



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:44 PM UTC

PDB ID : 3KZ4 / pdb_00003kz4
Title : Crystal Structure of the Rotavirus Double Layered Particle
Authors : McClain, B.; Settembre, E.C.; Bellamy, A.R.; Harrison, S.C.
Deposited on : 2009-12-07
Resolution : 3.80 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:

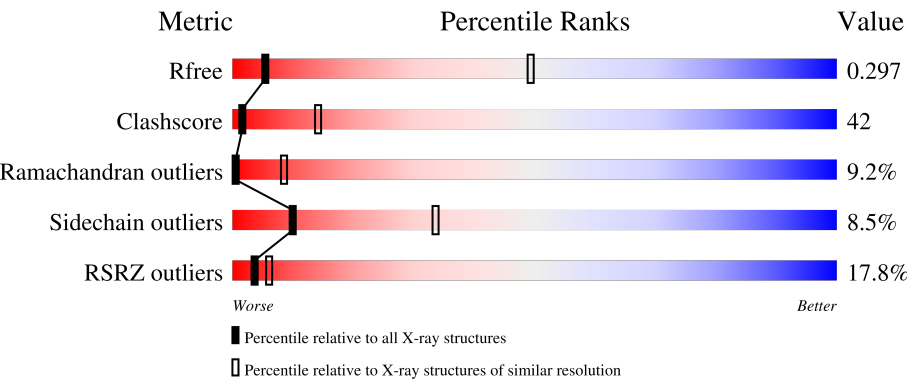
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



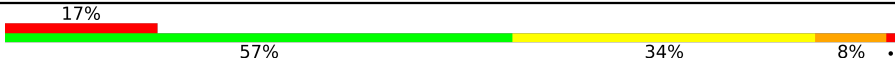
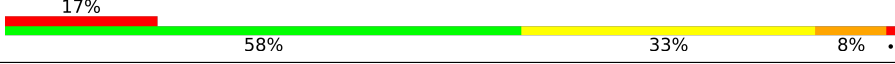
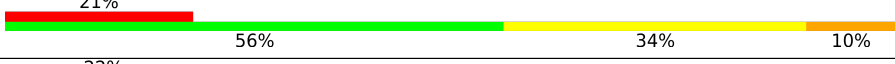
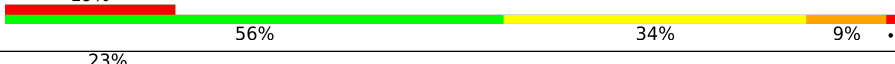
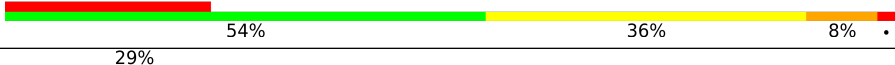
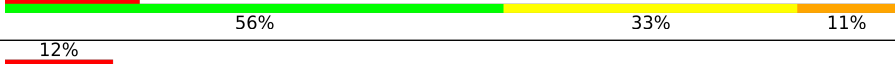
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	880	11% 14%47%24%11%
1	B	880	7% 16%47%26%8%
2	C	397	15% 59%31%9%
2	D	397	21% 55%34%11%
2	E	397	22% 56%33%9%

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Mol	Chain	Length	Quality of chain
2	F	397	
2	G	397	
2	H	397	
2	I	397	
2	J	397	
2	K	397	
2	L	397	
2	M	397	
2	N	397	
2	O	397	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 54109 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6374	4049	1099	1190	36			
1	B	810	Total	C	N	O	S	0	0	0
			6624	4211	1138	1239	36			

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	D	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	E	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	F	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	G	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	H	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	I	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	J	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	K	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	L	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	M	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	N	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

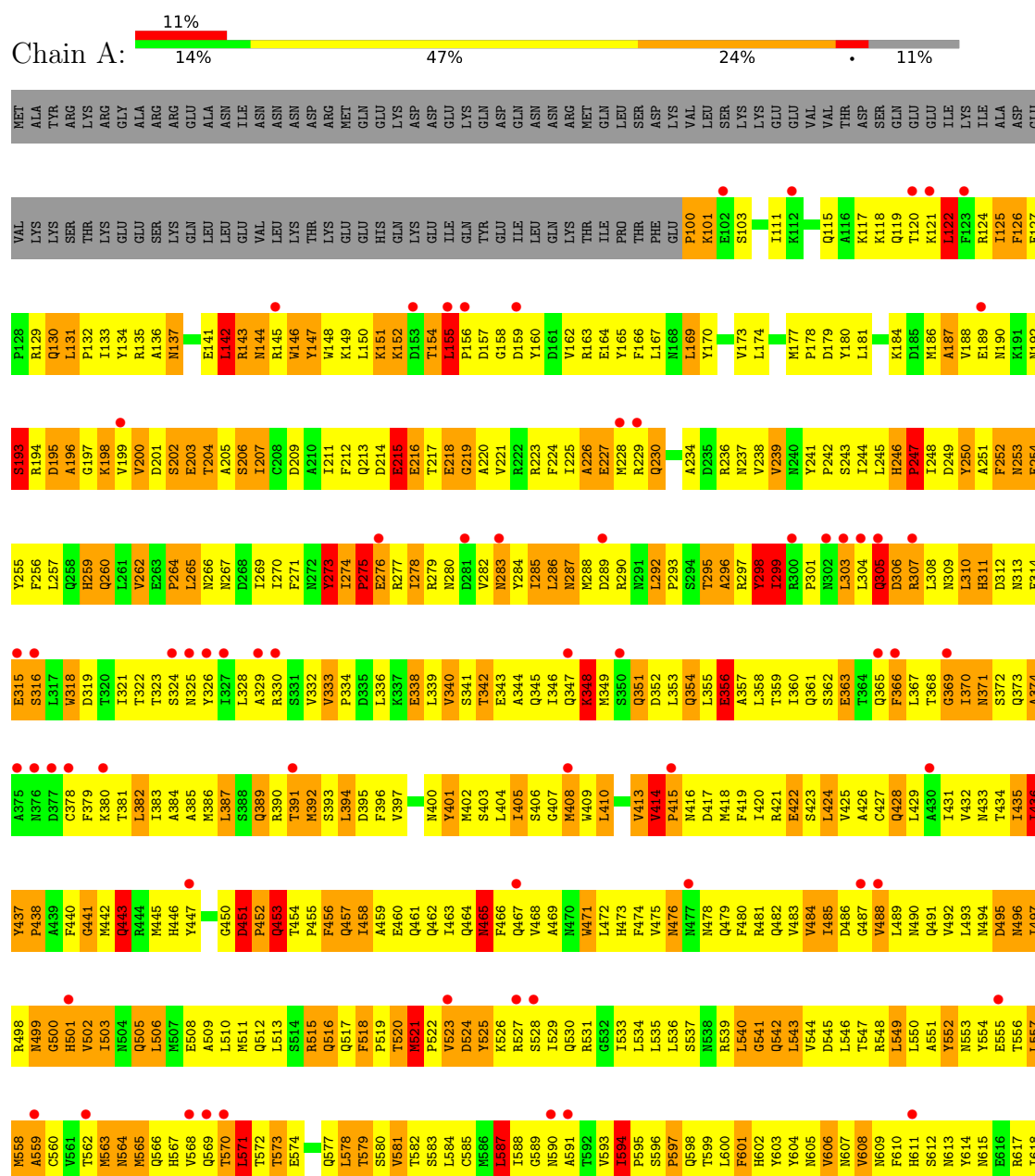
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

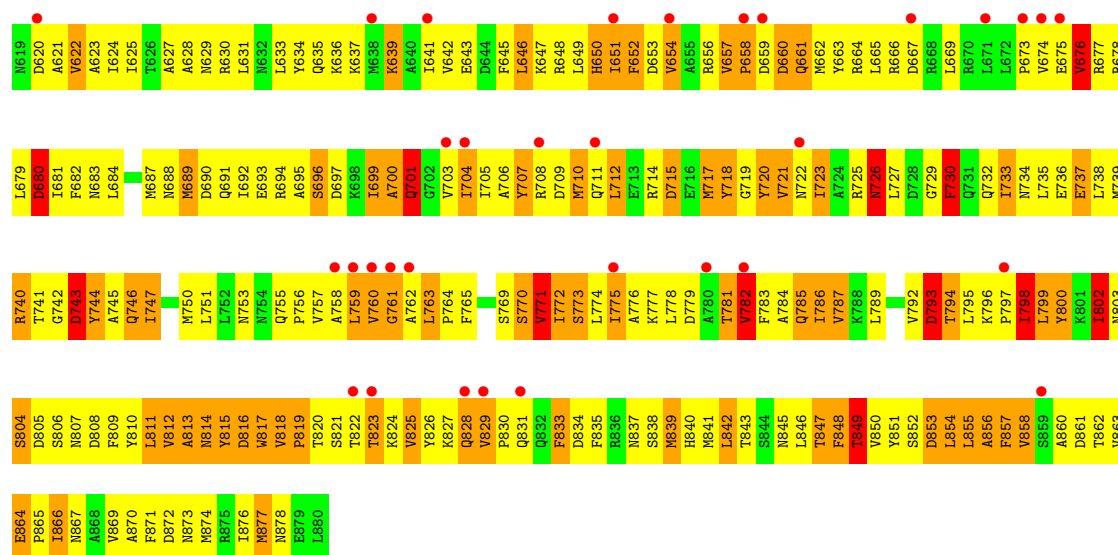
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	O	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

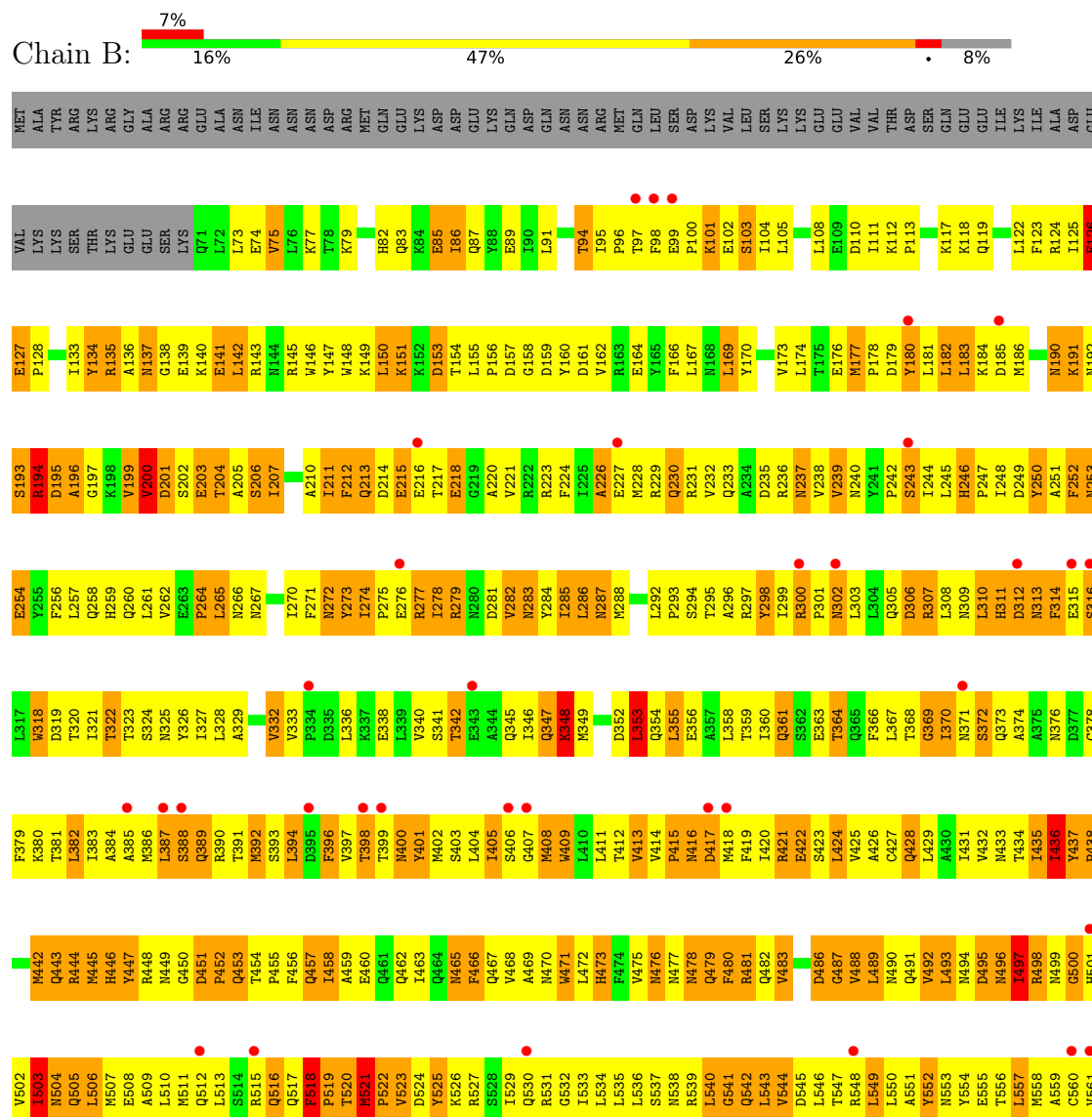
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

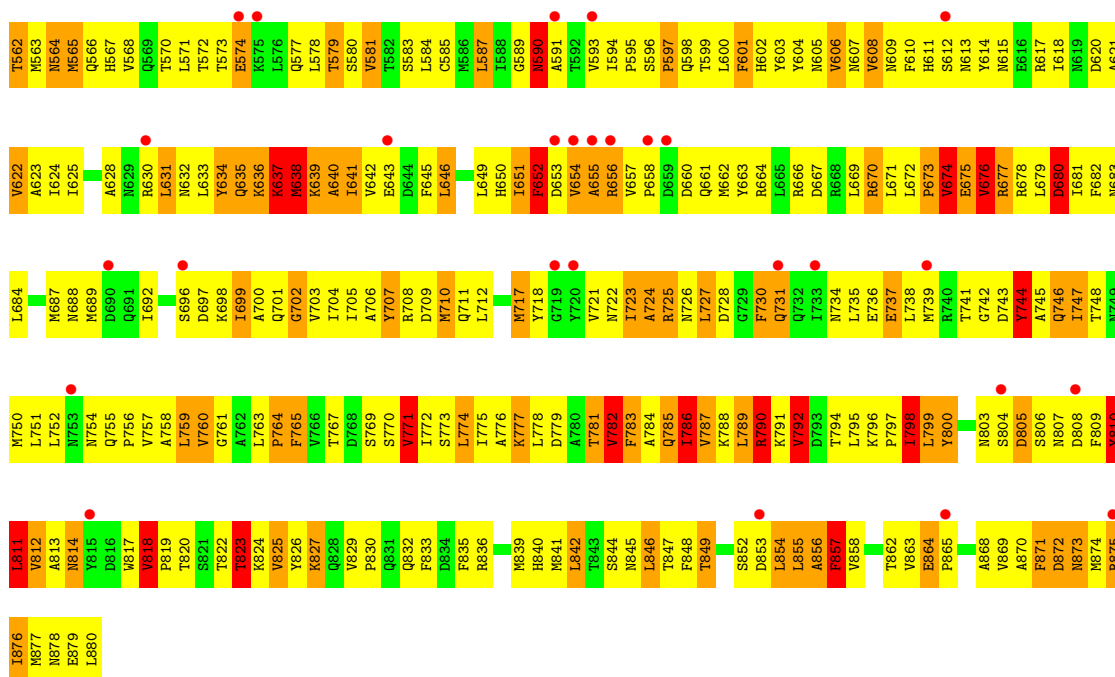
• Molecule 1: Inner capsid protein VP2



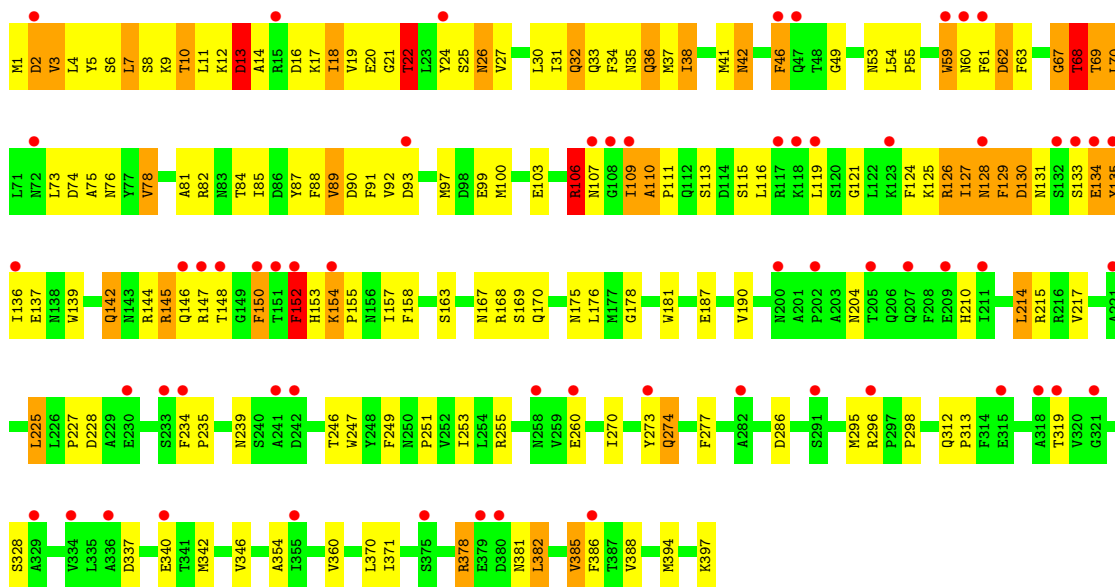


- Molecule 1: Inner capsid protein VP2



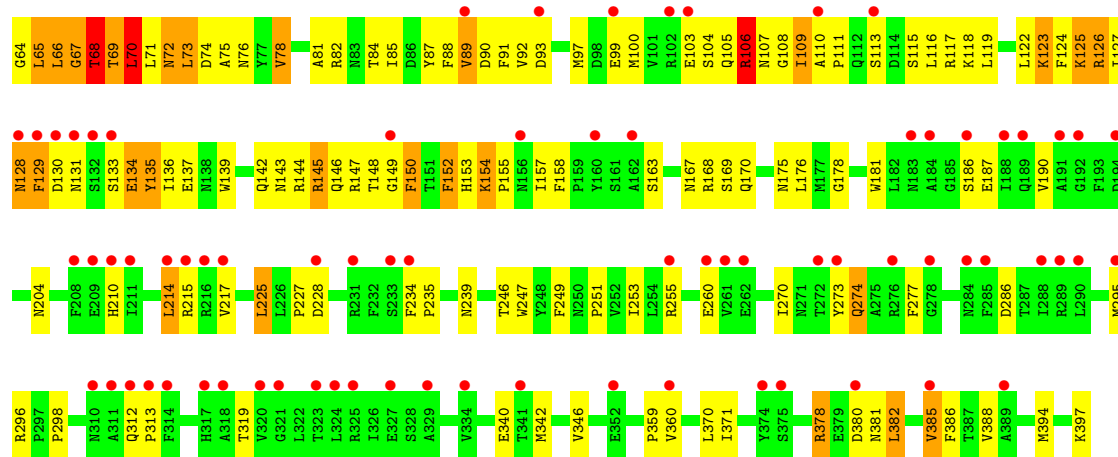


• Molecule 2: Intermediate capsid protein VP6

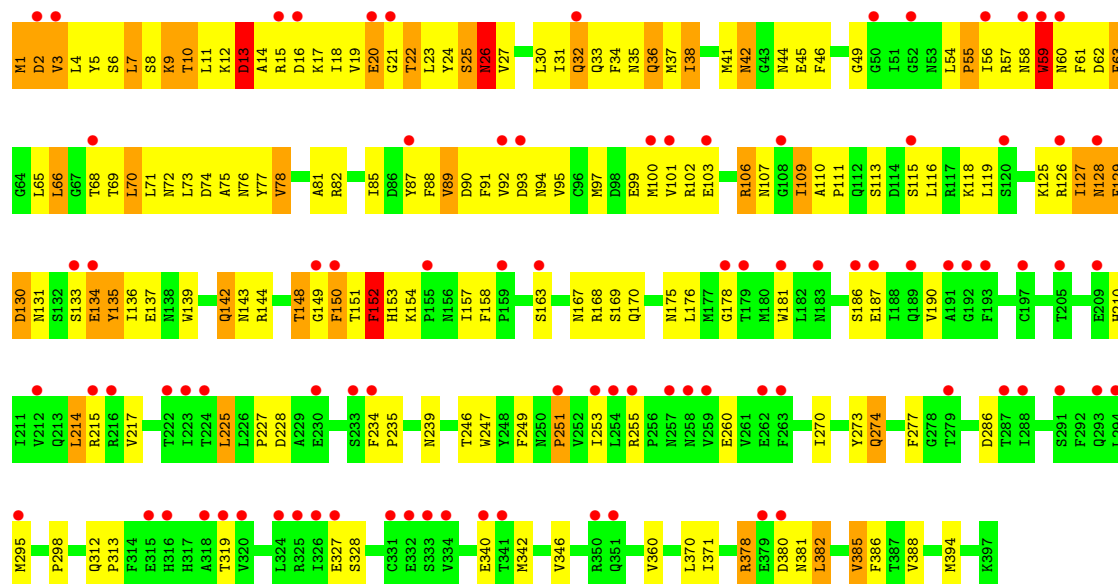


• Molecule 2: Intermediate capsid protein VP6

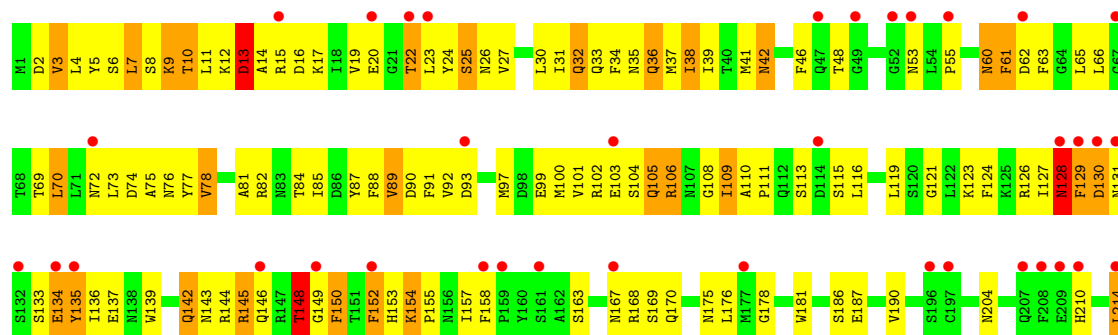


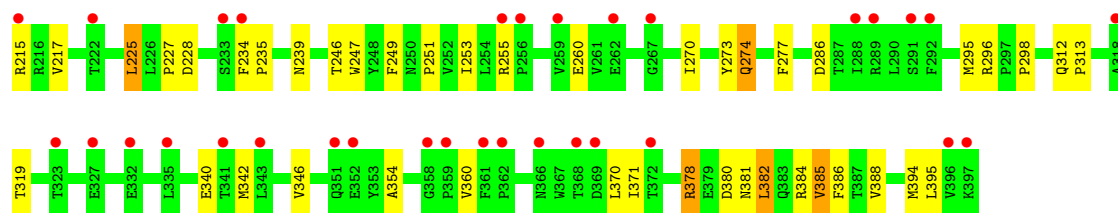


• Molecule 2: Intermediate capsid protein VP6

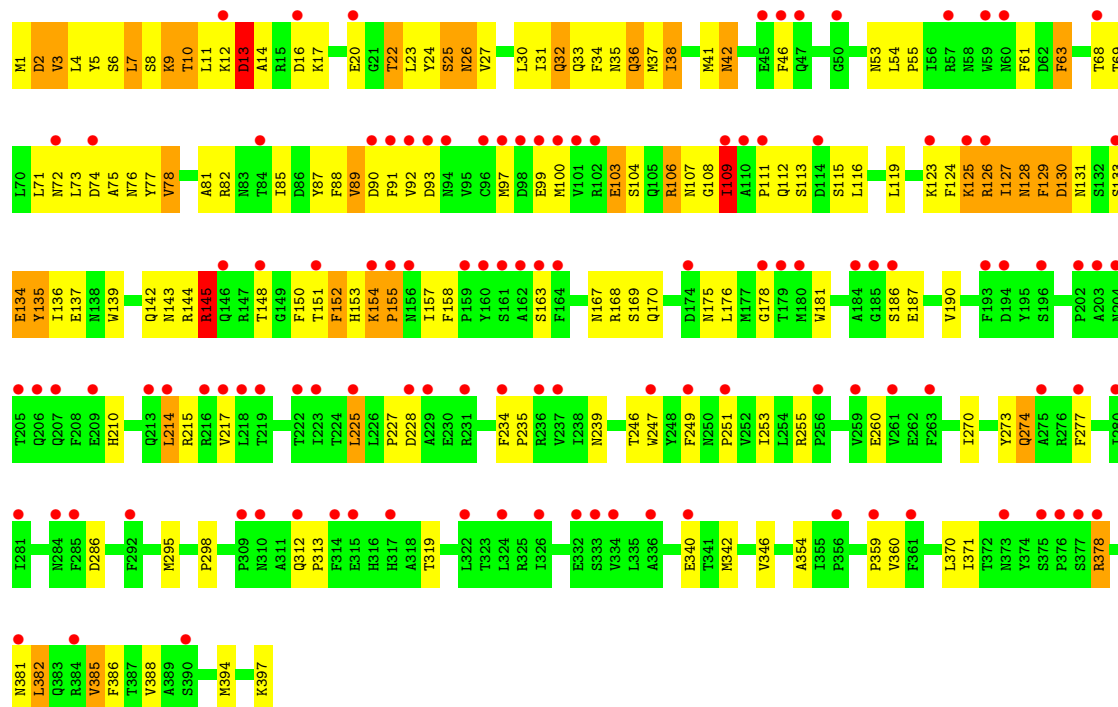


• Molecule 2: Intermediate capsid protein VP6

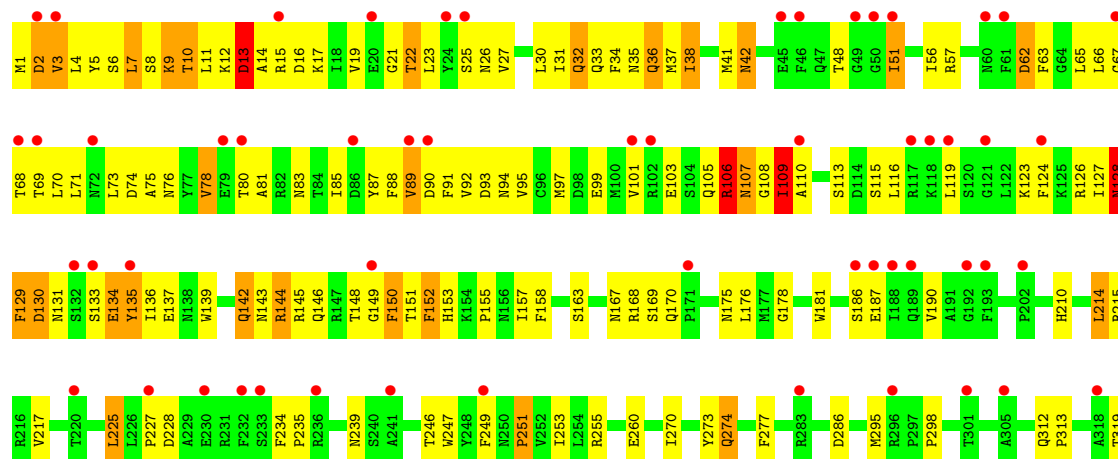




• Molecule 2: Intermediate capsid protein VP6

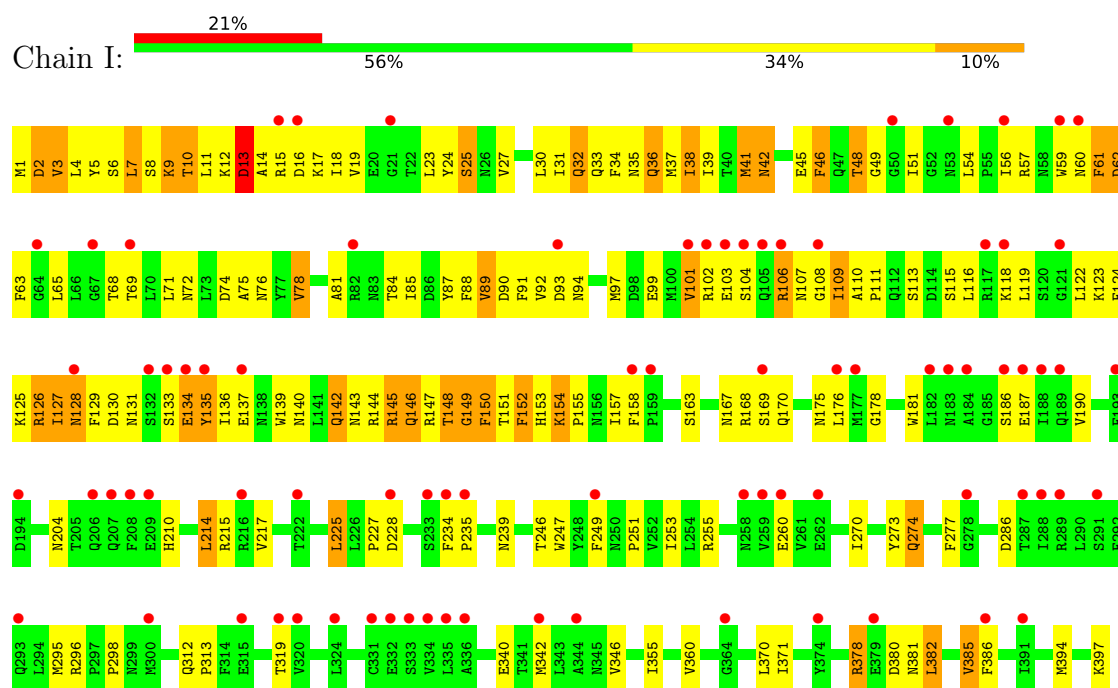


• Molecule 2: Intermediate capsid protein VP6

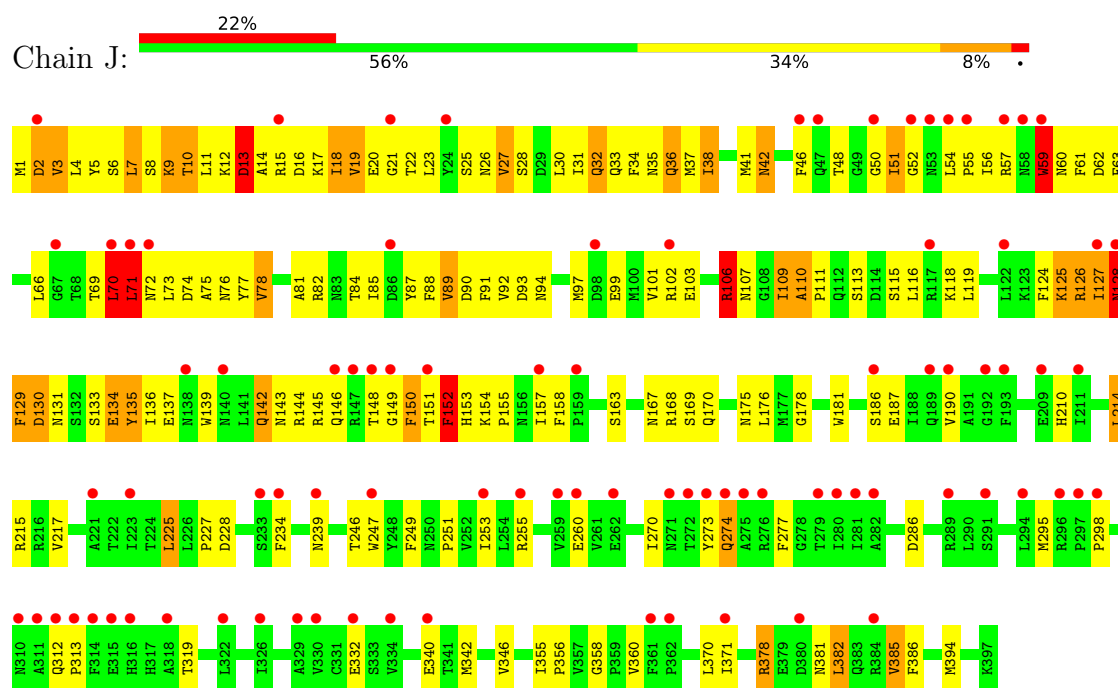




• Molecule 2: Intermediate capsid protein VP6

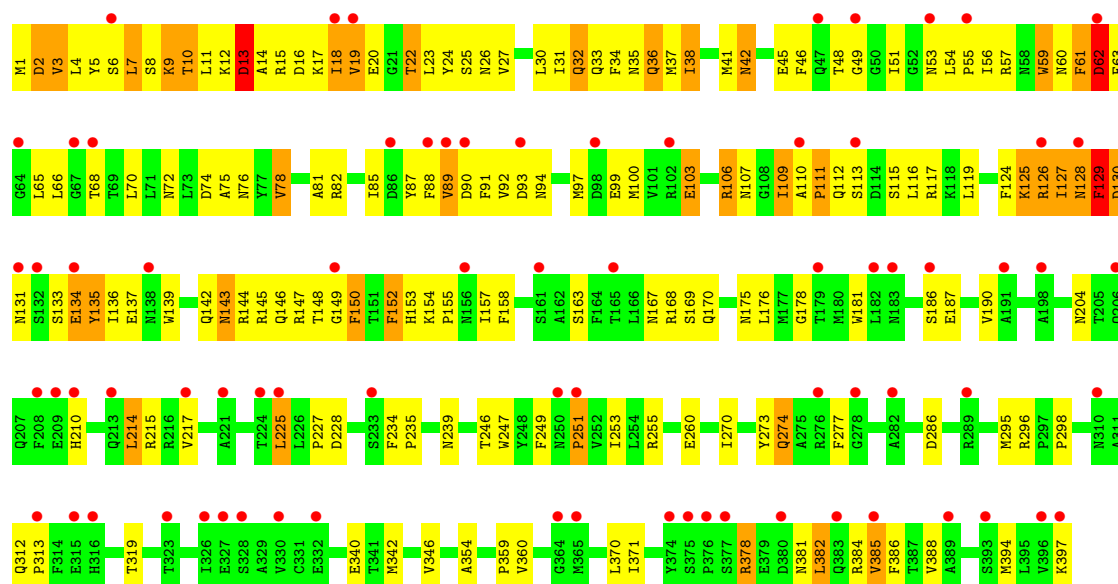


• Molecule 2: Intermediate capsid protein VP6



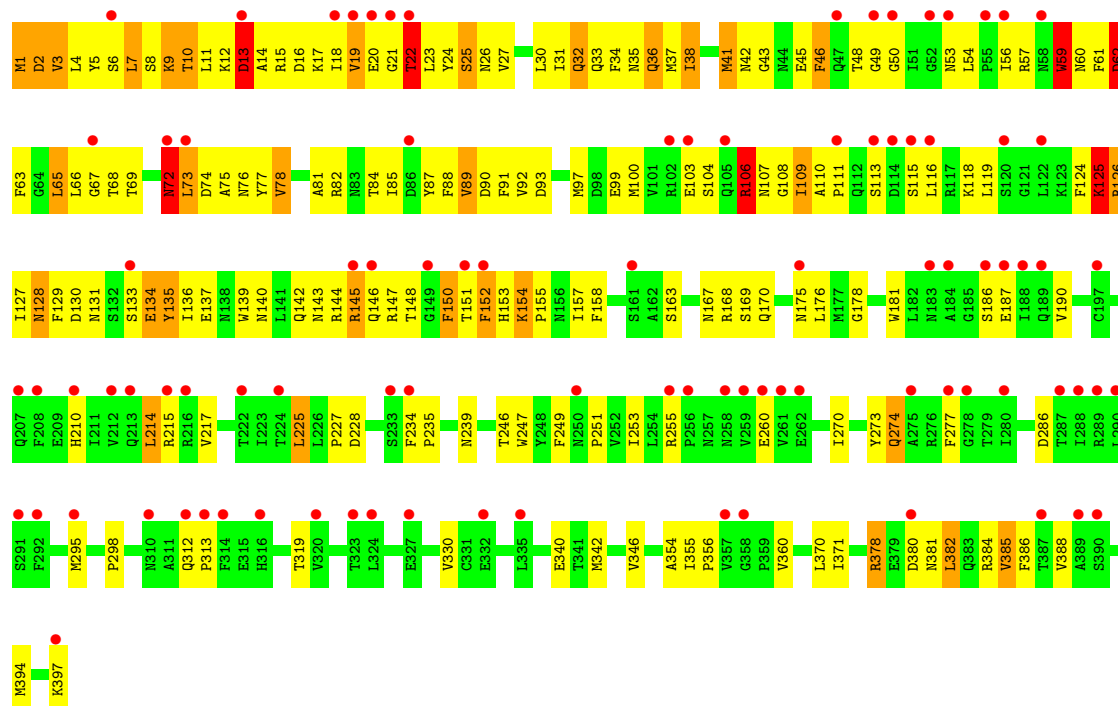
• Molecule 2: Intermediate capsid protein VP6





