J:105:ASN:CB	2.47	0.45
2:J:545:PHE:O	2:J:546:TYR:C	2.60	0.45
2:K:71:GLU:O	2:K:75:VAL:HG23	2.16	0.45
1:B:102:ILE:HD12	1:B:132:HIS:CE1	2.51	0.45
1:B:216:GLU:HG2	1:B:221:GLU:N	2.29	0.45
1:D:43:LYS:CD	1:D:372:ASP:HA	2.44	0.45
2:G:570:LYS:HD2	2:I:86:ARG:NH2	2.32	0.45
2:H:80:TRP:CH2	2:H:133:SER:HA	2.51	0.45
2:H:724:TYR:CZ	2:H:728:LYS:HE2	2.52	0.45
2:I:435:TYR:HB3	2:I:438:PHE:CD1	2.51	0.45
2:I:563:GLN:CG	2:I:660:LYS:HA	2.46	0.45
2:J:99:ILE:HG22	2:J:100:ALA:N	2.30	0.45
2:J:456:HIS:O	2:J:457:ARG:C	2.59	0.45
2:L:541:ASP:OD1	2:L:542:GLY:N	2.50	0.45
1:C:106:VAL:HG23	1:C:107:ILE:N	2.32	0.45
1:F:256:GLN:HA	1:F:261:LEU:HD23	1.99	0.45
2:H:91:ILE:CG1	2:H:92:SER:N	2.80	0.45
2:I:672:ASP:HA	2:I:736:TYR:OH	2.17	0.45
2:J:160:ILE:HG12	2:J:220:GLN:HB3	1.99	0.45
2:J:163:LYS:HG2	2:J:221:LEU:CD2	2.47	0.45
2:J:294:THR:C	2:J:296:GLY:H	2.23	0.45
2:J:374:ALA:O	2:J:375:GLY:C	2.60	0.45
2:K:530:LEU:HG	2:K:536:ILE:HD12	1.98	0.45
2:L:618:LEU:C	2:L:618:LEU:HD12	2.41	0.45
1:B:338:ARG:HD2	1:B:470:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LEU:HD13	1:C:420:TRP:NE1	2.31	0.45
1:D:380:GLU:HB2	1:D:424:LEU:H	1.82	0.45
1:E:84:LEU:HB3	1:E:125:PHE:HE2	1.82	0.45
1:E:128:LYS:CG	1:E:129:THR:N	2.80	0.45
2:G:99:ILE:HG22	2:G:100:ALA:N	2.32	0.45
2:G:163:LYS:HD2	2:G:223:GLU:HG3	1.98	0.45
2:G:589:ASP:OD1	2:G:633:GLY:N	2.50	0.45
2:G:683:ASN:O	2:G:686:VAL:HG22	2.16	0.45
2:I:724:TYR:CZ	2:I:728:LYS:HE2	2.51	0.45
2:J:60:LYS:HG3	2:J:61:VAL:N	2.31	0.45
2:K:160:ILE:HG12	2:K:220:GLN:HB3	1.99	0.45
2:L:277:PHE:CD1	2:L:277:PHE:C	2.95	0.45
1:B:173:ILE:O	1:B:212:PRO:HB3	2.17	0.45
1:B:219:THR:HG22	1:B:219:THR:O	2.17	0.45
1:B:345:GLN:NE2	1:B:354:GLY:HA2	2.31	0.45
1:D:128:LYS:CG	1:D:129:THR:N	2.80	0.45
1:D:359:THR:O	1:D:363:LEU:HB2	2.17	0.45
1:E:102:ILE:HD12	1:E:132:HIS:CE1	2.51	0.45
1:E:336:TYR:HB2	1:E:470:GLU:HB3	1.98	0.45
1:F:197:SER:O	1:F:201:LYS:CB	2.65	0.45
2:J:510:GLU:OE1	2:J:547:THR:HG23	2.17	0.45
2:J:537:ILE:HG23	2:J:537:ILE:O	2.17	0.45
2:L:303:LYS:HD2	2:L:330:LEU:HD21	1.98	0.45
2:L:513:THR:HG23	2:L:513:THR:O	2.17	0.45
1:B:128:LYS:CG	1:B:129:THR:N	2.80	0.45
1:B:145:MET:SD	1:B:438:VAL:HG11	2.56	0.45
1:C:43:LYS:O	1:C:45:THR:HG23	2.17	0.45
1:D:405:ARG:HH12	1:D:409:VAL:HA	1.81	0.45
2:G:390:LYS:CD	2:G:435:TYR:CE1	2.89	0.45
2:H:335:GLU:OE1	2:H:335:GLU:N	2.44	0.45
2:J:413:LYS:C	2:J:415:LYS:N	2.74	0.45
2:K:443:MET:HE1	2:K:525:ALA:HA	1.99	0.45
2:K:563:GLN:CG	2:K:660:LYS:HA	2.45	0.45
1:B:312:THR:HG21	1:B:427:GLY:HA3	1.99	0.45
1:F:370:MET:HE2	1:F:410:GLY:O	2.16	0.45
2:G:607:PHE:C	2:G:609:GLU:H	2.25	0.45
2:I:385:LEU:O	2:I:387:THR:HG23	2.16	0.45
2:I:460:LYS:HE3	2:I:487:VAL:HG11	1.99	0.45
2:I:689:LEU:O	2:I:689:LEU:HD13	2.17	0.45
2:K:80:TRP:CH2	2:K:133:SER:HA	2.52	0.45
2:K:262:LYS:HB3	2:K:266:GLU:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:98:PHE:CD2	2:L:99:ILE:HG12	2.52	0.45
1:A:178:LYS:CA	1:A:181:LYS:CB	2.88	0.45
1:B:370:MET:HE1	1:B:412:PRO:HB3	1.99	0.45
1:C:47:ALA:HB2	1:C:338:ARG:HH21	1.82	0.45
2:K:89:VAL:HG12	2:K:90:LEU:N	2.31	0.45
2:K:330:LEU:O	2:K:331:VAL:C	2.60	0.45
2:K:446:GLU:HG2	2:K:448:VAL:HG23	1.99	0.45
2:K:667:VAL:O	2:K:667:VAL:HG12	2.17	0.45
2:K:689:LEU:O	2:K:689:LEU:HD13	2.17	0.45
2:L:174:VAL:HG22	2:L:201:MET:O	2.17	0.45
2:L:575:THR:HG21	2:L:584:ALA:HB2	2.00	0.45
1:A:69:THR:CG2	1:A:70:SER:N	2.78	0.44
1:B:168:MET:HE1	1:B:429:PRO:HA	1.99	0.44
1:D:336:TYR:HB3	1:D:338:ARG:CZ	2.47	0.44
1:E:350:GLN:HB2	1:E:353:LEU:HD12	1.99	0.44
1:F:106:VAL:HG22	1:F:166:GLU:OE1	2.16	0.44
2:G:545:PHE:O	2:G:546:TYR:C	2.60	0.44
2:G:701:ASP:OD2	2:G:761:PHE:CE2	2.70	0.44
2:I:283:TYR:OH	2:I:312:ILE:HD11	2.18	0.44
2:I:609:GLU:CG	2:I:610:ARG:N	2.79	0.44
2:K:91:ILE:CG1	2:K:92:SER:N	2.81	0.44
2:K:273:MET:HA	2:K:273:MET:HE3	2.00	0.44
2:K:294:THR:C	2:K:296:GLY:H	2.25	0.44
2:K:618:LEU:C	2:K:618:LEU:HD12	2.42	0.44
2:K:745:THR:HG22	2:K:746:PRO:HD2	1.98	0.44
2:L:652:MET:O	2:L:656:LEU:HB2	2.17	0.44
1:A:173:ILE:CB	1:B:173:ILE:HG22	2.47	0.44
1:A:359:THR:O	1:A:363:LEU:HB2	2.17	0.44
1:B:338:ARG:HA	1:B:338:ARG:HE	1.83	0.44
1:F:165:VAL:HG22	1:F:166:GLU:N	2.33	0.44
1:F:209:PRO:O	1:F:210:GLU:CB	2.66	0.44
2:G:142:ASN:ND2	2:G:237:ILE:HD11	2.33	0.44
2:G:262:LYS:HB3	2:G:266:GLU:CB	2.45	0.44
2:H:160:ILE:HG12	2:H:220:GLN:HB3	2.00	0.44
2:H:530:LEU:HG	2:H:536:ILE:HD12	1.99	0.44
2:I:163:LYS:HG3	2:I:221:LEU:HG	2.00	0.44
2:J:593:VAL:CG2	2:J:628:LEU:HD12	2.47	0.44
1:A:57:VAL:O	1:A:334:LYS:HG3	2.18	0.44
1:B:200:SER:O	1:B:203:ARG:HG3	2.14	0.44
1:C:399:ALA:HA	1:C:403:MET:HE3	2.00	0.44
1:E:234:PHE:CZ	1:E:392:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:643:VAL:O	2:G:644:LYS:CB	2.65	0.44
2:H:97:CYS:HA	2:H:143:GLY:HA3	1.99	0.44
2:H:513:THR:HG23	2:H:513:THR:O	2.16	0.44
2:I:188:LEU:HD23	2:I:200:MET:SD	2.57	0.44
2:I:375:GLY:HA2	2:I:504:ASP:OD1	2.17	0.44
2:J:66:LYS:HG3	2:J:105:ASN:ND2	2.33	0.44
2:J:163:LYS:HG3	2:J:221:LEU:HG	2.00	0.44
1:B:180:ARG:HD3	1:B:207:LEU:CD2	2.48	0.44
1:C:336:TYR:CZ	1:C:472:TYR:CE1	3.06	0.44
1:D:152:ILE:O	1:D:155:GLY:N	2.50	0.44
1:D:338:ARG:HA	1:D:338:ARG:HE	1.82	0.44
1:E:166:GLU:HG3	1:E:168:MET:HE2	1.99	0.44
2:G:174:VAL:CG2	2:G:201:MET:O	2.65	0.44
2:G:200:MET:HG3	2:G:207:ILE:HD11	2.00	0.44
2:G:294:THR:C	2:G:296:GLY:N	2.76	0.44
2:G:566:VAL:HG13	2:G:570:LYS:HD3	1.98	0.44
2:I:513:THR:O	2:I:513:THR:HG23	2.18	0.44
2:J:114:GLN:O	2:J:118:GLN:HB2	2.16	0.44