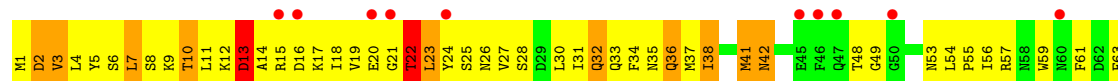
• Molecule 2: Intermediate capsid protein VP6

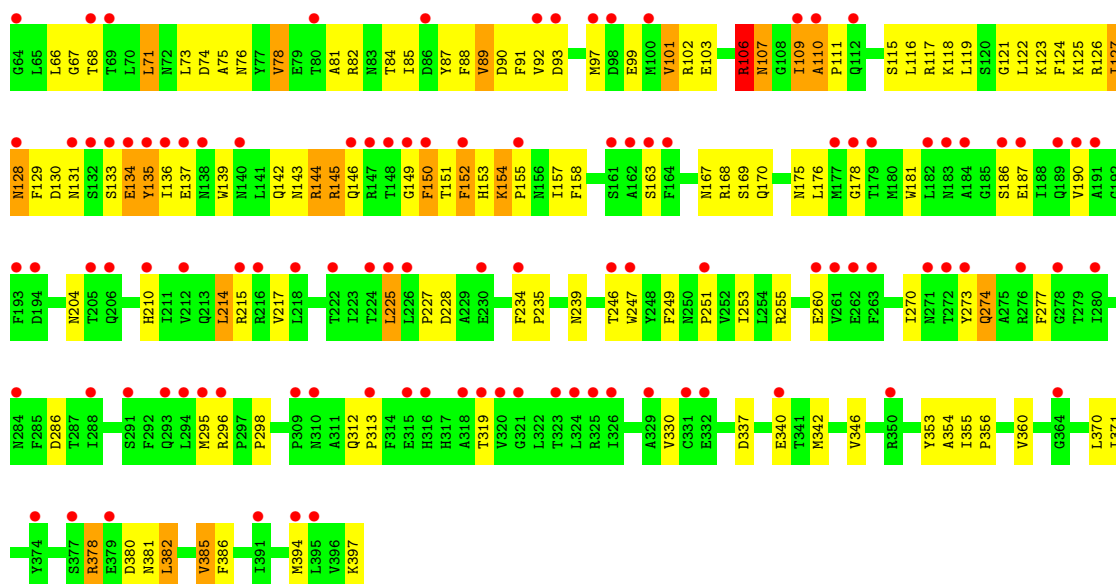
Chain L: 23% 54% 36% 8%



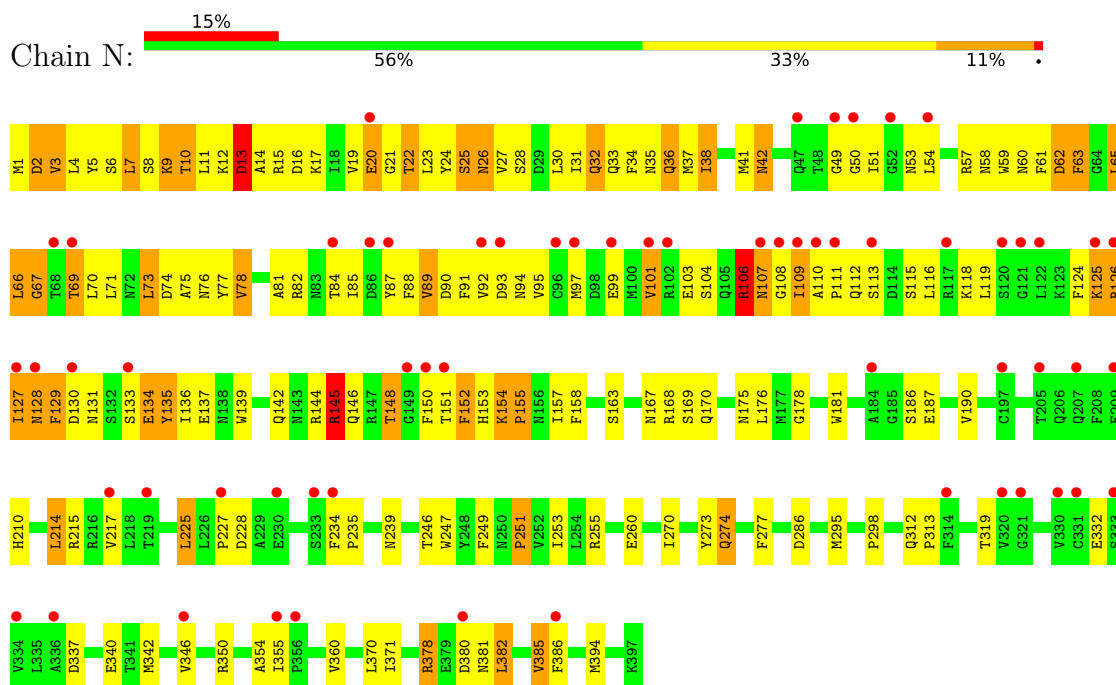
• Molecule 2: Intermediate capsid protein VP6

Chain M: 29% 56% 36% 8%

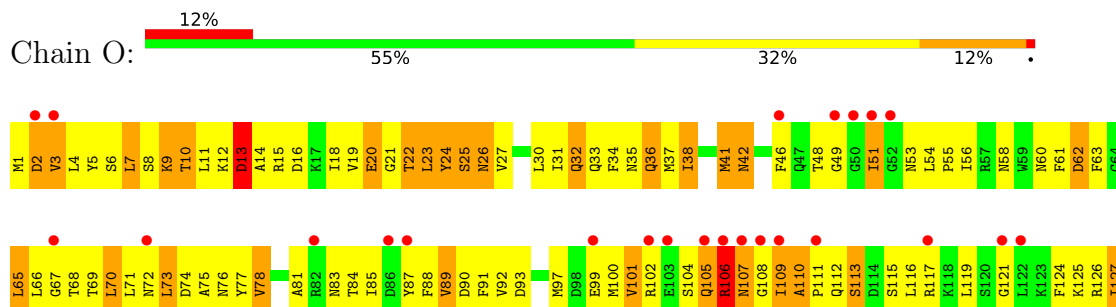


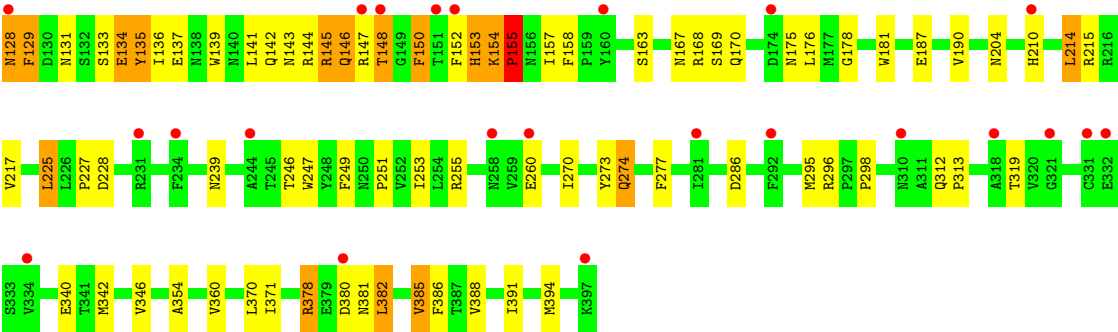


• Molecule 2: Intermediate capsid protein VP6



• Molecule 2: Intermediate capsid protein VP6





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	740.75Å 1198.07Å 1345.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	15.9 (30.00-3.80) 15.9 (30.00-3.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.49 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.328 , 0.339 0.290 , 0.297	Depositor DCC
R_{free} test set	47880 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	167.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	54109	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/6491	1.23	83/8806 (0.9%)
1	B	0.58	0/6745	1.21	75/9149 (0.8%)
2	C	0.62	1/3232 (0.0%)	1.05	17/4397 (0.4%)
2	D	0.63	1/3232 (0.0%)	1.03	12/4397 (0.3%)
2	E	0.62	1/3232 (0.0%)	1.04	16/4397 (0.4%)
2	F	0.62	1/3232 (0.0%)	1.02	11/4397 (0.3%)
2	G	0.61	1/3232 (0.0%)	1.03	13/4397 (0.3%)
2	H	0.62	1/3232 (0.0%)	1.00	10/4397 (0.2%)
2	I	0.63	1/3232 (0.0%)	1.03	13/4397 (0.3%)
2	J	0.62	1/3232 (0.0%)	1.04	17/4397 (0.4%)
2	K	0.63	2/3232 (0.1%)	1.03	16/4397 (0.4%)
2	L	0.62	1/3232 (0.0%)	1.03	15/4397 (0.3%)
2	M	0.63	1/3232 (0.0%)	1.05	13/4397 (0.3%)
2	N	0.62	1/3232 (0.0%)	1.03	13/4397 (0.3%)
2	O	0.64	2/3232 (0.1%)	1.08	19/4397 (0.4%)
All	All	0.61	15/55252 (0.0%)	1.08	343/75116 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	247	TRP	NE1-CE2	-5.55	1.31	1.37
2	K	154	LYS	CA-CB	5.55	1.57	1.52
2	I	247	TRP	NE1-CE2	-5.51	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	247	TRP	NE1-CE2	-5.49	1.31	1.37
2	O	154	LYS	CA-CB	5.45	1.57	1.52
2	L	247	TRP	NE1-CE2	-5.44	1.31	1.37
2	N	247	TRP	NE1-CE2	-5.44	1.31	1.37
2	O	247	TRP	NE1-CE2	-5.44	1.31	1.37
2	H	247	TRP	NE1-CE2	-5.39	1.31	1.37
2	K	247	TRP	NE1-CE2	-5.36	1.31	1.37
2	E	247	TRP	NE1-CE2	-5.32	1.31	1.37
2	M	247	TRP	NE1-CE2	-5.21	1.31	1.37
2	J	247	TRP	NE1-CE2	-5.16	1.31	1.37
2	D	247	TRP	NE1-CE2	-5.14	1.31	1.37
2	G	247	TRP	NE1-CE2	-5.02	1.31	1.37

All (343) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	LEU	N-CA-C	-20.02	90.51	112.93
1	B	636	LYS	N-CA-C	-12.91	94.53	110.41
1	B	497	ILE	N-CA-C	-12.47	95.47	111.05
1	B	75	VAL	N-CA-C	-11.82	101.12	112.83
1	A	298	TYR	N-CA-C	11.39	131.01	114.16
1	A	657	VAL	CA-C-N	10.80	133.34	119.84
1	A	657	VAL	C-N-CA	10.80	133.34	119.84
2	N	127	ILE	N-CA-C	10.57	121.00	112.12
2	O	153	HIS	N-CA-C	10.40	125.09	107.93
1	A	273	TYR	CA-CB-CG	10.12	132.12	113.90
1	B	398	THR	N-CA-C	10.11	123.24	111.11
2	O	154	LYS	CA-C-N	9.81	132.11	119.84
2	O	154	LYS	C-N-CA	9.81	132.11	119.84
1	B	842	LEU	N-CA-C	9.72	124.36	108.52
1	A	200	VAL	N-CA-C	9.65	122.62	107.28
2	M	144	ARG	N-CA-C	-9.38	100.42	112.23
1	B	273	TYR	CA-CB-CG	9.24	130.53	113.90
1	A	817	TRP	N-CA-C	9.23	120.89	107.88
1	B	518	PHE	N-CA-C	9.14	118.66	108.14
1	B	825	VAL	N-CA-C	9.02	121.97	108.80
1	A	825	VAL	N-CA-C	9.01	121.88	108.46
1	B	811	LEU	N-CA-C	-8.94	96.21	109.62
1	B	518	PHE	CA-C-N	8.91	130.98	119.84
1	B	518	PHE	C-N-CA	8.91	130.98	119.84
1	A	437	TYR	CA-C-N	8.90	130.96	119.84
1	A	437	TYR	C-N-CA	8.90	130.96	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	422	GLU	N-CA-C	8.71	120.46	110.97
1	B	353	LEU	N-CA-C	8.67	122.85	111.75
1	B	77	LYS	N-CA-C	-8.62	99.28	113.50
1	A	155	LEU	CA-C-N	8.56	130.54	119.84
1	A	155	LEU	C-N-CA	8.56	130.54	119.84
1	A	279	ARG	N-CA-C	-8.53	101.99	111.28
2	O	154	LYS	N-CA-C	-8.47	94.86	112.40
2	C	154	LYS	CA-C-N	8.45	129.58	120.11
2	C	154	LYS	C-N-CA	8.45	129.58	120.11
2	M	127	ILE	N-CA-C	8.40	119.37	111.48
1	B	818	VAL	CA-C-N	8.38	129.70	119.98
1	B	818	VAL	C-N-CA	8.38	129.70	119.98
1	A	639	LYS	N-CA-C	-8.37	92.98	110.80
1	B	127	GLU	N-CA-C	-8.24	99.61	110.40
2	E	71	LEU	N-CA-C	-8.01	102.14	111.03
2	O	146	GLN	N-CA-C	7.96	122.77	110.42
1	B	726	ASN	N-CA-C	7.85	121.27	107.61
1	A	818	VAL	CA-C-N	7.84	129.65	119.84
1	A	818	VAL	C-N-CA	7.84	129.65	119.84
1	A	763	LEU	N-CA-C	7.60	120.55	108.23
2	K	127	ILE	N-CA-C	7.60	118.50	112.12
1	A	719	GLY	N-CA-C	-7.45	100.46	112.31
2	K	68	THR	N-CA-C	-7.43	103.78	112.92
2	E	26	ASN	N-CA-C	-7.42	104.07	113.72
2	O	26	ASN	N-CA-C	-7.41	102.49	113.61
1	B	486	ASP	N-CA-C	7.36	121.35	110.46
1	A	842	LEU	N-CA-C	7.35	121.11	109.50
2	N	87	TYR	N-CA-C	-7.29	104.52	113.41
2	J	27	VAL	N-CA-C	7.25	120.16	113.20
2	M	87	TYR	N-CA-C	-7.24	104.58	113.41
1	B	523	VAL	N-CA-C	7.23	118.02	110.72
1	B	367	LEU	N-CA-C	-7.21	103.43	113.37
2	J	87	TYR	N-CA-C	-7.20	104.63	113.41
2	G	87	TYR	N-CA-C	-7.19	104.64	113.41
2	D	87	TYR	N-CA-C	-7.13	104.72	113.41
1	B	587	LEU	N-CA-C	7.12	121.68	112.92
2	I	149	GLY	N-CA-C	7.11	121.03	111.72
2	O	87	TYR	N-CA-C	-7.08	104.78	113.41
2	D	66	LEU	N-CA-C	7.06	119.91	108.41
2	L	43	GLY	N-CA-C	-7.03	106.06	113.58
1	B	864	GLU	CA-C-N	7.03	128.62	119.84
1	B	864	GLU	C-N-CA	7.03	128.62	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	LEU	N-CA-C	7.02	122.40	113.55
1	A	594	ILE	CA-C-N	7.02	128.61	119.84
1	A	594	ILE	C-N-CA	7.02	128.61	119.84
2	L	87	TYR	N-CA-C	-7.01	104.86	113.41
2	I	87	TYR	N-CA-C	-7.01	104.86	113.41
2	E	87	TYR	N-CA-C	-6.99	104.88	113.41
2	K	270	ILE	N-CA-C	-6.94	105.84	111.81
2	D	46	PHE	N-CA-C	6.93	120.45	109.50
2	C	87	TYR	N-CA-C	-6.93	104.96	113.41
2	D	270	ILE	N-CA-C	-6.91	105.86	111.81
1	A	746	GLN	N-CA-C	-6.91	103.68	111.14
1	B	846	LEU	N-CA-C	6.90	120.00	108.13
2	N	270	ILE	N-CA-C	-6.89	105.89	111.81
2	I	270	ILE	N-CA-C	-6.87	105.90	111.81
2	F	87	TYR	N-CA-C	-6.87	105.03	113.41
2	H	87	TYR	N-CA-C	-6.86	105.04	113.41
2	M	270	ILE	N-CA-C	-6.85	105.92	111.81
2	J	270	ILE	N-CA-C	-6.85	105.92	111.81
2	K	87	TYR	N-CA-C	-6.84	105.06	113.41
2	G	270	ILE	N-CA-C	-6.83	105.93	111.81
2	F	270	ILE	N-CA-C	-6.83	105.94	111.81
1	A	435	ILE	N-CA-C	6.82	117.85	112.12
1	A	562	THR	N-CA-C	-6.82	104.85	113.72
2	E	270	ILE	N-CA-C	-6.81	105.95	111.81
2	O	270	ILE	N-CA-C	-6.81	105.95	111.81
1	B	798	ILE	N-CA-C	6.80	118.39	108.53
2	H	135	TYR	N-CA-C	6.76	118.73	111.36
2	H	270	ILE	N-CA-C	-6.75	106.00	111.81
2	E	113	SER	N-CA-C	6.74	119.00	110.24
2	E	135	TYR	N-CA-C	6.71	118.68	111.36
2	C	270	ILE	N-CA-C	-6.71	106.04	111.81
2	J	113	SER	N-CA-C	6.64	118.88	110.24
2	L	68	THR	N-CA-C	-6.64	103.57	112.94
2	I	154	LYS	CA-C-N	6.63	128.12	119.84
2	I	154	LYS	C-N-CA	6.63	128.12	119.84
2	J	135	TYR	N-CA-C	6.62	118.58	111.36
2	L	270	ILE	N-CA-C	-6.61	106.12	111.81
1	A	792	VAL	N-CA-C	6.59	117.79	108.17
1	B	200	VAL	N-CA-C	6.57	123.01	109.34
2	D	135	TYR	N-CA-C	6.56	118.51	111.36
1	B	79	LYS	N-CA-C	-6.56	105.03	113.16
1	A	296	ALA	N-CA-C	6.55	119.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	135	TYR	N-CA-C	6.55	118.50	111.36
2	C	113	SER	N-CA-C	6.54	119.25	110.35
1	B	151	LYS	N-CA-C	-6.52	99.89	110.20
2	I	135	TYR	N-CA-C	6.52	118.47	111.36
1	B	199	VAL	N-CA-C	6.51	118.30	108.80
2	M	110	ALA	CA-C-N	6.50	126.41	119.85
2	M	110	ALA	C-N-CA	6.50	126.41	119.85
2	E	127	ILE	N-CA-C	6.48	119.86	113.71
2	N	26	ASN	N-CA-C	-6.47	105.39	113.28
1	A	710	MET	N-CA-C	6.46	118.37	108.42
1	B	82	HIS	N-CA-C	-6.46	97.05	110.80
2	D	63	PHE	N-CA-C	6.46	120.02	109.24
2	L	135	TYR	N-CA-C	6.46	118.40	111.36
1	B	348	LYS	N-CA-C	-6.45	104.67	112.54
1	A	274	ILE	CA-C-N	6.45	127.90	119.84
1	A	274	ILE	C-N-CA	6.45	127.90	119.84
2	G	68	THR	N-CA-C	-6.42	105.30	113.01
2	C	135	TYR	N-CA-C	6.42	118.35	111.36
1	A	798	ILE	N-CA-C	6.41	118.26	108.71
1	B	272	ASN	N-CA-C	6.38	119.22	111.82
1	A	435	ILE	CB-CA-C	-6.36	104.67	110.91
1	B	213	GLN	N-CA-C	6.35	121.19	113.38
2	K	135	TYR	N-CA-C	6.34	118.27	111.36
2	O	113	SER	N-CA-C	6.34	118.48	110.24
1	B	503	ILE	N-CA-C	6.33	122.52	109.34
1	A	456	PHE	N-CA-C	-6.32	101.89	111.56
2	C	18	ILE	N-CA-C	6.30	115.94	106.42
2	F	135	TYR	N-CA-C	6.28	118.21	111.36
2	D	154	LYS	CA-C-N	6.28	127.69	119.84
2	D	154	LYS	C-N-CA	6.28	127.69	119.84
2	G	135	TYR	N-CA-C	6.28	118.20	111.36
1	B	394	LEU	N-CA-C	6.27	119.79	108.69
2	C	18	ILE	CB-CA-C	-6.27	104.89	111.23
1	B	274	ILE	N-CA-C	6.26	114.72	107.89
2	J	46	PHE	N-CA-C	6.26	119.22	109.52
1	B	744	TYR	N-CA-C	-6.25	104.23	113.61
1	A	796	LYS	CA-C-N	6.22	126.57	119.92
1	A	796	LYS	C-N-CA	6.22	126.57	119.92
1	A	453	GLN	N-CA-C	-6.20	97.59	110.80
2	N	135	TYR	N-CA-C	6.20	118.12	111.36
2	L	46	PHE	N-CA-C	6.19	119.11	109.52
1	A	285	ILE	N-CA-C	6.17	117.01	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	ALA	N-CA-C	6.15	118.78	111.71
1	A	451	ASP	CA-C-N	6.14	127.52	119.84
1	A	451	ASP	C-N-CA	6.14	127.52	119.84
1	B	462	GLN	N-CA-C	6.13	117.94	109.54
2	O	135	TYR	N-CA-C	6.13	118.04	111.36
1	B	150	LEU	N-CA-C	6.12	118.61	109.25
1	B	637	LYS	N-CA-C	-6.12	97.76	110.80
2	I	46	PHE	N-CA-C	6.12	118.71	109.23
2	L	73	LEU	N-CA-C	6.10	119.46	110.30
2	O	110	ALA	CA-C-N	6.05	126.02	119.78
2	O	110	ALA	C-N-CA	6.05	126.02	119.78
1	A	483	VAL	N-CA-C	6.04	116.57	108.11
2	G	109	ILE	N-CA-C	6.03	116.21	110.42
2	K	154	LYS	CA-C-N	6.03	127.38	119.84
2	K	154	LYS	C-N-CA	6.03	127.38	119.84
1	B	469	ALA	N-CA-C	6.03	118.64	111.71
1	A	813	ALA	N-CA-C	-6.03	104.78	111.71
1	A	793	ASP	N-CA-C	-6.01	97.99	110.80
2	J	59	TRP	N-CA-C	6.01	119.28	109.24
1	A	151	LYS	N-CA-C	-6.01	99.35	108.67
1	A	363	GLU	N-CA-C	6.01	120.15	112.34
1	A	776	ALA	N-CA-C	-6.01	106.04	113.19
2	N	10	THR	N-CA-C	-5.94	104.43	111.03
2	G	127	ILE	N-CA-C	5.93	121.69	109.34
2	J	110	ALA	CA-C-N	5.93	126.26	119.92
2	J	110	ALA	C-N-CA	5.93	126.26	119.92
1	B	760	VAL	N-CA-C	5.90	118.11	108.97
1	B	445	MET	N-CA-C	-5.88	106.34	112.93
1	B	232	VAL	N-CA-C	5.88	116.07	106.72
2	N	113	SER	N-CA-C	5.87	117.87	110.24
1	A	397	VAL	N-CA-C	-5.87	101.37	108.53
2	C	46	PHE	N-CA-C	5.85	118.59	109.52
1	A	100	PRO	CA-C-N	5.85	132.71	121.54
1	A	100	PRO	C-N-CA	5.85	132.71	121.54
2	D	113	SER	N-CA-C	5.84	118.29	110.35
1	B	800	TYR	N-CA-C	5.83	118.89	107.57
1	B	409	TRP	N-CA-C	-5.83	104.62	110.97
2	C	127	ILE	N-CA-C	5.83	121.46	109.34
1	B	652	PHE	N-CA-C	5.80	118.99	109.72
1	A	436	ILE	N-CA-C	5.79	118.75	112.96
2	E	66	LEU	N-CA-C	5.79	118.64	108.75
2	I	113	SER	N-CA-C	5.78	117.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	10	THR	N-CA-C	-5.77	104.62	111.03
2	E	68	THR	N-CA-C	-5.75	103.73	112.99
2	M	68	THR	N-CA-C	-5.75	104.94	112.41
1	A	433	ASN	N-CA-C	5.75	119.47	112.23
1	B	651	ILE	N-CA-C	5.75	121.29	109.34
2	I	10	THR	N-CA-C	-5.75	104.65	111.03
2	O	10	THR	N-CA-C	-5.74	104.65	111.03
2	K	19	VAL	N-CA-C	5.73	116.62	108.42
1	B	871	PHE	N-CA-C	-5.72	104.90	112.34
1	A	587	LEU	N-CA-C	5.72	119.39	111.55
1	B	565	MET	N-CA-C	5.71	116.75	107.32
2	H	10	THR	N-CA-C	-5.71	104.69	111.03
1	A	414	VAL	CA-C-N	5.69	126.96	119.84
1	A	414	VAL	C-N-CA	5.69	126.96	119.84
2	E	152	PHE	N-CA-C	5.69	117.92	108.13
1	A	760	VAL	N-CA-C	5.68	118.01	108.81
1	A	394	LEU	N-CA-C	5.67	117.48	107.61
1	A	578	LEU	N-CA-C	-5.66	105.64	112.54
1	B	541	GLY	N-CA-C	-5.66	105.92	112.83
2	L	10	THR	N-CA-C	-5.66	104.75	111.03
2	G	69	THR	N-CA-C	5.65	117.89	111.11
1	A	541	GLY	N-CA-C	-5.65	105.95	112.73
2	M	10	THR	N-CA-C	-5.65	104.76	111.03
1	A	652	PHE	N-CA-C	5.63	118.71	109.76
2	C	10	THR	N-CA-C	-5.62	104.79	111.03
2	L	113	SER	N-CA-C	5.62	117.99	110.35
1	B	823	THR	N-CA-C	5.62	117.38	108.79
1	A	802	ILE	N-CA-C	5.60	116.06	107.77
1	A	465	ASN	N-CA-C	-5.60	98.87	110.80
2	J	10	THR	N-CA-C	-5.60	104.82	111.03
2	J	18	ILE	CB-CA-C	-5.60	105.10	111.59
1	A	184	LYS	N-CA-C	-5.58	104.61	111.75
1	B	814	ASN	N-CA-C	-5.57	106.52	113.38
1	A	858	VAL	N-CA-C	5.57	115.90	108.27
2	G	154	LYS	CA-C-N	5.57	126.80	119.84
2	G	154	LYS	C-N-CA	5.57	126.80	119.84
2	J	70	LEU	N-CA-C	5.57	122.66	110.80
2	O	155	PRO	CA-C-N	-5.57	114.24	123.37
2	O	155	PRO	C-N-CA	-5.57	114.24	123.37
2	K	61	PHE	N-CA-C	5.56	118.52	109.06
1	B	480	PHE	N-CA-C	-5.56	105.80	112.58
1	B	273	TYR	CB-CA-C	-5.54	99.39	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	GLU	N-CA-C	5.54	122.60	110.80
1	B	364	THR	N-CA-C	-5.54	105.73	112.88
2	C	68	THR	N-CA-C	-5.54	105.73	113.37
2	N	63	PHE	N-CA-C	5.53	118.58	109.72
1	A	812	VAL	N-CA-C	5.53	117.44	111.58
2	D	10	THR	N-CA-C	-5.53	104.90	111.03
1	B	243	SER	N-CA-C	5.52	116.65	108.86
2	J	127	ILE	N-CA-C	5.52	120.82	109.34
1	A	794	THR	N-CA-C	-5.52	105.76	113.37
2	F	10	THR	N-CA-C	-5.51	104.92	111.03
2	J	152	PHE	N-CA-C	5.47	117.71	109.23
2	J	71	LEU	N-CA-C	-5.45	105.75	112.72
1	B	285	ILE	N-CA-C	5.44	116.42	108.58
1	A	115	GLN	N-CA-C	-5.44	101.41	110.17
1	A	292	LEU	N-CA-C	5.44	116.54	109.64
1	A	726	ASN	N-CA-C	5.44	121.32	114.31
1	B	444	ARG	N-CA-C	-5.43	106.63	113.20
1	A	761	GLY	N-CA-C	5.42	118.52	110.60
2	G	113	SER	N-CA-C	5.42	117.72	110.35
1	A	299	ILE	CB-CA-C	-5.42	102.40	111.29
2	K	10	THR	N-CA-C	-5.41	105.03	111.03
2	C	152	PHE	N-CA-C	5.39	118.25	109.24
2	F	113	SER	N-CA-C	5.39	118.10	110.50
1	A	305	GLN	N-CA-C	5.38	117.03	110.41
1	A	800	TYR	N-CA-C	5.37	117.34	108.49
1	B	300	ARG	CA-C-N	5.36	124.98	119.56
1	B	300	ARG	C-N-CA	5.36	124.98	119.56
2	F	154	LYS	CA-C-N	5.36	126.54	119.84
2	F	154	LYS	C-N-CA	5.36	126.54	119.84
2	G	10	THR	N-CA-C	-5.36	105.08	111.03
2	C	110	ALA	CA-C-N	5.35	125.33	120.03
2	C	110	ALA	C-N-CA	5.35	125.33	120.03
2	H	144	ARG	N-CA-C	-5.35	106.80	113.38
2	J	394	MET	N-CA-C	-5.34	106.26	112.89
1	A	833	PHE	N-CA-C	5.34	118.87	107.70
2	O	127	ILE	N-CA-C	5.34	120.45	109.34
1	A	348	LYS	N-CA-C	-5.34	105.57	111.71
1	B	279	ARG	N-CA-C	-5.33	105.47	111.28
2	E	394	MET	N-CA-C	-5.33	106.28	112.89
1	B	94	THR	N-CA-C	-5.33	106.01	112.88
2	M	154	LYS	CA-C-N	5.32	126.49	119.84
2	M	154	LYS	C-N-CA	5.32	126.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	763	LEU	CA-C-N	5.31	126.48	119.84
1	A	763	LEU	C-N-CA	5.31	126.48	119.84
2	F	106	ARG	N-CA-C	-5.29	100.55	109.07
2	D	394	MET	N-CA-C	-5.29	106.34	112.89
2	L	154	LYS	CA-C-N	5.29	126.45	119.84
2	L	154	LYS	C-N-CA	5.29	126.45	119.84
2	H	394	MET	N-CA-C	-5.28	106.34	112.89
1	B	810	TYR	N-CA-C	5.26	119.41	112.25
2	K	18	ILE	N-CA-C	5.25	115.07	106.72
2	G	394	MET	N-CA-C	-5.25	106.39	112.89
2	N	394	MET	N-CA-C	-5.24	106.39	112.89
2	M	394	MET	N-CA-C	-5.24	106.39	112.89
2	K	394	MET	N-CA-C	-5.23	106.41	112.89
2	L	394	MET	N-CA-C	-5.23	106.41	112.89
2	O	46	PHE	N-CA-C	5.22	117.62	109.52
2	N	187	GLU	N-CA-C	5.22	118.08	109.72
2	C	187	GLU	N-CA-C	5.20	118.04	109.72
2	F	187	GLU	N-CA-C	5.20	118.03	109.72
2	I	187	GLU	N-CA-C	5.20	118.03	109.72
1	B	137	ASN	N-CA-C	-5.19	105.60	112.24
2	E	63	PHE	N-CA-C	5.19	118.05	109.85
2	E	187	GLU	N-CA-C	5.19	118.02	109.72
1	A	146	TRP	N-CA-C	5.18	116.96	108.52
2	F	394	MET	N-CA-C	-5.18	106.47	112.89
2	K	187	GLU	N-CA-C	5.18	118.00	109.72
1	B	126	PHE	N-CA-C	5.17	117.33	108.90
1	B	771	VAL	N-CA-C	-5.17	104.94	110.36
2	O	394	MET	N-CA-C	-5.16	106.49	112.89
2	L	59	TRP	N-CA-C	5.16	117.48	108.76
2	H	251	PRO	O-C-N	5.16	129.40	123.06
2	I	59	TRP	N-CA-C	5.16	117.22	109.23
2	L	187	GLU	N-CA-C	5.16	117.97	109.72
1	A	250	TYR	N-CA-C	-5.15	105.10	111.33
2	H	187	GLU	N-CA-C	5.14	117.95	109.72
2	I	394	MET	N-CA-C	-5.14	106.52	112.89
1	B	83	GLN	N-CA-C	-5.13	105.38	110.97
2	H	113	SER	N-CA-C	5.13	117.32	110.35
2	O	187	GLU	N-CA-C	5.12	117.91	109.72
2	L	384	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	122	LEU	N-CA-C	-5.11	102.30	109.96
2	K	251	PRO	O-C-N	5.10	129.34	123.06
2	M	187	GLU	N-CA-C	5.09	117.87	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	746	GLN	N-CA-C	-5.09	102.97	111.37
1	B	211	ILE	CB-CA-C	-5.09	105.46	111.97
2	G	187	GLU	N-CA-C	5.08	117.86	109.72
2	E	59	TRP	N-CA-C	5.08	117.70	109.06
2	C	394	MET	N-CA-C	-5.08	106.59	112.89
1	B	250	TYR	N-CA-C	-5.08	105.01	111.11
2	D	187	GLU	N-CA-C	5.08	117.84	109.72
2	H	384	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	829	VAL	N-CA-C	5.06	113.91	108.95
1	A	374	ALA	N-CA-C	5.06	116.48	111.07
2	I	127	ILE	N-CA-C	5.05	119.85	109.34
2	E	251	PRO	O-C-N	5.04	129.26	123.06
1	A	499	ASN	N-CA-C	5.04	116.77	111.28
2	F	384	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	A	740	ARG	N-CA-C	-5.03	105.99	112.68
2	J	187	GLU	N-CA-C	5.03	117.77	109.72
2	N	154	LYS	CA-C-N	5.03	126.12	119.84
2	N	154	LYS	C-N-CA	5.03	126.12	119.84
2	N	251	PRO	O-C-N	5.03	129.24	123.06
2	K	129	PHE	N-CA-C	5.02	116.05	108.07
1	A	523	VAL	N-CA-C	5.01	119.76	109.34
2	K	113	SER	N-CA-C	5.00	117.56	110.50
1	B	717	MET	N-CA-C	5.00	117.62	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

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	6374	0	6394	1069	0
1	B	6624	0	6652	1209	0
2	C	3162	0	3101	185	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3162	0	3101	195	0
2	E	3162	0	3101	181	0
2	F	3162	0	3101	174	0
2	G	3162	0	3101	160	0
2	H	3162	0	3101	189	0
2	I	3162	0	3101	230	0
2	J	3162	0	3101	203	0
2	K	3162	0	3101	182	0
2	L	3162	0	3101	192	0
2	M	3162	0	3101	190	0
2	N	3162	0	3101	205	0
2	O	3162	0	3101	183	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
3	O	1	0	0	0	0
All	All	54109	0	53359	4504	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 42.

All (4504) 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:B:771:VAL:HB	1:B:809:PHE:HB3	1.23	1.18
1:A:333:VAL:HG11	1:A:380:LYS:HA	1.27	1.15
1:B:442:MET:HE1	1:B:463:ILE:HG12	1.29	1.15
1:A:428:GLN:OE1	1:A:456:PHE:HB2	1.46	1.13
1:B:717:MET:HE1	1:B:830:PRO:HD2	1.25	1.13
2:G:145:ARG:HB3	2:G:145:ARG:HH11	1.10	1.12
2:H:83:ASN:ND2	2:I:122:LEU:HB2	1.65	1.11
1:A:451:ASP:HB3	1:A:452:PRO:HD2	1.14	1.11
1:B:432:VAL:HA	1:B:436:ILE:HD11	1.18	1.11
1:B:734:ASN:HB3	1:B:737:GLU:HB2	1.28	1.10
1:B:718:TYR:HB3	1:B:721:VAL:HG21	1.33	1.10
1:A:270:ILE:HD11	1:A:292:LEU:HD11	1.31	1.09
1:B:548:ARG:NH1	1:B:878:ASN:H	1.50	1.09
2:L:22:THR:HG23	2:L:73:LEU:HD12	1.35	1.08
1:A:699:ILE:HG12	1:A:700:ALA:H	1.18	1.07
2:G:145:ARG:HD2	2:I:143:ASN:HA	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TRP:HA	1:A:321:ILE:HD12	1.34	1.07
1:B:200:VAL:HG21	1:B:243:SER:HB3	1.13	1.07
1:B:790:ARG:HE	1:B:790:ARG:HA	0.98	1.06
2:N:106:ARG:H	2:N:106:ARG:HD3	1.17	1.06
1:B:318:TRP:HA	1:B:321:ILE:HD12	1.37	1.06
1:A:658:PRO:HG2	1:B:348:LYS:HG2	1.38	1.05
1:B:498:ARG:HB2	2:I:32:GLN:HE22	1.15	1.05
1:A:721:VAL:HG12	1:A:722:ASN:H	1.18	1.04
1:B:510:LEU:HD11	1:B:537:SER:HA	1.36	1.04
1:A:199:VAL:HG12	1:A:200:VAL:H	1.20	1.04
1:B:457:GLN:HG3	1:B:458:ILE:H	1.22	1.03
1:B:646:LEU:HA	1:B:649:LEU:HD12	1.40	1.03
1:A:428:GLN:NE2	1:A:455:PRO:HB2	1.73	1.03
1:A:451:ASP:CB	1:A:452:PRO:HD2	1.84	1.03
1:B:274:ILE:HG23	1:B:278:ILE:HD11	1.40	1.03
1:A:510:LEU:HD22	1:A:540:LEU:HD13	1.39	1.02
1:B:444:ARG:HH21	1:B:520:THR:HG23	1.20	1.02
1:A:310:LEU:H	1:A:310:LEU:HD12	1.21	1.02
1:B:743:ASP:C	1:B:744:TYR:HD2	1.67	1.02
1:B:457:GLN:HB2	1:B:476:ASN:ND2	1.75	1.02
1:A:513:LEU:HA	1:A:516:GLN:NE2	1.75	1.01
1:B:224:PHE:O	1:B:228:MET:HG2	1.61	1.01
1:B:573:THR:HG22	1:B:574:GLU:H	0.88	1.01
1:A:521:MET:HB3	1:A:522:PRO:HD3	1.39	1.01
1:B:790:ARG:HE	1:B:790:ARG:CA	1.70	1.00
1:A:506:LEU:HD23	1:A:544:VAL:HA	1.40	1.00
2:C:106:ARG:H	2:C:106:ARG:HD3	1.26	1.00
1:B:573:THR:HG22	1:B:574:GLU:N	1.71	0.99
1:A:705:ILE:HA	1:A:823:THR:HG22	1.43	0.99
1:B:674:VAL:HG21	1:B:679:LEU:HD13	1.44	0.99
1:B:473:HIS:HB2	2:I:126:ARG:HH22	1.21	0.99
1:B:510:LEU:HD22	1:B:540:LEU:HD13	1.42	0.99
1:B:573:THR:CG2	1:B:574:GLU:H	1.71	0.99
2:L:42:ASN:HA	2:L:61:PHE:HB2	1.43	0.98
1:B:371:ASN:HD22	1:B:583:SER:HB3	1.28	0.98
1:B:204:THR:HG23	1:B:244:ILE:HG22	1.44	0.98
2:H:106:ARG:HD3	2:H:106:ARG:H	1.26	0.98
1:A:275:PRO:HB2	1:A:278:ILE:HD11	1.45	0.98
1:B:265:LEU:HB3	1:B:296:ALA:HB1	1.46	0.98
1:B:435:ILE:HG22	1:B:436:ILE:H	1.29	0.98
2:J:106:ARG:HD3	2:J:106:ARG:H	1.23	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:ALA:HB2	1:B:827:LYS:HB2	1.45	0.97
1:B:700:ALA:CB	1:B:827:LYS:HB2	1.95	0.97
1:A:540:LEU:O	1:A:544:VAL:HG23	1.64	0.97
1:A:270:ILE:HG23	1:A:854:LEU:HD21	1.46	0.96
1:A:192:ASN:O	1:A:193:SER:HB3	1.65	0.96
1:B:200:VAL:HG21	1:B:243:SER:CB	1.96	0.96
2:H:83:ASN:HD21	2:I:122:LEU:HB2	1.30	0.96
1:A:660:ASP:HB3	1:B:539:ARG:HD2	1.43	0.96
1:A:588:ILE:HG22	1:A:589:GLY:H	1.28	0.96
1:B:458:ILE:HD12	1:B:459:ALA:N	1.81	0.95
1:A:563:MET:HE2	1:A:563:MET:HA	1.48	0.95
1:B:435:ILE:O	1:B:438:PRO:HD2	1.67	0.95
2:I:145:ARG:NH1	2:I:145:ARG:HB3	1.82	0.95
1:A:563:MET:HA	1:A:563:MET:CE	1.98	0.94
1:A:510:LEU:HD11	1:A:537:SER:HA	1.46	0.94
1:A:779:ASP:HA	1:A:798:ILE:CD1	1.98	0.93
1:B:446:HIS:O	1:B:447:TYR:HB2	1.68	0.93
2:O:27:VAL:O	2:O:31:ILE:HG12	1.66	0.93
1:A:643:GLU:HG2	1:A:662:MET:HE1	1.46	0.93
1:B:764:PRO:O	1:B:765:PHE:HB3	1.65	0.93
1:A:371:ASN:C	1:A:373:GLN:H	1.71	0.93
1:B:518:PHE:HB3	1:B:519:PRO:HD2	1.49	0.93
1:A:225:ILE:HA	1:A:228:MET:HE2	1.50	0.93
1:B:790:ARG:HA	1:B:790:ARG:NE	1.84	0.92
1:A:428:GLN:HE21	1:A:455:PRO:HB2	1.30	0.92
2:G:145:ARG:HB3	2:G:145:ARG:NH1	1.84	0.92
1:B:126:PHE:H	1:B:126:PHE:HD2	1.09	0.92
1:B:190:ASN:HD21	1:B:193:SER:HB3	1.31	0.92
1:B:722:ASN:HD22	1:B:824:LYS:HA	1.35	0.92
1:B:513:LEU:HA	1:B:516:GLN:CD	1.95	0.92
2:G:6:SER:OG	2:G:128:ASN:HA	1.70	0.92
1:A:779:ASP:HA	1:A:798:ILE:HD12	1.50	0.91
1:B:428:GLN:HB2	1:B:456:PHE:CD1	2.05	0.91
1:B:513:LEU:HA	1:B:516:GLN:NE2	1.85	0.91
1:B:366:PHE:C	1:B:368:THR:H	1.76	0.91
1:B:803:ASN:H	1:B:807:ASN:HD21	1.17	0.91
1:A:661:GLN:HE21	1:B:348:LYS:NZ	1.67	0.91
1:B:166:PHE:HE2	1:B:689:MET:HA	1.34	0.91
1:B:454:THR:HG21	1:B:476:ASN:ND2	1.86	0.91
1:B:459:ALA:HB1	1:B:463:ILE:HD11	1.51	0.90
1:A:588:ILE:HG22	1:A:589:GLY:N	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:135:TYR:CZ	2:I:342:MET:HE3	2.07	0.90
2:L:88:PHE:O	2:L:92:VAL:HG23	1.72	0.90
1:A:126:PHE:N	1:A:126:PHE:HD2	1.68	0.90
1:A:339:LEU:HD22	1:A:588:ILE:HA	1.53	0.90
2:L:106:ARG:H	2:L:106:ARG:HD3	1.37	0.90
2:N:145:ARG:O	2:N:146:GLN:HG3	1.71	0.90
2:C:88:PHE:O	2:C:92:VAL:HG23	1.72	0.89
1:B:509:ALA:O	1:B:513:LEU:HG	1.71	0.89
1:A:169:LEU:O	1:A:173:VAL:HG23	1.73	0.89
1:A:244:ILE:HD13	1:A:835:PHE:HE1	1.38	0.89
1:A:521:MET:HA	1:A:521:MET:HE3	1.54	0.89
1:A:660:ASP:HB3	1:B:539:ARG:HH11	1.38	0.89
2:K:106:ARG:H	2:K:106:ARG:HD3	1.37	0.89
1:A:366:PHE:C	1:A:368:THR:H	1.76	0.88
1:A:855:LEU:O	1:A:857:PHE:N	2.06	0.88
1:B:457:GLN:O	1:B:459:ALA:N	2.05	0.88
1:A:216:GLU:H	1:A:216:GLU:CD	1.81	0.88
1:B:457:GLN:HB2	1:B:476:ASN:CG	1.98	0.88
1:A:486:ASP:HB2	1:A:490:ASN:HD22	1.38	0.88
1:B:99:GLU:HB3	1:B:100:PRO:HD3	1.54	0.88
1:B:658:PRO:HB2	1:B:661:GLN:HG2	1.56	0.88
1:B:874:MET:O	1:B:875:ARG:HB2	1.73	0.88
2:M:88:PHE:O	2:M:92:VAL:HG23	1.74	0.88
1:A:194:ARG:HH11	1:A:229:ARG:HG2	1.39	0.88
2:J:106:ARG:HD3	2:J:106:ARG:N	1.87	0.88
1:B:803:ASN:H	1:B:807:ASN:ND2	1.72	0.87
1:B:182:LEU:HD11	1:B:847:THR:H	1.38	0.87
1:B:297:ARG:HG3	1:B:848:PHE:HD2	1.40	0.87
1:A:428:GLN:HB2	1:A:456:PHE:CD1	2.09	0.86
1:A:509:ALA:O	1:A:513:LEU:HG	1.75	0.86
1:B:447:TYR:O	1:B:448:ARG:HG2	1.73	0.86
2:D:88:PHE:O	2:D:92:VAL:HG23	1.73	0.86
2:O:88:PHE:O	2:O:92:VAL:HG23	1.72	0.86
2:I:76:ASN:H	2:M:76:ASN:HB2	1.37	0.86
1:B:451:ASP:H	1:B:452:PRO:HD3	1.39	0.86
1:B:413:VAL:HG12	1:B:414:VAL:N	1.88	0.86
2:N:88:PHE:O	2:N:92:VAL:HG23	1.74	0.86
1:B:473:HIS:HB2	2:I:126:ARG:NH2	1.91	0.86
1:B:745:ALA:HB1	1:B:748:THR:HB	1.57	0.86
2:H:88:PHE:O	2:H:92:VAL:HG23	1.73	0.86
2:I:24:TYR:O	2:I:27:VAL:HG22	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LEU:O	1:B:544:VAL:HG23	1.75	0.86
1:B:182:LEU:HD23	1:B:183:LEU:H	1.40	0.86
1:A:150:LEU:HD12	1:A:696:SER:HB2	1.58	0.86
1:A:275:PRO:HB2	1:A:278:ILE:CD1	2.04	0.86
2:E:88:PHE:O	2:E:92:VAL:HG23	1.75	0.86
2:J:88:PHE:O	2:J:92:VAL:HG23	1.75	0.85
1:A:451:ASP:HB3	1:A:452:PRO:CD	2.03	0.85
2:I:88:PHE:O	2:I:92:VAL:HG23	1.76	0.85
1:B:590:ASN:N	1:B:590:ASN:HD22	1.74	0.85
2:C:150:PHE:HB2	2:C:152:PHE:CE1	2.11	0.85
2:F:88:PHE:O	2:F:92:VAL:HG23	1.75	0.85
2:M:106:ARG:HD3	2:M:106:ARG:H	1.40	0.85
1:B:126:PHE:HD2	1:B:126:PHE:N	1.73	0.85
2:G:88:PHE:O	2:G:92:VAL:HG23	1.75	0.85
2:H:6:SER:OG	2:H:128:ASN:HA	1.77	0.85
2:M:6:SER:OG	2:M:128:ASN:HA	1.76	0.85
1:A:239:VAL:HG22	1:A:846:LEU:HG	1.58	0.84
1:B:723:ILE:HG22	1:B:724:ALA:H	1.40	0.84
1:A:445:MET:C	1:A:447:TYR:H	1.84	0.84
1:B:306:ASP:O	1:B:308:LEU:N	2.10	0.84
1:B:518:PHE:HD2	2:H:69:THR:HB	1.40	0.84
2:K:88:PHE:O	2:K:92:VAL:HG23	1.76	0.84
1:A:660:ASP:HB3	1:B:539:ARG:CD	2.05	0.84
1:B:415:PRO:HG2	1:B:480:PHE:HD1	1.42	0.84
1:B:701:GLN:HB2	1:B:826:TYR:HD2	1.40	0.84
1:B:825:VAL:HG12	1:B:826:TYR:N	1.91	0.84
2:L:144:ARG:O	2:L:145:ARG:HB2	1.74	0.84
1:A:125:ILE:N	1:A:125:ILE:HD12	1.92	0.84
1:B:523:VAL:C	1:B:525:TYR:H	1.85	0.84
1:B:743:ASP:CG	1:B:745:ALA:H	1.85	0.84
1:A:570:THR:HG22	1:A:571:LEU:H	1.42	0.84
1:B:200:VAL:CG2	1:B:243:SER:HB3	2.05	0.84
1:B:498:ARG:NH1	2:J:25:SER:HB3	1.92	0.84
1:B:735:LEU:HG	1:B:760:VAL:O	1.78	0.84
1:B:471:TRP:HB2	1:B:512:GLN:OE1	1.77	0.84
1:A:126:PHE:N	1:A:126:PHE:CD2	2.42	0.84
1:B:503:ILE:HD11	1:B:548:ARG:HG2	1.58	0.84
2:F:82:ARG:NH1	2:H:144:ARG:HD2	1.93	0.84
2:I:76:ASN:HB2	2:M:76:ASN:HB2	1.57	0.84
1:A:771:VAL:HG13	1:A:772:ILE:H	1.43	0.84
1:B:717:MET:HE1	1:B:830:PRO:CD	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLN:HB2	1:A:528:SER:OG	1.78	0.83
1:B:124:ARG:C	1:B:125:ILE:HD12	2.02	0.83
1:B:428:GLN:HG2	1:B:429:LEU:N	1.92	0.83
1:B:435:ILE:HG22	1:B:436:ILE:N	1.93	0.83
2:L:23:LEU:HD21	2:N:36:GLN:OE1	1.76	0.83
1:B:743:ASP:C	1:B:744:TYR:CD2	2.54	0.83
1:A:158:GLY:H	1:A:762:ALA:HB3	1.43	0.83
1:B:454:THR:HG21	1:B:476:ASN:HD21	1.39	0.83
2:I:23:LEU:HD23	2:I:24:TYR:N	1.94	0.83
1:A:474:PHE:O	1:A:478:ASN:HB2	1.77	0.83
1:B:126:PHE:N	1:B:126:PHE:CD2	2.43	0.83
1:B:799:LEU:HD22	1:B:800:TYR:N	1.93	0.83
1:A:471:TRP:HB2	1:A:512:GLN:OE1	1.79	0.83
1:A:524:ASP:O	1:A:526:LYS:N	2.10	0.83
1:A:647:LYS:HG3	1:A:654:VAL:HG21	1.59	0.83
1:B:272:ASN:C	1:B:274:ILE:H	1.87	0.82
2:H:135:TYR:CZ	2:H:342:MET:HE3	2.14	0.82
2:O:6:SER:OG	2:O:128:ASN:HA	1.80	0.82
2:I:38:ILE:HG22	2:I:42:ASN:HD21	1.42	0.82
1:B:516:GLN:HA	1:B:518:PHE:HE1	1.41	0.82
1:B:590:ASN:HD22	1:B:590:ASN:H	1.25	0.82
1:A:461:GLN:HA	2:F:32:GLN:HE22	1.43	0.82
1:B:549:LEU:HD13	1:B:877:MET:HE2	1.61	0.82
1:B:428:GLN:HA	1:B:431:ILE:HD12	1.61	0.82
2:F:150:PHE:HB2	2:F:152:PHE:CE1	2.15	0.82
1:A:486:ASP:HB2	1:A:490:ASN:ND2	1.94	0.81
1:A:734:ASN:HB3	1:A:737:GLU:HG2	1.61	0.81
1:B:722:ASN:HB2	1:B:824:LYS:HB3	1.62	0.81
2:H:109:ILE:HG13	2:H:109:ILE:O	1.79	0.81
1:B:454:THR:CG2	1:B:476:ASN:HD21	1.92	0.81
1:A:406:SER:O	1:A:409:TRP:HB3	1.81	0.81
1:B:494:ASN:ND2	1:B:495:ASP:H	1.79	0.81
1:B:769:SER:HB3	1:B:807:ASN:OD1	1.80	0.81
2:L:22:THR:HB	2:N:128:ASN:O	1.79	0.81
1:A:712:LEU:HB3	1:A:721:VAL:O	1.79	0.81
1:B:218:GLU:HG3	1:B:221:VAL:HG23	1.62	0.81
1:B:193:SER:HB2	1:B:226:ALA:HA	1.62	0.81
1:B:725:ARG:H	1:B:725:ARG:HD2	1.44	0.81
1:B:498:ARG:HB2	2:I:32:GLN:NE2	1.94	0.81
1:B:511:MET:CE	2:J:70:LEU:HG	2.09	0.81
1:B:537:SER:O	1:B:540:LEU:HB3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:76:ASN:HB2	2:J:76:ASN:HB2	1.60	0.81
1:A:459:ALA:O	1:A:462:GLN:HB2	1.81	0.81
1:B:118:LYS:HG2	1:B:119:GLN:H	1.46	0.81
2:I:76:ASN:CB	2:M:76:ASN:HB2	2.11	0.81
1:A:712:LEU:HG	1:A:819:PRO:HB2	1.61	0.81
1:B:315:GLU:HB3	1:B:571:LEU:HD11	1.61	0.80
2:D:128:ASN:O	2:E:22:THR:HB	1.82	0.80
2:E:24:TYR:O	2:E:27:VAL:HG22	1.82	0.80
2:O:67:GLY:O	2:O:69:THR:N	2.14	0.80
1:A:660:ASP:O	1:A:662:MET:N	2.14	0.80
1:B:510:LEU:CD1	1:B:537:SER:HA	2.11	0.80
1:A:362:SER:HB2	1:A:365:GLN:NE2	1.97	0.80
1:A:699:ILE:HG12	1:A:700:ALA:N	1.97	0.80
2:L:150:PHE:HB2	2:L:152:PHE:CE1	2.17	0.80
1:A:546:LEU:HD21	1:A:588:ILE:CD1	2.12	0.80
1:A:126:PHE:HD2	1:A:126:PHE:H	1.26	0.80
1:A:270:ILE:CD1	1:A:292:LEU:HD11	2.10	0.80
1:B:239:VAL:HG23	1:B:844:SER:O	1.81	0.80
1:A:769:SER:HB3	1:A:807:ASN:OD1	1.82	0.80
1:B:293:PRO:C	1:B:295:THR:H	1.90	0.80
2:N:144:ARG:O	2:N:145:ARG:HB2	1.81	0.80
1:B:563:MET:HA	1:B:563:MET:HE3	1.64	0.80
1:B:869:VAL:CG1	1:B:873:ASN:HA	2.11	0.80
1:A:371:ASN:C	1:A:373:GLN:N	2.37	0.79
1:A:437:TYR:N	1:A:438:PRO:HD2	1.97	0.79
1:B:393:SER:O	1:B:394:LEU:HD23	1.82	0.79
1:B:506:LEU:HD23	1:B:544:VAL:HA	1.62	0.79
1:A:199:VAL:HG12	1:A:200:VAL:N	1.97	0.79
1:A:303:LEU:HA	1:A:615:ASN:ND2	1.97	0.79
1:A:694:ARG:HG2	1:A:701:GLN:HE22	1.46	0.79
1:B:790:ARG:HG3	1:B:791:LYS:H	1.48	0.79
2:L:104:SER:O	2:L:108:GLY:HA3	1.82	0.79
1:A:869:VAL:HG11	1:A:873:ASN:HA	1.64	0.79
2:I:57:ARG:HH11	2:I:94:ASN:HD21	1.31	0.79
1:B:744:TYR:CD2	1:B:744:TYR:N	2.38	0.79
1:A:721:VAL:HG12	1:A:722:ASN:N	1.98	0.79
2:K:6:SER:OG	2:K:128:ASN:HA	1.82	0.79
1:A:711:GLN:C	1:A:712:LEU:HD23	2.08	0.79
1:B:457:GLN:HG3	1:B:458:ILE:N	1.98	0.79
1:B:465:ASN:HD22	1:B:468:VAL:HG23	1.47	0.79
1:A:480:PHE:CD2	1:A:493:LEU:HB3	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:VAL:HG23	1:A:607:ASN:H	1.46	0.79
1:B:673:PRO:O	1:B:674:VAL:HG13	1.83	0.79
2:H:2:ASP:HB2	2:H:128:ASN:HD21	1.46	0.79
2:N:50:GLY:O	2:N:51:ILE:HG23	1.83	0.79
1:A:869:VAL:CG1	1:A:873:ASN:HA	2.12	0.79
1:B:277:ARG:O	1:B:278:ILE:HG12	1.83	0.79
1:B:548:ARG:HH11	1:B:878:ASN:H	1.28	0.78
2:J:128:ASN:O	2:K:22:THR:HB	1.83	0.78
2:H:105:GLN:C	2:H:107:ASN:H	1.91	0.78
2:M:145:ARG:O	2:M:146:GLN:HG3	1.83	0.78
1:A:305:GLN:O	1:A:307:ARG:HG3	1.82	0.78
1:A:428:GLN:HG2	1:A:429:LEU:N	1.98	0.78
1:A:118:LYS:HG2	1:A:119:GLN:N	1.98	0.78
1:B:457:GLN:C	1:B:459:ALA:H	1.91	0.78
1:A:480:PHE:HD2	1:A:493:LEU:HB3	1.49	0.78
1:B:606:VAL:HG23	1:B:607:ASN:H	1.46	0.78
1:A:639:LYS:O	1:A:643:GLU:HG3	1.84	0.78
1:B:111:ILE:C	1:B:113:PRO:HD3	2.09	0.78
2:I:42:ASN:HA	2:I:61:PHE:HB2	1.66	0.78
1:B:702:GLY:HA3	1:B:759:LEU:O	1.84	0.77
2:N:144:ARG:NH2	2:N:146:GLN:HE22	1.81	0.77
1:B:374:ALA:HB1	1:B:580:SER:HB3	1.66	0.77
1:B:562:THR:HB	1:B:611:HIS:CD2	2.20	0.77
1:B:779:ASP:HA	1:B:798:ILE:CD1	2.14	0.77
1:B:406:SER:O	1:B:409:TRP:HB3	1.84	0.77
1:B:491:GLN:CD	1:B:564:ASN:HB3	2.08	0.77
2:E:93:ASP:O	2:E:97:MET:HG3	1.84	0.77
2:H:106:ARG:H	2:H:106:ARG:CD	1.98	0.77
2:I:128:ASN:HD22	2:J:19:VAL:HB	1.49	0.77
2:K:93:ASP:O	2:K:97:MET:HG3	1.85	0.77
2:M:22:THR:HG23	2:M:73:LEU:HD12	1.66	0.77
1:A:817:TRP:CG	1:A:818:VAL:H	2.02	0.77
1:B:764:PRO:O	1:B:765:PHE:CB	2.33	0.77
1:A:471:TRP:O	1:A:475:VAL:HG23	1.85	0.77
1:B:169:LEU:O	1:B:173:VAL:HG23	1.84	0.77
1:B:855:LEU:O	1:B:857:PHE:N	2.17	0.77
1:B:204:THR:CG2	1:B:244:ILE:HG22	2.14	0.77
1:B:435:ILE:C	1:B:436:ILE:HG12	2.08	0.77
2:M:139:TRP:NE1	2:M:143:ASN:HD21	1.81	0.77
2:H:93:ASP:O	2:H:97:MET:HG3	1.85	0.77
1:B:166:PHE:CE2	1:B:689:MET:HA	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:HG3	1:B:221:VAL:CG2	2.15	0.76
1:B:503:ILE:O	1:B:505:GLN:HG2	1.85	0.76
1:B:573:THR:O	1:B:574:GLU:HG2	1.84	0.76
1:B:744:TYR:HD2	1:B:744:TYR:N	1.77	0.76
2:F:17:LYS:HG2	2:H:130:ASP:HA	1.67	0.76
1:A:405:ILE:HG21	1:A:536:LEU:HG	1.67	0.76
1:A:614:TYR:O	1:A:618:ILE:HG12	1.85	0.76
1:B:200:VAL:HG23	1:B:242:PRO:O	1.86	0.76
1:B:731:GLN:HG2	2:D:62:ASP:HB2	1.67	0.76
1:A:548:ARG:HH12	1:A:878:ASN:H	1.34	0.76
1:A:563:MET:HE3	1:A:611:HIS:CD2	2.20	0.76
1:A:122:LEU:HG	1:A:201:ASP:OD2	1.84	0.76
1:A:461:GLN:HA	2:F:32:GLN:NE2	2.00	0.76
1:A:588:ILE:CG2	1:A:589:GLY:H	1.99	0.76
1:B:133:ILE:HD12	1:B:145:ARG:HB2	1.66	0.76
1:B:678:ARG:O	1:B:681:ILE:HG22	1.85	0.76
2:C:24:TYR:O	2:C:27:VAL:HG22	1.86	0.76
2:D:67:GLY:O	2:D:68:THR:HG23	1.85	0.76
2:I:110:ALA:HB1	2:I:111:PRO:CD	2.16	0.76
1:A:158:GLY:H	1:A:762:ALA:CB	1.99	0.76
1:A:678:ARG:O	1:A:681:ILE:HG22	1.86	0.76
1:B:199:VAL:HG12	1:B:200:VAL:N	2.00	0.76
1:B:701:GLN:HA	1:B:761:GLY:O	1.85	0.76
2:G:93:ASP:O	2:G:97:MET:HG3	1.85	0.76
1:A:503:ILE:HD13	1:A:547:THR:HB	1.68	0.76
1:B:675:GLU:HB3	1:B:678:ARG:HG2	1.68	0.76
1:A:244:ILE:HD13	1:A:835:PHE:CE1	2.21	0.76
1:A:428:GLN:HA	1:A:431:ILE:HD12	1.68	0.76
1:B:96:PRO:O	1:B:652:PHE:HB3	1.84	0.76
2:I:93:ASP:O	2:I:97:MET:HG3	1.86	0.76
2:M:135:TYR:CZ	2:M:342:MET:HE3	2.21	0.76
1:A:310:LEU:H	1:A:310:LEU:CD1	1.97	0.75
1:B:518:PHE:CB	1:B:519:PRO:HD2	2.14	0.75
1:A:501:HIS:C	1:A:503:ILE:HG13	2.11	0.75
2:C:145:ARG:HB3	2:C:145:ARG:NH1	2.02	0.75
2:F:104:SER:HB3	2:F:108:GLY:CA	2.16	0.75
1:B:781:THR:O	1:B:783:PHE:N	2.19	0.75
1:A:371:ASN:HA	1:A:374:ALA:HB3	1.68	0.75
1:A:457:GLN:HB2	1:A:476:ASN:HD21	1.52	0.75
2:E:135:TYR:CZ	2:E:342:MET:HE3	2.21	0.75
2:L:19:VAL:HG23	2:N:128:ASN:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:12:LYS:C	2:J:14:ALA:H	1.94	0.75
2:J:93:ASP:O	2:J:97:MET:HG3	1.87	0.75
1:B:251:ALA:HA	2:N:69:THR:HG21	1.69	0.75
1:B:498:ARG:CB	2:I:32:GLN:HE22	1.97	0.75
1:A:694:ARG:HG2	1:A:701:GLN:NE2	2.01	0.74
1:B:511:MET:HE3	2:J:70:LEU:HG	1.67	0.74
2:C:38:ILE:HG22	2:C:42:ASN:HD21	1.51	0.74
1:B:698:LYS:O	1:B:699:ILE:HB	1.86	0.74
2:I:76:ASN:HB2	2:M:76:ASN:CB	2.17	0.74
1:A:148:TRP:CZ3	1:A:246:HIS:HB2	2.22	0.74
1:A:537:SER:O	1:A:540:LEU:HB3	1.87	0.74
1:B:491:GLN:HG3	1:B:565:MET:H	1.50	0.74
2:J:128:ASN:HB3	2:K:19:VAL:HG23	1.69	0.74
2:N:57:ARG:HH11	2:N:94:ASN:HD21	1.33	0.74
1:A:492:VAL:HG13	1:A:558:MET:SD	2.27	0.74
1:A:647:LYS:CG	1:A:654:VAL:HG21	2.17	0.74
1:B:482:GLN:HB2	1:B:493:LEU:HD22	1.70	0.74
1:B:675:GLU:HB3	1:B:678:ARG:CG	2.17	0.74
1:B:688:ASN:O	1:B:692:ILE:HD12	1.87	0.74
1:B:614:TYR:O	1:B:618:ILE:HG12	1.87	0.74
2:O:150:PHE:HB2	2:O:152:PHE:CE1	2.23	0.74
1:A:306:ASP:C	1:A:308:LEU:H	1.95	0.74
2:D:23:LEU:HD23	2:D:24:TYR:N	2.03	0.74
2:D:93:ASP:O	2:D:97:MET:HG3	1.87	0.74
2:I:75:ALA:HB3	2:M:76:ASN:HA	1.68	0.74
2:L:93:ASP:O	2:L:97:MET:HG3	1.88	0.74
1:A:286:LEU:HD23	1:A:286:LEU:H	1.52	0.74
1:A:784:ALA:O	1:A:787:VAL:HG23	1.88	0.74
1:A:802:ILE:HA	1:A:807:ASN:HD21	1.52	0.74
1:B:190:ASN:ND2	1:B:193:SER:HB3	2.03	0.74
1:B:783:PHE:HD1	1:B:783:PHE:H	1.33	0.74
2:C:82:ARG:CZ	2:E:144:ARG:HD2	2.18	0.74
2:D:24:TYR:O	2:D:27:VAL:HG22	1.88	0.74
2:H:12:LYS:C	2:H:14:ALA:H	1.95	0.74
1:A:405:ILE:CG2	1:A:536:LEU:HG	2.18	0.74
1:A:428:GLN:HB2	1:A:456:PHE:HD1	1.51	0.74
1:B:366:PHE:C	1:B:368:THR:N	2.46	0.74
2:E:54:LEU:HD12	2:E:55:PRO:HD2	1.70	0.74
1:A:164:GLU:O	1:A:167:LEU:HB3	1.87	0.74
1:A:252:PHE:HD2	1:A:684:LEU:HD21	1.52	0.74
1:A:301:PRO:O	1:A:303:LEU:HD23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:LEU:HD11	1:B:537:SER:CA	2.15	0.74
2:D:6:SER:OG	2:D:128:ASN:HA	1.87	0.74
1:B:368:THR:HG22	1:B:371:ASN:HD21	1.51	0.73
1:B:433:ASN:ND2	1:B:446:HIS:HB3	2.02	0.73
2:J:150:PHE:HB2	2:J:152:PHE:CE1	2.22	0.73
1:A:117:LYS:O	1:A:179:ASP:HB2	1.88	0.73
1:A:275:PRO:CB	1:A:278:ILE:HD11	2.18	0.73
1:B:254:GLU:HG2	2:N:69:THR:HB	1.68	0.73
2:G:106:ARG:HD3	2:G:106:ARG:H	1.53	0.73
2:G:12:LYS:C	2:G:14:ALA:H	1.96	0.73
2:I:12:LYS:C	2:I:14:ALA:H	1.95	0.73
2:M:144:ARG:HD2	2:N:82:ARG:NH1	2.02	0.73
1:A:277:ARG:HD3	1:A:559:ALA:HB2	1.71	0.73
1:A:660:ASP:CB	1:B:539:ARG:HD2	2.19	0.73
1:B:257:LEU:O	1:B:260:GLN:HG3	1.88	0.73
2:C:93:ASP:O	2:C:97:MET:HG3	1.87	0.73
2:F:42:ASN:HA	2:F:61:PHE:HB2	1.70	0.73
2:H:109:ILE:HB	2:H:380:ASP:HB3	1.68	0.73
1:A:310:LEU:HD12	1:A:310:LEU:N	2.00	0.73
1:B:540:LEU:HD23	1:B:541:GLY:N	2.03	0.73
2:E:12:LYS:C	2:E:14:ALA:H	1.96	0.73
2:M:12:LYS:C	2:M:14:ALA:H	1.96	0.73
2:N:93:ASP:O	2:N:97:MET:HG3	1.87	0.73
1:A:499:ASN:HA	1:A:505:GLN:NE2	2.04	0.73
1:B:265:LEU:HB3	1:B:296:ALA:CB	2.17	0.73
2:I:145:ARG:HB3	2:I:145:ARG:HH11	1.50	0.73
2:N:24:TYR:O	2:N:27:VAL:HG22	1.89	0.73
1:A:245:LEU:HB3	1:A:249:ASP:HB2	1.71	0.73
1:A:286:LEU:HD23	1:A:286:LEU:N	2.04	0.73
1:B:703:VAL:HG13	1:B:824:LYS:O	1.89	0.73
2:F:93:ASP:O	2:F:97:MET:HG3	1.87	0.73
2:M:93:ASP:O	2:M:97:MET:HG3	1.88	0.73
1:A:631:LEU:HB3	1:A:633:LEU:HD13	1.69	0.73
1:A:661:GLN:HE21	1:B:348:LYS:HZ1	1.37	0.73
1:B:503:ILE:O	1:B:505:GLN:N	2.22	0.73
1:B:674:VAL:HG23	1:B:679:LEU:HD22	1.69	0.73
1:B:770:SER:HB2	1:B:773:SER:OG	1.88	0.73
1:B:771:VAL:HB	1:B:809:PHE:CB	2.11	0.73
2:F:145:ARG:O	2:F:146:GLN:HG2	1.89	0.73
2:J:11:LEU:O	2:J:14:ALA:HB3	1.89	0.73
1:B:277:ARG:O	1:B:279:ARG:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ILE:C	1:B:594:ILE:HD12	2.13	0.73
1:B:701:GLN:O	1:B:826:TYR:HB3	1.89	0.73
2:D:12:LYS:C	2:D:14:ALA:H	1.95	0.73
2:D:63:PHE:CD2	2:D:84:THR:HG23	2.24	0.73
2:F:23:LEU:HD21	2:H:36:GLN:OE1	1.89	0.73
2:H:27:VAL:O	2:H:31:ILE:HG12	1.88	0.73
1:B:436:ILE:HG13	1:B:437:TYR:H	1.54	0.72
1:B:471:TRP:O	1:B:475:VAL:HG23	1.88	0.72
2:H:106:ARG:HD3	2:H:106:ARG:N	2.03	0.72
1:B:498:ARG:HH12	2:J:25:SER:HB3	1.52	0.72
1:B:521:MET:HB2	1:B:522:PRO:CD	2.19	0.72
1:B:712:LEU:CD1	1:B:722:ASN:HB3	2.18	0.72
1:A:510:LEU:CD1	1:A:537:SER:HA	2.20	0.72