2:J:256:ILE:O	2:J:256:ILE:HG13	2.18	0.44
2:K:142:ASN:ND2	2:K:237:ILE:HD11	2.33	0.44
2:K:298:TYR:OH	2:K:712:PRO:HG2	2.17	0.44
2:K:601:GLU:O	2:K:605:LYS:HG3	2.18	0.44
2:L:593:VAL:CG2	2:L:628:LEU:HD12	2.48	0.44
2:L:696:THR:HB	2:L:697:PRO:HD2	1.98	0.44
1:A:75:MET:O	1:A:78:ASP:HB2	2.18	0.44
1:C:102:ILE:HD13	1:C:147:THR:HB	1.99	0.44
1:C:312:THR:HG21	1:C:427:GLY:HA3	2.00	0.44
1:D:297:ILE:O	1:D:301:GLY:HA3	2.17	0.44
2:G:186:GLN:HG3	2:G:320:TYR:CD1	2.52	0.44
2:I:43:TYR:OH	2:I:79:ILE:HG22	2.18	0.44
2:I:66:LYS:HE3	2:I:105:ASN:HB2	1.99	0.44
2:I:147:GLY:O	2:I:151:GLU:HG3	2.18	0.44
2:I:446:GLU:HG2	2:I:448:VAL:HG23	1.99	0.44
2:I:459:LEU:O	2:I:463:GLU:HB2	2.17	0.44
2:J:493:LYS:HD3	2:J:521:THR:OG1	2.17	0.44
2:J:730:VAL:HG21	2:J:754:ALA:CB	2.45	0.44
2:K:253:ASP:CB	2:K:255:LYS:HE2	2.46	0.44
2:K:368:GLY:O	2:K:373:GLY:HA3	2.18	0.44
2:L:179:LEU:HB2	2:L:180:PRO:CD	2.47	0.44
2:L:675:PHE:O	2:L:676:ARG:C	2.59	0.44
2:L:730:VAL:HG22	2:L:750:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.85	0.44
1:C:108:GLN:H	1:D:108:GLN:HE22	1.65	0.44
1:D:273:ASP:O	1:D:274:THR:HB	2.17	0.44
1:D:369:THR:OG1	1:D:372:ASP:OD1	2.35	0.44
1:E:69:THR:CG2	1:E:70:SER:N	2.76	0.44
1:E:220:SER:O	1:E:221:GLU:HB2	2.18	0.44
2:G:540:LYS:CE	2:G:692:GLY:O	2.66	0.44
2:G:551:LEU:HD12	2:G:708:LEU:CD1	2.48	0.44
2:H:114:GLN:HA	2:H:117:THR:HB	1.98	0.44
2:H:114:GLN:O	2:H:118:GLN:HB2	2.18	0.44
2:I:488:SER:HB3	2:I:491:PRO:HG3	1.98	0.44
2:K:588:VAL:O	2:K:589:ASP:C	2.59	0.44
1:B:47:ALA:HB2	1:B:338:ARG:HH21	1.82	0.44
1:B:226:SER:OG	1:B:351:LEU:CD2	2.65	0.44
1:C:102:ILE:HD12	1:C:132:HIS:CE1	2.53	0.44
1:C:238:ARG:NH2	1:C:304:THR:HG21	2.32	0.44
1:D:43:LYS:HE2	1:D:371:ASN:O	2.17	0.44
1:D:399:ALA:HA	1:D:403:MET:HE3	1.99	0.44
1:E:413:PRO:C	1:E:415:GLU:N	2.75	0.44
1:E:444:ARG:O	1:E:448:GLU:HB2	2.17	0.44
1:F:104:GLY:HA2	1:F:134:VAL:O	2.17	0.44
2:G:390:LYS:HD2	2:G:435:TYR:CD1	2.50	0.44
2:G:541:ASP:OD1	2:G:542:GLY:N	2.51	0.44
2:H:575:THR:HG21	2:H:584:ALA:HB2	2.00	0.44
2:I:309:LYS:C	2:I:311:GLY:H	2.26	0.44
2:I:495:ILE:HG13	2:I:512:ILE:O	2.18	0.44
2:J:125:ARG:O	2:J:129:LYS:HG3	2.18	0.44
2:J:455:LYS:NZ	2:J:479:LEU:HD12	2.33	0.44
2:L:481:ILE:O	2:L:481:ILE:HG22	2.18	0.44
1:A:108:GLN:HE22	1:B:108:GLN:H	1.66	0.44
1:C:251:LEU:HD21	1:C:419:ASN:HA	1.99	0.44
1:D:75:MET:O	1:D:78:ASP:HB2	2.17	0.44
1:E:370:MET:HE1	1:E:412:PRO:HB3	1.98	0.44
2:I:92:SER:HB3	2:I:98:PHE:HA	1.99	0.44
1:A:152:ILE:HA	1:A:157:CYS:O	2.17	0.44
1:B:81:ARG:HH11	1:B:122:GLY:HA3	1.83	0.44
1:B:203:ARG:HG3	1:B:204:PHE:N	2.33	0.44
1:C:220:SER:O	1:C:221:GLU:HB2	2.17	0.44
1:C:338:ARG:HG3	1:C:470:GLU:HB2	1.99	0.44
1:C:350:GLN:HB2	1:C:353:LEU:HD12	1.99	0.44
1:E:74:LEU:O	1:E:167:LEU:HD21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLN:H	1:F:108:GLN:HE22	1.66	0.44
1:E:228:ASP:HA	1:E:303:VAL:HG23	2.00	0.44
1:E:256:GLN:HA	1:E:261:LEU:HD23	2.00	0.44
2:G:429:LEU:O	2:G:429:LEU:HD13	2.18	0.44
2:G:578:PHE:CE2	2:G:678:VAL:HG21	2.53	0.44
2:H:651:ASP:O	2:H:654:SER:N	2.49	0.44
2:I:98:PHE:CD2	2:I:99:ILE:HG12	2.53	0.44
2:K:708:LEU:HD22	2:K:708:LEU:N	2.33	0.44
1:A:297:ILE:O	1:A:301:GLY:HA3	2.17	0.43
1:A:412:PRO:O	1:A:413:PRO:C	2.61	0.43
1:B:180:ARG:NE	1:B:203:ARG:HE	2.16	0.43
1:B:285:SER:OG	1:B:288:GLN:HB2	2.18	0.43
1:B:347:PRO:HA	1:B:351:LEU:HB3	2.00	0.43
1:C:47:ALA:CB	1:C:338:ARG:NH2	2.81	0.43
1:C:102:ILE:CD1	1:C:147:THR:HB	2.47	0.43
1:C:378:PHE:HB2	1:C:417:PHE:CZ	2.53	0.43
1:D:336:TYR:CZ	1:D:472:TYR:CE1	3.06	0.43
1:E:166:GLU:CG	1:E:168:MET:HE2	2.48	0.43
1:E:335:ALA:HB2	1:E:442:ALA:HB1	2.00	0.43
1:F:106:VAL:HG23	1:F:107:ILE:N	2.32	0.43
2:H:163:LYS:HG2	2:H:221:LEU:CD2	2.47	0.43
2:H:645:ARG:O	2:H:646:LYS:C	2.61	0.43
2:K:66:LYS:HE3	2:K:105:ASN:CB	2.48	0.43
2:K:89:VAL:CG1	2:K:90:LEU:N	2.81	0.43
2:K:380:SER:HB2	2:K:387:THR:HG21	1.98	0.43
2:K:398:ASP:O	2:K:399:ARG:C	2.59	0.43
2:K:560:ARG:O	2:K:564:GLU:HG3	2.18	0.43
2:K:667:VAL:HG12	2:K:676:ARG:HE	1.83	0.43
1:A:188:LYS:HD2	1:A:192:MET:C	2.43	0.43
1:A:312:THR:HG21	1:A:427:GLY:HA3	2.00	0.43
1:A:321:MET:CE	1:A:329:MET:HG3	2.47	0.43
1:D:370:MET:HE1	1:D:412:PRO:HB3	1.99	0.43
1:E:339:ASP:OD2	1:E:366:ALA:HA	2.18	0.43
1:F:260:LEU:HD13	1:F:420:TRP:NE1	2.32	0.43
2:G:253:ASP:CB	2:G:255:LYS:HE2	2.48	0.43
2:G:546:TYR:CE1	2:G:694:LEU:HD11	2.53	0.43
2:I:60:LYS:HG3	2:I:61:VAL:N	2.33	0.43
2:I:380:SER:HB2	2:I:387:THR:HG21	2.00	0.43
2:I:487:VAL:O	2:I:487:VAL:CG1	2.65	0.43
2:J:115:GLU:O	2:J:119:LEU:HD13	2.18	0.43
2:J:174:VAL:HG21	2:J:201:MET:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:172:PRO:O	2:K:173:GLU:C	2.61	0.43
2:L:164:ASP:OD1	2:L:165:ARG:N	2.51	0.43
1:A:47:ALA:HB2	1:A:338:ARG:NH2	2.32	0.43
1:A:177:ARG:NH1	1:A:209:PRO:CG	2.72	0.43
1:B:211:LEU:HB3	1:B:212:PRO:HD2	1.95	0.43
1:B:251:LEU:HD21	1:B:419:ASN:HA	1.99	0.43
1:D:321:MET:CE	1:D:329:MET:HG3	2.47	0.43
1:E:145:MET:SD	1:E:438:VAL:HG11	2.59	0.43
1:E:216:GLU:HG2	1:E:221:GLU:N	2.33	0.43
1:F:312:THR:HG21	1:F:427:GLY:CA	2.49	0.43
2:G:309:LYS:C	2:G:311:GLY:H	2.25	0.43
2:G:404:VAL:HG13	2:G:426:PHE:HE1	1.83	0.43
2:G:730:VAL:HG21	2:G:754:ALA:CB	2.46	0.43
2:H:179:LEU:HB2	2:H:180:PRO:CD	2.48	0.43
2:I:80:TRP:CH2	2:I:133:SER:HA	2.53	0.43
2:L:91:ILE:CG1	2:L:92:SER:N	2.82	0.43
2:L:200:MET:HG3	2:L:207:ILE:HD11	2.00	0.43
1:A:251:LEU:HD21	1:A:419:ASN:HA	2.00	0.43
1:A:273:ASP:O	1:A:274:THR:HB	2.17	0.43
1:B:212:PRO:HB2	1:B:213:ALA:H	1.60	0.43
1:C:101:ILE:HB	1:C:131:ALA:HB2	2.00	0.43