2:N:12:LYS:C	2:N:14:ALA:H	1.94	0.72
1:B:492:VAL:HG11	1:B:558:MET:HG2	1.71	0.72
1:B:516:GLN:HA	1:B:518:PHE:CE1	2.25	0.72
1:B:630:ARG:O	1:B:631:LEU:HG	1.90	0.72
1:B:799:LEU:HD22	1:B:800:TYR:H	1.52	0.72
2:J:106:ARG:HG2	2:J:107:ASN:H	1.54	0.72
1:A:420:ILE:HG12	1:A:423:SER:HB2	1.69	0.72
1:A:496:ASN:HD22	1:A:498:ARG:HB2	1.53	0.72
1:A:629:ASN:O	1:A:631:LEU:N	2.17	0.72
1:B:499:ASN:O	1:B:500:GLY:C	2.33	0.72
1:B:615:ASN:O	1:B:618:ILE:HB	1.90	0.72
2:J:144:ARG:HD2	2:K:82:ARG:NH1	2.05	0.72
2:M:122:LEU:HB2	2:O:83:ASN:ND2	2.04	0.72
2:F:22:THR:HB	2:H:128:ASN:O	1.89	0.72
1:B:156:PRO:HB2	1:B:161:ASP:HB3	1.72	0.72
1:B:444:ARG:NH2	1:B:520:THR:HG23	2.03	0.72
2:K:12:LYS:C	2:K:14:ALA:H	1.96	0.72
1:A:239:VAL:CG2	1:A:846:LEU:HG	2.19	0.72
1:A:613:ASN:HD22	1:A:649:LEU:CD2	2.03	0.72
1:B:752:LEU:C	1:B:754:ASN:H	1.95	0.72
1:A:605:ASN:O	1:A:608:VAL:HB	1.90	0.72
1:A:146:TRP:O	1:A:833:PHE:HB3	1.89	0.72
1:A:721:VAL:CG1	1:A:722:ASN:H	2.01	0.72
1:B:551:ALA:O	1:B:555:GLU:HB2	1.90	0.72
1:B:825:VAL:HG12	1:B:826:TYR:H	1.53	0.72
2:C:12:LYS:C	2:C:14:ALA:H	1.96	0.72
2:D:145:ARG:O	2:D:146:GLN:HG3	1.90	0.72
2:I:135:TYR:OH	2:I:340:GLU:OE1	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:MET:O	1:A:447:TYR:N	2.23	0.71
1:B:355:LEU:HG	1:B:356:GLU:N	2.05	0.71
1:B:473:HIS:HB3	2:I:126:ARG:HH12	1.54	0.71
2:D:11:LEU:O	2:D:14:ALA:HB3	1.90	0.71
1:A:735:LEU:HG	1:A:760:VAL:O	1.89	0.71
1:A:764:PRO:O	1:A:797:PRO:HD2	1.91	0.71
1:B:422:GLU:HA	1:B:425:VAL:HG23	1.72	0.71
1:B:480:PHE:CE2	1:B:493:LEU:HB2	2.24	0.71
2:F:12:LYS:C	2:F:14:ALA:H	1.96	0.71
2:J:130:ASP:HA	2:K:17:LYS:HG2	1.71	0.71
2:O:93:ASP:O	2:O:97:MET:HG3	1.90	0.71
1:B:156:PRO:CB	1:B:161:ASP:HB3	2.20	0.71
2:C:144:ARG:HD2	2:D:82:ARG:CZ	2.20	0.71
2:L:6:SER:OG	2:L:128:ASN:HA	1.91	0.71
2:O:12:LYS:C	2:O:14:ALA:H	1.96	0.71
1:A:246:HIS:HB3	1:A:249:ASP:OD2	1.90	0.71
1:A:709:ASP:HB3	1:A:820:THR:HG23	1.73	0.71
1:B:194:ARG:O	1:B:196:ALA:N	2.23	0.71
1:B:428:GLN:OE1	1:B:456:PHE:HB2	1.90	0.71
2:I:11:LEU:O	2:I:14:ALA:HB3	1.91	0.71
2:I:150:PHE:HB2	2:I:152:PHE:CE1	2.25	0.71
1:A:236:ARG:HB2	1:A:238:VAL:HG23	1.72	0.71
1:B:166:PHE:CE2	1:B:689:MET:HG3	2.24	0.71
1:B:791:LYS:O	1:B:792:VAL:HG22	1.91	0.71
2:K:11:LEU:O	2:K:14:ALA:HB3	1.91	0.71
1:A:530:GLN:HA	1:A:533:ILE:HD12	1.71	0.71
1:B:605:ASN:O	1:B:608:VAL:HB	1.91	0.71
2:K:38:ILE:HG22	2:K:42:ASN:HD21	1.56	0.71
1:A:194:ARG:NH1	1:A:229:ARG:HG2	2.05	0.71
1:B:523:VAL:C	1:B:525:TYR:N	2.47	0.71
2:N:11:LEU:O	2:N:14:ALA:HB3	1.91	0.71
2:N:38:ILE:HG22	2:N:42:ASN:HD21	1.56	0.71
1:B:277:ARG:HG2	1:B:278:ILE:H	1.54	0.71
1:B:717:MET:CE	1:B:830:PRO:HD2	2.15	0.71
2:H:116:LEU:HD12	2:H:119:LEU:HB2	1.73	0.71
2:O:11:LEU:O	2:O:14:ALA:HB3	1.90	0.71
1:A:283:ASN:O	1:A:863:VAL:HG23	1.91	0.71
2:G:36:GLN:OE1	2:H:23:LEU:HD21	1.91	0.71
1:A:496:ASN:ND2	1:A:498:ARG:HB2	2.06	0.71
1:A:510:LEU:HD11	1:A:537:SER:CA	2.21	0.71
1:B:548:ARG:HH12	1:B:878:ASN:H	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:LEU:HD12	1:B:722:ASN:HB3	1.72	0.71
2:G:4:LEU:HA	2:G:7:LEU:HD12	1.73	0.71
2:K:53:ASN:HD22	2:K:354:ALA:HB3	1.56	0.71
2:M:11:LEU:O	2:M:14:ALA:HB3	1.91	0.71
1:A:312:ASP:O	1:A:313:ASN:HB3	1.90	0.70
1:A:415:PRO:HG2	1:A:480:PHE:CD1	2.26	0.70
1:B:374:ALA:HB1	1:B:580:SER:HA	1.71	0.70
2:L:82:ARG:CZ	2:N:144:ARG:HD2	2.21	0.70
1:A:729:GLY:C	1:A:730:PHE:HD1	1.98	0.70
1:B:164:GLU:O	1:B:167:LEU:HB3	1.90	0.70
2:D:4:LEU:HA	2:D:7:LEU:HD12	1.73	0.70
2:M:150:PHE:HB2	2:M:152:PHE:CE1	2.26	0.70
1:A:615:ASN:O	1:A:618:ILE:HB	1.89	0.70
1:B:477:ASN:ND2	2:I:39:ILE:HG21	2.06	0.70
1:B:518:PHE:CD2	2:H:69:THR:HB	2.24	0.70
2:J:106:ARG:H	2:J:106:ARG:CD	2.03	0.70
2:J:109:ILE:HD12	2:J:109:ILE:O	1.91	0.70
1:B:259:HIS:CD2	1:B:677:ARG:HG3	2.25	0.70
2:C:11:LEU:O	2:C:14:ALA:HB3	1.90	0.70
2:K:54:LEU:HD12	2:K:55:PRO:HD2	1.71	0.70
2:N:4:LEU:HA	2:N:7:LEU:HD12	1.73	0.70
1:A:506:LEU:CD2	1:A:544:VAL:HA	2.18	0.70
1:A:551:ALA:O	1:A:555:GLU:HB2	1.92	0.70
1:B:230:GLN:HA	1:B:242:PRO:HD3	1.73	0.70
1:A:131:LEU:HD12	1:A:132:PRO:HD2	1.74	0.70
1:A:467:GLN:HB2	1:A:515:ARG:HD2	1.72	0.70
1:A:762:ALA:O	1:A:763:LEU:HG	1.92	0.70
1:B:508:GLU:HG2	1:B:512:GLN:NE2	2.07	0.70
1:B:790:ARG:HG3	1:B:791:LYS:N	2.05	0.70
2:J:116:LEU:HD12	2:J:119:LEU:HB2	1.74	0.70
2:L:12:LYS:C	2:L:14:ALA:H	1.96	0.70
2:N:167:ASN:HD22	2:N:178:GLY:HA2	1.57	0.70
1:A:508:GLU:C	1:A:512:GLN:HE21	2.00	0.70
1:A:783:PHE:HD1	1:A:783:PHE:H	1.38	0.70
2:C:167:ASN:HD22	2:C:178:GLY:HA2	1.57	0.70
2:D:153:HIS:NE2	2:E:153:HIS:NE2	2.39	0.70
2:G:167:ASN:HD22	2:G:178:GLY:HA2	1.57	0.70
1:A:482:GLN:OE1	1:A:493:LEU:HD22	1.90	0.70
1:A:503:ILE:C	1:A:505:GLN:H	1.98	0.70
1:A:560:CYS:HB2	1:A:603:TYR:HD2	1.57	0.70
1:A:793:ASP:C	1:A:795:LEU:H	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:CG1	1:B:297:ARG:HB3	2.21	0.70
1:B:786:ILE:HG13	1:B:787:VAL:H	1.56	0.70
2:K:167:ASN:HD22	2:K:178:GLY:HA2	1.57	0.70
2:O:154:LYS:N	2:O:155:PRO:CD	2.54	0.70
1:B:393:SER:N	1:B:573:THR:HG23	2.06	0.70
1:B:708:ARG:O	1:B:709:ASP:C	2.35	0.70
1:B:857:PHE:H	1:B:857:PHE:HD1	1.40	0.70
2:C:4:LEU:HA	2:C:7:LEU:HD12	1.74	0.70
2:J:38:ILE:HG22	2:J:42:ASN:HD21	1.56	0.70
2:J:167:ASN:HD22	2:J:178:GLY:HA2	1.57	0.70
2:O:167:ASN:HD22	2:O:178:GLY:HA2	1.57	0.70
1:A:396:PHE:HB3	1:A:578:LEU:CD1	2.22	0.70
1:A:401:TYR:HA	1:A:404:LEU:HD13	1.73	0.70
1:A:436:ILE:HD11	1:A:437:TYR:CD1	2.27	0.70
1:B:721:VAL:CG1	1:B:799:LEU:HD21	2.22	0.70
2:C:6:SER:OG	2:C:128:ASN:HA	1.92	0.70
2:E:38:ILE:HG22	2:E:42:ASN:HD21	1.57	0.70
1:A:781:THR:O	1:A:783:PHE:N	2.24	0.69
1:B:318:TRP:CA	1:B:321:ILE:HD12	2.19	0.69
1:B:670:ARG:O	1:B:671:LEU:HD23	1.92	0.69
1:B:791:LYS:O	1:B:792:VAL:HG13	1.91	0.69
1:B:805:ASP:C	1:B:807:ASN:H	1.99	0.69
2:D:239:ASN:HD22	2:D:246:THR:HG22	1.57	0.69
2:O:4:LEU:HA	2:O:7:LEU:HD12	1.74	0.69
1:A:589:GLY:C	1:A:591:ALA:H	1.99	0.69
1:B:590:ASN:H	1:B:590:ASN:ND2	1.90	0.69
2:C:22:THR:OG1	2:C:26:ASN:ND2	2.25	0.69
2:F:104:SER:HB3	2:F:108:GLY:HA2	1.74	0.69
2:O:106:ARG:H	2:O:106:ARG:HD3	1.56	0.69
1:A:437:TYR:H	1:A:438:PRO:HD2	1.56	0.69
1:A:548:ARG:HH11	1:A:877:MET:HA	1.56	0.69
1:B:182:LEU:HD11	1:B:847:THR:N	2.07	0.69
2:C:239:ASN:HD22	2:C:246:THR:HG22	1.58	0.69
2:D:150:PHE:HB2	2:D:152:PHE:CE1	2.27	0.69
2:K:150:PHE:HB2	2:K:152:PHE:CE1	2.27	0.69
2:L:11:LEU:O	2:L:14:ALA:HB3	1.93	0.69
2:L:239:ASN:HD22	2:L:246:THR:HG22	1.58	0.69
2:N:106:ARG:HD3	2:N:106:ARG:N	2.01	0.69
1:A:275:PRO:HB2	1:A:278:ILE:CG1	2.22	0.69
2:F:110:ALA:HB1	2:F:111:PRO:CD	2.22	0.69
2:I:109:ILE:HD12	2:I:109:ILE:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:167:ASN:HD22	2:I:178:GLY:HA2	1.57	0.69
2:J:22:THR:O	2:J:72:ASN:HA	1.92	0.69
2:E:11:LEU:O	2:E:14:ALA:HB3	1.91	0.69
2:G:11:LEU:O	2:G:14:ALA:HB3	1.92	0.69
2:M:167:ASN:HD22	2:M:178:GLY:HA2	1.57	0.69
1:A:634:TYR:HB2	1:B:875:ARG:HH22	1.57	0.69
1:B:374:ALA:HB1	1:B:580:SER:CB	2.23	0.69
2:E:5:TYR:CE2	2:E:131:ASN:HA	2.27	0.69
2:F:167:ASN:HD22	2:F:178:GLY:HA2	1.57	0.69
2:N:116:LEU:HD12	2:N:119:LEU:HB2	1.74	0.69
1:A:540:LEU:HD23	1:A:541:GLY:N	2.08	0.69
1:A:588:ILE:CG2	1:A:589:GLY:N	2.56	0.69
1:A:666:ARG:CG	1:A:667:ASP:N	2.55	0.69
1:A:803:ASN:HD22	1:A:805:ASP:HB3	1.58	0.69
1:B:772:ILE:HG23	1:B:773:SER:N	2.06	0.69
1:A:322:THR:HG22	1:A:390:ARG:HB2	1.75	0.69
1:A:451:ASP:CB	1:A:452:PRO:CD	2.68	0.69
1:A:664:ARG:HD3	1:B:538:ASN:OD1	1.92	0.69
1:A:689:MET:HA	1:A:692:ILE:HD13	1.73	0.69
1:B:368:THR:HA	1:B:579:THR:HG23	1.75	0.69
1:B:442:MET:HE1	1:B:463:ILE:CG1	2.17	0.69
1:B:783:PHE:N	1:B:783:PHE:CD1	2.60	0.69
2:D:106:ARG:H	2:D:106:ARG:HD3	1.58	0.69
2:E:109:ILE:HB	2:E:380:ASP:HB3	1.74	0.69
2:E:150:PHE:HB2	2:E:152:PHE:CE1	2.27	0.69
1:A:118:LYS:HG2	1:A:119:GLN:H	1.57	0.69
1:A:546:LEU:HD21	1:A:588:ILE:HD13	1.73	0.69
1:A:757:VAL:HG12	1:A:758:ALA:H	1.57	0.69
1:B:118:LYS:HG2	1:B:119:GLN:N	2.08	0.69
1:B:812:VAL:HG13	1:B:813:ALA:H	1.57	0.69
2:E:116:LEU:HD12	2:E:119:LEU:HB2	1.73	0.69
2:F:11:LEU:O	2:F:14:ALA:HB3	1.93	0.69
1:B:457:GLN:CG	1:B:458:ILE:H	1.89	0.69
1:B:633:LEU:O	1:B:633:LEU:HD23	1.92	0.69
2:H:239:ASN:HD22	2:H:246:THR:HG22	1.58	0.69
2:I:6:SER:OG	2:I:128:ASN:HA	1.92	0.69
2:K:106:ARG:HG2	2:K:107:ASN:H	1.56	0.69
2:K:144:ARG:O	2:K:145:ARG:HB2	1.92	0.69
2:L:167:ASN:HD22	2:L:178:GLY:HA2	1.57	0.69
2:M:116:LEU:HD12	2:M:119:LEU:HB2	1.75	0.69
2:O:109:ILE:HD12	2:O:109:ILE:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASP:O	1:A:308:LEU:N	2.25	0.68
1:A:570:THR:HG22	1:A:571:LEU:N	2.07	0.68
1:A:658:PRO:HG3	1:B:345:GLN:HA	1.75	0.68
1:B:166:PHE:O	1:B:169:LEU:HB2	1.93	0.68
1:B:805:ASP:O	1:B:807:ASN:N	2.26	0.68
1:A:366:PHE:N	1:A:366:PHE:CD1	2.60	0.68
1:A:661:GLN:NE2	1:B:348:LYS:NZ	2.39	0.68
1:A:807:ASN:O	1:A:809:PHE:N	2.26	0.68
1:B:264:PRO:O	1:B:265:LEU:HB2	1.92	0.68
2:F:6:SER:OG	2:F:128:ASN:HA	1.92	0.68
2:H:106:ARG:O	2:H:107:ASN:HB2	1.93	0.68
2:J:4:LEU:HA	2:J:7:LEU:HD12	1.75	0.68
2:L:116:LEU:HD12	2:L:119:LEU:HB2	1.75	0.68
2:E:167:ASN:HD22	2:E:178:GLY:HA2	1.57	0.68
2:F:4:LEU:HA	2:F:7:LEU:HD12	1.75	0.68
2:L:110:ALA:HB1	2:L:111:PRO:CD	2.23	0.68
1:B:548:ARG:NH1	1:B:878:ASN:N	2.35	0.68
2:C:116:LEU:HD12	2:C:119:LEU:HB2	1.75	0.68
2:D:116:LEU:HD12	2:D:119:LEU:HB2	1.75	0.68
2:F:116:LEU:HD12	2:F:119:LEU:HB2	1.75	0.68
2:F:153:HIS:NE2	2:H:153:HIS:NE2	2.41	0.68
2:H:11:LEU:O	2:H:14:ALA:HB3	1.93	0.68
2:N:239:ASN:HD22	2:N:246:THR:HG22	1.58	0.68
1:A:318:TRP:CA	1:A:321:ILE:HD12	2.19	0.68
2:I:116:LEU:HD12	2:I:119:LEU:HB2	1.75	0.68
1:B:180:TYR:HD1	1:B:181:LEU:N	1.91	0.68
1:B:288:MET:HE2	1:B:288:MET:HA	1.75	0.68
2:I:239:ASN:HD22	2:I:246:THR:HG22	1.59	0.68
2:M:153:HIS:NE2	2:N:153:HIS:NE2	2.40	0.68
1:A:396:PHE:HB3	1:A:578:LEU:HD12	1.76	0.68
1:A:660:ASP:CB	1:B:539:ARG:HH11	2.04	0.68
1:B:431:ILE:HA	1:B:435:ILE:HD12	1.76	0.68
1:B:545:ASP:HB3	1:B:877:MET:SD	2.34	0.68
1:B:855:LEU:O	1:B:858:VAL:HG23	1.94	0.68
2:M:4:LEU:HA	2:M:7:LEU:HD12	1.75	0.68
1:A:659:ASP:O	1:A:662:MET:HB2	1.94	0.68
2:H:4:LEU:HA	2:H:7:LEU:HD12	1.76	0.68
2:I:4:LEU:HA	2:I:7:LEU:HD12	1.74	0.68
2:N:65:LEU:O	2:N:66:LEU:HD23	1.94	0.68
1:B:498:ARG:HB3	1:B:505:GLN:HE22	1.59	0.68
1:B:869:VAL:HG11	1:B:873:ASN:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:167:ASN:HD22	2:H:178:GLY:HA2	1.57	0.68
2:J:239:ASN:HD22	2:J:246:THR:HG22	1.58	0.68
1:A:136:ALA:O	1:A:137:ASN:HB3	1.94	0.68
1:A:587:LEU:HD13	1:A:587:LEU:O	1.94	0.68
1:B:143:ARG:HG3	1:B:216:GLU:OE2	1.92	0.68
1:B:246:HIS:CD2	1:B:248:ILE:H	2.11	0.68
1:B:492:VAL:HG11	1:B:558:MET:CG	2.22	0.68
1:B:530:GLN:HA	1:B:533:ILE:HD12	1.76	0.68
2:D:167:ASN:HD22	2:D:178:GLY:HA2	1.57	0.68
2:M:239:ASN:HD22	2:M:246:THR:HG22	1.59	0.68
1:A:589:GLY:O	1:A:591:ALA:N	2.26	0.67
1:A:629:ASN:C	1:A:631:LEU:H	2.02	0.67
1:A:710:MET:HE2	1:A:824:LYS:HE2	1.75	0.67
2:H:76:ASN:HB2	2:J:76:ASN:CB	2.23	0.67
2:I:9:LYS:O	2:I:13:ASP:HB2	1.94	0.67
1:A:188:VAL:O	1:A:198:LYS:HA	1.93	0.67
1:A:436:ILE:HD12	1:A:436:ILE:C	2.18	0.67
1:A:738:LEU:C	1:A:740:ARG:H	2.02	0.67
1:B:125:ILE:HD12	1:B:125:ILE:N	2.10	0.67
1:B:258:GLN:HB3	2:N:71:LEU:HB2	1.76	0.67
1:B:721:VAL:HG12	1:B:722:ASN:N	2.08	0.67
2:G:239:ASN:HD22	2:G:246:THR:HG22	1.58	0.67
2:K:117:ARG:HH21	2:M:57:ARG:NH1	1.90	0.67
1:A:270:ILE:HG23	1:A:854:LEU:CD2	2.22	0.67
2:N:135:TYR:CZ	2:N:342:MET:HE3	2.30	0.67
1:A:306:ASP:HB3	1:A:310:LEU:CD1	2.24	0.67
1:B:305:GLN:HE21	1:B:564:ASN:CG	2.03	0.67
1:B:605:ASN:HD21	1:B:855:LEU:HD12	1.58	0.67
1:B:745:ALA:O	1:B:748:THR:N	2.28	0.67
2:D:38:ILE:HD12	2:D:65:LEU:HD23	1.75	0.67
2:E:4:LEU:HA	2:E:7:LEU:HD12	1.75	0.67
2:F:19:VAL:HG23	2:H:128:ASN:HB3	1.77	0.67
2:H:76:ASN:H	2:J:76:ASN:HB2	1.60	0.67
2:I:104:SER:O	2:I:108:GLY:HA3	1.94	0.67
2:K:116:LEU:HD12	2:K:119:LEU:HB2	1.76	0.67
2:L:4:LEU:HA	2:L:7:LEU:HD12	1.75	0.67
2:N:73:LEU:N	2:N:73:LEU:HD23	2.09	0.67
1:A:136:ALA:O	1:A:137:ASN:CB	2.43	0.67
1:A:310:LEU:O	1:A:318:TRP:HD1	1.76	0.67
1:B:183:LEU:HD12	1:B:844:SER:HB3	1.77	0.67
2:I:63:PHE:CD2	2:I:84:THR:HG23	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:239:ASN:HD22	2:O:246:THR:HG22	1.58	0.67
1:A:571:LEU:O	1:A:571:LEU:HD13	1.94	0.67
1:B:869:VAL:HG22	1:B:875:ARG:HA	1.76	0.67
2:F:239:ASN:HD22	2:F:246:THR:HG22	1.58	0.67
2:K:239:ASN:HD22	2:K:246:THR:HG22	1.58	0.67
1:B:666:ARG:CG	1:B:667:ASP:N	2.57	0.67
1:B:782:VAL:HG11	1:B:796:LYS:O	1.94	0.67
1:B:791:LYS:C	1:B:792:VAL:HG13	2.20	0.67
2:O:9:LYS:O	2:O:13:ASP:HB2	1.95	0.67
1:B:108:LEU:HD22	1:B:108:LEU:N	2.10	0.67
1:B:154:THR:O	1:B:155:LEU:HD23	1.94	0.67
1:B:394:LEU:C	1:B:396:PHE:H	2.02	0.67
2:I:76:ASN:N	2:M:76:ASN:HB2	2.09	0.67
2:K:4:LEU:HA	2:K:7:LEU:HD12	1.75	0.67
1:A:219:GLY:O	1:A:221:VAL:N	2.28	0.67
1:A:223:ARG:O	1:A:226:ALA:HB3	1.95	0.67
1:A:839:MET:HG2	1:A:840:HIS:H	1.60	0.67
1:B:371:ASN:ND2	1:B:583:SER:HB3	2.06	0.67
2:G:116:LEU:HD12	2:G:119:LEU:HB2	1.76	0.67
2:K:9:LYS:O	2:K:13:ASP:HB2	1.95	0.67
1:A:409:TRP:HH2	1:A:547:THR:HG1	1.42	0.67
1:A:521:MET:HB3	1:A:522:PRO:CD	2.22	0.67
1:A:556:THR:O	1:A:557:LEU:C	2.38	0.67
1:A:650:HIS:O	1:A:651:ILE:HB	1.94	0.67
1:B:200:VAL:HG12	1:B:201:ASP:N	2.08	0.67
1:B:700:ALA:HB1	1:B:827:LYS:HB2	1.75	0.67
1:B:771:VAL:HG12	1:B:772:ILE:N	2.09	0.67
1:A:252:PHE:CD2	1:A:684:LEU:HD21	2.30	0.66
2:L:62:ASP:CG	2:L:62:ASP:O	2.37	0.66
2:O:116:LEU:HD12	2:O:119:LEU:HB2	1.76	0.66
1:A:524:ASP:OD1	1:A:525:TYR:N	2.27	0.66
1:B:229:ARG:HD2	1:B:230:GLN:HE22	1.60	0.66
1:B:672:LEU:HB3	1:B:673:PRO:HD2	1.77	0.66
2:D:99:GLU:O	2:D:99:GLU:HG2	1.94	0.66
2:D:99:GLU:OE1	2:D:116:LEU:HD22	1.94	0.66
2:O:49:GLY:HA2	2:O:54:LEU:HD23	1.77	0.66
1:B:825:VAL:CG1	1:B:826:TYR:N	2.57	0.66
2:E:239:ASN:HD22	2:E:246:THR:HG22	1.59	0.66
1:A:246:HIS:CD2	1:A:248:ILE:H	2.14	0.66
1:A:508:GLU:HG2	1:A:512:GLN:NE2	2.10	0.66
1:B:508:GLU:CD	2:J:71:LEU:HB3	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:ALA:HB2	1:B:824:LYS:HE3	1.77	0.66
2:C:153:HIS:NE2	2:E:153:HIS:NE2	2.43	0.66
2:E:14:ALA:O	2:E:18:ILE:HD12	1.95	0.66
1:A:701:GLN:HG2	1:A:826:TYR:CD2	2.31	0.66
1:B:374:ALA:HB1	1:B:580:SER:CA	2.25	0.66
2:D:144:ARG:O	2:D:145:ARG:HB2	1.94	0.66
2:L:153:HIS:NE2	2:M:153:HIS:NE2	2.44	0.66
1:A:443:GLN:CD	1:A:521:MET:HG2	2.21	0.66
1:A:454:THR:HB	1:A:457:GLN:HB3	1.78	0.66
1:A:513:LEU:O	1:A:516:GLN:OE1	2.14	0.66
1:A:653:ASP:HB3	1:A:656:ARG:HB2	1.77	0.66
1:B:396:PHE:HB2	1:B:578:LEU:HD11	1.77	0.66
2:E:23:LEU:HD23	2:E:24:TYR:N	2.11	0.66
2:N:9:LYS:O	2:N:13:ASP:HB2	1.96	0.66
2:N:150:PHE:HB2	2:N:152:PHE:CE1	2.30	0.66
1:A:277:ARG:HD3	1:A:559:ALA:CB	2.25	0.66
1:B:594:ILE:HB	1:B:595:PRO:CD	2.26	0.66
1:B:825:VAL:CG1	1:B:826:TYR:H	2.08	0.66
1:B:349:MET:O	1:B:353:LEU:HB2	1.94	0.66
2:C:2:ASP:HB2	2:C:128:ASN:HD21	1.60	0.66
2:J:5:TYR:CE2	2:J:131:ASN:HA	2.31	0.66
2:M:9:LYS:O	2:M:13:ASP:HB2	1.96	0.66
2:N:4:LEU:HA	2:N:7:LEU:CD1	2.26	0.66
1:A:506:LEU:HD21	1:A:543:LEU:C	2.20	0.66
1:A:717:MET:HE1	1:A:830:PRO:O	1.95	0.66
1:B:140:LYS:O	1:B:142:LEU:N	2.29	0.66
1:B:445:MET:O	1:B:447:TYR:N	2.23	0.66
1:B:504:ASN:O	1:B:507:MET:N	2.29	0.66
2:C:22:THR:HG23	2:C:73:LEU:HD12	1.78	0.66
2:G:145:ARG:HH11	2:G:145:ARG:CB	2.00	0.66
2:I:110:ALA:HB1	2:I:111:PRO:HD2	1.77	0.66
1:B:170:TYR:HE1	1:B:681:ILE:HG23	1.60	0.66
1:B:194:ARG:NE	1:B:194:ARG:HA	2.11	0.66
2:O:4:LEU:HA	2:O:7:LEU:CD1	2.26	0.66
1:A:166:PHE:O	1:A:169:LEU:HB2	1.96	0.65
2:C:150:PHE:HB2	2:C:152:PHE:HE1	1.61	0.65
2:D:9:LYS:O	2:D:13:ASP:HB2	1.94	0.65
2:F:26:ASN:OD1	2:H:33:GLN:HB2	1.97	0.65
2:I:109:ILE:HB	2:I:380:ASP:HB3	1.79	0.65
2:N:150:PHE:HB2	2:N:152:PHE:HE1	1.61	0.65
1:A:603:TYR:O	1:A:606:VAL:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:LEU:HA	2:C:7:LEU:CD1	2.27	0.65
2:C:54:LEU:HD12	2:C:55:PRO:HD2	1.77	0.65
2:G:128:ASN:O	2:H:22:THR:HB	1.95	0.65
2:L:135:TYR:CZ	2:L:342:MET:HE3	2.31	0.65
1:A:660:ASP:O	1:A:661:GLN:C	2.38	0.65
1:A:755:GLN:O	1:A:757:VAL:HG23	1.96	0.65
1:A:849:THR:HB	1:A:851:TYR:HE1	1.61	0.65
1:B:322:THR:HB	1:B:390:ARG:HH11	1.61	0.65
1:B:396:PHE:HE1	1:B:398:THR:HA	1.60	0.65
1:B:642:VAL:O	1:B:646:LEU:HG	1.96	0.65
2:D:109:ILE:HB	2:D:380:ASP:HB3	1.78	0.65
2:G:9:LYS:O	2:G:13:ASP:HB2	1.96	0.65
2:J:12:LYS:HG2	2:J:16:ASP:OD2	1.95	0.65
2:K:46:PHE:HE2	2:K:119:LEU:HD21	1.62	0.65
2:M:144:ARG:HD2	2:N:82:ARG:CZ	2.27	0.65
2:C:9:LYS:O	2:C:13:ASP:HB2	1.96	0.65
1:A:308:LEU:O	1:A:309:ASN:C	2.39	0.65
1:A:711:GLN:O	1:A:712:LEU:HD23	1.96	0.65
1:A:871:PHE:O	1:A:871:PHE:HD1	1.80	0.65
1:A:501:HIS:O	1:A:503:ILE:HG13	1.97	0.65
2:D:22:THR:O	2:D:72:ASN:HA	1.95	0.65
2:G:4:LEU:HA	2:G:7:LEU:CD1	2.26	0.65
2:I:150:PHE:HB2	2:I:152:PHE:CZ	2.32	0.65
1:A:516:GLN:OE1	1:A:516:GLN:N	2.28	0.65
1:A:622:VAL:HG11	1:A:673:PRO:O	1.97	0.65
1:A:642:VAL:O	1:A:646:LEU:HG	1.96	0.65
1:B:492:VAL:O	1:B:493:LEU:C	2.40	0.65
2:H:9:LYS:O	2:H:13:ASP:HB2	1.97	0.65
2:I:130:ASP:HA	2:J:17:LYS:HG2	1.78	0.65
2:I:153:HIS:NE2	2:K:153:HIS:NE2	2.45	0.65
2:N:12:LYS:C	2:N:14:ALA:N	2.54	0.65
1:A:142:LEU:O	1:A:144:ASN:N	2.28	0.65
1:A:658:PRO:CG	1:B:348:LYS:HG2	2.23	0.65
1:A:782:VAL:O	1:A:785:GLN:HG2	1.97	0.65
1:A:803:ASN:C	1:A:805:ASP:H	2.05	0.65
1:B:170:TYR:CE1	1:B:681:ILE:HG23	2.31	0.65
1:B:401:TYR:HA	1:B:404:LEU:HD13	1.79	0.65
1:A:779:ASP:CA	1:A:798:ILE:HD12	2.26	0.65
1:B:236:ARG:O	1:B:237:ASN:HB2	1.97	0.65
1:B:315:GLU:CB	1:B:571:LEU:HD11	2.25	0.65
1:B:745:ALA:O	1:B:746:GLN:C	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:PHE:HA	1:A:274:ILE:HD12	1.79	0.65
1:B:96:PRO:HG2	1:B:657:VAL:HG22	1.79	0.65
1:B:298:TYR:HD1	1:B:299:ILE:N	1.94	0.65
1:B:508:GLU:C	1:B:512:GLN:HE21	2.05	0.65
2:J:135:TYR:CZ	2:J:342:MET:HE3	2.32	0.65
2:N:12:LYS:HG2	2:N:16:ASP:OD2	1.96	0.65
1:B:180:TYR:C	1:B:180:TYR:CD1	2.75	0.64
1:B:378:CYS:HB2	1:B:580:SER:HB2	1.79	0.64
2:E:9:LYS:O	2:E:13:ASP:HB2	1.97	0.64
2:F:9:LYS:O	2:F:13:ASP:HB2	1.97	0.64
2:I:4:LEU:HA	2:I:7:LEU:CD1	2.27	0.64
2:J:57:ARG:HH11	2:J:94:ASN:HD21	1.46	0.64
1:B:314:PHE:CZ	1:B:664:ARG:HG2	2.32	0.64
1:B:603:TYR:O	1:B:606:VAL:HG22	1.97	0.64
2:D:4:LEU:HA	2:D:7:LEU:CD1	2.27	0.64
2:D:106:ARG:HG2	2:D:107:ASN:H	1.62	0.64
2:L:9:LYS:O	2:L:13:ASP:HB2	1.96	0.64
1:A:802:ILE:HA	1:A:807:ASN:ND2	2.12	0.64
2:O:104:SER:HB3	2:O:108:GLY:HA2	1.79	0.64
1:A:714:ARG:HA	1:A:720:TYR:HB3	1.78	0.64
1:A:863:VAL:HG12	1:A:864:GLU:H	1.61	0.64
2:D:110:ALA:HB1	2:D:111:PRO:CD	2.28	0.64
2:L:27:VAL:O	2:L:31:ILE:HG12	1.97	0.64
1:A:414:VAL:HB	1:A:419:PHE:HE1	1.62	0.64
1:A:834:ASP:O	1:A:838:SER:HB2	1.97	0.64
1:B:124:ARG:HB2	1:B:249:ASP:CG	2.22	0.64
1:B:182:LEU:CD2	1:B:183:LEU:H	2.08	0.64
1:B:491:GLN:NE2	1:B:566:GLN:HG2	2.12	0.64
1:B:606:VAL:HG23	1:B:607:ASN:N	2.11	0.64
2:J:144:ARG:NH2	2:J:146:GLN:HE22	1.96	0.64
1:A:246:HIS:O	1:A:249:ASP:N	2.31	0.64
1:A:548:ARG:HB3	1:A:876:ILE:HG23	1.78	0.64
1:B:371:ASN:C	1:B:373:GLN:N	2.52	0.64
1:B:645:PHE:HD2	1:B:646:LEU:HD23	1.62	0.64
1:B:718:TYR:HB3	1:B:721:VAL:CG2	2.18	0.64
2:F:109:ILE:HB	2:F:380:ASP:HB3	1.79	0.64
2:J:4:LEU:HA	2:J:7:LEU:CD1	2.28	0.64
2:J:9:LYS:O	2:J:13:ASP:HB2	1.98	0.64
2:K:12:LYS:HG2	2:K:16:ASP:OD2	1.97	0.64
2:M:139:TRP:NE1	2:M:143:ASN:ND2	2.46	0.64
1:A:246:HIS:HD2	1:A:248:ILE:HB	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:CYS:SG	1:A:584:LEU:HD13	2.38	0.64
1:A:770:SER:O	1:A:771:VAL:C	2.40	0.64
1:B:703:VAL:HG22	1:B:825:VAL:HG22	1.78	0.64
2:F:38:ILE:HG22	2:F:42:ASN:HD21	1.62	0.64
2:J:8:SER:C	2:J:10:THR:N	2.55	0.64