1:F:428:HIS:CG	1:F:428:HIS:O	2.68	0.43
2:G:471:ILE:HG22	2:G:472:PHE:N	2.33	0.43
2:G:756:SER:HB3	2:G:757:PRO:HD2	2.01	0.43
2:H:91:ILE:HD11	2:H:237:ILE:HG23	2.01	0.43
2:H:628:LEU:O	2:H:629:GLY:C	2.56	0.43
2:I:618:LEU:C	2:I:618:LEU:HD12	2.44	0.43
2:J:179:LEU:HB2	2:J:180:PRO:HD2	2.01	0.43
2:J:188:LEU:N	2:J:189:PRO:CD	2.82	0.43
2:K:359:LYS:NZ	2:K:471:ILE:HD12	2.33	0.43
2:L:114:GLN:O	2:L:118:GLN:HB2	2.19	0.43
2:L:718:PHE:CD2	2:L:760:LYS:HD2	2.54	0.43
1:A:197:SER:HA	1:A:200:SER:CB	2.48	0.43
1:B:174:ARG:HD2	1:B:178:LYS:CG	2.48	0.43
1:B:244:TYR:O	1:B:245:ALA:C	2.61	0.43
1:D:326:ALA:O	1:D:331:TYR:HB2	2.17	0.43
1:E:93:VAL:HG21	1:E:319:LEU:HD22	2.00	0.43
1:F:146:THR:HG21	1:F:342:TYR:HE2	1.83	0.43
2:I:701:ASP:OD2	2:I:761:PHE:CE2	2.71	0.43
2:L:172:PRO:O	2:L:173:GLU:C	2.62	0.43
1:B:326:ALA:O	1:B:331:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:SER:OG	1:D:127:ASP:O	2.33	0.43
1:D:115:VAL:HG11	1:D:165:VAL:HG11	2.01	0.43
1:D:146:THR:HG21	1:D:342:TYR:HE2	1.84	0.43
1:D:256:GLN:HA	1:D:261:LEU:HD23	2.00	0.43
1:D:335:ALA:HB2	1:D:442:ALA:HB1	2.01	0.43
1:E:336:TYR:HB3	1:E:338:ARG:CZ	2.49	0.43
1:F:217:PHE:C	1:F:219:THR:H	2.26	0.43
1:F:336:TYR:HB3	1:F:338:ARG:CZ	2.49	0.43
2:G:71:GLU:O	2:G:75:VAL:HG23	2.18	0.43
2:G:174:VAL:HG21	2:G:201:MET:O	2.18	0.43
2:I:160:ILE:HG12	2:I:220:GLN:HB3	2.00	0.43
2:I:294:THR:C	2:I:296:GLY:H	2.26	0.43
2:J:481:ILE:HG22	2:J:481:ILE:O	2.18	0.43
2:K:253:ASP:HB2	2:K:255:LYS:CE	2.46	0.43
2:L:256:ILE:O	2:L:256:ILE:HG13	2.19	0.43
1:A:117:ARG:CZ	1:A:121:LEU:HD21	2.49	0.43
1:A:175:HIS:HE2	1:A:212:PRO:HG3	1.82	0.43
1:B:84:LEU:HB3	1:B:125:PHE:HE2	1.84	0.43
1:C:143:GLN:HA	1:C:342:TYR:OH	2.18	0.43
1:D:310:PHE:O	1:D:312:THR:HG23	2.18	0.43
1:E:251:LEU:HD21	1:E:419:ASN:HA	2.01	0.43
1:F:63:PRO:HB2	1:F:65:LEU:HD21	2.01	0.43
1:F:76:PRO:O	1:F:165:VAL:HG21	2.18	0.43
1:F:228:ASP:HA	1:F:303:VAL:HG23	2.01	0.43
1:F:341:MET:HE3	1:F:361:LYS:HB3	2.01	0.43
2:G:418:THR:HB	2:G:421:GLU:H	1.83	0.43
2:H:98:PHE:C	2:H:99:ILE:HG12	2.43	0.43
2:H:186:GLN:HG3	2:H:320:TYR:CD1	2.54	0.43
2:H:446:GLU:HG2	2:H:448:VAL:HG23	2.00	0.43
2:H:589:ASP:OD1	2:H:589:ASP:C	2.62	0.43
2:I:91:ILE:HD11	2:I:237:ILE:HG23	2.00	0.43
2:I:748:GLN:O	2:I:752:ASP:HB2	2.18	0.43
2:J:232:PRO:O	2:J:233:GLU:C	2.62	0.43
2:J:481:ILE:HG13	2:J:512:ILE:HB	2.00	0.43
2:J:500:PHE:CE2	2:J:508:LEU:HD23	2.54	0.43
2:K:500:PHE:CE2	2:K:508:LEU:HD23	2.53	0.43
1:A:102:ILE:HD12	1:A:132:HIS:NE2	2.34	0.43
1:A:208:ALA:CB	1:A:209:PRO:HD2	2.49	0.43
1:B:88:LEU:HD21	1:B:95:LYS:HE2	2.01	0.43
1:B:297:ILE:O	1:B:301:GLY:HA3	2.18	0.43
1:C:74:LEU:HD11	1:C:269:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ILE:HA	1:D:157:CYS:O	2.19	0.43
1:D:165:VAL:HG22	1:D:166:GLU:N	2.32	0.43
1:E:238:ARG:NH2	1:E:304:THR:HG21	2.34	0.43
1:F:65:LEU:HG	1:F:71:TYR:CE2	2.54	0.43
2:G:256:ILE:HG23	2:G:256:ILE:O	2.19	0.43
2:G:530:LEU:HG	2:G:536:ILE:HD12	2.00	0.43
2:G:610:ARG:HG3	2:G:744:PHE:HD1	1.84	0.43
2:I:154:ILE:HG12	2:I:188:LEU:HD12	2.01	0.43
2:I:610:ARG:HH22	2:I:687:MET:HE1	1.82	0.43
2:K:147:GLY:O	2:K:148:GLY:C	2.59	0.43
2:L:121:GLN:CG	2:L:324:SER:OG	2.63	0.43
2:L:702:ILE:HG23	2:L:706:PHE:HD2	1.84	0.43
1:A:91:THR:HG21	1:A:319:LEU:HD23	2.01	0.43
1:A:141:ALA:HB3	1:A:434:GLY:HA3	2.01	0.43
1:B:176:SER:HA	1:B:179:MET:CG	2.49	0.43
1:C:228:ASP:HA	1:C:303:VAL:HG23	2.01	0.43
1:C:310:PHE:CE2	1:C:312:THR:HG22	2.54	0.43
1:C:342:TYR:CE1	1:C:465:HIS:CG	3.07	0.43
1:D:164:GLY:HA3	1:D:431:GLY:O	2.17	0.43
1:D:226:SER:O	1:D:230:LEU:N	2.48	0.43
1:D:350:GLN:HB2	1:D:353:LEU:HD12	2.01	0.43
1:F:238:ARG:NH2	1:F:304:THR:HG21	2.34	0.43
2:G:232:PRO:O	2:G:233:GLU:C	2.60	0.43
2:H:154:ILE:HG12	2:H:188:LEU:HD12	2.01	0.43
2:I:263:GLY:O	2:I:267:LYS:HD2	2.19	0.43
2:I:273:MET:HE2	2:I:279:ARG:HG2	2.01	0.43
2:L:160:ILE:HG12	2:L:220:GLN:HB3	2.01	0.43
2:L:290:VAL:O	2:L:291:ARG:C	2.62	0.43
2:L:390:LYS:HD2	2:L:435:TYR:CD1	2.52	0.43
2:L:551:LEU:HD12	2:L:708:LEU:CD1	2.49	0.43
1:E:217:PHE:O	1:E:219:THR:N	2.51	0.43
2:G:263:GLY:O	2:G:267:LYS:HD2	2.19	0.43
2:G:443:MET:HE1	2:G:525:ALA:HA	2.01	0.43
2:H:147:GLY:O	2:H:148:GLY:C	2.62	0.43
2:H:487:VAL:O	2:H:487:VAL:CG1	2.67	0.43
2:J:245:ILE:CG2	2:J:249:LYS:HE3	2.48	0.43
2:L:380:SER:HB2	2:L:387:THR:HG21	1.99	0.43
1:A:84:LEU:HB3	1:A:125:PHE:HE2	1.84	0.42
1:A:102:ILE:HD13	1:A:147:THR:HB	2.00	0.42
1:B:175:HIS:NE2	1:B:212:PRO:HA	2.34	0.42
1:B:180:ARG:CD	1:B:203:ARG:HB2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:SER:OG	1:F:351:LEU:CD2	2.67	0.42
2:G:487:VAL:O	2:G:487:VAL:CG1	2.67	0.42
2:G:595:VAL:O	2:G:595:VAL:HG12	2.19	0.42
2:G:629:GLY:C	2:G:631:LYS:N	2.57	0.42
2:H:142:ASN:ND2	2:H:237:ILE:HD11	2.35	0.42
2:H:537:ILE:O	2:H:537:ILE:HG23	2.19	0.42
2:I:142:ASN:ND2	2:I:237:ILE:HD11	2.34	0.42
2:I:698:ALA:HA	2:I:761:PHE:CE1	2.54	0.42
2:J:652:MET:HA	2:J:655:ILE:HG22	2.01	0.42
2:K:119:LEU:O	2:K:120:SER:C	2.62	0.42
2:K:262:LYS:HB3	2:K:266:GLU:CG	2.49	0.42
2:L:169:LEU:HD12	2:L:217:LEU:HD23	2.01	0.42
1:B:200:SER:C	1:B:203:ARG:HG2	2.42	0.42
1:C:117:ARG:CZ	1:C:121:LEU:HD21	2.48	0.42
1:D:52:ARG:HH21	1:D:322:ALA:CB	2.31	0.42
1:D:102:ILE:HD13	1:D:147:THR:HB	2.01	0.42
1:D:378:PHE:HB2	1:D:417:PHE:CZ	2.54	0.42
1:E:380:GLU:HG2	1:E:386:ILE:HD11	2.01	0.42
1:F:297:ILE:O	1:F:301:GLY:HA3	2.20	0.42
2:G:732:ARG:O	2:G:736:TYR:CD2	2.72	0.42
2:I:543:PRO:HB2	2:I:606:VAL:HG11	2.00	0.42
2:K:359:LYS:HZ1	2:K:471:ILE:HD12	1.84	0.42
2:K:543:PRO:HB2	2:K:606:VAL:HG11	2.01	0.42
2:K:607:PHE:C	2:K:609:GLU:H	2.27	0.42
2:L:66:LYS:HE3	2:L:105:ASN:CB	2.48	0.42
2:L:294:THR:C	2:L:296:GLY:N	2.76	0.42
2:L:563:GLN:O	2:L:660:LYS:HB2	2.19	0.42
2:L:627:PHE:CD1	2:L:652:MET:HE2	2.54	0.42
1:A:67:SER:CB	1:A:168:MET:HB2	2.49	0.42
1:A:344:SER:OG	1:B:127:ASP:O	2.31	0.42
1:A:360:PRO:O	1:A:361:LYS:C	2.62	0.42
1:B:380:GLU:HB2	1:B:424:LEU:H	1.83	0.42
1:E:347:PRO:HA	1:E:351:LEU:HB3	2.00	0.42
2:H:40:HIS:CE1	2:H:57:PRO:CD	3.02	0.42
2:H:92:SER:HB3	2:H:98:PHE:HA	2.02	0.42
2:H:540:LYS:HE3	2:H:692:GLY:O	2.20	0.42
2:H:595:VAL:O	2:H:595:VAL:HG12	2.19	0.42
2:I:610:ARG:HG3	2:I:744:PHE:HD1	1.85	0.42
2:I:683:ASN:O	2:I:686:VAL:HG22	2.18	0.42
2:K:330:LEU:O	2:K:332:MET:N	2.53	0.42
2:L:64:LEU:O	2:L:102:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:OG	1:A:311:LEU:C	2.63	0.42
1:B:213:ALA:C	1:B:214:VAL:HG23	2.44	0.42
1:B:262:SER:HB3	1:B:443:ASN:HD21	1.84	0.42
1:C:43:LYS:CE	1:C:371:ASN:O	2.68	0.42
1:C:128:LYS:O	1:C:130:PRO:HD3	2.19	0.42
1:C:344:SER:HB3	1:D:128:LYS:C	2.42	0.42
1:D:362:VAL:HG13	1:D:363:LEU:N	2.35	0.42
1:E:220:SER:O	1:E:221:GLU:CB	2.66	0.42
1:E:273:ASP:O	1:E:274:THR:HB	2.20	0.42
1:E:412:PRO:O	1:E:413:PRO:C	2.62	0.42
2:G:145:CYS:HB3	2:G:169:LEU:CD2	2.49	0.42
2:G:667:VAL:HG12	2:G:676:ARG:NE	2.35	0.42
2:H:540:LYS:CE	2:H:692:GLY:O	2.67	0.42
2:J:290:VAL:O	2:J:291:ARG:C	2.62	0.42
2:K:593:VAL:CG2	2:K:628:LEU:HD12	2.49	0.42
1:A:345:GLN:O	1:B:127:ASP:HB3	2.20	0.42
1:B:341:MET:HE3	1:B:361:LYS:HB3	2.02	0.42
2:G:92:SER:HB3	2:G:98:PHE:HA	2.01	0.42
2:I:147:GLY:O	2:I:148:GLY:C	2.62	0.42
2:J:294:THR:C	2:J:296:GLY:N	2.77	0.42
2:J:359:LYS:NZ	2:J:442:ASP:O	2.50	0.42
2:L:390:LYS:HA	2:L:432:GLN:O	2.19	0.42
2:L:610:ARG:CD	2:L:743:GLN:O	2.63	0.42
2:L:683:ASN:O	2:L:686:VAL:HG22	2.19	0.42
1:A:69:THR:CG2	1:A:70:SER:H	2.32	0.42
1:B:93:VAL:HG21	1:B:319:LEU:HD22	2.02	0.42
1:B:205:ASN:O	1:B:206:PHE:CB	2.68	0.42
1:E:260:LEU:O	1:E:262:SER:N	2.52	0.42
2:G:311:GLY:O	2:G:314:GLN:O	2.37	0.42
2:G:507:GLN:HA	2:G:534:LYS:HD3	2.02	0.42
2:H:460:LYS:HE3	2:H:487:VAL:HG11	2.02	0.42
2:J:40:HIS:CE1	2:J:57:PRO:CD	3.02	0.42
2:J:359:LYS:NZ	2:J:471:ILE:HD12	2.35	0.42
2:K:730:VAL:HG21	2:K:754:ALA:CB	2.48	0.42
2:L:263:GLY:O	2:L:267:LYS:HD2	2.20	0.42
2:L:273:MET:HE3	2:L:273:MET:HA	2.00	0.42
2:L:354:PHE:CE2	2:L:522:SER:HB3	2.54	0.42
2:L:622:MET:O	2:L:627:PHE:N	2.52	0.42
2:L:652:MET:HA	2:L:655:ILE:HG22	2.02	0.42
2:L:667:VAL:HG12	2:L:676:ARG:NE	2.35	0.42
1:A:102:ILE:CD1	1:A:147:THR:HB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:N	1:A:172:PRO:CD	2.82	0.42
1:A:179:MET:C	1:A:181:LYS:N	2.76	0.42
1:A:195:ARG:C	1:A:197:SER:H	2.27	0.42
1:A:318:MET:HE2	1:A:439:MET:SD	2.59	0.42
1:C:59:GLY:HA3	1:C:439:MET:SD	2.59	0.42
1:D:280:GLY:HA3	1:D:425:SER:O	2.18	0.42
1:D:377:GLU:O	1:D:455:VAL:HA	2.19	0.42
1:D:413:PRO:C	1:D:415:GLU:N	2.75	0.42
1:E:312:THR:HG21	1:E:427:GLY:HA3	2.02	0.42
2:G:89:VAL:HG12	2:G:90:LEU:N	2.34	0.42
2:G:262:LYS:HB3	2:G:266:GLU:CG	2.50	0.42
2:G:537:ILE:HG23	2:G:537:ILE:O	2.20	0.42
2:G:560:ARG:O	2:G:564:GLU:HG3	2.19	0.42
2:G:740:TYR:HD1	2:G:740:TYR:HA	1.75	0.42
2:H:481:ILE:HG22	2:H:481:ILE:O	2.19	0.42
2:I:368:GLY:C	2:I:370:GLY:H	2.27	0.42
2:I:471:ILE:HG22	2:I:472:PHE:N	2.34	0.42
2:I:652:MET:HA	2:I:655:ILE:HG22	2.02	0.42
2:J:572:ASP:OD1	2:J:585:ALA:HB3	2.20	0.42
1:B:196:LEU:HA	1:B:199:ILE:CD1	2.49	0.42
1:B:362:VAL:HG13	1:B:363:LEU:N	2.35	0.42
1:C:132:HIS:HB2	1:D:136:MET:HB2	2.00	0.42
1:C:380:GLU:HA	1:C:386:ILE:HD11	2.00	0.42
1:C:413:PRO:O	1:C:415:GLU:N	2.52	0.42
1:D:106:VAL:HG23	1:D:107:ILE:N	2.34	0.42
1:D:247:ARG:HH22	1:D:417:PHE:HB3	1.85	0.42
2:G:367:LEU:HD11	2:G:462:VAL:HG21	2.01	0.42
2:G:612:GLY:O	2:G:744:PHE:CZ	2.72	0.42
2:H:593:VAL:HG22	2:H:622:MET:HE2	2.01	0.42
2:H:708:LEU:HD22	2:H:708:LEU:N	2.34	0.42
2:I:587:LEU:O	2:I:591:VAL:HG23	2.20	0.42
2:I:650:SER:O	2:I:653:ASP:HB2	2.20	0.42
2:J:262:LYS:HB3	2:J:266:GLU:CB	2.47	0.42
2:J:263:GLY:O	2:J:267:LYS:HD2	2.19	0.42
2:J:595:VAL:HA	2:J:598:HIS:HB2	2.01	0.42
2:L:404:VAL:HG13	2:L:426:PHE:HE1	1.85	0.42
2:L:745:THR:HG22	2:L:746:PRO:HD2	2.01	0.42
1:B:174:ARG:HD2	1:B:178:LYS:HG2	1.94	0.42
1:B:176:SER:C	1:B:178:LYS:N	2.70	0.42
1:B:370:MET:HE2	1:B:410:GLY:O	2.20	0.42
1:C:91:THR:HG21	1:C:319:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:THR:HG21	1:E:342:TYR:HE2	1.84	0.42
1:F:47:ALA:HB2	1:F:338:ARG:NH2	2.35	0.42
2:G:488:SER:HB3	2:G:491:PRO:HG3	2.02	0.42
2:H:279:ARG:NH1	2:H:313:GLU:OE1	2.53	0.42
2:I:413:LYS:C	2:I:415:LYS:N	2.77	0.42
2:J:488:SER:HB3	2:J:491:PRO:HG3	2.01	0.42
2:L:549:ARG:NH2	2:L:687:MET:SD	2.92	0.42
1:A:256:GLN:HA	1:A:261:LEU:HD23	2.02	0.42
1:B:66:LEU:O	1:B:69:THR:CG2	2.67	0.42
1:B:174:ARG:CZ	1:B:178:LYS:HE2	2.50	0.42
1:B:194:GLN:O	1:B:198:LEU:HD11	2.19	0.42
1:B:335:ALA:HB2	1:B:442:ALA:HB1	2.01	0.42
1:E:359:THR:CB	1:E:360:PRO:HD3	2.48	0.42
1:F:251:LEU:HG	1:F:419:ASN:O	2.20	0.42
2:G:87:SER:OG	2:G:88:ALA:N	2.51	0.42
2:H:171:THR:OG1	2:H:200:MET:O	2.38	0.42
2:H:250:GLY:O	2:H:255:LYS:HG2	2.20	0.42
2:J:446:GLU:OE1	2:J:455:LYS:HE2	2.19	0.42
2:K:724:TYR:CZ	2:K:728:LYS:HE2	2.55	0.42
1:A:63:PRO:HB2	1:A:65:LEU:HD21	2.02	0.41
1:B:234:PHE:CE1	1:B:392:ALA:HB2	2.55	0.41
1:C:217:PHE:HD1	1:C:219:THR:H	1.67	0.41
1:C:273:ASP:O	1:C:274:THR:HB	2.20	0.41
1:D:81:ARG:HH11	1:D:122:GLY:HA3	1.85	0.41
1:D:238:ARG:NH2	1:D:304:THR:HG21	2.35	0.41