2:M:42:ASN:HA	2:M:61:PHE:HB3	1.80	0.64
2:N:128:ASN:O	2:N:129:PHE:HB3	1.98	0.64
1:A:606:VAL:HG23	1:A:607:ASN:N	2.13	0.64
1:B:182:LEU:HD11	1:B:847:THR:HA	1.78	0.64
1:B:389:GLN:HA	1:B:389:GLN:OE1	1.98	0.64
1:B:492:VAL:HG13	1:B:565:MET:SD	2.38	0.64
1:B:721:VAL:HG12	1:B:722:ASN:H	1.63	0.64
2:F:135:TYR:CZ	2:F:342:MET:HE3	2.33	0.64
2:M:12:LYS:HG2	2:M:16:ASP:OD2	1.98	0.64
1:A:360:ILE:HG23	1:A:363:GLU:HB2	1.78	0.64
1:A:563:MET:HE3	1:A:611:HIS:NE2	2.13	0.64
2:D:54:LEU:HD12	2:D:55:PRO:HD2	1.79	0.64
2:G:106:ARG:HG2	2:G:107:ASN:H	1.62	0.64
2:D:12:LYS:HG2	2:D:16:ASP:OD2	1.98	0.64
2:E:4:LEU:HA	2:E:7:LEU:CD1	2.28	0.64
2:H:57:ARG:HH11	2:H:94:ASN:HD21	1.44	0.64
2:K:4:LEU:HA	2:K:7:LEU:CD1	2.28	0.64
2:O:14:ALA:O	2:O:18:ILE:HD12	1.97	0.64
1:A:158:GLY:N	1:A:762:ALA:HB3	2.13	0.63
1:A:371:ASN:HB3	1:A:583:SER:HB2	1.80	0.63
1:A:784:ALA:O	1:A:785:GLN:C	2.41	0.63
1:B:491:GLN:HE22	1:B:566:GLN:HG2	1.63	0.63
1:B:498:ARG:CB	1:B:505:GLN:HE22	2.10	0.63
2:I:19:VAL:CG2	2:K:128:ASN:HB3	2.27	0.63
2:J:110:ALA:HB1	2:J:111:PRO:CD	2.28	0.63
2:L:12:LYS:HG2	2:L:16:ASP:OD2	1.98	0.63
2:M:27:VAL:O	2:M:31:ILE:HG12	1.97	0.63
1:A:772:ILE:O	1:A:775:ILE:HG13	1.98	0.63
1:B:346:ILE:O	1:B:349:MET:HB3	1.97	0.63
1:B:442:MET:HG2	1:B:443:GLN:H	1.63	0.63
1:B:645:PHE:CD2	1:B:646:LEU:HD23	2.33	0.63
2:F:4:LEU:HA	2:F:7:LEU:CD1	2.29	0.63
2:J:71:LEU:HG	2:J:72:ASN:OD1	1.98	0.63
2:K:8:SER:C	2:K:10:THR:N	2.55	0.63
2:M:4:LEU:HA	2:M:7:LEU:CD1	2.28	0.63
1:A:491:GLN:OE1	1:A:564:ASN:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ILE:C	1:B:286:LEU:HD13	2.22	0.63
1:B:396:PHE:CE1	1:B:398:THR:HA	2.33	0.63
1:B:730:PHE:N	1:B:730:PHE:CD1	2.67	0.63
1:B:772:ILE:O	1:B:775:ILE:HB	1.98	0.63
2:F:110:ALA:HB1	2:F:111:PRO:HD2	1.80	0.63
2:I:145:ARG:HH11	2:I:145:ARG:CB	2.12	0.63
1:A:560:CYS:HB2	1:A:603:TYR:CD2	2.33	0.63
1:A:721:VAL:HG11	1:A:799:LEU:HD22	1.81	0.63
1:B:305:GLN:HG3	1:B:564:ASN:HD21	1.62	0.63
1:B:415:PRO:CB	1:B:480:PHE:HB2	2.28	0.63
1:B:503:ILE:HD11	1:B:548:ARG:CG	2.26	0.63
1:B:722:ASN:ND2	1:B:824:LYS:HA	2.10	0.63
2:D:109:ILE:HD12	2:D:109:ILE:O	1.99	0.63
2:F:12:LYS:HG2	2:F:16:ASP:OD2	1.99	0.63
2:O:141:LEU:HD12	2:O:148:THR:HG21	1.80	0.63
1:A:262:VAL:HG12	1:A:297:ARG:HB3	1.80	0.63
1:B:498:ARG:HD3	2:I:32:GLN:HE21	1.63	0.63
2:C:12:LYS:C	2:C:14:ALA:N	2.56	0.63
2:F:104:SER:O	2:F:105:GLN:HB2	1.98	0.63
2:L:346:VAL:HG21	2:L:385:VAL:HG13	1.81	0.63
1:A:197:GLY:O	1:A:198:LYS:C	2.42	0.63
1:A:521:MET:HA	1:A:521:MET:CE	2.26	0.63
1:B:231:ARG:HB3	1:B:240:ASN:HB2	1.80	0.63
1:B:422:GLU:HA	1:B:425:VAL:CG2	2.29	0.63
1:B:492:VAL:HG11	1:B:558:MET:SD	2.38	0.63
1:B:587:LEU:HG	1:B:587:LEU:O	1.97	0.63
1:B:701:GLN:HB2	1:B:826:TYR:CD2	2.29	0.63
1:B:735:LEU:HD21	1:B:759:LEU:HB3	1.80	0.63
1:A:513:LEU:HA	1:A:516:GLN:HE22	1.64	0.63
2:C:12:LYS:HG2	2:C:16:ASP:OD2	1.99	0.63
2:L:24:TYR:O	2:L:27:VAL:HG22	1.98	0.63
2:L:85:ILE:O	2:L:89:VAL:HG23	1.99	0.63
2:O:12:LYS:HG2	2:O:16:ASP:OD2	1.99	0.63
2:O:85:ILE:O	2:O:89:VAL:HG23	1.99	0.63
1:A:180:TYR:CD1	1:A:180:TYR:C	2.75	0.63
1:A:795:LEU:O	1:A:797:PRO:HD3	1.98	0.63
1:B:127:GLU:OE1	1:B:151:LYS:HE2	1.98	0.63
1:B:549:LEU:HD13	1:B:877:MET:CE	2.28	0.63
1:B:818:VAL:HG12	1:B:819:PRO:HD2	1.80	0.63
2:K:346:VAL:HG21	2:K:385:VAL:HG13	1.81	0.63
2:N:106:ARG:H	2:N:106:ARG:CD	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:147:ARG:HG2	2:O:148:THR:N	2.13	0.63
1:A:601:PHE:HD1	1:A:601:PHE:H	1.46	0.63
1:A:744:TYR:C	1:A:746:GLN:H	2.07	0.63
1:A:147:TYR:CE2	1:A:717:MET:HE2	2.34	0.62
1:A:328:LEU:HD11	1:A:606:VAL:HG21	1.80	0.62
1:A:416:ASN:HB3	1:A:424:LEU:CD2	2.29	0.62
1:B:274:ILE:HG23	1:B:278:ILE:CD1	2.24	0.62
1:B:457:GLN:CG	1:B:458:ILE:N	2.53	0.62
2:I:12:LYS:HG2	2:I:16:ASP:OD2	1.99	0.62
2:I:85:ILE:O	2:I:89:VAL:HG23	1.99	0.62
2:M:12:LYS:C	2:M:14:ALA:N	2.57	0.62
2:N:49:GLY:HA2	2:N:54:LEU:HD23	1.81	0.62
2:N:346:VAL:HG21	2:N:385:VAL:HG13	1.81	0.62
2:O:8:SER:C	2:O:10:THR:N	2.55	0.62
1:A:200:VAL:O	1:A:204:THR:OG1	2.17	0.62
1:A:721:VAL:HG13	1:A:800:TYR:O	1.98	0.62
1:A:810:TYR:O	1:A:812:VAL:N	2.32	0.62
1:B:95:ILE:HG22	1:B:97:THR:OG1	1.99	0.62
1:B:199:VAL:CG1	1:B:200:VAL:N	2.62	0.62
1:B:451:ASP:N	1:B:452:PRO:HD3	2.13	0.62
1:B:494:ASN:ND2	1:B:495:ASP:N	2.46	0.62
1:B:704:ILE:O	1:B:823:THR:OG1	2.17	0.62
1:B:812:VAL:HG22	1:B:813:ALA:N	2.13	0.62
2:D:68:THR:O	2:D:69:THR:C	2.41	0.62
2:J:346:VAL:HG21	2:J:385:VAL:HG13	1.81	0.62
2:O:135:TYR:CZ	2:O:342:MET:HE3	2.34	0.62
2:O:346:VAL:HG21	2:O:385:VAL:HG13	1.81	0.62
1:A:360:ILE:CG2	1:A:363:GLU:HB2	2.29	0.62
1:A:472:LEU:O	1:A:476:ASN:HB2	1.99	0.62
1:A:545:ASP:HA	1:A:548:ARG:HD2	1.80	0.62
1:A:839:MET:HE3	1:A:840:HIS:CA	2.29	0.62
1:B:596:SER:HB2	1:B:599:THR:OG1	1.99	0.62
2:C:135:TYR:CZ	2:C:342:MET:HE3	2.33	0.62
2:E:8:SER:C	2:E:10:THR:N	2.55	0.62
2:H:346:VAL:HG21	2:H:385:VAL:HG13	1.81	0.62
2:J:144:ARG:HD2	2:K:82:ARG:CZ	2.28	0.62
2:K:12:LYS:C	2:K:14:ALA:N	2.56	0.62
2:K:48:THR:HG22	2:K:115:SER:OG	1.98	0.62
2:O:135:TYR:OH	2:O:340:GLU:OE1	2.17	0.62
1:A:503:ILE:CD1	1:A:547:THR:HB	2.29	0.62
1:B:122:LEU:HD11	1:B:200:VAL:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ILE:HG12	2:I:68:THR:HG23	1.82	0.62
1:B:681:ILE:O	1:B:684:LEU:HB3	1.99	0.62
1:B:723:ILE:O	1:B:824:LYS:HD2	2.00	0.62
2:C:21:GLY:O	2:C:22:THR:O	2.17	0.62
2:E:149:GLY:C	2:E:150:PHE:CD1	2.77	0.62
1:B:494:ASN:CG	1:B:495:ASP:H	2.07	0.62
2:C:8:SER:O	2:C:11:LEU:N	2.33	0.62
2:E:116:LEU:HA	2:E:119:LEU:HD12	1.81	0.62
2:H:109:ILE:O	2:H:109:ILE:CG1	2.48	0.62
2:I:346:VAL:HG21	2:I:385:VAL:HG13	1.81	0.62
2:L:4:LEU:HA	2:L:7:LEU:CD1	2.28	0.62
2:L:12:LYS:C	2:L:14:ALA:N	2.56	0.62
1:A:763:LEU:HD23	1:A:764:PRO:HD3	1.80	0.62
1:B:432:VAL:HA	1:B:436:ILE:CD1	2.12	0.62
1:B:692:ILE:HD12	1:B:692:ILE:H	1.63	0.62
1:B:717:MET:HE3	1:B:718:TYR:HE1	1.64	0.62
2:J:85:ILE:O	2:J:89:VAL:HG23	1.99	0.62
2:K:62:ASP:CG	2:K:62:ASP:O	2.42	0.62
1:A:366:PHE:C	1:A:368:THR:N	2.48	0.62
1:B:140:LYS:C	1:B:142:LEU:H	2.06	0.62
1:B:371:ASN:HA	1:B:374:ALA:HB3	1.82	0.62
1:B:435:ILE:O	1:B:436:ILE:HG12	2.00	0.62
2:D:12:LYS:C	2:D:14:ALA:N	2.56	0.62
2:F:8:SER:C	2:F:10:THR:N	2.55	0.62
1:A:596:SER:O	1:A:600:LEU:HD12	1.99	0.62
2:F:346:VAL:HG21	2:F:385:VAL:HG13	1.81	0.62
2:H:4:LEU:HA	2:H:7:LEU:CD1	2.28	0.62
2:H:76:ASN:CB	2:J:76:ASN:HB2	2.30	0.62
2:I:8:SER:C	2:I:10:THR:N	2.56	0.62
2:I:23:LEU:HD23	2:I:24:TYR:H	1.65	0.62
2:J:22:THR:HG22	2:J:73:LEU:HD12	1.81	0.62
2:L:38:ILE:HD12	2:L:65:LEU:CD2	2.29	0.62
2:N:8:SER:O	2:N:11:LEU:N	2.33	0.62
1:B:634:TYR:O	1:B:635:GLN:HG2	1.99	0.62
2:G:46:PHE:HE2	2:G:119:LEU:HD21	1.63	0.62
2:H:12:LYS:HG2	2:H:16:ASP:OD2	2.00	0.62
2:M:346:VAL:HG21	2:M:385:VAL:HG13	1.81	0.62
2:O:23:LEU:HD23	2:O:24:TYR:N	2.14	0.62
1:A:163:ARG:HH22	1:A:736:GLU:CD	2.07	0.62
1:A:587:LEU:C	1:A:588:ILE:HG13	2.24	0.62
1:A:692:ILE:H	1:A:692:ILE:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASN:HA	1:B:842:LEU:O	2.00	0.62
1:B:477:ASN:O	1:B:478:ASN:C	2.43	0.62
1:B:591:ALA:O	1:B:877:MET:HE3	1.98	0.62
1:B:722:ASN:O	1:B:824:LYS:HB2	1.99	0.62
2:D:27:VAL:O	2:D:31:ILE:HG12	1.99	0.62
2:L:109:ILE:HD12	2:L:109:ILE:O	1.99	0.62
1:B:503:ILE:HG21	1:B:544:VAL:HG13	1.80	0.61
1:B:839:MET:SD	1:B:839:MET:C	2.83	0.61
2:E:12:LYS:HG2	2:E:16:ASP:OD2	1.99	0.61
1:A:568:VAL:HG12	1:A:569:GLN:N	2.14	0.61
1:B:277:ARG:C	1:B:278:ILE:HG12	2.23	0.61
1:B:863:VAL:HG12	1:B:864:GLU:H	1.65	0.61
2:G:27:VAL:O	2:G:31:ILE:HG12	2.01	0.61
2:L:22:THR:HG23	2:L:73:LEU:CD1	2.23	0.61
2:M:116:LEU:HA	2:M:119:LEU:HD12	1.82	0.61
2:M:145:ARG:HB3	2:M:145:ARG:CZ	2.31	0.61
2:N:66:LEU:HD13	2:N:77:TYR:OH	2.00	0.61
1:A:362:SER:CB	1:A:365:GLN:NE2	2.63	0.61
1:A:447:TYR:OH	1:A:458:ILE:HG23	2.01	0.61
1:B:94:THR:O	1:B:316:SER:HB3	2.01	0.61
1:B:182:LEU:HD21	1:B:846:LEU:HA	1.82	0.61
1:B:194:ARG:HA	1:B:194:ARG:CZ	2.30	0.61
1:B:415:PRO:HG2	1:B:480:PHE:CD1	2.30	0.61
1:B:428:GLN:HB2	1:B:456:PHE:HD1	1.61	0.61
2:D:23:LEU:HD23	2:D:24:TYR:H	1.62	0.61
2:D:346:VAL:HG21	2:D:385:VAL:HG13	1.81	0.61
2:E:8:SER:O	2:E:11:LEU:N	2.34	0.61
2:E:346:VAL:HG21	2:E:385:VAL:HG13	1.81	0.61
2:J:12:LYS:C	2:J:14:ALA:N	2.55	0.61
2:G:12:LYS:HG2	2:G:16:ASP:OD2	1.99	0.61
2:J:116:LEU:HA	2:J:119:LEU:HD12	1.82	0.61
2:K:8:SER:O	2:K:11:LEU:N	2.34	0.61
2:O:38:ILE:HG22	2:O:42:ASN:HD21	1.64	0.61
1:A:389:GLN:HG3	1:A:389:GLN:O	2.00	0.61
1:A:765:PHE:CD1	1:A:765:PHE:C	2.79	0.61
1:B:521:MET:HB2	1:B:522:PRO:HD2	1.81	0.61
2:E:12:LYS:C	2:E:14:ALA:N	2.56	0.61
2:G:38:ILE:HG22	2:G:42:ASN:HD21	1.64	0.61
2:G:128:ASN:HB3	2:H:19:VAL:HG23	1.81	0.61
2:I:116:LEU:HA	2:I:119:LEU:HD12	1.82	0.61
2:L:8:SER:O	2:L:11:LEU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:63:PHE:CD2	2:M:84:THR:HG23	2.35	0.61
2:O:8:SER:O	2:O:11:LEU:N	2.34	0.61
1:B:297:ARG:HG3	1:B:848:PHE:CD2	2.29	0.61
1:B:556:THR:O	1:B:557:LEU:C	2.44	0.61
2:D:85:ILE:O	2:D:89:VAL:HG23	2.01	0.61
1:A:135:ARG:O	1:A:136:ALA:C	2.44	0.61
1:B:545:ASP:HA	1:B:548:ARG:HD2	1.82	0.61
1:A:257:LEU:HD13	1:A:843:THR:O	2.01	0.61
1:A:282:VAL:O	1:A:284:TYR:N	2.34	0.61
1:A:443:GLN:O	1:A:445:MET:N	2.34	0.61
1:A:450:GLY:O	1:A:451:ASP:HB2	2.01	0.61
1:B:496:ASN:HB3	1:B:498:ARG:HB3	1.83	0.61
2:D:8:SER:C	2:D:10:THR:N	2.54	0.61
2:O:147:ARG:O	2:O:148:THR:HB	1.99	0.61
2:O:150:PHE:N	2:O:150:PHE:CD1	2.69	0.61
1:A:125:ILE:HD13	1:A:126:PHE:HE2	1.66	0.61
1:A:729:GLY:C	1:A:730:PHE:CD1	2.78	0.61
1:B:272:ASN:C	1:B:274:ILE:N	2.54	0.61
2:H:108:GLY:C	2:H:110:ALA:H	2.09	0.61
2:J:6:SER:OG	2:J:128:ASN:HA	2.00	0.61
2:L:72:ASN:ND2	2:N:126:ARG:HH11	1.99	0.61
2:O:116:LEU:HA	2:O:119:LEU:HD12	1.82	0.61
1:A:701:GLN:HB3	1:A:826:TYR:HD2	1.66	0.61
1:B:96:PRO:O	1:B:320:THR:HG21	1.99	0.61
1:B:523:VAL:O	1:B:525:TYR:N	2.34	0.61
1:B:744:TYR:O	1:B:745:ALA:HB3	2.00	0.61
1:B:870:ALA:C	1:B:872:ASP:N	2.56	0.61
2:G:346:VAL:HG21	2:G:385:VAL:HG13	1.81	0.61
2:I:19:VAL:HG23	2:K:128:ASN:HB3	1.83	0.61
2:J:8:SER:O	2:J:11:LEU:N	2.34	0.61
2:K:152:PHE:N	2:K:152:PHE:CD1	2.69	0.61
2:L:8:SER:C	2:L:10:THR:N	2.55	0.61
2:M:8:SER:C	2:M:10:THR:N	2.55	0.61
2:N:116:LEU:HA	2:N:119:LEU:HD12	1.82	0.61
1:A:434:THR:O	1:A:434:THR:HG22	2.00	0.60
1:A:570:THR:CG2	1:A:571:LEU:H	2.12	0.60
1:A:817:TRP:CG	1:A:818:VAL:N	2.65	0.60
1:B:133:ILE:CD1	1:B:145:ARG:HB2	2.31	0.60
1:B:153:ASP:CG	1:B:153:ASP:O	2.43	0.60
1:B:180:TYR:CD1	1:B:181:LEU:N	2.68	0.60
1:B:333:VAL:HG11	1:B:380:LYS:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:GLN:CB	1:B:493:LEU:HD22	2.30	0.60
1:B:673:PRO:C	1:B:674:VAL:HG22	2.26	0.60
2:E:150:PHE:HB2	2:E:152:PHE:CZ	2.37	0.60
2:N:109:ILE:HB	2:N:380:ASP:HB3	1.82	0.60
1:A:319:ASP:OD2	1:A:571:LEU:HB3	2.00	0.60
1:A:403:SER:HA	1:A:582:THR:OG1	2.00	0.60
1:A:503:ILE:C	1:A:505:GLN:N	2.55	0.60
1:A:631:LEU:HB3	1:A:633:LEU:CD1	2.31	0.60
1:A:817:TRP:CH2	1:A:819:PRO:HA	2.36	0.60
1:B:156:PRO:HB2	1:B:161:ASP:CB	2.30	0.60
1:B:503:ILE:HD13	1:B:544:VAL:CG1	2.31	0.60
1:B:527:ARG:O	1:B:531:ARG:CG	2.49	0.60
1:B:779:ASP:HA	1:B:798:ILE:HD11	1.82	0.60
2:C:346:VAL:HG21	2:C:385:VAL:HG13	1.81	0.60
2:F:109:ILE:HD12	2:F:109:ILE:O	2.01	0.60
2:H:142:GLN:HE21	2:H:143:ASN:N	1.98	0.60
2:L:150:PHE:HB2	2:L:152:PHE:HE1	1.60	0.60
2:M:49:GLY:HA2	2:M:54:LEU:CD2	2.31	0.60
1:A:122:LEU:HD11	1:A:200:VAL:HG12	1.82	0.60
1:A:625:ILE:O	1:A:628:ALA:HB3	2.00	0.60
1:A:757:VAL:HG12	1:A:758:ALA:N	2.17	0.60
1:A:779:ASP:HA	1:A:798:ILE:HD11	1.80	0.60
1:B:118:LYS:CG	1:B:119:GLN:H	2.13	0.60
1:B:684:LEU:O	1:B:687:MET:HG2	2.02	0.60
2:D:133:SER:O	2:D:135:TYR:N	2.35	0.60
2:G:12:LYS:C	2:G:14:ALA:N	2.57	0.60
1:A:355:LEU:HD13	1:A:363:GLU:HG2	1.83	0.60
1:B:424:LEU:HD12	1:B:424:LEU:O	2.01	0.60
2:E:57:ARG:HH11	2:E:94:ASN:HD21	1.49	0.60
2:I:153:HIS:NE2	2:J:153:HIS:NE2	2.50	0.60
2:M:5:TYR:CE2	2:M:131:ASN:HA	2.37	0.60
2:M:8:SER:O	2:M:11:LEU:N	2.34	0.60
1:B:266:ASN:O	1:B:267:ASN:C	2.45	0.60
1:B:275:PRO:HD2	1:B:278:ILE:HD11	1.83	0.60
1:B:875:ARG:HD3	1:B:878:ASN:HD22	1.66	0.60
2:E:133:SER:O	2:E:135:TYR:N	2.35	0.60
2:F:12:LYS:C	2:F:14:ALA:N	2.56	0.60
2:L:116:LEU:HA	2:L:119:LEU:HD12	1.83	0.60
2:O:24:TYR:HB2	2:O:71:LEU:HD12	1.83	0.60
1:A:437:TYR:CD2	1:A:442:MET:HG3	2.36	0.60
1:B:389:GLN:NE2	1:B:567:HIS:HA	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:TYR:O	1:B:608:VAL:HG23	2.00	0.60
2:D:8:SER:O	2:D:11:LEU:N	2.34	0.60
2:E:129:PHE:CD1	2:E:129:PHE:C	2.80	0.60
2:H:8:SER:O	2:H:11:LEU:N	2.34	0.60
2:N:27:VAL:O	2:N:30:LEU:N	2.34	0.60
2:N:157:ILE:HG12	2:N:214:LEU:HD13	1.84	0.60
1:A:203:GLU:O	1:A:207:ILE:HG13	2.02	0.60
1:B:371:ASN:HD22	1:B:583:SER:CB	2.10	0.60
1:B:674:VAL:CG2	1:B:679:LEU:HD13	2.27	0.60
1:B:874:MET:O	1:B:875:ARG:CB	2.50	0.60
2:E:85:ILE:O	2:E:89:VAL:HG23	2.01	0.60
2:F:104:SER:HB3	2:F:108:GLY:HA3	1.84	0.60
2:H:23:LEU:H	2:H:26:ASN:ND2	2.00	0.60
2:I:68:THR:HG22	2:I:69:THR:N	2.16	0.60
2:L:73:LEU:HD22	2:L:77:TYR:CD2	2.36	0.60
2:M:145:ARG:HB3	2:M:145:ARG:NH1	2.16	0.60
1:A:237:ASN:OD1	1:A:237:ASN:O	2.20	0.60
1:A:326:TYR:CD1	1:A:384:ALA:HB1	2.36	0.60
1:A:492:VAL:CG1	1:A:558:MET:SD	2.90	0.60
1:A:546:LEU:CD1	1:A:584:LEU:HD23	2.32	0.60
1:A:727:LEU:HD12	1:A:727:LEU:O	2.02	0.60
1:B:274:ILE:CG2	1:B:278:ILE:HD11	2.25	0.60
1:B:387:LEU:HD23	1:B:554:TYR:CE1	2.36	0.60
1:B:743:ASP:OD2	1:B:745:ALA:HA	2.01	0.60
2:C:133:SER:O	2:C:135:TYR:N	2.34	0.60
2:D:116:LEU:HA	2:D:119:LEU:HD12	1.82	0.60
2:F:133:SER:O	2:F:135:TYR:N	2.35	0.60
2:G:157:ILE:HG12	2:G:214:LEU:HD13	1.84	0.60
2:J:110:ALA:HB1	2:J:111:PRO:HD2	1.83	0.60
2:K:5:TYR:CE2	2:K:131:ASN:HA	2.37	0.60
2:K:116:LEU:HA	2:K:119:LEU:HD12	1.84	0.60
2:M:274:GLN:N	2:M:274:GLN:HE21	2.00	0.60
1:A:666:ARG:HG3	1:A:667:ASP:N	2.14	0.60
1:A:822:THR:C	1:A:823:THR:HG23	2.26	0.60
1:B:435:ILE:CG2	1:B:436:ILE:H	2.09	0.60
1:B:502:VAL:O	1:B:504:ASN:N	2.35	0.60
1:B:723:ILE:O	1:B:724:ALA:HB2	2.01	0.60
1:B:868:ALA:C	1:B:876:ILE:HG23	2.26	0.60
2:D:38:ILE:HG22	2:D:42:ASN:HD21	1.67	0.60
2:E:157:ILE:HG12	2:E:214:LEU:HD13	1.84	0.60
2:H:8:SER:C	2:H:10:THR:N	2.56	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:14:ALA:C	2:J:16:ASP:H	2.10	0.60
2:J:133:SER:O	2:J:135:TYR:N	2.35	0.60
2:J:274:GLN:N	2:J:274:GLN:HE21	2.00	0.60
1:A:535:LEU:O	1:A:539:ARG:HG2	2.02	0.60
1:B:555:GLU:OE2	1:B:871:PHE:HE2	1.85	0.60
1:B:601:PHE:H	1:B:601:PHE:HD1	1.47	0.60
1:B:675:GLU:O	1:B:676:VAL:C	2.44	0.60
2:F:157:ILE:HG12	2:F:214:LEU:HD13	1.84	0.60
2:G:73:LEU:HD22	2:G:77:TYR:CD2	2.37	0.60
2:H:5:TYR:CE2	2:H:131:ASN:HA	2.37	0.60
2:I:12:LYS:C	2:I:14:ALA:N	2.56	0.60
2:K:133:SER:O	2:K:135:TYR:N	2.35	0.60
2:M:152:PHE:N	2:M:152:PHE:CD1	2.70	0.60
1:A:604:TYR:O	1:A:608:VAL:HG23	2.01	0.59
1:B:482:GLN:HG3	1:B:482:GLN:O	2.02	0.59
1:B:508:GLU:OE2	2:J:71:LEU:HB3	2.02	0.59
1:B:535:LEU:O	1:B:539:ARG:HG2	2.01	0.59
2:C:85:ILE:O	2:C:89:VAL:HG23	2.01	0.59
2:C:274:GLN:N	2:C:274:GLN:HE21	2.00	0.59
2:D:128:ASN:ND2	2:E:19:VAL:HG21	2.17	0.59
2:G:111:PRO:HB3	2:G:116:LEU:HD23	1.83	0.59
2:G:135:TYR:CZ	2:G:342:MET:HE3	2.37	0.59
2:H:133:SER:O	2:H:135:TYR:N	2.35	0.59
2:N:8:SER:C	2:N:10:THR:N	2.55	0.59
1:A:577:GLN:O	1:A:581:VAL:HG23	2.01	0.59
1:B:122:LEU:HG	1:B:201:ASP:CG	2.27	0.59
1:B:513:LEU:HA	1:B:516:GLN:OE1	2.01	0.59
2:D:76:ASN:HB2	2:L:76:ASN:HB2	1.83	0.59
2:H:152:PHE:N	2:H:152:PHE:CD1	2.69	0.59
2:I:60:ASN:C	2:I:61:PHE:CD1	2.80	0.59
2:I:157:ILE:HG12	2:I:214:LEU:HD13	1.84	0.59
2:L:19:VAL:CG2	2:N:128:ASN:HB3	2.32	0.59
2:M:24:TYR:O	2:M:27:VAL:HG22	2.02	0.59
1:A:246:HIS:CD2	1:A:248:ILE:HB	2.36	0.59
1:A:548:ARG:HH11	1:A:877:MET:CA	2.14	0.59
1:A:643:GLU:CG	1:A:662:MET:HE1	2.26	0.59
1:A:744:TYR:O	1:A:746:GLN:N	2.35	0.59
1:A:747:ILE:HD11	1:A:786:ILE:HG21	1.85	0.59
1:B:363:GLU:HA	1:B:363:GLU:OE1	2.02	0.59
1:B:401:TYR:O	1:B:404:LEU:HB2	2.02	0.59
1:B:787:VAL:O	1:B:788:LYS:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:VAL:HG12	1:B:864:GLU:N	2.17	0.59
2:C:14:ALA:C	2:C:16:ASP:H	2.10	0.59
2:C:131:ASN:HD22	2:C:131:ASN:N	1.99	0.59
2:G:8:SER:C	2:G:10:THR:N	2.56	0.59
2:G:85:ILE:O	2:G:89:VAL:HG23	2.01	0.59
2:H:274:GLN:N	2:H:274:GLN:HE21	2.00	0.59
2:M:133:SER:O	2:M:135:TYR:N	2.35	0.59
2:N:85:ILE:O	2:N:89:VAL:HG23	2.02	0.59
2:N:274:GLN:N	2:N:274:GLN:HE21	2.00	0.59
1:A:703:VAL:HG21	1:A:797:PRO:HB3	1.84	0.59
1:B:543:LEU:HD23	1:B:546:LEU:HD12	1.84	0.59
2:F:23:LEU:HD11	2:H:36:GLN:HB2	1.85	0.59
1:A:415:PRO:HB3	1:A:479:GLN:HA	1.84	0.59
1:A:545:ASP:O	1:A:548:ARG:N	2.35	0.59
1:A:700:ALA:O	1:A:701:GLN:HB2	2.02	0.59
1:A:839:MET:HG2	1:A:840:HIS:N	2.16	0.59
1:B:383:ILE:HD11	1:B:550:LEU:CD2	2.32	0.59
2:D:70:LEU:HD12	2:D:71:LEU:N	2.17	0.59
2:L:53:ASN:HD22	2:L:354:ALA:HB3	1.66	0.59
2:L:157:ILE:HG12	2:L:214:LEU:HD13	1.84	0.59
1:A:371:ASN:O	1:A:373:GLN:N	2.36	0.59
1:A:548:ARG:NH1	1:A:877:MET:HA	2.17	0.59
1:A:744:TYR:C	1:A:746:GLN:N	2.60	0.59
1:B:141:GLU:O	1:B:142:LEU:HB2	2.03	0.59
1:B:368:THR:O	1:B:371:ASN:ND2	2.36	0.59
1:B:393:SER:HB3	1:B:573:THR:HG21	1.84	0.59
2:D:104:SER:O	2:D:108:GLY:HA3	2.02	0.59
2:M:74:ASP:OD2	2:M:76:ASN:HB3	2.03	0.59
2:M:135:TYR:OH	2:M:340:GLU:OE1	2.20	0.59
2:O:274:GLN:HE21	2:O:274:GLN:N	2.00	0.59
1:A:160:TYR:CZ	1:A:635:GLN:HB2	2.38	0.59
1:A:803:ASN:H	1:A:807:ASN:ND2	2.00	0.59
1:B:190:ASN:HD21	1:B:193:SER:CB	2.10	0.59
1:B:498:ARG:HH22	2:J:25:SER:H	1.49	0.59
2:C:5:TYR:CE2	2:C:131:ASN:HA	2.36	0.59
2:D:157:ILE:HG12	2:D:214:LEU:HD13	1.84	0.59
2:J:157:ILE:HG12	2:J:214:LEU:HD13	1.84	0.59
2:K:157:ILE:HG12	2:K:214:LEU:HD13	1.84	0.59
2:L:130:ASP:HA	2:M:17:LYS:HG2	1.83	0.59
1:A:368:THR:HG21	1:A:582:THR:HB	1.83	0.59
1:A:413:VAL:HG12	1:A:414:VAL:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLN:HG3	2:F:39:ILE:HD11	1.84	0.59
1:B:506:LEU:HD21	1:B:543:LEU:C	2.27	0.59
2:D:76:ASN:H	2:L:76:ASN:HB2	1.67	0.59
2:E:274:GLN:N	2:E:274:GLN:HE21	2.00	0.59
2:H:157:ILE:HG12	2:H:214:LEU:HD13	1.84	0.59
2:J:124:PHE:O	2:J:127:ILE:HG13	2.03	0.59
1:A:322:THR:HG21	1:A:390:ARG:HA	1.83	0.59
1:A:467:GLN:HE21	1:A:511:MET:HG2	1.67	0.59
1:A:520:THR:HG21	1:A:526:LYS:HD3	1.85	0.59
1:A:545:ASP:HA	1:A:548:ARG:CD	2.33	0.59
1:A:633:LEU:C	1:A:635:GLN:H	2.11	0.59
1:A:771:VAL:HG22	1:A:772:ILE:N	2.18	0.59
1:B:833:PHE:CZ	1:B:835:PHE:HA	2.38	0.59
2:F:8:SER:O	2:F:11:LEU:N	2.36	0.59
2:F:274:GLN:N	2:F:274:GLN:HE21	2.00	0.59
2:G:71:LEU:HG	2:G:72:ASN:N	2.17	0.59
2:G:152:PHE:CD1	2:G:152:PHE:N	2.71	0.59
2:H:85:ILE:O	2:H:89:VAL:HG23	2.03	0.59
2:L:274:GLN:HE21	2:L:274:GLN:N	2.00	0.59
2:O:4:LEU:HG	2:O:391:ILE:HG21	1.85	0.59
2:O:12:LYS:C	2:O:14:ALA:N	2.57	0.59
1:A:242:PRO:HA	1:A:841:MET:SD	2.42	0.59
1:A:401:TYR:O	1:A:404:LEU:HB2	2.02	0.59
1:A:546:LEU:HD11	1:A:588:ILE:HD12	1.83	0.59
1:A:722:ASN:HD22	1:A:824:LYS:HA	1.68	0.59
1:A:810:TYR:CD1	1:A:811:LEU:N	2.71	0.59
1:B:803:ASN:N	1:B:807:ASN:ND2	2.48	0.59
2:I:152:PHE:N	2:I:152:PHE:CD1	2.70	0.59
2:M:38:ILE:HG22	2:M:42:ASN:HD21	1.67	0.59
2:N:14:ALA:C	2:N:16:ASP:H	2.10	0.59
2:N:109:ILE:HD12	2:N:109:ILE:O	2.03	0.59
2:O:100:MET:HG3	2:O:388:VAL:HG11	1.85	0.59
1:A:437:TYR:CE2	1:A:442:MET:HG3	2.37	0.58
1:A:484:VAL:HG12	1:A:485:ILE:H	1.68	0.58
1:A:501:HIS:C	1:A:503:ILE:H	2.09	0.58
1:A:571:LEU:HD23	1:B:531:ARG:NH2	2.17	0.58
1:A:803:ASN:O	1:A:805:ASP:N	2.36	0.58
1:B:326:TYR:CD1	1:B:384:ALA:HB1	2.37	0.58
1:B:745:ALA:HB1	1:B:748:THR:CB	2.31	0.58
2:F:14:ALA:C	2:F:16:ASP:H	2.11	0.58