1:E:102:ILE:HD12	1:E:132:HIS:NE2	2.35	0.41
1:E:262:SER:HB3	1:E:443:ASN:HD21	1.85	0.41
2:G:330:LEU:O	2:G:331:VAL:C	2.63	0.41
2:H:89:VAL:HG12	2:H:90:LEU:N	2.34	0.41
2:J:61:VAL:HG23	2:J:97:CYS:SG	2.59	0.41
2:J:300:ALA:N	2:J:301:PRO:CD	2.82	0.41
2:J:669:SER:HB3	2:J:672:ASP:OD1	2.20	0.41
1:A:111:LYS:HE2	1:B:213:ALA:HB3	2.03	0.41
1:A:121:LEU:HB2	2:H:420:PHE:HZ	1.84	0.41
1:A:347:PRO:HA	1:A:351:LEU:HB3	2.02	0.41
1:B:198:LEU:HA	1:B:201:LYS:HZ3	1.85	0.41
1:D:47:ALA:HB2	1:D:338:ARG:NH2	2.35	0.41
1:D:60:VAL:HG22	1:D:61:ARG:H	1.84	0.41
2:G:76:MET:O	2:G:77:ASN:C	2.62	0.41
2:G:163:LYS:HG2	2:G:221:LEU:CD2	2.49	0.41
2:G:531:LYS:C	2:G:533:GLY:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:540:LYS:HE3	2:G:692:GLY:O	2.21	0.41
2:G:575:THR:HG21	2:G:584:ALA:HB2	2.01	0.41
2:G:708:LEU:HD22	2:G:708:LEU:N	2.35	0.41
2:H:611:PHE:N	2:H:611:PHE:CD1	2.88	0.41
2:H:667:VAL:HG12	2:H:676:ARG:HE	1.84	0.41
2:H:672:ASP:HA	2:H:736:TYR:OH	2.20	0.41
2:I:592:GLY:O	2:I:596:ALA:N	2.50	0.41
2:I:708:LEU:HD22	2:I:708:LEU:N	2.35	0.41
2:J:330:LEU:O	2:J:331:VAL:C	2.63	0.41
2:K:628:LEU:HB3	2:K:631:LYS:HB2	2.02	0.41
2:K:649:ASN:HB3	2:K:652:MET:HB2	2.01	0.41
2:L:43:TYR:OH	2:L:79:ILE:HG22	2.20	0.41
2:L:163:LYS:HD2	2:L:223:GLU:HG3	2.02	0.41
2:L:382:ASP:OD1	2:L:383:LYS:HD3	2.20	0.41
2:L:740:TYR:O	2:L:742:LYS:N	2.53	0.41
1:A:382:PHE:O	1:A:385:GLN:HB3	2.20	0.41
1:C:256:GLN:HA	1:C:261:LEU:HD23	2.02	0.41
1:F:247:ARG:HH22	1:F:417:PHE:HB3	1.85	0.41
2:G:49:VAL:HG21	2:G:249:LYS:HG3	2.02	0.41
2:G:60:LYS:HG3	2:G:61:VAL:H	1.84	0.41
2:G:379:VAL:O	2:G:383:LYS:HD3	2.19	0.41
2:H:117:THR:HG23	2:H:325:GLN:HA	2.02	0.41
2:H:122:GLU:O	2:H:126:ILE:HG12	2.20	0.41
2:H:125:ARG:O	2:H:129:LYS:HG3	2.20	0.41
2:H:683:ASN:O	2:H:686:VAL:HG22	2.21	0.41
2:I:595:VAL:HA	2:I:598:HIS:HB2	2.03	0.41
2:J:708:LEU:N	2:J:708:LEU:HD22	2.35	0.41
2:K:279:ARG:NH1	2:K:313:GLU:CD	2.78	0.41
2:K:400:GLY:O	2:K:404:VAL:HG12	2.20	0.41
2:L:99:ILE:HG22	2:L:100:ALA:N	2.35	0.41
2:L:545:PHE:O	2:L:546:TYR:C	2.63	0.41
1:A:128:LYS:C	1:B:344:SER:HB3	2.43	0.41
1:B:109:GLU:O	1:B:112:THR:N	2.48	0.41
1:C:362:VAL:HG13	1:C:363:LEU:N	2.36	0.41
1:D:165:VAL:HG23	1:D:315:ALA:HB2	2.01	0.41
1:D:345:GLN:NE2	1:D:354:GLY:HA2	2.34	0.41
1:D:382:PHE:O	1:D:383:SER:C	2.64	0.41
1:E:127:ASP:HB3	1:F:345:GLN:O	2.20	0.41
1:E:216:GLU:HG2	1:E:221:GLU:C	2.45	0.41
1:E:294:PRO:O	1:E:298:LYS:HE2	2.19	0.41
2:G:718:PHE:CD2	2:G:760:LYS:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:531:LYS:C	2:H:533:GLY:N	2.78	0.41
2:H:543:PRO:HB2	2:H:606:VAL:HG11	2.01	0.41
2:H:561:ILE:CD1	2:H:677:LEU:HD11	2.51	0.41
2:H:698:ALA:HA	2:H:761:PHE:CE1	2.56	0.41
2:I:262:LYS:HB3	2:I:266:GLU:CB	2.50	0.41
2:I:443:MET:HE1	2:I:525:ALA:HA	2.02	0.41
2:I:530:LEU:HG	2:I:536:ILE:HD12	2.02	0.41
2:I:581:PRO:HD2	2:I:709:GLY:O	2.21	0.41
2:I:652:MET:O	2:I:656:LEU:HB2	2.21	0.41
2:J:262:LYS:HB3	2:J:266:GLU:CG	2.50	0.41
2:K:460:LYS:HE3	2:K:487:VAL:HG11	2.01	0.41
2:K:698:ALA:HA	2:K:761:PHE:CE1	2.54	0.41
2:L:163:LYS:HG3	2:L:221:LEU:HG	2.02	0.41
1:C:345:GLN:NE2	1:C:354:GLY:HA2	2.35	0.41
1:E:280:GLY:HA3	1:E:425:SER:O	2.20	0.41
1:F:91:THR:HG21	1:F:319:LEU:HD23	2.01	0.41
1:F:234:PHE:O	1:F:235:ALA:C	2.62	0.41
2:G:701:ASP:OD1	2:G:718:PHE:HB2	2.19	0.41
2:H:443:MET:HE1	2:H:525:ALA:HA	2.02	0.41
2:I:298:TYR:HA	2:I:299:PRO:HD3	1.95	0.41
2:J:443:MET:HE1	2:J:525:ALA:HA	2.01	0.41
2:J:687:MET:HE3	2:J:747:CYS:HB3	2.03	0.41
2:K:513:THR:HG23	2:K:513:THR:O	2.19	0.41
2:K:610:ARG:HH22	2:K:687:MET:HE1	1.81	0.41
2:K:687:MET:HE3	2:K:747:CYS:HB3	2.02	0.41
2:L:66:LYS:HG3	2:L:105:ASN:ND2	2.36	0.41
2:L:80:TRP:CH2	2:L:133:SER:HA	2.55	0.41
2:L:418:THR:HB	2:L:421:GLU:H	1.85	0.41
2:L:493:LYS:HD3	2:L:521:THR:OG1	2.21	0.41
1:A:91:THR:HG21	1:A:319:LEU:CD2	2.50	0.41
1:A:326:ALA:O	1:A:331:TYR:HB2	2.21	0.41
1:A:380:GLU:HB2	1:A:424:LEU:H	1.86	0.41
1:B:142:ASN:HA	1:B:145:MET:HE3	2.02	0.41
1:D:229:ARG:NH1	2:J:223:GLU:OE1	2.53	0.41
1:D:262:SER:HB3	1:D:443:ASN:HD21	1.84	0.41
1:E:94:PRO:HG2	1:E:97:VAL:HG12	2.03	0.41
1:E:244:TYR:O	1:E:245:ALA:C	2.61	0.41
1:F:342:TYR:CE1	1:F:465:HIS:CD2	3.08	0.41
2:G:359:LYS:NZ	2:G:471:ILE:HD12	2.34	0.41
2:H:742:LYS:CB	2:H:744:PHE:CE2	3.03	0.41
2:I:245:ILE:CG2	2:I:249:LYS:HE3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:76:MET:O	2:J:77:ASN:C	2.63	0.41
2:J:154:ILE:HG12	2:J:188:LEU:HD12	2.02	0.41
2:J:540:LYS:HE3	2:J:692:GLY:O	2.20	0.41
2:K:620:THR:C	2:K:622:MET:N	2.78	0.41
2:L:147:GLY:O	2:L:148:GLY:C	2.63	0.41
2:L:552:ALA:HB3	2:L:553:PRO:CD	2.48	0.41
2:L:667:VAL:HG12	2:L:676:ARG:HE	1.85	0.41
1:A:179:MET:C	1:A:181:LYS:H	2.28	0.41
1:B:63:PRO:HB2	1:B:65:LEU:HD21	2.03	0.41
1:C:234:PHE:CE1	1:C:392:ALA:HB2	2.55	0.41
1:C:335:ALA:HB2	1:C:442:ALA:HB1	2.01	0.41
1:C:347:PRO:HA	1:C:351:LEU:HB3	2.02	0.41
1:D:43:LYS:O	1:D:45:THR:HG23	2.21	0.41
1:D:341:MET:HE3	1:D:361:LYS:HB3	2.02	0.41
1:E:57:VAL:HG21	1:E:321:MET:SD	2.60	0.41
1:F:66:LEU:O	1:F:69:THR:HB	2.21	0.41
1:F:166:GLU:CG	1:F:168:MET:HE2	2.51	0.41
2:G:500:PHE:CE2	2:G:508:LEU:HD23	2.56	0.41
2:G:632:SER:HA	2:G:635:GLY:O	2.20	0.41
2:H:154:ILE:HG23	2:H:187:ARG:HD2	2.03	0.41
2:H:718:PHE:CD2	2:H:760:LYS:HD2	2.55	0.41
2:J:256:ILE:O	2:J:256:ILE:HG23	2.21	0.41
2:J:303:LYS:HD2	2:J:330:LEU:HD21	2.02	0.41
2:K:456:HIS:O	2:K:457:ARG:C	2.62	0.41
2:K:572:ASP:OD1	2:K:585:ALA:HB3	2.21	0.41
2:L:58:ASN:O	2:L:59:SER:HB3	2.21	0.41