2:F:116:LEU:HA	2:F:119:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:153:HIS:NE2	2:H:153:HIS:NE2	2.51	0.58
2:H:116:LEU:HA	2:H:119:LEU:HD12	1.84	0.58
1:A:428:GLN:NE2	1:A:455:PRO:CB	2.59	0.58
1:A:508:GLU:O	1:A:512:GLN:HG3	2.02	0.58
1:A:571:LEU:HD23	1:B:531:ARG:CZ	2.32	0.58
1:B:437:TYR:CD2	1:B:443:GLN:HB3	2.38	0.58
1:B:463:ILE:HG21	1:B:468:VAL:HG11	1.84	0.58
1:B:717:MET:HE3	1:B:718:TYR:CE1	2.37	0.58
1:B:875:ARG:HD3	1:B:878:ASN:ND2	2.18	0.58
2:C:157:ILE:HG12	2:C:214:LEU:HD13	1.84	0.58
2:D:14:ALA:C	2:D:16:ASP:H	2.11	0.58
2:G:274:GLN:HE21	2:G:274:GLN:N	2.00	0.58
2:H:22:THR:HG23	2:H:73:LEU:HD12	1.83	0.58
1:A:420:ILE:CD1	1:A:422:GLU:HG3	2.33	0.58
1:A:661:GLN:HG3	1:B:348:LYS:HZ1	1.67	0.58
1:B:111:ILE:HG22	1:B:113:PRO:HD3	1.84	0.58
1:B:112:LYS:N	1:B:113:PRO:HD3	2.18	0.58
1:B:190:ASN:O	1:B:192:ASN:N	2.37	0.58
1:B:223:ARG:O	1:B:226:ALA:HB3	2.03	0.58
1:B:421:ARG:O	1:B:425:VAL:HG23	2.02	0.58
1:B:501:HIS:C	1:B:503:ILE:N	2.60	0.58
2:C:67:GLY:C	2:C:69:THR:H	2.09	0.58
2:D:274:GLN:HE21	2:D:274:GLN:N	2.00	0.58
2:E:152:PHE:N	2:E:152:PHE:CD1	2.71	0.58
2:K:14:ALA:C	2:K:16:ASP:H	2.11	0.58
2:K:260:GLU:HG2	2:K:274:GLN:HG3	1.85	0.58
2:L:5:TYR:CE2	2:L:131:ASN:HA	2.37	0.58
2:M:85:ILE:O	2:M:89:VAL:HG23	2.02	0.58
2:M:157:ILE:HG12	2:M:214:LEU:HD13	1.84	0.58
1:B:653:ASP:O	1:B:654:VAL:C	2.46	0.58
2:C:8:SER:C	2:C:10:THR:N	2.55	0.58
2:D:130:ASP:HA	2:E:17:LYS:HG2	1.84	0.58
2:F:5:TYR:CE2	2:F:131:ASN:HA	2.38	0.58
2:G:133:SER:O	2:G:135:TYR:N	2.35	0.58
2:I:10:THR:O	2:I:14:ALA:HB2	2.04	0.58
2:K:145:ARG:O	2:K:146:GLN:HG2	2.02	0.58
2:L:17:LYS:HG2	2:N:130:ASP:HA	1.84	0.58
1:A:244:ILE:O	1:A:245:LEU:HD23	2.03	0.58
1:A:259:HIS:CD2	1:A:677:ARG:HG3	2.38	0.58
1:B:218:GLU:O	1:B:221:VAL:HG23	2.03	0.58
2:F:130:ASP:HA	2:G:17:LYS:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:116:LEU:HA	2:G:119:LEU:HD12	1.84	0.58
2:L:74:ASP:OD2	2:L:76:ASN:HB3	2.03	0.58
2:O:157:ILE:HG12	2:O:214:LEU:HD13	1.84	0.58
1:A:160:TYR:OH	1:A:635:GLN:HB2	2.04	0.58
1:A:188:VAL:HG12	1:A:189:GLU:N	2.17	0.58
1:A:306:ASP:C	1:A:308:LEU:N	2.56	0.58
1:B:508:GLU:O	1:B:512:GLN:HG3	2.04	0.58
2:E:22:THR:HG23	2:E:73:LEU:HD12	1.86	0.58
2:K:49:GLY:HA3	2:K:55:PRO:O	2.03	0.58
2:M:128:ASN:O	2:N:22:THR:HB	2.03	0.58
2:N:133:SER:O	2:N:135:TYR:N	2.36	0.58
1:A:839:MET:HE3	1:A:840:HIS:N	2.18	0.58
1:B:371:ASN:HB3	1:B:583:SER:HB2	1.86	0.58
1:B:772:ILE:CG2	1:B:773:SER:N	2.66	0.58
2:C:116:LEU:HA	2:C:119:LEU:HD12	1.84	0.58
2:D:99:GLU:CD	2:D:116:LEU:HD22	2.28	0.58
2:F:85:ILE:O	2:F:89:VAL:HG23	2.04	0.58
2:I:260:GLU:HG2	2:I:274:GLN:HG3	1.86	0.58
2:J:5:TYR:HE2	2:J:131:ASN:HA	1.69	0.58
2:K:85:ILE:O	2:K:89:VAL:HG23	2.02	0.58
2:O:260:GLU:HG2	2:O:274:GLN:HG3	1.86	0.58
1:A:467:GLN:HE22	1:A:511:MET:HE3	1.69	0.58
1:A:613:ASN:HD22	1:A:649:LEU:HD23	1.69	0.58
1:B:340:VAL:HB	1:B:587:LEU:HD12	1.84	0.58
1:B:416:ASN:O	1:B:418:MET:N	2.36	0.58
2:F:260:GLU:HG2	2:F:274:GLN:HG3	1.86	0.58
2:G:8:SER:O	2:G:11:LEU:N	2.36	0.58
2:J:116:LEU:HD12	2:J:119:LEU:HD12	1.86	0.58
2:L:133:SER:O	2:L:135:TYR:N	2.36	0.58
2:L:150:PHE:HA	2:M:397:LYS:HZ1	1.68	0.58
2:N:116:LEU:HD12	2:N:119:LEU:HD12	1.86	0.58
1:A:303:LEU:HA	1:A:615:ASN:HD22	1.67	0.58
1:A:304:LEU:N	1:A:615:ASN:HD21	2.02	0.58
1:A:365:GLN:HB2	1:A:366:PHE:CZ	2.39	0.58
1:A:420:ILE:CG1	1:A:423:SER:HB2	2.32	0.58
1:A:568:VAL:HG12	1:A:569:GLN:H	1.68	0.58
1:A:771:VAL:O	1:A:772:ILE:C	2.46	0.58
1:B:140:LYS:C	1:B:142:LEU:N	2.60	0.58
1:B:190:ASN:HB2	1:B:199:VAL:HG23	1.85	0.58
1:B:459:ALA:O	1:B:463:ILE:HG13	2.03	0.58
1:B:492:VAL:HG21	1:B:558:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:SER:O	1:B:827:LYS:HE3	2.04	0.58
2:C:7:LEU:O	2:C:11:LEU:HG	2.04	0.58
2:C:260:GLU:HG2	2:C:274:GLN:HG3	1.86	0.58
2:J:10:THR:O	2:J:14:ALA:HB2	2.04	0.58
2:O:14:ALA:C	2:O:16:ASP:H	2.11	0.58
2:O:133:SER:O	2:O:135:TYR:N	2.36	0.58
1:A:390:ARG:HD2	1:A:570:THR:HG21	1.84	0.58
1:A:803:ASN:H	1:A:807:ASN:HD22	1.50	0.58
1:B:491:GLN:HE22	1:B:566:GLN:CG	2.16	0.58
2:I:38:ILE:HG22	2:I:42:ASN:ND2	2.16	0.57
2:I:274:GLN:N	2:I:274:GLN:HE21	2.00	0.57
2:K:53:ASN:HD22	2:K:354:ALA:CB	2.17	0.57
2:K:274:GLN:N	2:K:274:GLN:HE21	2.01	0.57
2:L:104:SER:HB3	2:L:108:GLY:HA2	1.86	0.57
1:A:527:ARG:O	1:A:531:ARG:CG	2.51	0.57
1:A:681:ILE:O	1:A:684:LEU:HB3	2.03	0.57
1:B:199:VAL:CG1	1:B:200:VAL:H	2.17	0.57
1:B:458:ILE:HD12	1:B:458:ILE:C	2.29	0.57
1:B:577:GLN:C	1:B:579:THR:N	2.60	0.57
2:D:260:GLU:HG2	2:D:274:GLN:HG3	1.86	0.57
2:I:8:SER:O	2:I:11:LEU:N	2.36	0.57
2:I:133:SER:O	2:I:135:TYR:N	2.36	0.57
2:K:65:LEU:C	2:K:66:LEU:HG	2.29	0.57
2:M:260:GLU:HG2	2:M:274:GLN:HG3	1.86	0.57
1:A:548:ARG:NH1	1:A:878:ASN:H	2.01	0.57
1:A:550:LEU:O	1:A:551:ALA:C	2.47	0.57
1:B:254:GLU:HG2	2:N:69:THR:CB	2.34	0.57
1:B:415:PRO:HB2	1:B:480:PHE:HB2	1.86	0.57
1:B:434:THR:HG22	1:B:434:THR:O	2.04	0.57
1:B:472:LEU:O	1:B:476:ASN:HB2	2.04	0.57
2:E:260:GLU:HG2	2:E:274:GLN:HG3	1.86	0.57
2:F:144:ARG:HD2	2:G:82:ARG:NH1	2.19	0.57
2:G:10:THR:O	2:G:14:ALA:HB2	2.05	0.57
2:K:8:SER:O	2:K:10:THR:N	2.38	0.57
2:K:10:THR:O	2:K:14:ALA:HB2	2.05	0.57
2:N:76:ASN:HB2	2:O:76:ASN:H	1.69	0.57
1:A:647:LYS:C	1:A:649:LEU:H	2.12	0.57
2:J:139:TRP:C	2:J:139:TRP:CD1	2.83	0.57
2:L:144:ARG:O	2:L:145:ARG:CB	2.48	0.57
1:A:127:GLU:OE2	1:A:151:LYS:HG2	2.03	0.57
1:A:428:GLN:CD	1:A:456:PHE:HB2	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HG22	1:A:506:LEU:HB2	1.86	0.57
1:A:738:LEU:O	1:A:740:ARG:N	2.37	0.57
1:A:771:VAL:CG1	1:A:809:PHE:HB3	2.34	0.57
1:B:504:ASN:O	1:B:505:GLN:C	2.46	0.57
2:C:116:LEU:HD12	2:C:119:LEU:HD12	1.86	0.57
2:H:12:LYS:C	2:H:14:ALA:N	2.56	0.57
2:J:129:PHE:CD1	2:J:129:PHE:C	2.82	0.57
2:K:7:LEU:O	2:K:11:LEU:HG	2.04	0.57
2:L:7:LEU:O	2:L:11:LEU:HG	2.05	0.57
2:L:145:ARG:O	2:L:146:GLN:HG3	2.04	0.57
1:A:783:PHE:O	1:A:786:ILE:HD12	2.05	0.57
1:B:117:LYS:HB2	1:B:179:ASP:OD2	2.04	0.57
1:B:371:ASN:C	1:B:373:GLN:H	2.11	0.57
1:B:466:PHE:O	1:B:467:GLN:C	2.47	0.57
1:B:786:ILE:HG13	1:B:787:VAL:HG23	1.87	0.57
1:B:817:TRP:CD1	1:B:818:VAL:N	2.73	0.57
2:N:5:TYR:CE2	2:N:131:ASN:HA	2.39	0.57
1:A:131:LEU:HD12	1:A:132:PRO:CD	2.35	0.57
1:A:259:HIS:ND1	1:A:260:GLN:N	2.52	0.57
1:A:722:ASN:C	1:A:723:ILE:HG13	2.29	0.57
1:B:246:HIS:HB3	1:B:249:ASP:OD2	2.05	0.57
1:B:518:PHE:N	1:B:518:PHE:CD1	2.72	0.57
1:B:535:LEU:O	1:B:539:ARG:CG	2.52	0.57
1:B:703:VAL:HG12	1:B:704:ILE:N	2.20	0.57
2:C:128:ASN:HB3	2:D:19:VAL:CG2	2.35	0.57
2:E:14:ALA:C	2:E:16:ASP:H	2.11	0.57
2:G:116:LEU:HD12	2:G:119:LEU:HD12	1.87	0.57
2:G:260:GLU:HG2	2:G:274:GLN:HG3	1.86	0.57
2:I:14:ALA:C	2:I:16:ASP:H	2.11	0.57
1:A:314:PHE:O	1:A:315:GLU:C	2.48	0.57
1:B:340:VAL:HB	1:B:587:LEU:CD1	2.35	0.57
1:B:473:HIS:CB	2:I:126:ARG:HH22	2.08	0.57
1:B:701:GLN:O	1:B:702:GLY:O	2.23	0.57
2:I:116:LEU:HD12	2:I:119:LEU:HD12	1.86	0.57
2:I:145:ARG:O	2:I:146:GLN:HG3	2.04	0.57
2:L:8:SER:C	2:L:10:THR:H	2.13	0.57
2:M:106:ARG:H	2:M:106:ARG:CD	2.14	0.57
2:O:150:PHE:HB2	2:O:152:PHE:HE1	1.70	0.57
1:A:122:LEU:HD11	1:A:201:ASP:HB2	1.85	0.57
1:A:187:ALA:O	1:A:188:VAL:HG23	2.04	0.57
1:A:420:ILE:CD1	1:A:423:SER:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:GLN:O	1:A:516:GLN:HG3	2.05	0.57
1:A:710:MET:CE	1:A:824:LYS:HE2	2.35	0.57
1:B:492:VAL:CG1	1:B:558:MET:SD	2.93	0.57
1:B:752:LEU:C	1:B:754:ASN:N	2.63	0.57
2:J:260:GLU:HG2	2:J:274:GLN:HG3	1.86	0.57
2:N:260:GLU:HG2	2:N:274:GLN:HG3	1.85	0.57
1:B:271:PHE:O	1:B:274:ILE:HB	2.05	0.57
1:B:312:ASP:O	1:B:313:ASN:HB2	2.05	0.57
1:B:396:PHE:CD1	1:B:396:PHE:C	2.83	0.57
2:C:150:PHE:HB2	2:C:152:PHE:CZ	2.40	0.57
2:E:27:VAL:O	2:E:31:ILE:HG12	2.05	0.57
2:E:35:ASN:HA	2:E:38:ILE:HD12	1.87	0.57
2:G:5:TYR:CE2	2:G:131:ASN:HA	2.40	0.57
2:G:24:TYR:O	2:G:27:VAL:HG22	2.03	0.57
2:H:7:LEU:O	2:H:11:LEU:HG	2.05	0.57
2:L:144:ARG:HD2	2:M:82:ARG:NH1	2.20	0.57
2:O:107:ASN:CG	2:O:107:ASN:O	2.48	0.57
1:A:180:TYR:HD1	1:A:181:LEU:N	2.03	0.56
1:A:597:PRO:HB3	1:A:860:ALA:CB	2.35	0.56
1:B:137:ASN:O	1:B:137:ASN:OD1	2.22	0.56
1:B:211:ILE:O	1:B:212:PHE:C	2.48	0.56
1:B:254:GLU:CG	2:N:69:THR:HB	2.35	0.56
1:B:775:ILE:N	1:B:775:ILE:HD12	2.20	0.56
1:B:790:ARG:CA	1:B:790:ARG:NE	2.47	0.56
2:D:41:MET:O	2:D:42:ASN:C	2.47	0.56
2:D:116:LEU:HD12	2:D:119:LEU:HD12	1.85	0.56
2:D:128:ASN:HB3	2:E:19:VAL:HG23	1.87	0.56
2:F:129:PHE:CD1	2:F:129:PHE:C	2.83	0.56
2:G:61:PHE:HA	2:G:63:PHE:HE1	1.70	0.56
2:G:135:TYR:OH	2:G:340:GLU:OE1	2.23	0.56
2:H:42:ASN:OD1	2:H:62:ASP:HA	2.05	0.56
2:K:14:ALA:O	2:K:18:ILE:HD12	2.05	0.56
2:N:74:ASP:OD2	2:N:76:ASN:HB3	2.05	0.56
1:A:226:ALA:O	1:A:228:MET:N	2.32	0.56
1:A:332:VAL:HG13	1:A:599:THR:CG2	2.36	0.56
1:A:703:VAL:HG22	1:A:825:VAL:HG22	1.87	0.56
1:A:721:VAL:HG13	1:A:800:TYR:C	2.29	0.56
1:B:97:THR:HA	1:B:320:THR:HG23	1.86	0.56
1:B:550:LEU:O	1:B:551:ALA:C	2.49	0.56
2:D:8:SER:C	2:D:10:THR:H	2.13	0.56
2:M:139:TRP:HE1	2:M:143:ASN:HD21	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:110:ALA:HB1	2:O:111:PRO:CD	2.35	0.56
1:A:275:PRO:O	1:A:278:ILE:HG13	2.05	0.56
1:A:305:GLN:O	1:A:307:ARG:N	2.38	0.56
1:A:420:ILE:HD12	1:A:422:GLU:HG3	1.87	0.56
1:A:649:LEU:O	1:A:650:HIS:O	2.24	0.56
1:B:322:THR:O	1:B:323:THR:C	2.48	0.56
1:B:368:THR:O	1:B:369:GLY:O	2.23	0.56
1:B:390:ARG:HG3	1:B:391:THR:H	1.69	0.56
1:B:393:SER:N	1:B:573:THR:CG2	2.68	0.56
1:B:409:TRP:CH2	1:B:413:VAL:HG21	2.40	0.56
2:D:8:SER:O	2:D:10:THR:N	2.38	0.56
2:D:10:THR:O	2:D:14:ALA:HB2	2.05	0.56
2:H:139:TRP:CD1	2:H:139:TRP:C	2.83	0.56
2:H:260:GLU:HG2	2:H:274:GLN:HG3	1.85	0.56
2:I:116:LEU:CD1	2:I:119:LEU:HD12	2.36	0.56
2:J:152:PHE:CD1	2:J:152:PHE:N	2.71	0.56
2:K:35:ASN:HA	2:K:38:ILE:HD12	1.87	0.56
2:L:14:ALA:C	2:L:16:ASP:H	2.12	0.56
2:N:24:TYR:O	2:N:26:ASN:N	2.38	0.56
1:A:209:ASP:O	1:A:213:GLN:HG3	2.05	0.56
1:A:308:LEU:HB2	1:A:614:TYR:OH	2.06	0.56
1:A:410:LEU:O	1:A:413:VAL:HB	2.05	0.56
1:B:153:ASP:O	1:B:153:ASP:OD1	2.22	0.56
1:B:606:VAL:O	1:B:607:ASN:C	2.47	0.56
2:G:2:ASP:HB2	2:G:128:ASN:HD21	1.71	0.56
2:H:10:THR:O	2:H:14:ALA:HB2	2.06	0.56
2:H:27:VAL:CG2	2:H:31:ILE:HD11	2.35	0.56
2:J:74:ASP:OD2	2:J:76:ASN:HB3	2.04	0.56
2:M:110:ALA:HB1	2:M:111:PRO:CD	2.36	0.56
2:M:150:PHE:N	2:M:150:PHE:CD1	2.74	0.56
1:A:190:ASN:OD1	1:A:192:ASN:N	2.38	0.56
1:B:303:LEU:HD13	1:B:562:THR:HG21	1.88	0.56
1:B:618:ILE:O	1:B:622:VAL:HG23	2.06	0.56
2:H:14:ALA:C	2:H:16:ASP:H	2.11	0.56
2:I:139:TRP:CD1	2:I:139:TRP:C	2.84	0.56
2:L:38:ILE:HD12	2:L:65:LEU:HD23	1.86	0.56
2:M:7:LEU:O	2:M:11:LEU:HG	2.06	0.56
2:M:10:THR:O	2:M:14:ALA:HB2	2.05	0.56
2:M:14:ALA:C	2:M:16:ASP:H	2.11	0.56
2:N:144:ARG:O	2:N:145:ARG:CB	2.52	0.56
2:O:116:LEU:HD12	2:O:119:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HB3	1:A:249:ASP:CB	2.34	0.56
1:A:516:GLN:CD	1:A:516:GLN:H	2.11	0.56
1:A:540:LEU:HD23	1:A:540:LEU:C	2.30	0.56
1:B:203:GLU:O	1:B:207:ILE:HG13	2.05	0.56
1:B:246:HIS:ND1	1:B:247:PRO:HD2	2.20	0.56
2:E:5:TYR:HE2	2:E:131:ASN:HA	1.69	0.56
2:E:109:ILE:HD12	2:E:109:ILE:O	2.05	0.56
2:F:150:PHE:HB2	2:F:152:PHE:HE1	1.70	0.56
2:I:76:ASN:H	2:M:76:ASN:CB	2.13	0.56
2:K:41:MET:O	2:K:42:ASN:C	2.49	0.56
2:L:260:GLU:HG2	2:L:274:GLN:HG3	1.86	0.56
2:M:8:SER:C	2:M:10:THR:H	2.13	0.56
1:B:392:MET:HA	1:B:573:THR:HG23	1.87	0.56
2:C:35:ASN:HA	2:C:38:ILE:HD12	1.88	0.56
2:D:38:ILE:HD12	2:D:65:LEU:CD2	2.35	0.56
2:E:8:SER:O	2:E:10:THR:N	2.39	0.56
2:F:7:LEU:O	2:F:11:LEU:HG	2.06	0.56
2:F:116:LEU:HD12	2:F:119:LEU:HD12	1.88	0.56
2:K:99:GLU:O	2:K:384:ARG:NH1	2.39	0.56
2:M:150:PHE:HB2	2:M:152:PHE:CZ	2.41	0.56
2:N:10:THR:O	2:N:14:ALA:HB2	2.06	0.56
1:A:319:ASP:OD2	1:A:571:LEU:CB	2.53	0.56
1:A:857:PHE:HD1	1:A:857:PHE:H	1.52	0.56
1:B:305:GLN:HE21	1:B:564:ASN:ND2	2.04	0.56
1:B:496:ASN:HB3	1:B:498:ARG:CB	2.35	0.56
2:D:139:TRP:C	2:D:139:TRP:CD1	2.84	0.56
2:K:57:ARG:NH1	2:K:94:ASN:HD21	2.03	0.56
2:M:35:ASN:HA	2:M:38:ILE:HD12	1.86	0.56
2:M:116:LEU:HD12	2:M:119:LEU:HD12	1.86	0.56
2:N:8:SER:C	2:N:10:THR:H	2.14	0.56
2:N:41:MET:O	2:N:42:ASN:C	2.49	0.56
2:O:7:LEU:O	2:O:11:LEU:HG	2.06	0.56
2:O:35:ASN:HA	2:O:38:ILE:HD12	1.88	0.56
1:A:389:GLN:NE2	1:A:568:VAL:H	2.04	0.56
1:A:404:LEU:CD2	1:A:435:ILE:HD11	2.36	0.56
1:A:461:GLN:HB3	2:F:32:GLN:NE2	2.20	0.56
1:A:496:ASN:O	1:A:497:ILE:C	2.49	0.56
1:A:852:SER:O	1:A:853:ASP:HB3	2.04	0.56
2:D:128:ASN:HB3	2:E:19:VAL:CG2	2.36	0.56
2:E:38:ILE:HG22	2:E:42:ASN:ND2	2.19	0.56
2:J:8:SER:O	2:J:10:THR:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:35:ASN:HA	2:J:38:ILE:HD12	1.87	0.56
2:J:50:GLY:O	2:J:51:ILE:HB	2.05	0.56
1:A:503:ILE:CG2	1:A:506:LEU:HB2	2.36	0.56
1:A:814:ASN:O	1:A:815:TYR:C	2.48	0.56
1:B:89:GLU:C	1:B:91:LEU:N	2.61	0.56
1:B:325:ASN:O	1:B:328:LEU:HB3	2.05	0.56
1:B:498:ARG:HG3	1:B:505:GLN:OE1	2.05	0.56
1:B:516:GLN:O	1:B:517:GLN:NE2	2.39	0.56
2:D:7:LEU:O	2:D:11:LEU:HG	2.06	0.56
2:N:7:LEU:O	2:N:11:LEU:HG	2.06	0.56
1:A:332:VAL:HG13	1:A:599:THR:HG22	1.87	0.55
1:A:440:PHE:O	1:A:442:MET:N	2.38	0.55
1:A:490:ASN:HB3	1:A:492:VAL:HG23	1.88	0.55
1:B:563:MET:SD	1:B:611:HIS:CD2	2.99	0.55
1:B:707:TYR:HE2	1:B:754:ASN:OD1	1.89	0.55
1:B:712:LEU:CB	1:B:819:PRO:HB2	2.36	0.55
1:B:763:LEU:HD22	1:B:764:PRO:CD	2.36	0.55
2:C:139:TRP:CD1	2:C:139:TRP:C	2.83	0.55
2:D:152:PHE:N	2:D:152:PHE:CD1	2.73	0.55
2:F:8:SER:C	2:F:10:THR:H	2.14	0.55
2:F:10:THR:O	2:F:14:ALA:HB2	2.05	0.55
2:G:14:ALA:C	2:G:16:ASP:H	2.11	0.55
2:I:57:ARG:NH1	2:I:94:ASN:HD21	2.02	0.55
2:I:145:ARG:HB3	2:I:145:ARG:CZ	2.35	0.55
2:O:41:MET:O	2:O:42:ASN:C	2.49	0.55
1:A:314:PHE:O	1:A:316:SER:N	2.38	0.55
1:A:346:ILE:O	1:A:349:MET:HB3	2.06	0.55
1:A:414:VAL:O	1:A:416:ASN:N	2.38	0.55
1:A:738:LEU:HA	1:A:741:THR:HG22	1.88	0.55
1:B:260:GLN:O	1:B:262:VAL:N	2.39	0.55
1:B:363:GLU:O	1:B:363:GLU:HG3	2.05	0.55
2:F:53:ASN:HD22	2:F:354:ALA:HB3	1.71	0.55
2:L:139:TRP:CD1	2:L:139:TRP:C	2.84	0.55
1:A:396:PHE:CB	1:A:578:LEU:HD12	2.37	0.55
1:A:535:LEU:O	1:A:539:ARG:CG	2.55	0.55
1:B:127:GLU:HB3	1:B:151:LYS:HE3	1.87	0.55
1:B:433:ASN:HD21	1:B:446:HIS:HB3	1.71	0.55
2:C:153:HIS:CD2	2:E:153:HIS:NE2	2.75	0.55
2:F:144:ARG:O	2:F:145:ARG:HB2	2.06	0.55
2:N:60:ASN:C	2:N:61:PHE:CD1	2.84	0.55
2:N:99:GLU:HG3	2:N:99:GLU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:116:LEU:CD1	2:N:119:LEU:HD12	2.36	0.55
2:O:8:SER:O	2:O:10:THR:N	2.40	0.55
1:A:275:PRO:HB2	1:A:278:ILE:HG13	1.87	0.55
1:A:606:VAL:O	1:A:607:ASN:C	2.46	0.55
1:A:725:ARG:HB3	1:A:828:GLN:OE1	2.06	0.55
1:A:804:SER:HB2	1:A:810:TYR:CB	2.35	0.55
1:B:428:GLN:HG3	1:B:456:PHE:HD1	1.70	0.55
1:B:577:GLN:C	1:B:579:THR:H	2.14	0.55
2:C:99:GLU:HG3	2:C:99:GLU:O	2.07	0.55
2:C:129:PHE:C	2:C:129:PHE:CD1	2.85	0.55
2:I:35:ASN:HA	2:I:38:ILE:HD12	1.87	0.55
2:J:116:LEU:CD1	2:J:119:LEU:HD12	2.36	0.55
2:O:8:SER:C	2:O:10:THR:H	2.14	0.55
1:A:150:LEU:HD12	1:A:696:SER:CB	2.34	0.55
1:B:392:MET:C	1:B:573:THR:HG23	2.32	0.55
1:B:413:VAL:HG12	1:B:414:VAL:H	1.69	0.55
2:G:106:ARG:HD3	2:G:106:ARG:N	2.22	0.55
2:H:105:GLN:C	2:H:107:ASN:N	2.58	0.55
2:J:128:ASN:HB3	2:K:19:VAL:CG2	2.36	0.55
2:N:6:SER:OG	2:N:128:ASN:HA	2.05	0.55
2:O:23:LEU:HD23	2:O:23:LEU:C	2.31	0.55
1:A:383:ILE:HD11	1:A:550:LEU:HD23	1.89	0.55
1:B:508:GLU:HG2	1:B:512:GLN:HE21	1.71	0.55
1:B:625:ILE:O	1:B:628:ALA:HB3	2.06	0.55
1:B:650:HIS:O	1:B:652:PHE:N	2.39	0.55
1:B:675:GLU:HB3	1:B:678:ARG:HG3	1.88	0.55
1:B:723:ILE:HG22	1:B:724:ALA:N	2.16	0.55
1:B:804:SER:HA	1:B:810:TYR:CZ	2.42	0.55
2:C:144:ARG:HD2	2:D:82:ARG:NH1	2.20	0.55
2:C:145:ARG:O	2:C:146:GLN:HG3	2.06	0.55
2:D:116:LEU:CD1	2:D:119:LEU:HD12	2.36	0.55
2:F:8:SER:O	2:F:10:THR:N	2.39	0.55
2:G:8:SER:C	2:G:10:THR:H	2.14	0.55
2:G:63:PHE:N	2:G:63:PHE:CD1	2.74	0.55
2:H:116:LEU:HD12	2:H:119:LEU:HD12	1.89	0.55
2:J:8:SER:C	2:J:10:THR:H	2.14	0.55
2:K:60:ASN:C	2:K:61:PHE:CD1	2.85	0.55
2:L:35:ASN:HA	2:L:38:ILE:HD12	1.87	0.55
2:L:116:LEU:HD12	2:L:119:LEU:HD12	1.87	0.55
2:O:10:THR:O	2:O:14:ALA:HB2	2.06	0.55
2:O:144:ARG:O	2:O:145:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:GLN:O	1:A:733:ILE:HG23	2.06	0.55
1:B:371:ASN:O	1:B:373:GLN:N	2.39	0.55
1:B:457:GLN:C	1:B:458:ILE:HG13	2.31	0.55
1:B:784:ALA:O	1:B:785:GLN:O	2.25	0.55
1:B:805:ASP:C	1:B:807:ASN:N	2.65	0.55
2:C:10:THR:O	2:C:14:ALA:HB2	2.06	0.55
2:C:82:ARG:NH1	2:E:144:ARG:HD2	2.21	0.55
2:E:8:SER:C	2:E:10:THR:H	2.14	0.55
2:H:99:GLU:HG3	2:H:99:GLU:O	2.07	0.55
2:I:89:VAL:O	2:I:91:PHE:N	2.40	0.55
2:L:8:SER:O	2:L:10:THR:N	2.39	0.55
2:N:139:TRP:CD1	2:N:139:TRP:C	2.84	0.55
2:O:49:GLY:HA2	2:O:54:LEU:CD2	2.37	0.55
1:A:389:GLN:O	1:A:389:GLN:CG	2.54	0.55
1:A:510:LEU:HD22	1:A:540:LEU:CD1	2.26	0.55
1:A:563:MET:O	1:A:565:MET:N	2.40	0.55
1:B:113:PRO:HG2	1:B:609:ASN:HB3	1.89	0.55
1:B:160:TYR:OH	1:B:635:GLN:HG3	2.07	0.55
1:B:710:MET:HE1	1:B:824:LYS:NZ	2.22	0.55
1:B:763:LEU:O	1:B:764:PRO:O	2.25	0.55
1:B:826:TYR:O	1:B:827:LYS:C	2.50	0.55
2:C:152:PHE:N	2:C:152:PHE:CD1	2.74	0.55
2:E:99:GLU:HG3	2:E:99:GLU:O	2.05	0.55
2:F:139:TRP:CD1	2:F:139:TRP:C	2.85	0.55
2:H:8:SER:O	2:H:10:THR:N	2.40	0.55
2:I:101:VAL:HB	2:I:355:ILE:HG21	1.88	0.55
2:I:153:HIS:NE2	2:J:153:HIS:CD2	2.75	0.55
2:J:38:ILE:HG22	2:J:42:ASN:ND2	2.22	0.55
2:K:35:ASN:HA	2:K:38:ILE:CD1	2.37	0.55
1:A:214:ASP:O	1:A:215:GLU:C	2.50	0.55
1:A:675:GLU:O	1:A:676:VAL:C	2.50	0.55
1:B:594:ILE:C	1:B:594:ILE:CD1	2.79	0.55
2:E:139:TRP:CD1	2:E:139:TRP:C	2.84	0.55
2:E:151:THR:C	2:E:152:PHE:CD1	2.84	0.55
2:G:8:SER:O	2:G:10:THR:N	2.40	0.55
2:G:139:TRP:C	2:G:139:TRP:CD1	2.85	0.55
2:I:124:PHE:C	2:I:126:ARG:H	2.14	0.55
2:L:10:THR:O	2:L:14:ALA:HB2	2.06	0.55
2:L:116:LEU:CD1	2:L:119:LEU:HD12	2.37	0.55
2:M:99:GLU:HG3	2:M:99:GLU:O	2.07	0.55
1:A:500:GLY:O	1:A:502:VAL:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ILE:N	1:B:360:ILE:HD12	2.22	0.55
1:B:654:VAL:O	1:B:656:ARG:N	2.39	0.55
1:B:698:LYS:O	1:B:699:ILE:CB	2.53	0.55
2:C:109:ILE:HG23	2:C:110:ALA:H	1.70	0.55
2:C:116:LEU:CD1	2:C:119:LEU:HD12	2.36	0.55
2:C:167:ASN:ND2	2:C:178:GLY:HA2	2.23	0.55
2:E:7:LEU:O	2:E:11:LEU:HG	2.07	0.55
2:F:144:ARG:O	2:F:145:ARG:CB	2.55	0.55
2:F:152:PHE:N	2:F:152:PHE:CD1	2.74	0.55
2:L:35:ASN:O	2:L:36:GLN:C	2.50	0.55
2:N:35:ASN:HA	2:N:38:ILE:HD12	1.89	0.55
1:A:142:LEU:O	1:A:143:ARG:HG2	2.08	0.54
1:A:289:ASP:C	1:A:290:ARG:HG2	2.32	0.54
1:A:369:GLY:O	1:A:370:ILE:C	2.49	0.54
1:A:501:HIS:C	1:A:503:ILE:N	2.62	0.54
1:A:525:TYR:O	1:A:529:ILE:HG13	2.05	0.54
1:A:705:ILE:HG22	1:A:757:VAL:O	2.07	0.54
1:A:793:ASP:C	1:A:795:LEU:N	2.63	0.54
1:B:195:ASP:O	1:B:197:GLY:N	2.39	0.54
1:B:245:LEU:HD12	1:B:250:TYR:HA	1.89	0.54
2:E:116:LEU:HD12	2:E:119:LEU:HD12	1.88	0.54
2:J:131:ASN:N	2:J:131:ASN:HD22	2.04	0.54
2:L:82:ARG:NH1	2:N:144:ARG:HD2	2.22	0.54
2:N:8:SER:O	2:N:10:THR:N	2.40	0.54
1:A:742:GLY:HA3	1:B:285:ILE:HD11	1.89	0.54
1:B:306:ASP:C	1:B:308:LEU:H	2.08	0.54
1:B:388:SER:O	1:B:389:GLN:HB2	2.07	0.54
1:B:779:ASP:HA	1:B:798:ILE:HG13	1.89	0.54
2:C:22:THR:HB	2:E:128:ASN:O	2.08	0.54
2:C:135:TYR:OH	2:C:340:GLU:OE1	2.24	0.54
2:D:144:ARG:HD2	2:E:82:ARG:CZ	2.36	0.54
2:G:35:ASN:HA	2:G:38:ILE:HD12	1.89	0.54
2:I:8:SER:C	2:I:10:THR:H	2.14	0.54
2:I:8:SER:O	2:I:10:THR:N	2.40	0.54
2:I:124:PHE:O	2:I:126:ARG:N	2.39	0.54
2:I:153:HIS:CD2	2:K:153:HIS:NE2	2.75	0.54
2:J:35:ASN:HA	2:J:38:ILE:CD1	2.37	0.54
2:O:30:LEU:O	2:O:31:ILE:C	2.51	0.54
2:O:35:ASN:HA	2:O:38:ILE:CD1	2.37	0.54
1:A:151:LYS:O	1:A:152:LYS:HB2	2.06	0.54