2:L:649:ASN:HB3	2:L:652:MET:HB2	2.02	0.41
2:L:710:PHE:CE2	2:L:716:GLY:C	2.99	0.41
1:A:335:ALA:HB2	1:A:442:ALA:HB1	2.03	0.41
1:A:336:TYR:CZ	1:A:472:TYR:CE1	3.09	0.41
1:B:456:ALA:HA	1:B:465:HIS:O	2.21	0.41
1:C:43:LYS:CD	1:C:372:ASP:HA	2.47	0.41
1:D:456:ALA:HA	1:D:465:HIS:O	2.21	0.41
1:E:60:VAL:HG22	1:E:61:ARG:H	1.86	0.41
1:E:217:PHE:C	1:E:219:THR:H	2.28	0.41
1:F:168:MET:HE3	1:F:312:THR:O	2.20	0.41
2:G:724:TYR:OH	2:G:728:LYS:HE2	2.21	0.41
2:I:71:GLU:O	2:I:75:VAL:HG23	2.20	0.41
2:I:73:SER:O	2:I:77:ASN:OD1	2.38	0.41
2:J:650:SER:O	2:J:653:ASP:HB2	2.19	0.41
2:L:162:THR:HA	2:L:222:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:186:GLN:HG3	2:L:320:TYR:CD1	2.56	0.41
2:L:531:LYS:C	2:L:533:GLY:H	2.29	0.41
2:L:564:GLU:OE2	2:L:740:TYR:OH	2.36	0.41
1:A:43:LYS:CD	1:A:372:ASP:HA	2.49	0.41
1:A:178:LYS:HA	1:A:181:LYS:HB3	1.97	0.41
1:A:214:VAL:CG1	1:A:215:SER:N	2.84	0.41
1:A:234:PHE:CE1	1:A:392:ALA:HB2	2.56	0.41
1:A:247:ARG:HH22	1:A:417:PHE:HB3	1.86	0.41
1:A:440:ALA:O	1:A:444:ARG:HG3	2.20	0.41
1:B:200:SER:OG	1:B:204:PHE:CD1	2.73	0.41
1:C:338:ARG:HB2	1:C:468:ILE:O	2.21	0.41
1:C:424:LEU:HD23	1:C:424:LEU:O	2.21	0.41
1:D:168:MET:HE1	1:D:429:PRO:HA	2.02	0.41
1:E:43:LYS:CD	1:E:372:ASP:HA	2.50	0.41
1:E:104:GLY:HA2	1:E:134:VAL:O	2.21	0.41
1:E:115:VAL:HG11	1:E:165:VAL:HG11	2.03	0.41
1:E:216:GLU:HB3	1:E:217:PHE:H	1.71	0.41
1:F:93:VAL:HG21	1:F:319:LEU:HD22	2.03	0.41
1:F:358:ALA:O	1:F:359:THR:C	2.63	0.41
2:G:89:VAL:CG1	2:G:90:LEU:N	2.84	0.41
2:G:413:LYS:C	2:G:415:LYS:N	2.78	0.41
2:G:543:PRO:HB2	2:G:606:VAL:HG11	2.03	0.41
2:H:43:TYR:OH	2:H:79:ILE:HG22	2.21	0.41
2:H:120:SER:OG	2:H:324:SER:HA	2.21	0.41
2:H:587:LEU:O	2:H:591:VAL:HG23	2.21	0.41
2:H:710:PHE:CE2	2:H:716:GLY:C	2.99	0.41
2:I:390:LYS:HA	2:I:432:GLN:O	2.21	0.41
2:J:91:ILE:HD11	2:J:237:ILE:HG23	2.02	0.41
2:J:179:LEU:HB2	2:J:180:PRO:CD	2.51	0.41
2:J:566:VAL:HG13	2:J:570:LYS:CD	2.47	0.41
2:J:667:VAL:HG12	2:J:676:ARG:NE	2.36	0.41
2:K:154:ILE:HG23	2:K:187:ARG:HD2	2.03	0.41
2:K:374:ALA:O	2:K:375:GLY:C	2.64	0.41
2:K:537:ILE:HG23	2:K:537:ILE:O	2.21	0.41
2:K:595:VAL:HA	2:K:598:HIS:HB2	2.03	0.41
2:L:154:ILE:HG13	2:L:191:MET:HE1	2.03	0.41
1:A:47:ALA:CB	1:A:338:ARG:NH2	2.84	0.41
1:A:341:MET:HE3	1:A:361:LYS:HD2	2.02	0.41
1:A:359:THR:CB	1:A:360:PRO:HD3	2.48	0.41
1:A:424:LEU:HD23	1:A:424:LEU:O	2.21	0.41
1:B:251:LEU:HG	1:B:419:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:ASP:OD1	1:C:374:ASP:N	2.54	0.41
1:C:411:LEU:HD23	1:C:412:PRO:O	2.21	0.41
1:D:380:GLU:HG2	1:D:386:ILE:HD11	2.03	0.41
1:D:440:ALA:O	1:D:444:ARG:HG3	2.22	0.41
1:E:128:LYS:O	1:E:130:PRO:HD3	2.20	0.41
1:E:241:GLN:C	1:E:243:GLU:N	2.79	0.41
1:F:264:VAL:O	1:F:264:VAL:HG13	2.21	0.41
2:G:273:MET:HA	2:G:273:MET:HE3	2.02	0.41
2:G:303:LYS:HD2	2:G:330:LEU:HD21	2.03	0.41
2:G:569:LYS:NZ	2:I:255:LYS:HB3	2.36	0.41
2:I:38:ARG:HB3	2:I:41:ILE:O	2.21	0.41
2:I:740:TYR:HD1	2:I:740:TYR:HA	1.73	0.41
2:J:552:ALA:O	2:J:553:PRO:C	2.64	0.41
2:K:174:VAL:HG22	2:K:201:MET:O	2.20	0.41
2:K:413:LYS:C	2:K:415:LYS:H	2.28	0.41
2:K:610:ARG:HG3	2:K:744:PHE:HD1	1.86	0.41
2:K:652:MET:O	2:K:656:LEU:HB2	2.21	0.41
2:L:247:PHE:O	2:L:251:LEU:HG	2.21	0.41
2:L:262:LYS:HB3	2:L:266:GLU:CB	2.50	0.41
2:L:543:PRO:HB2	2:L:606:VAL:HG11	2.03	0.41
1:A:142:ASN:HA	1:A:145:MET:HE3	2.03	0.40
1:A:178:LYS:C	1:A:181:LYS:HB3	2.46	0.40
1:B:398:PHE:HD1	1:B:403:MET:HE2	1.85	0.40
1:C:63:PRO:HB2	1:C:65:LEU:HD21	2.03	0.40
1:C:377:GLU:O	1:C:455:VAL:HA	2.21	0.40
1:D:65:LEU:HG	1:D:71:TYR:CE2	2.56	0.40
1:D:312:THR:OG1	1:D:428:HIS:C	2.65	0.40
1:F:429:PRO:O	1:F:430:PHE:C	2.63	0.40
2:G:159:ARG:N	2:G:159:ARG:HD2	2.36	0.40
2:G:256:ILE:O	2:G:256:ILE:HG13	2.21	0.40
2:I:306:ASP:O	2:I:309:LYS:N	2.54	0.40
2:J:742:LYS:CB	2:J:744:PHE:CZ	3.04	0.40
2:K:114:GLN:O	2:K:118:GLN:HB2	2.21	0.40
2:L:256:ILE:O	2:L:256:ILE:HG23	2.21	0.40
2:L:319:GLY:O	2:L:320:TYR:C	2.64	0.40
2:L:607:PHE:C	2:L:609:GLU:H	2.29	0.40
2:L:756:SER:HB3	2:L:757:PRO:HD2	2.03	0.40
1:A:128:LYS:O	1:A:130:PRO:HD3	2.22	0.40
1:A:238:ARG:NH2	1:A:304:THR:HG21	2.36	0.40
1:B:141:ALA:HB2	1:B:431:GLY:C	2.45	0.40
1:B:169:SER:O	1:B:170:ASP:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.88	0.40
1:D:216:GLU:CD	1:D:220:SER:HA	2.46	0.40
1:D:220:SER:O	1:D:221:GLU:HB2	2.20	0.40
1:E:402:TYR:CZ	2:K:227:PRO:HB3	2.56	0.40
1:F:47:ALA:CB	1:F:338:ARG:NH2	2.84	0.40
1:F:251:LEU:HD21	1:F:419:ASN:HA	2.03	0.40
1:F:337:LEU:HD13	1:F:337:LEU:HA	1.90	0.40
1:F:360:PRO:O	1:F:363:LEU:N	2.54	0.40
2:G:179:LEU:C	2:G:179:LEU:CD1	2.94	0.40
2:G:179:LEU:HD12	2:G:179:LEU:O	2.21	0.40
2:G:610:ARG:CD	2:G:743:GLN:O	2.64	0.40
2:G:652:MET:HA	2:G:655:ILE:HG22	2.03	0.40
2:G:698:ALA:HA	2:G:761:PHE:CE1	2.56	0.40
2:H:368:GLY:C	2:H:370:GLY:H	2.29	0.40
2:H:593:VAL:HG22	2:H:622:MET:HE1	2.00	0.40
2:H:620:THR:C	2:H:622:MET:N	2.79	0.40
2:I:191:MET:HE3	2:I:191:MET:HB2	1.88	0.40
2:I:649:ASN:HB3	2:I:652:MET:HB2	2.04	0.40
2:J:169:LEU:O	2:J:207:ILE:N	2.45	0.40
2:J:546:TYR:CE1	2:J:694:LEU:HD11	2.56	0.40
2:K:179:LEU:HB2	2:K:180:PRO:HD2	2.03	0.40
2:K:273:MET:HE2	2:K:279:ARG:HG2	2.03	0.40
2:K:343:TYR:O	2:K:347:VAL:HG23	2.21	0.40
1:A:263:ASP:OD1	1:A:263:ASP:N	2.54	0.40
1:A:350:GLN:HB2	1:A:353:LEU:HD12	2.03	0.40
1:A:362:VAL:HG13	1:A:363:LEU:N	2.37	0.40
1:B:52:ARG:HH21	1:B:322:ALA:CB	2.34	0.40
1:B:217:PHE:HD1	1:B:219:THR:H	1.70	0.40
1:E:166:GLU:HB2	1:E:430:PHE:O	2.22	0.40
1:E:225:HIS:HA	1:E:296:PHE:HB3	2.03	0.40
1:E:380:GLU:HA	1:E:386:ILE:HD11	2.03	0.40
1:F:57:VAL:HG21	1:F:321:MET:SD	2.62	0.40
2:G:611:PHE:N	2:G:611:PHE:CD1	2.89	0.40
2:G:652:MET:O	2:G:656:LEU:HB2	2.22	0.40
2:J:319:GLY:O	2:J:320:TYR:C	2.63	0.40
2:J:446:GLU:HG2	2:J:448:VAL:HG23	2.04	0.40
2:K:459:LEU:O	2:K:463:GLU:HB2	2.21	0.40
2:K:667:VAL:HG12	2:K:676:ARG:NE	2.36	0.40
2:L:628:LEU:HD23	2:L:631:LYS:HG3	2.03	0.40
2:L:742:LYS:CB	2:L:744:PHE:CZ	3.04	0.40
1:A:114:ASN:O	1:A:115:VAL:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:PHE:CE1	1:A:456:ALA:HB3	2.56	0.40
1:B:321:MET:CE	1:B:329:MET:HG3	2.50	0.40
1:B:374:ASP:OD1	1:B:374:ASP:N	2.54	0.40
1:C:429:PRO:O	1:C:430:PHE:C	2.64	0.40
1:E:102:ILE:HD13	1:E:147:THR:HB	2.02	0.40
1:E:342:TYR:CE1	1:E:465:HIS:CD2	3.10	0.40
2:H:413:LYS:C	2:H:415:LYS:N	2.79	0.40
2:I:179:LEU:HB2	2:I:180:PRO:HD2	2.03	0.40
2:J:540:LYS:CE	2:J:692:GLY:O	2.69	0.40
2:J:689:LEU:O	2:J:689:LEU:HD13	2.22	0.40
2:K:188:LEU:N	2:K:189:PRO:CD	2.85	0.40
2:K:540:LYS:CE	2:K:692:GLY:O	2.70	0.40
2:L:540:LYS:CE	2:L:692:GLY:O	2.69	0.40
1:C:106:VAL:HG22	1:C:166:GLU:CD	2.46	0.40
1:C:456:ALA:HA	1:C:465:HIS:O	2.22	0.40
1:F:294:PRO:O	1:F:298:LYS:HE2	2.22	0.40
1:F:380:GLU:HB2	1:F:424:LEU:H	1.86	0.40
2:G:188:LEU:N	2:G:189:PRO:CD	2.83	0.40
2:H:283:TYR:OH	2:H:312:ILE:HD11	2.21	0.40
2:H:667:VAL:HG12	2:H:676:ARG:NE	2.37	0.40
2:H:756:SER:HB3	2:H:757:PRO:HD2	2.03	0.40
2:I:481:ILE:O	2:I:481:ILE:HG22	2.21	0.40
2:J:147:GLY:O	2:J:148:GLY:C	2.64	0.40
2:J:172:PRO:O	2:J:173:GLU:C	2.65	0.40
2:J:667:VAL:HG12	2:J:667:VAL:O	2.21	0.40
2:K:98:PHE:C	2:K:99:ILE:HG12	2.46	0.40
2:K:163:LYS:HG2	2:K:221:LEU:CD2	2.51	0.40
2:K:163:LYS:HE3	2:K:221:LEU:HB3	2.04	0.40
2:K:367:LEU:HB2	2:K:446:GLU:HA	2.03	0.40
2:L:198:LEU:O	2:L:199:ASP:C	2.64	0.40
2:L:367:LEU:HB2	2:L:446:GLU:HA	2.04	0.40
2:L:541:ASP:OD1	2:L:541:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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	430/457 (94%)	353 (82%)	61 (14%)	16 (4%)	2	21
1	B	415/457 (91%)	347 (84%)	54 (13%)	14 (3%)	3	23
1	C	417/457 (91%)	355 (85%)	48 (12%)	14 (3%)	3	23
1	D	420/457 (92%)	347 (83%)	59 (14%)	14 (3%)	3	24
1	E	419/457 (92%)	357 (85%)	48 (12%)	14 (3%)	3	24
1	F	421/457 (92%)	357 (85%)	53 (13%)	11 (3%)	4	27
2	G	723/727 (99%)	613 (85%)	91 (13%)	19 (3%)	4	27
2	H	723/727 (99%)	619 (86%)	87 (12%)	17 (2%)	4	29
2	I	710/727 (98%)	621 (88%)	82 (12%)	7 (1%)	12	45
2	J	710/727 (98%)	608 (86%)	95 (13%)	7 (1%)	12	45
2	K	710/727 (98%)	614 (86%)	87 (12%)	9 (1%)	9	39
2	L	710/727 (98%)	617 (87%)	86 (12%)	7 (1%)	12	45
All	All	6808/7104 (96%)	5808 (85%)	851 (12%)	149 (2%)	5	30

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
1	A	208	ALA
1	A	216	GLU
1	A	221	GLU
1	B	49	PRO
1	B	170	ASP
1	B	206	PHE
1	B	212	PRO
1	B	214	VAL
1	B	215	SER
1	B	216	GLU
1	B	221	GLU
1	C	49	PRO
1	C	170	ASP
1	C	206	PHE
1	C	214	VAL
1	D	49	PRO
1	D	170	ASP

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Mol	Chain	Res	Type
1	D	211	LEU
1	D	214	VAL
1	D	221	GLU
1	E	49	PRO
1	E	170	ASP
1	E	208	ALA
1	E	209	PRO
1	E	212	PRO
1	E	214	VAL
1	F	49	PRO
1	F	170	ASP
1	F	210	GLU
1	F	212	PRO
1	F	214	VAL
1	F	221	GLU
2	G	637	TYR
2	G	638	ILE
2	G	641	GLU
2	H	643	VAL
2	H	646	LYS
1	A	189	ALA
1	A	215	SER
1	B	176	SER
1	C	212	PRO
1	C	221	GLU
1	E	216	GLU
1	E	221	GLU
2	G	630	ARG
2	G	642	GLY
2	G	644	LYS
2	G	741	GLY
2	H	630	ARG
2	H	632	SER
2	H	639	TYR
1	A	46	LEU
1	A	198	LEU
1	A	212	PRO
1	A	213	ALA
1	C	216	GLU
1	C	338	ARG
1	C	414	LEU
1	D	46	LEU

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Mol	Chain	Res	Type
1	D	274	THR
1	E	46	LEU
1	F	46	LEU
1	F	414	LEU
2	G	195	PRO
2	G	645	ARG
2	G	652	MET
2	H	631	LYS
2	H	634	LYS
2	J	195	PRO
2	K	195	PRO
2	L	741	GLY
1	A	191	SER
1	A	220	SER
1	A	274	THR
1	B	204	PHE
1	B	338	ARG
1	C	46	LEU
1	C	220	SER
1	C	274	THR
1	D	210	GLU
1	D	212	PRO
1	E	217	PHE
1	F	220	SER
1	F	274	THR
2	G	702	ILE
2	I	195	PRO
1	A	209	PRO
1	B	274	THR
1	B	414	LEU
1	D	209	PRO
1	D	216	GLU
1	D	338	ARG
1	E	261	LEU
1	E	274	THR
2	G	299	PRO
2	G	629	GLY
2	H	195	PRO
2	I	258	PRO
2	I	608	GLY
2	J	258	PRO
2	K	310	THR

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Mol	Chain	Res	Type
2	L	195	PRO
2	L	299	PRO
2	L	702	ILE
1	A	211	LEU
1	A	338	ARG
1	B	129	THR
1	C	207	LEU
1	D	129	THR
1	D	220	SER
1	E	338	ARG
1	F	360	PRO
2	G	258	PRO
2	H	299	PRO
2	J	299	PRO
2	J	544	GLY
2	J	702	ILE
2	K	258	PRO
2	K	702	ILE
2	L	544	GLY
2	H	258	PRO
2	H	608	GLY
2	I	544	GLY
2	K	299	PRO
2	K	544	GLY
1	E	281	ILE
2	G	256	ILE
2	G	643	VAL
2	H	544	GLY
2	H	741	GLY
2	I	299	PRO
2	I	741	GLY
2	K	741	GLY
2	L	258	PRO
2	G	257	SER
2	G	608	GLY
2	H	256	ILE
2	H	467	PRO
2	I	257	SER
2	J	257	SER
1	C	333	PRO
2	G	232	PRO
2	H	257	SER

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Mol	Chain	Res	Type
2	J	256	ILE
2	K	257	SER
2	K	608	GLY
2	H	592	GLY
2	L	257	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	345/365 (94%)	324 (94%)	21 (6%)	17	45
1	B	334/365 (92%)	309 (92%)	25 (8%)	12	39
1	C	305/365 (84%)	289 (95%)	16 (5%)	21	48
1	D	305/365 (84%)	289 (95%)	16 (5%)	21	48
1	E	305/365 (84%)	285 (93%)	20 (7%)	15	43
1	F	305/365 (84%)	289 (95%)	16 (5%)	21	48
2	G	580/603 (96%)	569 (98%)	11 (2%)	50	67
2	H	580/603 (96%)	564 (97%)	16 (3%)	38	60
2	I	591/603 (98%)	578 (98%)	13 (2%)	45	65
2	J	591/603 (98%)	576 (98%)	15 (2%)	42	63
2	K	591/603 (98%)	576 (98%)	15 (2%)	42	63
2	L	591/603 (98%)	578 (98%)	13 (2%)	45	65