1:A:166:PHE:CE2	1:A:689:MET:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:SER:HB2	1:A:573:THR:HG21	1.90	0.54
1:A:717:MET:SD	1:A:829:VAL:HG22	2.47	0.54
1:A:730:PHE:CD1	1:A:730:PHE:N	2.75	0.54
1:A:863:VAL:HG12	1:A:864:GLU:N	2.22	0.54
1:A:871:PHE:O	1:A:871:PHE:CD1	2.60	0.54
2:E:35:ASN:HA	2:E:38:ILE:CD1	2.37	0.54
2:H:116:LEU:CD1	2:H:119:LEU:HD12	2.38	0.54
2:H:150:PHE:HB2	2:H:152:PHE:CE1	2.43	0.54
2:I:49:GLY:HA2	2:I:54:LEU:HD21	1.90	0.54
2:M:8:SER:O	2:M:10:THR:N	2.40	0.54
2:O:116:LEU:CD1	2:O:119:LEU:HD12	2.37	0.54
2:O:144:ARG:O	2:O:146:GLN:N	2.41	0.54
1:A:111:ILE:O	1:A:111:ILE:HG23	2.07	0.54
1:A:404:LEU:O	1:A:405:ILE:C	2.50	0.54
1:A:549:LEU:HD13	1:A:877:MET:HE3	1.89	0.54
1:B:305:GLN:NE2	1:B:564:ASN:CG	2.65	0.54
1:B:404:LEU:O	1:B:407:GLY:N	2.40	0.54
2:C:8:SER:O	2:C:10:THR:N	2.40	0.54
2:C:16:ASP:HB3	2:E:131:ASN:O	2.06	0.54
2:D:110:ALA:HB1	2:D:111:PRO:HD2	1.89	0.54
2:F:65:LEU:O	2:F:66:LEU:HD23	2.08	0.54
2:M:139:TRP:CD1	2:M:139:TRP:C	2.84	0.54
2:N:42:ASN:HA	2:N:61:PHE:HB2	1.88	0.54
1:A:386:MET:HE2	1:A:480:PHE:HZ	1.73	0.54
1:A:530:GLN:HA	1:A:533:ILE:CD1	2.37	0.54
1:A:663:TYR:O	1:A:666:ARG:HG2	2.08	0.54
1:B:323:THR:O	1:B:326:TYR:HB3	2.08	0.54
1:B:326:TYR:CD1	1:B:384:ALA:CB	2.91	0.54
1:B:370:ILE:O	1:B:373:GLN:HB3	2.08	0.54
1:B:394:LEU:C	1:B:396:PHE:N	2.65	0.54
1:B:480:PHE:O	1:B:481:ARG:C	2.49	0.54
1:B:481:ARG:HG2	2:I:65:LEU:HD12	1.89	0.54
2:E:10:THR:O	2:E:14:ALA:HB2	2.07	0.54
2:F:35:ASN:HA	2:F:38:ILE:HD12	1.90	0.54
2:H:74:ASP:OD2	2:H:76:ASN:HB3	2.07	0.54
2:J:14:ALA:C	2:J:16:ASP:N	2.65	0.54
2:K:8:SER:C	2:K:10:THR:H	2.14	0.54
1:A:688:ASN:O	1:A:689:MET:C	2.51	0.54
1:B:666:ARG:HG3	1:B:667:ASP:N	2.20	0.54
1:B:698:LYS:C	1:B:699:ILE:HD13	2.33	0.54
2:E:116:LEU:CD1	2:E:119:LEU:HD12	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:167:ASN:ND2	2:E:178:GLY:HA2	2.22	0.54
2:G:14:ALA:C	2:G:16:ASP:N	2.66	0.54
2:I:167:ASN:ND2	2:I:178:GLY:HA2	2.22	0.54
2:J:7:LEU:O	2:J:11:LEU:HG	2.06	0.54
2:N:110:ALA:HB1	2:N:111:PRO:CD	2.37	0.54
2:O:139:TRP:C	2:O:139:TRP:CD1	2.85	0.54
2:O:158:PHE:HE2	2:O:214:LEU:HD22	1.73	0.54
1:A:120:THR:HA	1:A:186:MET:HE1	1.88	0.54
1:A:217:THR:HG22	1:A:217:THR:O	2.07	0.54
1:B:428:GLN:HG2	1:B:429:LEU:H	1.71	0.54
1:B:501:HIS:C	1:B:503:ILE:H	2.15	0.54
1:B:875:ARG:CD	1:B:878:ASN:HD22	2.20	0.54
2:C:35:ASN:HA	2:C:38:ILE:CD1	2.38	0.54
2:H:35:ASN:HA	2:H:38:ILE:HD12	1.89	0.54
2:I:106:ARG:H	2:I:106:ARG:HD3	1.72	0.54
2:J:30:LEU:O	2:J:31:ILE:C	2.51	0.54
2:J:99:GLU:HG3	2:J:99:GLU:O	2.08	0.54
2:M:139:TRP:HE1	2:M:143:ASN:ND2	2.04	0.54
1:A:311:HIS:HB3	1:A:318:TRP:NE1	2.23	0.54
1:A:645:PHE:HD2	1:A:646:LEU:HD23	1.72	0.54
1:A:650:HIS:O	1:A:651:ILE:CB	2.56	0.54
1:A:701:GLN:HG2	1:A:826:TYR:CE2	2.43	0.54
2:C:8:SER:C	2:C:10:THR:H	2.14	0.54
2:C:35:ASN:O	2:C:36:GLN:C	2.51	0.54
2:C:60:ASN:C	2:C:61:PHE:CD1	2.85	0.54
2:F:158:PHE:HE2	2:F:214:LEU:HD22	1.73	0.54
2:H:8:SER:C	2:H:10:THR:H	2.14	0.54
2:M:167:ASN:ND2	2:M:178:GLY:HA2	2.23	0.54
1:A:178:PRO:HD2	1:A:256:PHE:CE2	2.43	0.54
1:A:642:VAL:HB	1:A:662:MET:HE2	1.90	0.54
1:B:427:CYS:O	1:B:431:ILE:HG13	2.08	0.54
2:C:153:HIS:O	2:C:154:LYS:C	2.50	0.54
2:D:167:ASN:ND2	2:D:178:GLY:HA2	2.23	0.54
2:G:116:LEU:CD1	2:G:119:LEU:HD12	2.38	0.54
2:K:14:ALA:C	2:K:16:ASP:N	2.65	0.54
2:K:158:PHE:HE2	2:K:214:LEU:HD22	1.73	0.54
2:L:72:ASN:ND2	2:N:126:ARG:NH1	2.56	0.54
2:L:128:ASN:O	2:M:22:THR:HB	2.08	0.54
1:A:273:TYR:O	1:A:273:TYR:CD2	2.61	0.54
1:A:298:TYR:O	1:A:299:ILE:HB	2.06	0.54
1:B:457:GLN:CB	1:B:476:ASN:ND2	2.63	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:SER:O	1:B:581:VAL:C	2.51	0.54
1:B:856:ALA:C	1:B:858:VAL:H	2.14	0.54
2:D:35:ASN:HA	2:D:38:ILE:HD12	1.89	0.54
2:I:7:LEU:O	2:I:11:LEU:HG	2.08	0.54
2:J:27:VAL:O	2:J:30:LEU:N	2.40	0.54
2:M:116:LEU:CD1	2:M:119:LEU:HD12	2.37	0.54
2:N:167:ASN:ND2	2:N:178:GLY:HA2	2.22	0.54
1:A:804:SER:HB2	1:A:810:TYR:HA	1.89	0.53
1:B:125:ILE:N	1:B:125:ILE:CD1	2.71	0.53
1:B:125:ILE:HB	1:B:126:PHE:CD2	2.43	0.53
1:B:184:LYS:C	1:B:186:MET:H	2.15	0.53
1:B:393:SER:CB	1:B:573:THR:HG21	2.38	0.53
1:B:457:GLN:O	1:B:458:ILE:HG13	2.08	0.53
1:B:503:ILE:HD13	1:B:544:VAL:HG12	1.88	0.53
1:B:862:THR:HG22	1:B:863:VAL:O	2.09	0.53
2:D:35:ASN:O	2:D:36:GLN:C	2.51	0.53
2:E:74:ASP:OD2	2:E:76:ASN:HB3	2.08	0.53
2:F:116:LEU:CD1	2:F:119:LEU:HD12	2.38	0.53
2:G:22:THR:OG1	2:G:26:ASN:ND2	2.41	0.53
2:G:150:PHE:HB2	2:G:152:PHE:CE1	2.43	0.53
2:H:23:LEU:N	2:H:26:ASN:ND2	2.57	0.53
2:H:135:TYR:OH	2:H:340:GLU:OE1	2.25	0.53
2:I:158:PHE:HE2	2:I:214:LEU:HD22	1.73	0.53
2:J:35:ASN:O	2:J:36:GLN:C	2.51	0.53
2:K:116:LEU:HD12	2:K:119:LEU:HD12	1.89	0.53
2:K:139:TRP:CD1	2:K:139:TRP:C	2.85	0.53
2:M:35:ASN:HA	2:M:38:ILE:CD1	2.38	0.53
1:B:252:PHE:O	1:B:254:GLU:N	2.40	0.53
1:B:467:GLN:HB3	1:B:512:GLN:HG2	1.90	0.53
2:G:46:PHE:CE2	2:G:119:LEU:HD21	2.43	0.53
2:G:128:ASN:HB3	2:H:19:VAL:CG2	2.37	0.53
2:K:150:PHE:HB2	2:K:152:PHE:CZ	2.42	0.53
2:K:167:ASN:ND2	2:K:178:GLY:HA2	2.22	0.53
2:L:153:HIS:NE2	2:N:153:HIS:NE2	2.55	0.53
2:N:89:VAL:O	2:N:91:PHE:N	2.41	0.53
1:B:449:ASN:HD21	1:B:455:PRO:CG	2.21	0.53
2:C:158:PHE:HE2	2:C:214:LEU:HD22	1.73	0.53
2:D:70:LEU:HD12	2:D:71:LEU:H	1.74	0.53
2:G:129:PHE:CD1	2:G:129:PHE:C	2.86	0.53
2:G:130:ASP:HA	2:H:17:LYS:HG2	1.90	0.53
2:K:215:ARG:HG3	2:K:371:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:41:MET:O	2:L:42:ASN:C	2.51	0.53
2:N:49:GLY:HA2	2:N:54:LEU:CD2	2.39	0.53
2:N:158:PHE:HE2	2:N:214:LEU:HD22	1.73	0.53
2:O:24:TYR:O	2:O:27:VAL:HG22	2.09	0.53
2:O:144:ARG:C	2:O:145:ARG:HG2	2.33	0.53
1:A:322:THR:O	1:A:323:THR:C	2.50	0.53
1:A:503:ILE:HG22	1:A:506:LEU:H	1.73	0.53
1:A:705:ILE:O	1:A:705:ILE:HG12	2.07	0.53
1:B:211:ILE:O	1:B:213:GLN:N	2.41	0.53
1:B:436:ILE:O	1:B:437:TYR:C	2.51	0.53
1:B:789:LEU:O	1:B:790:ARG:C	2.51	0.53
2:E:116:LEU:HA	2:E:119:LEU:CD1	2.38	0.53
2:I:35:ASN:HA	2:I:38:ILE:CD1	2.38	0.53
2:J:150:PHE:HB2	2:J:152:PHE:CZ	2.42	0.53
2:K:30:LEU:O	2:K:31:ILE:C	2.52	0.53
2:L:38:ILE:O	2:L:42:ASN:OD1	2.27	0.53
2:O:215:ARG:HG3	2:O:371:ILE:O	2.09	0.53
1:A:542:GLN:O	1:A:545:ASP:HB2	2.08	0.53
1:B:94:THR:HG23	1:B:658:PRO:HG3	1.90	0.53
1:B:122:LEU:HD11	1:B:200:VAL:HG12	1.88	0.53
1:B:170:TYR:CE1	1:B:681:ILE:CG2	2.92	0.53
1:B:182:LEU:HD23	1:B:183:LEU:N	2.15	0.53
1:B:199:VAL:HG12	1:B:200:VAL:H	1.70	0.53
1:B:246:HIS:CE1	1:B:247:PRO:HD2	2.44	0.53
1:B:293:PRO:C	1:B:295:THR:N	2.60	0.53
1:B:457:GLN:C	1:B:459:ALA:N	2.57	0.53
1:B:497:ILE:HG23	2:I:68:THR:HG23	1.89	0.53
2:C:130:ASP:C	2:C:131:ASN:HD22	2.17	0.53
2:D:144:ARG:HD2	2:E:82:ARG:NH1	2.23	0.53
2:G:99:GLU:O	2:G:99:GLU:HG3	2.09	0.53
2:H:14:ALA:C	2:H:16:ASP:N	2.66	0.53
2:H:149:GLY:C	2:H:150:PHE:CD1	2.87	0.53
2:H:158:PHE:HE2	2:H:214:LEU:HD22	1.73	0.53
2:I:215:ARG:HG3	2:I:371:ILE:O	2.09	0.53
2:J:116:LEU:HA	2:J:119:LEU:CD1	2.38	0.53
2:K:35:ASN:O	2:K:36:GLN:C	2.51	0.53
2:L:63:PHE:N	2:L:63:PHE:CD1	2.75	0.53
2:L:158:PHE:HE2	2:L:214:LEU:HD22	1.73	0.53
2:N:215:ARG:HG3	2:N:371:ILE:O	2.09	0.53
1:A:311:HIS:NE2	1:A:566:GLN:NE2	2.54	0.53
1:A:384:ALA:O	1:A:385:ALA:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:HD22	1:A:584:LEU:HD21	1.90	0.53
1:A:560:CYS:CB	1:A:603:TYR:HD2	2.21	0.53
1:B:133:ILE:HD11	1:B:147:TYR:CE1	2.43	0.53
1:B:200:VAL:HB	1:B:204:THR:HG21	1.89	0.53
1:B:298:TYR:CD1	1:B:299:ILE:N	2.75	0.53
1:B:428:GLN:CG	1:B:456:PHE:HD1	2.21	0.53
1:B:442:MET:O	1:B:443:GLN:C	2.50	0.53
1:B:498:ARG:HG3	1:B:505:GLN:HE22	1.73	0.53
1:B:770:SER:HB3	1:B:772:ILE:HG22	1.90	0.53
2:F:99:GLU:HG3	2:F:99:GLU:O	2.08	0.53
1:A:226:ALA:C	1:A:228:MET:H	2.15	0.53
1:A:545:ASP:O	1:A:546:LEU:C	2.51	0.53
1:A:642:VAL:HG13	1:A:665:LEU:HD23	1.90	0.53
1:A:750:MET:HE2	1:A:757:VAL:HG21	1.91	0.53
2:D:116:LEU:HA	2:D:119:LEU:CD1	2.39	0.53
2:E:158:PHE:HE2	2:E:214:LEU:HD22	1.73	0.53
2:G:158:PHE:HE2	2:G:214:LEU:HD22	1.73	0.53
2:H:35:ASN:O	2:H:36:GLN:C	2.51	0.53
2:J:158:PHE:HE2	2:J:214:LEU:HD22	1.73	0.53
2:K:131:ASN:HD22	2:K:131:ASN:N	2.05	0.53
2:L:215:ARG:HG3	2:L:371:ILE:O	2.09	0.53
2:N:35:ASN:HA	2:N:38:ILE:CD1	2.38	0.53
2:O:167:ASN:ND2	2:O:178:GLY:HA2	2.22	0.53
1:A:238:VAL:HG12	1:A:239:VAL:N	2.24	0.53
1:A:487:GLY:O	1:A:488:VAL:HG23	2.08	0.53
1:A:491:GLN:HB3	1:A:564:ASN:HB3	1.90	0.53
1:A:629:ASN:C	1:A:631:LEU:N	2.61	0.53
1:B:400:ASN:ND2	1:B:403:SER:OG	2.41	0.53
1:B:415:PRO:O	1:B:416:ASN:C	2.52	0.53
1:B:436:ILE:O	1:B:438:PRO:N	2.42	0.53
1:B:498:ARG:CB	2:I:32:GLN:NE2	2.66	0.53
2:C:30:LEU:O	2:C:31:ILE:C	2.52	0.53
2:E:35:ASN:O	2:E:36:GLN:C	2.52	0.53
2:E:110:ALA:HB1	2:E:111:PRO:CD	2.39	0.53
2:F:144:ARG:HD2	2:G:82:ARG:CZ	2.38	0.53
2:I:99:GLU:HG3	2:I:99:GLU:O	2.09	0.53
2:I:116:LEU:HA	2:I:119:LEU:CD1	2.38	0.53
2:I:144:ARG:HD2	2:J:82:ARG:NH1	2.24	0.53
2:N:35:ASN:O	2:N:36:GLN:C	2.51	0.53
2:O:74:ASP:OD2	2:O:76:ASN:HB3	2.09	0.53
1:A:271:PHE:O	1:A:274:ILE:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASN:O	1:A:328:LEU:HB3	2.09	0.53
1:A:460:GLU:C	1:A:462:GLN:H	2.16	0.53
1:A:771:VAL:HA	1:A:802:ILE:HD11	1.91	0.53
1:A:853:ASP:O	1:A:854:LEU:CB	2.56	0.53
1:A:876:ILE:HG22	1:A:877:MET:HG2	1.89	0.53
1:B:190:ASN:O	1:B:190:ASN:CG	2.52	0.53
1:B:548:ARG:HD3	1:B:877:MET:H	1.73	0.53
1:B:755:GLN:O	1:B:757:VAL:HG23	2.08	0.53
1:B:785:GLN:O	1:B:786:ILE:C	2.51	0.53
1:B:786:ILE:O	1:B:788:LYS:N	2.41	0.53
2:C:215:ARG:HG3	2:C:371:ILE:O	2.09	0.53
2:H:167:ASN:ND2	2:H:178:GLY:HA2	2.23	0.53
2:H:215:ARG:HG3	2:H:371:ILE:O	2.09	0.53
2:I:45:GLU:C	2:I:46:PHE:CD1	2.87	0.53
2:K:46:PHE:CE2	2:K:119:LEU:HD21	2.41	0.53
2:K:116:LEU:CD1	2:K:119:LEU:HD12	2.39	0.53
2:L:30:LEU:O	2:L:31:ILE:C	2.52	0.53
2:M:145:ARG:NH1	2:M:145:ARG:CB	2.71	0.53
2:M:158:PHE:HE2	2:M:214:LEU:HD22	1.74	0.53
2:N:31:ILE:O	2:N:34:PHE:HB3	2.09	0.53
2:O:32:GLN:O	2:O:33:GLN:C	2.52	0.53
2:O:89:VAL:O	2:O:91:PHE:N	2.42	0.53
1:A:363:GLU:C	1:A:366:PHE:HE1	2.16	0.53
1:A:661:GLN:NE2	1:B:348:LYS:HZ2	2.06	0.53
1:A:769:SER:O	1:A:770:SER:C	2.51	0.53
1:B:182:LEU:CD2	1:B:183:LEU:N	2.71	0.53
1:B:387:LEU:O	1:B:389:GLN:N	2.42	0.53
1:B:501:HIS:ND1	1:B:548:ARG:HG2	2.24	0.53
1:B:508:GLU:OE2	2:J:70:LEU:HD23	2.09	0.53
1:B:642:VAL:O	1:B:645:PHE:HB3	2.09	0.53
1:B:654:VAL:HG12	1:B:655:ALA:N	2.24	0.53
1:B:655:ALA:C	1:B:657:VAL:H	2.17	0.53
1:B:708:ARG:O	1:B:710:MET:N	2.42	0.53
2:D:35:ASN:HA	2:D:38:ILE:CD1	2.39	0.53
2:F:167:ASN:ND2	2:F:178:GLY:HA2	2.22	0.53
2:G:215:ARG:HG3	2:G:371:ILE:O	2.09	0.53
2:J:215:ARG:HG3	2:J:371:ILE:O	2.09	0.53
2:M:215:ARG:HG3	2:M:371:ILE:O	2.09	0.53
2:O:99:GLU:O	2:O:99:GLU:HG3	2.09	0.53
1:A:297:ARG:HG3	1:A:848:PHE:CE2	2.43	0.52
1:A:323:THR:O	1:A:326:TYR:HB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:TYR:CD1	1:A:401:TYR:N	2.75	0.52
1:A:660:ASP:C	1:A:662:MET:N	2.66	0.52
1:A:721:VAL:CG1	1:A:799:LEU:HD22	2.39	0.52
1:A:794:THR:O	1:A:794:THR:HG22	2.08	0.52
1:B:437:TYR:HD2	1:B:443:GLN:HB3	1.73	0.52
1:B:442:MET:CE	1:B:463:ILE:HG12	2.19	0.52
1:B:499:ASN:O	1:B:500:GLY:O	2.27	0.52
1:B:654:VAL:O	1:B:657:VAL:HG23	2.08	0.52
1:B:742:GLY:O	1:B:744:TYR:CE2	2.62	0.52
2:C:150:PHE:HA	2:D:397:LYS:HZ1	1.74	0.52
2:I:37:MET:O	2:I:38:ILE:C	2.53	0.52
2:K:89:VAL:O	2:K:91:PHE:N	2.43	0.52
2:L:152:PHE:N	2:L:152:PHE:CD1	2.77	0.52
2:N:14:ALA:C	2:N:16:ASP:N	2.65	0.52
1:A:255:TYR:O	1:A:259:HIS:HB3	2.08	0.52
1:A:365:GLN:C	1:A:366:PHE:CG	2.88	0.52
1:A:424:LEU:HD12	1:A:424:LEU:O	2.08	0.52
1:A:618:ILE:HD13	1:A:645:PHE:CZ	2.44	0.52
1:B:135:ARG:O	1:B:138:GLY:N	2.43	0.52
1:B:326:TYR:CE1	1:B:384:ALA:HB3	2.44	0.52
1:B:384:ALA:O	1:B:385:ALA:C	2.50	0.52
1:B:478:ASN:C	1:B:480:PHE:H	2.17	0.52
1:B:540:LEU:HD23	1:B:540:LEU:C	2.34	0.52
1:B:663:TYR:O	1:B:666:ARG:HG2	2.09	0.52
2:I:35:ASN:O	2:I:36:GLN:C	2.52	0.52
2:I:41:MET:O	2:I:42:ASN:C	2.52	0.52
2:L:61:PHE:O	2:L:62:ASP:HB3	2.07	0.52
2:M:14:ALA:C	2:M:16:ASP:N	2.66	0.52
2:M:30:LEU:O	2:M:31:ILE:C	2.52	0.52
2:M:48:THR:O	2:M:56:ILE:HA	2.10	0.52
2:O:35:ASN:O	2:O:36:GLN:C	2.52	0.52
1:A:225:ILE:HA	1:A:228:MET:CE	2.32	0.52
1:A:329:ALA:O	1:A:333:VAL:HG23	2.10	0.52
1:A:340:VAL:HB	1:A:587:LEU:CD2	2.39	0.52
1:A:658:PRO:HB2	1:A:660:ASP:OD1	2.09	0.52
1:B:311:HIS:CD2	1:B:566:GLN:OE1	2.62	0.52
1:B:525:TYR:O	1:B:529:ILE:HG13	2.08	0.52
1:B:807:ASN:C	1:B:809:PHE:N	2.66	0.52
2:C:381:ASN:O	2:C:385:VAL:HB	2.10	0.52
2:D:42:ASN:HA	2:D:61:PHE:HB2	1.92	0.52
2:D:158:PHE:HE2	2:D:214:LEU:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:ARG:HG3	2:D:371:ILE:O	2.09	0.52
2:G:35:ASN:O	2:G:36:GLN:C	2.52	0.52
2:H:150:PHE:HB2	2:H:152:PHE:CZ	2.44	0.52
2:M:41:MET:O	2:M:42:ASN:C	2.52	0.52
2:M:101:VAL:HG23	2:M:102:ARG:N	2.24	0.52
2:M:116:LEU:HA	2:M:119:LEU:CD1	2.38	0.52
2:O:110:ALA:HB1	2:O:111:PRO:HD2	1.90	0.52
2:O:116:LEU:HA	2:O:119:LEU:CD1	2.39	0.52
1:A:326:TYR:CD1	1:A:384:ALA:CB	2.92	0.52
1:A:361:GLN:HG3	1:A:362:SER:H	1.75	0.52
1:A:555:GLU:OE2	1:A:871:PHE:CE2	2.63	0.52
1:B:89:GLU:C	1:B:91:LEU:H	2.16	0.52
1:B:296:ALA:C	1:B:297:ARG:HG2	2.35	0.52
1:B:418:MET:HB3	1:B:567:HIS:NE2	2.24	0.52
1:B:431:ILE:O	1:B:435:ILE:HB	2.09	0.52
1:B:689:MET:HA	1:B:692:ILE:HD13	1.91	0.52
2:C:14:ALA:C	2:C:16:ASP:N	2.65	0.52
2:D:24:TYR:CZ	2:D:68:THR:HG22	2.44	0.52
2:E:14:ALA:C	2:E:16:ASP:N	2.66	0.52
2:E:135:TYR:OH	2:E:342:MET:HE3	2.09	0.52
2:F:30:LEU:O	2:F:31:ILE:C	2.53	0.52
2:F:35:ASN:O	2:F:36:GLN:C	2.53	0.52
2:G:35:ASN:HA	2:G:38:ILE:CD1	2.39	0.52
2:I:74:ASP:OD2	2:I:76:ASN:HB3	2.08	0.52
2:J:150:PHE:HB2	2:J:152:PHE:HE1	1.73	0.52
2:L:167:ASN:ND2	2:L:178:GLY:HA2	2.22	0.52
2:M:31:ILE:O	2:M:34:PHE:HB3	2.09	0.52
2:M:35:ASN:O	2:M:36:GLN:C	2.51	0.52
2:O:23:LEU:HB3	2:O:26:ASN:HD21	1.73	0.52
1:A:383:ILE:O	1:A:384:ALA:C	2.53	0.52
1:A:421:ARG:O	1:A:425:VAL:HG23	2.10	0.52
1:A:636:LYS:O	1:A:637:LYS:C	2.52	0.52
1:A:742:GLY:O	1:A:743:ASP:O	2.28	0.52
1:A:872:ASP:OD2	1:A:874:MET:HB2	2.10	0.52
1:B:277:ARG:NH1	1:B:559:ALA:HB2	2.25	0.52
1:B:340:VAL:O	1:B:587:LEU:HD11	2.09	0.52
1:B:563:MET:HE3	1:B:563:MET:CA	2.35	0.52
2:D:32:GLN:O	2:D:33:GLN:C	2.52	0.52
2:D:74:ASP:OD2	2:D:76:ASN:HB3	2.09	0.52
2:F:150:PHE:HB2	2:F:152:PHE:CZ	2.44	0.52
2:F:381:ASN:O	2:F:385:VAL:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:381:ASN:O	2:G:385:VAL:HB	2.10	0.52
2:K:53:ASN:ND2	2:K:354:ALA:HB3	2.25	0.52
2:N:116:LEU:HA	2:N:119:LEU:CD1	2.39	0.52
1:A:464:GLN:O	1:A:465:ASN:HB2	2.08	0.52
1:B:527:ARG:O	1:B:531:ARG:HG2	2.08	0.52
1:B:527:ARG:HG3	1:B:527:ARG:HH11	1.74	0.52
1:B:558:MET:O	1:B:561:VAL:HG23	2.09	0.52
1:B:763:LEU:HD22	1:B:764:PRO:HD2	1.92	0.52
1:B:811:LEU:N	1:B:811:LEU:HD23	2.24	0.52
2:E:30:LEU:O	2:E:31:ILE:C	2.51	0.52
2:E:215:ARG:HG3	2:E:371:ILE:O	2.09	0.52
2:F:215:ARG:HG3	2:F:371:ILE:O	2.09	0.52
2:G:7:LEU:O	2:G:11:LEU:HG	2.09	0.52
2:H:57:ARG:NH1	2:H:94:ASN:HD21	2.07	0.52
2:M:21:GLY:O	2:M:22:THR:O	2.28	0.52
2:M:37:MET:O	2:M:38:ILE:C	2.53	0.52
2:N:32:GLN:O	2:N:33:GLN:C	2.53	0.52
2:O:153:HIS:O	2:O:154:LYS:C	2.52	0.52
1:B:326:TYR:HD1	1:B:384:ALA:HB1	1.75	0.52
1:B:570:THR:HG22	1:B:571:LEU:H	1.75	0.52
1:B:632:ASN:O	1:B:634:TYR:N	2.38	0.52
1:B:639:LYS:O	1:B:640:ALA:C	2.52	0.52
1:B:771:VAL:CG1	1:B:772:ILE:N	2.71	0.52
2:E:32:GLN:O	2:E:33:GLN:C	2.52	0.52
2:F:5:TYR:HE2	2:F:131:ASN:HA	1.75	0.52
2:I:14:ALA:O	2:I:18:ILE:HD12	2.10	0.52
2:J:167:ASN:ND2	2:J:178:GLY:HA2	2.23	0.52
2:J:381:ASN:O	2:J:385:VAL:HB	2.10	0.52
2:K:381:ASN:O	2:K:385:VAL:HB	2.10	0.52
2:L:381:ASN:O	2:L:385:VAL:HB	2.10	0.52
2:N:12:LYS:O	2:N:14:ALA:N	2.43	0.52
2:N:381:ASN:O	2:N:385:VAL:HB	2.10	0.52
2:O:381:ASN:O	2:O:385:VAL:HB	2.10	0.52
1:A:786:ILE:O	1:A:789:LEU:N	2.43	0.52
1:B:812:VAL:HG23	1:B:817:TRP:CZ3	2.45	0.52
2:D:23:LEU:HD22	2:D:25:SER:OG	2.10	0.52
2:G:153:HIS:O	2:G:154:LYS:C	2.53	0.52
2:L:31:ILE:O	2:L:34:PHE:HB3	2.10	0.52
2:M:89:VAL:O	2:M:91:PHE:N	2.43	0.52
1:A:163:ARG:NH2	1:A:736:GLU:OE2	2.42	0.52
1:A:323:THR:OG1	1:A:390:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLN:HB3	1:A:512:GLN:HG2	1.92	0.52
1:B:314:PHE:N	1:B:314:PHE:CD1	2.77	0.52
1:B:444:ARG:HH22	1:B:520:THR:HA	1.75	0.52
1:B:540:LEU:HA	1:B:543:LEU:HB2	1.92	0.52
1:B:583:SER:O	1:B:584:LEU:C	2.53	0.52
1:B:723:ILE:CG2	1:B:724:ALA:H	2.13	0.52
2:I:135:TYR:OH	2:I:342:MET:HE3	2.09	0.52
2:K:32:GLN:O	2:K:33:GLN:C	2.53	0.52
2:K:99:GLU:O	2:K:99:GLU:HG3	2.10	0.52
2:L:35:ASN:HA	2:L:38:ILE:CD1	2.39	0.52
2:L:37:MET:O	2:L:38:ILE:C	2.53	0.52
2:L:106:ARG:HD3	2:L:106:ARG:N	2.17	0.52
2:L:110:ALA:HB1	2:L:111:PRO:HD2	1.92	0.52
1:A:205:ALA:O	1:A:206:SER:C	2.52	0.52
1:A:428:GLN:CD	1:A:456:PHE:N	2.67	0.52
1:A:494:ASN:CG	1:A:495:ASP:N	2.67	0.52
1:A:516:GLN:C	1:A:518:PHE:H	2.18	0.52
2:F:35:ASN:HA	2:F:38:ILE:CD1	2.40	0.52
2:F:135:TYR:OH	2:F:340:GLU:OE1	2.28	0.52
2:H:128:ASN:O	2:H:129:PHE:HB3	2.09	0.52
2:H:151:THR:C	2:H:152:PHE:CD1	2.88	0.52
2:L:32:GLN:O	2:L:33:GLN:C	2.52	0.52
2:M:131:ASN:HD22	2:M:131:ASN:N	2.07	0.52
1:A:310:LEU:O	1:A:318:TRP:CD1	2.62	0.51
1:A:647:LYS:C	1:A:649:LEU:N	2.68	0.51
1:A:769:SER:O	1:A:771:VAL:N	2.43	0.51
1:B:235:ASP:O	1:B:236:ARG:HB2	2.10	0.51
1:B:286:LEU:HD22	1:B:286:LEU:N	2.25	0.51
1:B:530:GLN:HA	1:B:533:ILE:CD1	2.40	0.51
1:B:563:MET:HA	1:B:563:MET:CE	2.39	0.51
2:C:116:LEU:HA	2:C:119:LEU:CD1	2.40	0.51
2:G:30:LEU:O	2:G:31:ILE:C	2.52	0.51
2:I:124:PHE:C	2:I:126:ARG:N	2.68	0.51
2:J:89:VAL:O	2:J:91:PHE:N	2.43	0.51
2:M:27:VAL:CG2	2:M:31:ILE:HD11	2.40	0.51
2:O:133:SER:O	2:O:136:ILE:HG22	2.10	0.51
1:A:125:ILE:N	1:A:125:ILE:CD1	2.63	0.51
1:A:269:ILE:HG21	1:A:298:TYR:HE2	1.76	0.51
1:A:286:LEU:O	1:A:287:ASN:HB2	2.09	0.51
1:A:431:ILE:HG23	1:A:435:ILE:HD12	1.91	0.51
1:B:378:CYS:SG	1:B:581:VAL:HA	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLU:O	1:B:425:VAL:N	2.43	0.51
1:B:653:ASP:O	1:B:653:ASP:CG	2.52	0.51
2:C:27:VAL:O	2:C:30:LEU:N	2.38	0.51
2:D:105:GLN:NE2	2:D:359:PRO:O	2.43	0.51
2:H:145:ARG:O	2:H:146:GLN:HG3	2.10	0.51
2:J:11:LEU:O	2:J:15:ARG:N	2.39	0.51
2:K:74:ASP:OD2	2:K:76:ASN:HB3	2.10	0.51
2:M:32:GLN:O	2:M:33:GLN:C	2.52	0.51
1:A:259:HIS:HD1	1:A:260:GLN:N	2.07	0.51
1:A:326:TYR:CE1	1:A:384:ALA:HB3	2.45	0.51
1:A:332:VAL:O	1:A:333:VAL:C	2.53	0.51
1:A:647:LYS:O	1:A:649:LEU:N	2.43	0.51
1:A:803:ASN:C	1:A:805:ASP:N	2.63	0.51
1:B:133:ILE:HD11	1:B:147:TYR:HE1	1.76	0.51
1:B:503:ILE:O	1:B:504:ASN:C	2.54	0.51
2:C:24:TYR:OH	2:C:68:THR:HG22	2.10	0.51
2:D:6:SER:O	2:D:8:SER:N	2.44	0.51
2:E:135:TYR:OH	2:E:340:GLU:OE1	2.28	0.51
2:G:32:GLN:O	2:G:33:GLN:C	2.53	0.51
2:H:76:ASN:N	2:J:76:ASN:HB2	2.24	0.51
2:H:148:THR:OG1	2:H:332:GLU:HG2	2.10	0.51
2:I:128:ASN:HD22	2:J:19:VAL:CB	2.21	0.51
2:L:116:LEU:HA	2:L:119:LEU:CD1	2.40	0.51
2:M:381:ASN:O	2:M:385:VAL:HB	2.10	0.51
2:N:37:MET:O	2:N:38:ILE:C	2.53	0.51
1:A:420:ILE:HG12	1:A:423:SER:CB	2.38	0.51
1:A:519:PRO:O	1:A:520:THR:HG23	2.10	0.51
1:A:645:PHE:CD2	1:A:646:LEU:HD23	2.44	0.51
1:B:442:MET:SD	1:B:463:ILE:HA	2.49	0.51
1:B:460:GLU:HG3	1:B:473:HIS:HD2	1.76	0.51
1:B:498:ARG:HG3	1:B:505:GLN:NE2	2.26	0.51
1:B:498:ARG:CG	1:B:505:GLN:HE22	2.23	0.51
1:B:639:LYS:O	1:B:642:VAL:HG23	2.10	0.51
1:B:699:ILE:HG13	1:B:763:LEU:O	2.10	0.51
1:B:779:ASP:HA	1:B:798:ILE:CG1	2.39	0.51
2:C:74:ASP:OD2	2:C:76:ASN:HB3	2.11	0.51
2:D:381:ASN:O	2:D:385:VAL:HB	2.10	0.51
2:E:6:SER:O	2:E:8:SER:N	2.44	0.51
2:E:89:VAL:O	2:E:91:PHE:N	2.44	0.51
2:G:89:VAL:O	2:G:91:PHE:N	2.44	0.51