All	All	5423/5808 (93%)	5226 (96%)	197 (4%)	31	56

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	93	VAL
1	A	102	ILE
1	A	103	PHE
1	A	149	VAL

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Mol	Chain	Res	Type
1	A	173	ILE
1	A	181	LYS
1	A	185	ASP
1	A	195	ARG
1	A	197	SER
1	A	239	LEU
1	A	247	ARG
1	A	263	ASP
1	A	337	LEU
1	A	346	ASP
1	A	348	LYS
1	A	389	ASN
1	A	423	SER
1	A	433	THR
1	A	438	VAL
1	A	443	ASN
1	B	56	VAL
1	B	93	VAL
1	B	102	ILE
1	B	103	PHE
1	B	149	VAL
1	B	173	ILE
1	B	174	ARG
1	B	177	ARG
1	B	181	LYS
1	B	184	LEU
1	B	194	GLN
1	B	198	LEU
1	B	207	LEU
1	B	239	LEU
1	B	247	ARG
1	B	263	ASP
1	B	337	LEU
1	B	348	LYS
1	B	389	ASN
1	B	391	LYS
1	B	405	ARG
1	B	423	SER
1	B	433	THR
1	B	438	VAL
1	B	443	ASN
1	C	56	VAL

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Mol	Chain	Res	Type
1	C	93	VAL
1	C	102	ILE
1	C	103	PHE
1	C	222	THR
1	C	239	LEU
1	C	247	ARG
1	C	263	ASP
1	C	337	LEU
1	C	346	ASP
1	C	348	LYS
1	C	389	ASN
1	C	405	ARG
1	C	433	THR
1	C	438	VAL
1	C	443	ASN
1	D	56	VAL
1	D	93	VAL
1	D	102	ILE
1	D	103	PHE
1	D	149	VAL
1	D	239	LEU
1	D	247	ARG
1	D	263	ASP
1	D	337	LEU
1	D	338	ARG
1	D	348	LYS
1	D	389	ASN
1	D	405	ARG
1	D	433	THR
1	D	438	VAL
1	D	443	ASN
1	E	44	LYS
1	E	56	VAL
1	E	93	VAL
1	E	102	ILE
1	E	103	PHE
1	E	222	THR
1	E	239	LEU
1	E	247	ARG
1	E	263	ASP
1	E	337	LEU
1	E	346	ASP

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Mol	Chain	Res	Type
1	E	348	LYS
1	E	389	ASN
1	E	391	LYS
1	E	405	ARG
1	E	415	GLU
1	E	423	SER
1	E	433	THR
1	E	438	VAL
1	E	443	ASN
1	F	56	VAL
1	F	93	VAL
1	F	102	ILE
1	F	103	PHE
1	F	149	VAL
1	F	239	LEU
1	F	247	ARG
1	F	263	ASP
1	F	337	LEU
1	F	348	LYS
1	F	389	ASN
1	F	391	LYS
1	F	405	ARG
1	F	423	SER
1	F	433	THR
1	F	438	VAL
2	G	119	LEU
2	G	230	LYS
2	G	430	THR
2	G	436	GLN
2	G	448	VAL
2	G	537	ILE
2	G	582	VAL
2	G	680	ARG
2	G	730	VAL
2	G	740	TYR
2	G	756	SER
2	H	173	GLU
2	H	230	LYS
2	H	430	THR
2	H	448	VAL
2	H	504	ASP
2	H	537	ILE

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Mol	Chain	Res	Type
2	H	582	VAL
2	H	589	ASP
2	H	593	VAL
2	H	597	LYS
2	H	652	MET
2	H	680	ARG
2	H	730	VAL
2	H	740	TYR
2	H	756	SER
2	H	762	TYR
2	I	173	GLU
2	I	230	LYS
2	I	397	LEU
2	I	430	THR
2	I	448	VAL
2	I	537	ILE
2	I	582	VAL
2	I	597	LYS
2	I	666	GLU
2	I	680	ARG
2	I	730	VAL
2	I	740	TYR
2	I	756	SER
2	J	119	LEU
2	J	173	GLU
2	J	230	LYS
2	J	397	LEU
2	J	430	THR
2	J	439	GLU
2	J	448	VAL
2	J	463	GLU
2	J	537	ILE
2	J	582	VAL
2	J	597	LYS
2	J	680	ARG
2	J	730	VAL
2	J	740	TYR
2	J	756	SER
2	K	173	GLU
2	K	230	LYS
2	K	397	LEU
2	K	430	THR

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Mol	Chain	Res	Type
2	K	448	VAL
2	K	474	SER
2	K	537	ILE
2	K	582	VAL
2	K	597	LYS
2	K	647	ASP
2	K	680	ARG
2	K	689	LEU
2	K	730	VAL
2	K	740	TYR
2	K	756	SER
2	L	173	GLU
2	L	230	LYS
2	L	430	THR
2	L	436	GLN
2	L	448	VAL
2	L	474	SER
2	L	504	ASP
2	L	537	ILE
2	L	582	VAL
2	L	680	ARG
2	L	713	CYS
2	L	740	TYR
2	L	756	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	205	ASN
1	A	249	HIS
1	A	279	ASN
1	A	288	GLN
1	A	385	GLN
1	A	418	ASN
1	B	108	GLN
1	B	205	ASN
1	B	249	HIS
1	B	288	GLN
1	B	350	GLN
1	B	385	GLN
1	B	418	ASN

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Mol	Chain	Res	Type
1	B	451	GLN
1	C	108	GLN
1	C	143	GLN
1	C	249	HIS
1	C	350	GLN
1	C	385	GLN
1	C	465	HIS
1	D	108	GLN
1	D	143	GLN
1	D	288	GLN
1	D	350	GLN
1	D	385	GLN
1	D	418	ASN
1	E	143	GLN
1	E	279	ASN
1	E	288	GLN
1	E	385	GLN
1	E	418	ASN
1	F	108	GLN
1	F	143	GLN
1	F	279	ASN
1	F	288	GLN
1	F	350	GLN
1	F	385	GLN
1	F	418	ASN
2	G	40	HIS
2	G	105	ASN
2	G	142	ASN
2	G	186	GLN
2	G	281	GLN
2	G	344	HIS
2	G	358	GLN
2	G	469	HIS
2	H	105	ASN
2	H	142	ASN
2	H	281	GLN
2	H	402	GLN
2	H	469	HIS
2	I	105	ASN
2	I	142	ASN
2	I	186	GLN
2	I	281	GLN

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Mol	Chain	Res	Type
2	I	358	GLN
2	I	469	HIS
2	J	105	ASN
2	J	186	GLN
2	J	281	GLN
2	J	358	GLN
2	J	409	ASN
2	J	469	HIS
2	K	40	HIS
2	K	105	ASN
2	K	142	ASN
2	K	186	GLN
2	K	281	GLN
2	K	358	GLN
2	K	409	ASN
2	K	469	HIS
2	L	40	HIS
2	L	55	ASN
2	L	105	ASN
2	L	142	ASN
2	L	186	GLN
2	L	281	GLN
2	L	358	GLN
2	L	469	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/457 (94%)	-0.25	2 (0%) 87 66	78, 115, 154, 202	0
1	B	419/457 (91%)	-0.37	1 (0%) 91 80	77, 114, 150, 211	0
1	C	421/457 (92%)	-0.33	0 100 100	74, 116, 181, 239	0
1	D	424/457 (92%)	-0.34	1 (0%) 91 80	78, 122, 186, 224	0
1	E	423/457 (92%)	-0.45	0 100 100	57, 91, 191, 228	0
1	F	425/457 (92%)	-0.42	0 100 100	59, 93, 186, 231	0
2	G	725/727 (99%)	-0.29	3 (0%) 88 70	68, 123, 180, 234	0
2	H	725/727 (99%)	-0.30	4 (0%) 85 64	76, 130, 186, 241	0
2	I	714/727 (98%)	-0.35	3 (0%) 88 70	86, 128, 184, 234	0
2	J	714/727 (98%)	-0.39	1 (0%) 92 85	78, 123, 183, 237	0
2	K	714/727 (98%)	-0.47	3 (0%) 88 70	66, 121, 178, 226	0
2	L	714/727 (98%)	-0.37	2 (0%) 90 75	67, 119, 179, 214	0
All	All	6850/7104 (96%)	-0.36	20 (0%) 90 75	57, 119, 181, 241	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	106	MET	3.1
2	J	551	LEU	2.9
2	L	731	ASP	2.8
1	A	421	GLY	2.7
2	I	588	VAL	2.6
2	I	538	VAL	2.5
2	K	588	VAL	2.5
2	H	652	MET	2.4
2	G	578	PHE	2.4
2	K	106	MET	2.3
1	A	453	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	176	LEU	2.3
1	B	170	ASP	2.3
2	H	633	GLY	2.2
1	D	210	GLU	2.2
2	G	593	VAL	2.2
2	K	555	MET	2.1
2	H	158	TYR	2.1
2	H	138	VAL	2.0
2	I	106	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.