2:H:5:TYR:HE2	2:H:131:ASN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:30:LEU:O	2:N:31:ILE:C	2.54	0.51
1:A:631:LEU:O	1:A:633:LEU:HD12	2.10	0.51
1:A:661:GLN:HG3	1:B:348:LYS:NZ	2.26	0.51
1:A:773:SER:HB3	1:A:778:LEU:HD12	1.91	0.51
1:B:104:ILE:HD12	1:B:327:ILE:HD12	1.92	0.51
1:B:548:ARG:HH11	1:B:878:ASN:N	2.04	0.51
1:B:705:ILE:HG22	1:B:707:TYR:CE1	2.45	0.51
2:D:89:VAL:O	2:D:91:PHE:N	2.43	0.51
2:H:31:ILE:O	2:H:34:PHE:HB3	2.11	0.51
2:K:155:PRO:O	2:K:186:SER:HB3	2.10	0.51
2:M:253:ILE:HD13	2:M:319:THR:HB	1.93	0.51
2:N:133:SER:O	2:N:136:ILE:HG22	2.11	0.51
2:O:106:ARG:HD3	2:O:106:ARG:N	2.23	0.51
1:A:252:PHE:O	1:A:254:GLU:N	2.44	0.51
1:A:427:CYS:O	1:A:431:ILE:HG13	2.11	0.51
1:A:443:GLN:NE2	1:A:521:MET:HB3	2.25	0.51
1:A:817:TRP:CD1	1:A:818:VAL:H	2.28	0.51
1:B:178:PRO:HD2	1:B:256:PHE:CE2	2.45	0.51
1:B:272:ASN:O	1:B:274:ILE:N	2.43	0.51
1:B:431:ILE:HG23	1:B:435:ILE:HD12	1.93	0.51
1:B:481:ARG:NH2	1:B:496:ASN:HD21	2.08	0.51
2:E:31:ILE:O	2:E:34:PHE:HB3	2.09	0.51
2:I:32:GLN:O	2:I:33:GLN:C	2.54	0.51
2:K:116:LEU:HA	2:K:119:LEU:CD1	2.41	0.51
2:L:89:VAL:O	2:L:91:PHE:N	2.43	0.51
2:L:153:HIS:O	2:L:154:LYS:C	2.54	0.51
2:N:66:LEU:O	2:N:67:GLY:C	2.53	0.51
2:O:60:ASN:C	2:O:61:PHE:CD1	2.89	0.51
1:A:158:GLY:O	1:A:162:VAL:HG23	2.09	0.51
1:A:159:ASP:O	1:A:162:VAL:HB	2.11	0.51
1:B:302:ASN:O	1:B:303:LEU:HD23	2.11	0.51
1:B:305:GLN:NE2	1:B:564:ASN:ND2	2.58	0.51
2:C:110:ALA:HB1	2:C:111:PRO:CD	2.41	0.51
2:D:360:VAL:O	2:D:378:ARG:HD3	2.11	0.51
2:E:41:MET:O	2:E:42:ASN:C	2.52	0.51
2:F:109:ILE:CB	2:F:380:ASP:HB3	2.40	0.51
2:H:381:ASN:O	2:H:385:VAL:HB	2.10	0.51
2:I:1:MET:C	2:I:3:VAL:N	2.67	0.51
2:J:32:GLN:O	2:J:33:GLN:C	2.54	0.51
2:J:253:ILE:HD13	2:J:319:THR:HB	1.92	0.51
2:K:106:ARG:HD3	2:K:106:ARG:N	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:253:ILE:HD13	2:K:319:THR:HB	1.93	0.51
2:O:31:ILE:O	2:O:34:PHE:HB3	2.11	0.51
2:O:54:LEU:HD12	2:O:55:PRO:HD2	1.93	0.51
2:O:253:ILE:HD13	2:O:319:THR:HB	1.93	0.51
1:A:326:TYR:HD1	1:A:384:ALA:HB1	1.75	0.51
1:A:772:ILE:O	1:A:773:SER:C	2.54	0.51
1:B:298:TYR:CD1	1:B:298:TYR:C	2.88	0.51
1:B:481:ARG:CZ	1:B:496:ASN:OD1	2.59	0.51
1:B:491:GLN:HG3	1:B:491:GLN:O	2.10	0.51
1:B:658:PRO:HD2	1:B:661:GLN:HG3	1.93	0.51
2:C:42:ASN:HA	2:C:61:PHE:HB2	1.92	0.51
2:E:381:ASN:O	2:E:385:VAL:HB	2.10	0.51
2:F:23:LEU:HD11	2:H:36:GLN:OE1	2.10	0.51
2:F:360:VAL:O	2:F:378:ARG:HD3	2.11	0.51
2:G:111:PRO:HB3	2:G:116:LEU:CD2	2.41	0.51
2:H:35:ASN:HA	2:H:38:ILE:CD1	2.41	0.51
2:I:14:ALA:C	2:I:16:ASP:N	2.66	0.51
2:I:381:ASN:O	2:I:385:VAL:HB	2.10	0.51
2:J:12:LYS:O	2:J:14:ALA:N	2.43	0.51
2:J:360:VAL:O	2:J:378:ARG:HD3	2.11	0.51
2:M:24:TYR:O	2:M:26:ASN:N	2.44	0.51
2:M:106:ARG:HG2	2:M:107:ASN:H	1.75	0.51
2:M:109:ILE:HB	2:M:380:ASP:HB3	1.93	0.51
2:M:360:VAL:O	2:M:378:ARG:HD3	2.11	0.51
2:O:1:MET:O	2:O:2:ASP:C	2.53	0.51
1:A:130:GLN:O	1:A:131:LEU:HB3	2.10	0.51
1:A:368:THR:O	1:A:368:THR:HG22	2.09	0.51
1:A:631:LEU:CB	1:A:633:LEU:HD13	2.38	0.51
1:B:608:VAL:O	1:B:609:ASN:C	2.54	0.51
1:B:712:LEU:HD11	1:B:722:ASN:HB3	1.93	0.51
1:B:869:VAL:N	1:B:876:ILE:HG23	2.26	0.51
2:C:17:LYS:HG2	2:E:130:ASP:HA	1.92	0.51
2:C:89:VAL:O	2:C:91:PHE:N	2.43	0.51
2:F:89:VAL:O	2:F:91:PHE:N	2.44	0.51
2:G:253:ILE:HD13	2:G:319:THR:HB	1.93	0.51
2:G:360:VAL:O	2:G:378:ARG:HD3	2.11	0.51
1:A:362:SER:HB2	1:A:365:GLN:HE22	1.72	0.51
1:A:527:ARG:O	1:A:531:ARG:HG2	2.10	0.51
1:A:546:LEU:HD11	1:A:584:LEU:HD23	1.93	0.51
1:A:601:PHE:O	1:A:602:HIS:C	2.54	0.51
1:A:618:ILE:O	1:A:622:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:GLN:O	1:A:761:GLY:O	2.29	0.51
1:B:140:LYS:HE2	1:B:805:ASP:OD2	2.10	0.51
2:C:41:MET:O	2:C:42:ASN:C	2.53	0.51
2:C:128:ASN:HB3	2:D:19:VAL:HG23	1.93	0.51
2:F:63:PHE:CD2	2:F:84:THR:HG23	2.46	0.51
2:F:74:ASP:OD2	2:F:76:ASN:HB3	2.11	0.51
2:G:41:MET:O	2:G:42:ASN:C	2.54	0.51
2:G:103:GLU:HG3	2:G:359:PRO:HD2	1.93	0.51
2:G:116:LEU:HA	2:G:119:LEU:CD1	2.40	0.51
2:J:153:HIS:NE2	2:K:153:HIS:NE2	2.59	0.51
2:K:129:PHE:C	2:K:129:PHE:CD1	2.89	0.51
1:A:508:GLU:O	1:A:512:GLN:NE2	2.45	0.50
1:A:555:GLU:OE1	1:A:871:PHE:HD2	1.93	0.50
1:A:676:VAL:O	1:A:680:ASP:HB2	2.10	0.50
1:A:706:ALA:C	1:A:708:ARG:H	2.19	0.50
1:A:775:ILE:C	1:A:777:LYS:H	2.19	0.50
1:B:178:PRO:HD2	1:B:256:PHE:CD2	2.45	0.50
1:B:509:ALA:O	1:B:513:LEU:CG	2.50	0.50
1:B:539:ARG:O	1:B:542:GLN:N	2.44	0.50
1:B:854:LEU:O	1:B:855:LEU:C	2.54	0.50
2:C:49:GLY:HA2	2:C:54:LEU:HD23	1.93	0.50
2:F:253:ILE:HD13	2:F:319:THR:HB	1.93	0.50
2:H:12:LYS:O	2:H:14:ALA:N	2.44	0.50
2:H:116:LEU:HA	2:H:119:LEU:CD1	2.40	0.50
2:K:11:LEU:O	2:K:15:ARG:N	2.38	0.50
2:L:99:GLU:O	2:L:99:GLU:HG3	2.10	0.50
2:N:135:TYR:OH	2:N:340:GLU:OE1	2.25	0.50
1:A:452:PRO:O	1:A:453:GLN:CB	2.58	0.50
1:A:467:GLN:NE2	1:A:511:MET:HG2	2.25	0.50
1:B:182:LEU:HD11	1:B:847:THR:CA	2.40	0.50
1:B:449:ASN:ND2	1:B:455:PRO:CG	2.75	0.50
1:B:527:ARG:O	1:B:531:ARG:HG3	2.10	0.50
1:B:671:LEU:O	1:B:672:LEU:HD23	2.10	0.50
1:B:783:PHE:O	1:B:784:ALA:C	2.54	0.50
2:C:133:SER:O	2:C:136:ILE:HG22	2.12	0.50
2:D:30:LEU:O	2:D:31:ILE:C	2.53	0.50
2:D:155:PRO:O	2:D:186:SER:HB3	2.11	0.50
2:I:133:SER:O	2:I:136:ILE:HG22	2.11	0.50
2:K:360:VAL:O	2:K:378:ARG:HD3	2.11	0.50
2:L:23:LEU:HD11	2:N:36:GLN:HB2	1.92	0.50
2:O:37:MET:O	2:O:38:ILE:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:TYR:HE1	1:B:300:ARG:HA	1.77	0.50
1:B:340:VAL:O	1:B:341:SER:C	2.54	0.50
1:B:518:PHE:CB	1:B:519:PRO:CD	2.89	0.50
1:B:739:MET:C	1:B:741:THR:H	2.19	0.50
1:B:878:ASN:OD1	1:B:878:ASN:O	2.29	0.50
2:D:253:ILE:HD13	2:D:319:THR:HB	1.93	0.50
2:E:56:ILE:O	2:E:56:ILE:HG22	2.11	0.50
2:F:61:PHE:N	2:F:61:PHE:CD1	2.79	0.50
2:H:89:VAL:O	2:H:91:PHE:N	2.44	0.50
2:J:37:MET:O	2:J:38:ILE:C	2.54	0.50
2:L:6:SER:O	2:L:8:SER:N	2.44	0.50
2:L:150:PHE:CD1	2:L:150:PHE:N	2.78	0.50
2:L:155:PRO:O	2:L:186:SER:HB3	2.11	0.50
2:N:23:LEU:O	2:N:26:ASN:ND2	2.43	0.50
1:A:199:VAL:CG1	1:A:200:VAL:H	2.07	0.50
1:A:436:ILE:CD1	1:A:437:TYR:CD1	2.94	0.50
1:A:545:ASP:OD1	1:A:877:MET:HA	2.11	0.50
1:A:822:THR:O	1:A:823:THR:HG23	2.12	0.50
1:B:498:ARG:HD3	2:I:32:GLN:NE2	2.26	0.50
1:B:596:SER:O	1:B:599:THR:HB	2.11	0.50
1:B:712:LEU:HB2	1:B:819:PRO:HB2	1.94	0.50
2:C:12:LYS:O	2:C:14:ALA:N	2.45	0.50
2:G:6:SER:O	2:G:8:SER:N	2.44	0.50
2:G:31:ILE:O	2:G:34:PHE:HB3	2.11	0.50
2:H:253:ILE:HD13	2:H:319:THR:HB	1.93	0.50
2:I:31:ILE:O	2:I:34:PHE:HB3	2.11	0.50
2:L:133:SER:O	2:L:136:ILE:HG22	2.12	0.50
2:L:253:ILE:HD13	2:L:319:THR:HB	1.93	0.50
2:N:1:MET:O	2:N:2:ASP:C	2.55	0.50
2:N:66:LEU:HD13	2:N:77:TYR:CZ	2.46	0.50
2:N:106:ARG:HG2	2:N:107:ASN:H	1.77	0.50
1:A:389:GLN:OE1	1:A:567:HIS:HA	2.11	0.50
1:A:634:TYR:HD1	1:A:635:GLN:HG3	1.76	0.50
1:B:402:MET:HE1	1:B:532:GLY:CA	2.42	0.50
1:B:428:GLN:NE2	1:B:455:PRO:HB2	2.26	0.50
1:B:710:MET:HE2	1:B:711:GLN:O	2.11	0.50
2:C:46:PHE:HE2	2:C:119:LEU:HD21	1.75	0.50
2:C:360:VAL:O	2:C:378:ARG:HD3	2.11	0.50
2:D:12:LYS:O	2:D:14:ALA:N	2.45	0.50
2:D:100:MET:HG3	2:D:388:VAL:HG11	1.93	0.50
2:D:124:PHE:O	2:D:127:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:14:ALA:C	2:F:16:ASP:N	2.66	0.50
2:G:124:PHE:O	2:G:127:ILE:HG13	2.11	0.50
2:I:1:MET:O	2:I:2:ASP:C	2.54	0.50
2:I:30:LEU:O	2:I:31:ILE:C	2.52	0.50
2:L:125:LYS:O	2:L:127:ILE:N	2.42	0.50
2:L:360:VAL:O	2:L:378:ARG:HD3	2.11	0.50
1:A:608:VAL:O	1:A:609:ASN:C	2.55	0.50
1:B:176:GLU:O	1:B:178:PRO:HD3	2.11	0.50
1:B:211:ILE:C	1:B:213:GLN:N	2.67	0.50
1:B:387:LEU:HD23	1:B:554:TYR:HE1	1.74	0.50
1:B:578:LEU:HA	1:B:581:VAL:CG2	2.42	0.50
1:B:872:ASP:CG	1:B:874:MET:H	2.20	0.50
2:E:150:PHE:CD1	2:E:150:PHE:N	2.80	0.50
2:E:253:ILE:HD13	2:E:319:THR:HB	1.93	0.50
2:F:32:GLN:O	2:F:33:GLN:C	2.54	0.50
2:F:73:LEU:HD22	2:F:77:TYR:CD2	2.46	0.50
2:G:167:ASN:ND2	2:G:178:GLY:HA2	2.22	0.50
2:I:6:SER:O	2:I:8:SER:N	2.44	0.50
2:J:6:SER:O	2:J:8:SER:N	2.45	0.50
2:L:11:LEU:O	2:L:15:ARG:N	2.39	0.50
2:L:89:VAL:C	2:L:91:PHE:H	2.20	0.50
2:O:11:LEU:O	2:O:15:ARG:N	2.40	0.50
1:A:229:ARG:O	1:A:242:PRO:CG	2.60	0.50
1:A:332:VAL:HG11	1:A:557:LEU:HD21	1.93	0.50
1:A:466:PHE:O	1:A:467:GLN:C	2.54	0.50
1:B:170:TYR:CE1	1:B:682:PHE:HB2	2.47	0.50
1:B:364:THR:HG22	1:B:364:THR:O	2.12	0.50
1:B:420:ILE:O	1:B:421:ARG:C	2.54	0.50
1:B:463:ILE:HG21	1:B:468:VAL:CG1	2.41	0.50
1:B:499:ASN:N	1:B:505:GLN:NE2	2.60	0.50
1:B:536:LEU:HD22	1:B:536:LEU:N	2.27	0.50
1:B:589:GLY:C	1:B:591:ALA:H	2.20	0.50
1:B:618:ILE:HD13	1:B:645:PHE:CZ	2.47	0.50
1:B:810:TYR:HA	1:B:812:VAL:HG12	1.92	0.50
2:C:31:ILE:O	2:C:34:PHE:HB3	2.12	0.50
2:C:37:MET:O	2:C:38:ILE:C	2.55	0.50
2:D:37:MET:O	2:D:38:ILE:C	2.55	0.50
2:D:133:SER:O	2:D:136:ILE:HG22	2.11	0.50
2:F:6:SER:O	2:F:8:SER:N	2.45	0.50
2:I:360:VAL:O	2:I:378:ARG:HD3	2.11	0.50
2:J:1:MET:C	2:J:3:VAL:N	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:124:PHE:O	2:K:126:ARG:N	2.45	0.50
2:N:104:SER:O	2:N:108:GLY:HA3	2.12	0.50
1:A:266:ASN:C	1:A:292:LEU:HD12	2.36	0.50
1:A:297:ARG:HG3	1:A:848:PHE:CD2	2.46	0.50
1:A:309:ASN:HA	1:A:311:HIS:CE1	2.47	0.50
1:A:554:TYR:CZ	1:A:558:MET:HE1	2.47	0.50
1:A:603:TYR:O	1:A:606:VAL:CG2	2.60	0.50
1:A:660:ASP:CA	1:B:539:ARG:HH11	2.24	0.50
1:A:704:ILE:HG23	1:A:758:ALA:HB2	1.94	0.50
1:B:113:PRO:HD2	1:B:609:ASN:HB3	1.94	0.50
1:B:141:GLU:O	1:B:142:LEU:CB	2.60	0.50
1:B:205:ALA:O	1:B:206:SER:C	2.55	0.50
1:B:392:MET:HB3	1:B:574:GLU:O	2.10	0.50
1:B:477:ASN:O	1:B:479:GLN:N	2.44	0.50
1:B:510:LEU:HD12	1:B:513:LEU:HD12	1.94	0.50
2:I:12:LYS:O	2:I:14:ALA:N	2.45	0.50
2:I:150:PHE:N	2:I:150:PHE:CD1	2.79	0.50
2:J:23:LEU:O	2:J:26:ASN:ND2	2.45	0.50
2:L:14:ALA:C	2:L:16:ASP:N	2.67	0.50
2:N:360:VAL:O	2:N:378:ARG:HD3	2.11	0.50
1:A:246:HIS:O	1:A:247:PRO:C	2.54	0.50
1:A:503:ILE:HG22	1:A:503:ILE:O	2.12	0.50
1:A:563:MET:HE2	1:A:563:MET:CA	2.31	0.50
1:A:613:ASN:HD22	1:A:649:LEU:HD21	1.75	0.50
1:B:436:ILE:CG1	1:B:437:TYR:H	2.21	0.50
1:B:444:ARG:HH21	1:B:520:THR:CG2	2.09	0.50
2:C:253:ILE:HD13	2:C:319:THR:HB	1.93	0.50
2:E:24:TYR:O	2:E:26:ASN:N	2.43	0.50
2:E:360:VAL:O	2:E:378:ARG:HD3	2.11	0.50
2:F:153:HIS:NE2	2:G:153:HIS:CD2	2.80	0.50
2:G:74:ASP:OD2	2:G:76:ASN:HB3	2.12	0.50
2:G:124:PHE:O	2:G:126:ARG:N	2.45	0.50
2:G:155:PRO:O	2:G:186:SER:HB3	2.12	0.50
2:G:273:TYR:C	2:G:274:GLN:HE21	2.20	0.50
2:H:32:GLN:O	2:H:33:GLN:C	2.54	0.50
2:J:63:PHE:N	2:J:63:PHE:CD1	2.80	0.50
2:J:153:HIS:O	2:J:154:LYS:C	2.53	0.50
2:N:253:ILE:HD13	2:N:319:THR:HB	1.93	0.50
1:A:284:TYR:OH	1:A:594:ILE:HG23	2.12	0.49
1:A:310:LEU:CD1	1:A:310:LEU:N	2.69	0.49
1:A:311:HIS:HA	1:A:318:TRP:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:MET:O	1:A:420:ILE:HG23	2.11	0.49
1:A:445:MET:C	1:A:447:TYR:N	2.54	0.49
1:A:465:ASN:HB3	1:A:468:VAL:HB	1.94	0.49
1:A:555:GLU:OE1	1:A:871:PHE:CD2	2.66	0.49
1:A:580:SER:O	1:A:581:VAL:C	2.55	0.49
1:A:674:VAL:HG12	1:A:678:ARG:HB2	1.93	0.49
1:A:774:LEU:HD12	1:A:774:LEU:O	2.11	0.49
1:B:85:GLU:O	1:B:86:ILE:C	2.54	0.49
1:B:108:LEU:C	1:B:110:ASP:N	2.67	0.49
1:B:402:MET:HE1	1:B:532:GLY:HA3	1.94	0.49
1:B:419:PHE:O	1:B:420:ILE:C	2.54	0.49
1:B:772:ILE:O	1:B:773:SER:C	2.54	0.49
2:E:101:VAL:HG23	2:E:102:ARG:N	2.27	0.49
2:H:135:TYR:OH	2:H:342:MET:HE3	2.10	0.49
2:J:60:ASN:C	2:J:61:PHE:CD1	2.90	0.49
2:K:133:SER:O	2:K:136:ILE:HG22	2.12	0.49
2:O:6:SER:O	2:O:8:SER:N	2.45	0.49
1:A:141:GLU:O	1:A:142:LEU:HB2	2.11	0.49
1:A:230:GLN:O	1:A:230:GLN:NE2	2.45	0.49
1:A:390:ARG:HG3	1:A:391:THR:N	2.26	0.49
1:A:416:ASN:C	1:A:418:MET:N	2.70	0.49
1:A:503:ILE:HG22	1:A:506:LEU:CB	2.42	0.49
1:A:779:ASP:OD1	1:A:779:ASP:N	2.43	0.49
1:B:134:TYR:CD2	1:B:803:ASN:HB2	2.47	0.49
1:B:267:ASN:N	1:B:292:LEU:HD12	2.27	0.49
1:B:322:THR:HG21	1:B:390:ARG:HA	1.94	0.49
1:B:601:PHE:O	1:B:602:HIS:C	2.53	0.49
1:B:639:LYS:O	1:B:642:VAL:N	2.44	0.49
2:C:106:ARG:HD3	2:C:106:ARG:N	2.10	0.49
2:D:14:ALA:C	2:D:16:ASP:N	2.66	0.49
2:E:37:MET:O	2:E:38:ILE:C	2.54	0.49
2:F:116:LEU:HA	2:F:119:LEU:CD1	2.42	0.49
2:G:133:SER:O	2:G:136:ILE:HG22	2.12	0.49
2:H:101:VAL:HB	2:H:355:ILE:HG21	1.94	0.49
2:H:360:VAL:O	2:H:378:ARG:HD3	2.11	0.49
2:J:41:MET:O	2:J:42:ASN:C	2.54	0.49
2:O:35:ASN:HD21	2:O:66:LEU:HD12	1.77	0.49
1:A:415:PRO:HD2	1:A:480:PHE:HE1	1.76	0.49
1:A:527:ARG:HH11	1:A:527:ARG:HG3	1.77	0.49
1:A:762:ALA:C	1:A:763:LEU:HG	2.37	0.49
1:A:867:ASN:CG	1:A:867:ASN:O	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASP:OD2	1:B:761:GLY:HA3	2.11	0.49
1:B:277:ARG:NH1	1:B:277:ARG:CB	2.75	0.49
1:B:287:ASN:O	1:B:288:MET:HE2	2.12	0.49
1:B:428:GLN:HE22	1:B:455:PRO:HB2	1.77	0.49
1:B:590:ASN:N	1:B:590:ASN:ND2	2.46	0.49
1:B:596:SER:O	1:B:597:PRO:C	2.55	0.49
1:B:735:LEU:CD2	1:B:759:LEU:HB3	2.42	0.49
2:C:32:GLN:O	2:C:33:GLN:C	2.54	0.49
2:E:12:LYS:O	2:E:14:ALA:N	2.45	0.49
2:E:22:THR:CG2	2:E:73:LEU:HD12	2.42	0.49
2:F:273:TYR:C	2:F:274:GLN:HE21	2.21	0.49
2:H:30:LEU:O	2:H:31:ILE:C	2.53	0.49
2:I:273:TYR:C	2:I:274:GLN:HE21	2.20	0.49
2:K:31:ILE:O	2:K:34:PHE:HB3	2.11	0.49
2:N:1:MET:C	2:N:3:VAL:N	2.69	0.49
2:O:14:ALA:C	2:O:16:ASP:N	2.66	0.49
2:O:273:TYR:C	2:O:274:GLN:HE21	2.21	0.49
1:A:149:LYS:NZ	1:A:697:ASP:OD1	2.45	0.49
1:A:224:PHE:O	1:A:225:ILE:C	2.55	0.49
1:A:771:VAL:HG12	1:A:809:PHE:HB3	1.93	0.49
1:B:428:GLN:CB	1:B:456:PHE:HD1	2.24	0.49
1:B:450:GLY:O	1:B:451:ASP:HB2	2.11	0.49
1:B:498:ARG:HH12	2:J:25:SER:CB	2.23	0.49
1:B:698:LYS:O	1:B:699:ILE:HD13	2.12	0.49
1:B:869:VAL:HG13	1:B:873:ASN:HA	1.92	0.49
2:J:89:VAL:C	2:J:91:PHE:H	2.21	0.49
2:J:144:ARG:O	2:J:145:ARG:HB2	2.12	0.49
2:K:37:MET:O	2:K:38:ILE:C	2.55	0.49
2:M:133:SER:O	2:M:136:ILE:HG22	2.13	0.49
1:A:117:LYS:HB2	1:A:179:ASP:CG	2.37	0.49
1:A:178:PRO:HD2	1:A:256:PHE:HE2	1.77	0.49
1:A:333:VAL:CG1	1:A:380:LYS:HA	2.19	0.49
1:A:415:PRO:HG2	1:A:480:PHE:HD1	1.73	0.49
1:A:718:TYR:N	1:A:718:TYR:CD1	2.80	0.49
1:B:122:LEU:O	1:B:123:PHE:HB3	2.12	0.49
1:B:174:LEU:O	1:B:177:MET:HB2	2.12	0.49
1:B:305:GLN:O	1:B:307:ARG:N	2.46	0.49
1:B:812:VAL:HA	1:B:817:TRP:HZ3	1.78	0.49
2:C:273:TYR:C	2:C:274:GLN:HE21	2.21	0.49
2:J:144:ARG:NH2	2:J:146:GLN:NE2	2.61	0.49
2:J:273:TYR:C	2:J:274:GLN:HE21	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:12:LYS:O	2:K:14:ALA:N	2.45	0.49
2:L:60:ASN:C	2:L:61:PHE:CD1	2.91	0.49
2:N:22:THR:OG1	2:N:26:ASN:ND2	2.40	0.49
2:N:89:VAL:C	2:N:91:PHE:H	2.21	0.49
2:O:63:PHE:N	2:O:63:PHE:CD1	2.81	0.49
1:A:101:LYS:C	1:A:103:SER:H	2.20	0.49
1:A:124:ARG:C	1:A:125:ILE:HD12	2.37	0.49
1:A:442:MET:HE3	1:A:463:ILE:CG2	2.43	0.49
1:B:150:LEU:HD12	1:B:696:SER:HA	1.93	0.49
1:B:603:TYR:O	1:B:606:VAL:CG2	2.61	0.49
2:C:6:SER:O	2:C:8:SER:N	2.45	0.49
2:C:89:VAL:C	2:C:91:PHE:H	2.21	0.49
2:C:153:HIS:CE1	2:D:153:HIS:CD2	3.01	0.49
2:F:12:LYS:O	2:F:14:ALA:N	2.45	0.49
2:H:126:ARG:C	2:H:127:ILE:HG13	2.37	0.49
2:H:155:PRO:O	2:H:186:SER:HB3	2.13	0.49
2:I:89:VAL:C	2:I:91:PHE:H	2.19	0.49
2:J:1:MET:O	2:J:2:ASP:C	2.54	0.49
2:J:31:ILE:O	2:J:34:PHE:HB3	2.13	0.49
2:J:115:SER:O	2:J:119:LEU:HG	2.13	0.49
2:O:360:VAL:O	2:O:378:ARG:HD3	2.11	0.49
1:A:147:TYR:N	1:A:147:TYR:CD1	2.80	0.49
1:A:389:GLN:HE22	1:A:568:VAL:H	1.60	0.49
1:A:452:PRO:O	1:A:453:GLN:HB3	2.13	0.49
1:A:457:GLN:O	1:A:459:ALA:N	2.45	0.49
1:A:524:ASP:C	1:A:526:LYS:N	2.71	0.49
1:A:548:ARG:O	1:A:551:ALA:HB3	2.12	0.49
1:A:854:LEU:O	1:A:856:ALA:N	2.46	0.49
1:B:447:TYR:C	1:B:448:ARG:HG2	2.38	0.49
1:B:544:VAL:HG11	1:B:548:ARG:HH21	1.78	0.49
1:B:674:VAL:O	1:B:675:GLU:C	2.54	0.49
2:E:115:SER:O	2:E:119:LEU:HG	2.13	0.49
2:F:150:PHE:N	2:F:150:PHE:CD1	2.80	0.49
2:G:153:HIS:NE2	2:H:153:HIS:CD2	2.81	0.49
2:I:5:TYR:CE2	2:I:131:ASN:HA	2.47	0.49
2:I:253:ILE:HD13	2:I:319:THR:HB	1.93	0.49
2:L:139:TRP:HE1	2:L:143:ASN:HD22	1.61	0.49
2:M:5:TYR:HE2	2:M:131:ASN:HA	1.77	0.49
1:A:539:ARG:O	1:A:542:GLN:N	2.44	0.49
1:A:557:LEU:O	1:A:558:MET:C	2.55	0.49
1:A:652:PHE:N	1:A:652:PHE:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:MET:O	1:A:665:LEU:CB	2.61	0.49
1:A:820:THR:HG22	1:A:820:THR:O	2.13	0.49
1:B:158:GLY:O	1:B:159:ASP:C	2.56	0.49
1:B:182:LEU:HD21	1:B:846:LEU:HD12	1.95	0.49
1:B:434:THR:C	1:B:435:ILE:HG13	2.37	0.49
1:B:487:GLY:O	1:B:488:VAL:HB	2.13	0.49
1:B:854:LEU:CD2	1:B:855:LEU:N	2.76	0.49
2:E:21:GLY:O	2:E:22:THR:O	2.31	0.49
2:E:110:ALA:HB1	2:E:111:PRO:HD2	1.95	0.49
2:F:72:ASN:ND2	2:H:126:ARG:NH1	2.60	0.49
2:H:37:MET:O	2:H:38:ILE:C	2.55	0.49
2:J:2:ASP:HB2	2:J:128:ASN:HD21	1.77	0.49
2:O:1:MET:C	2:O:3:VAL:N	2.68	0.49
2:O:89:VAL:C	2:O:91:PHE:H	2.21	0.49
2:O:109:ILE:HB	2:O:380:ASP:HB3	1.94	0.49
1:A:192:ASN:O	1:A:193:SER:CB	2.49	0.49
1:A:870:ALA:C	1:A:872:ASP:H	2.20	0.49
1:B:87:GLN:C	1:B:89:GLU:N	2.68	0.49
1:B:139:GLU:O	1:B:141:GLU:N	2.46	0.49
1:B:428:GLN:O	1:B:432:VAL:HG23	2.13	0.49
1:B:501:HIS:O	1:B:503:ILE:HG13	2.12	0.49
1:B:676:VAL:O	1:B:680:ASP:HB2	2.13	0.49
1:B:845:ASN:HB3	1:B:848:PHE:HE1	1.77	0.49
2:F:46:PHE:CE2	2:F:119:LEU:HD21	2.48	0.49
2:F:101:VAL:HG23	2:F:102:ARG:N	2.27	0.49
2:G:42:ASN:HA	2:G:61:PHE:HB2	1.94	0.49
2:H:6:SER:O	2:H:8:SER:N	2.46	0.49
2:I:144:ARG:NH2	2:I:146:GLN:HE22	2.10	0.49
2:J:101:VAL:HG23	2:J:102:ARG:N	2.27	0.49
2:J:150:PHE:N	2:J:150:PHE:CD1	2.81	0.49
2:L:12:LYS:O	2:L:14:ALA:N	2.45	0.49
2:L:273:TYR:C	2:L:274:GLN:HE21	2.21	0.49
1:A:311:HIS:HE2	1:A:566:GLN:HE22	1.59	0.49
1:A:597:PRO:HB3	1:A:860:ALA:HB3	1.94	0.49
1:A:646:LEU:HD23	1:A:646:LEU:N	2.28	0.49
1:A:666:ARG:HG2	1:A:667:ASP:H	1.78	0.49
1:B:277:ARG:NH1	1:B:277:ARG:HB2	2.28	0.49
1:B:422:GLU:OE1	1:B:422:GLU:N	2.46	0.49
1:B:473:HIS:CB	2:I:126:ARG:NH2	2.69	0.49
1:B:587:LEU:O	1:B:587:LEU:CG	2.60	0.49
2:C:106:ARG:HG2	2:C:107:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:273:TYR:C	2:D:274:GLN:HE21	2.21	0.49
2:E:1:MET:C	2:E:3:VAL:N	2.68	0.49
2:F:37:MET:O	2:F:38:ILE:C	2.56	0.49
2:F:41:MET:O	2:F:42:ASN:C	2.56	0.49
2:G:12:LYS:O	2:G:14:ALA:N	2.46	0.49
2:K:59:TRP:N	2:K:59:TRP:CD1	2.79	0.49
2:K:273:TYR:C	2:K:274:GLN:HE21	2.21	0.49
2:M:12:LYS:O	2:M:14:ALA:N	2.46	0.49
2:M:273:TYR:C	2:M:274:GLN:HE21	2.20	0.49
2:O:125:LYS:C	2:O:127:ILE:H	2.21	0.49
1:A:122:LEU:HD11	1:A:201:ASP:CB	2.43	0.48
1:A:179:ASP:HA	1:A:677:ARG:NH2	2.27	0.48
1:A:271:PHE:CA	1:A:274:ILE:HD12	2.43	0.48
1:A:404:LEU:O	1:A:407:GLY:N	2.46	0.48
1:B:302:ASN:ND2	1:B:615:ASN:HB3	2.27	0.48
1:B:404:LEU:O	1:B:405:ILE:C	2.55	0.48
1:B:643:GLU:HG2	1:B:662:MET:HE1	1.95	0.48
1:B:785:GLN:O	1:B:787:VAL:N	2.46	0.48
2:C:1:MET:C	2:C:3:VAL:N	2.70	0.48
2:C:3:VAL:O	2:C:4:LEU:C	2.56	0.48
2:E:273:TYR:C	2:E:274:GLN:HE21	2.21	0.48
2:G:23:LEU:C	2:G:23:LEU:HD23	2.38	0.48
2:G:115:SER:O	2:G:119:LEU:HG	2.13	0.48
2:G:295:MET:HE3	2:G:298:PRO:HD3	1.96	0.48
2:I:49:GLY:HA2	2:I:54:LEU:CD2	2.43	0.48
2:K:1:MET:O	2:K:2:ASP:C	2.54	0.48
2:K:1:MET:C	2:K:3:VAL:N	2.68	0.48
2:M:151:THR:C	2:M:152:PHE:CD1	2.91	0.48
2:O:69:THR:O	2:O:70:LEU:O	2.31	0.48
1:A:529:ILE:O	1:A:533:ILE:HG13	2.12	0.48
1:B:137:ASN:O	1:B:137:ASN:CG	2.55	0.48
1:B:473:HIS:O	1:B:477:ASN:ND2	2.46	0.48
1:B:583:SER:O	1:B:587:LEU:HB3	2.12	0.48
2:I:122:LEU:C	2:I:124:PHE:H	2.21	0.48
2:K:6:SER:O	2:K:8:SER:N	2.46	0.48
2:K:14:ALA:C	2:K:18:ILE:HD12	2.39	0.48
2:L:109:ILE:HB	2:L:380:ASP:HB3	1.94	0.48
2:L:135:TYR:OH	2:L:340:GLU:OE1	2.30	0.48
2:M:6:SER:O	2:M:8:SER:N	2.45	0.48
2:M:38:ILE:HG22	2:M:42:ASN:ND2	2.27	0.48
2:N:21:GLY:O	2:N:22:THR:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:53:ASN:ND2	2:N:354:ALA:HB3	2.28	0.48
2:O:48:THR:O	2:O:56:ILE:HA	2.12	0.48
1:A:434:THR:O	1:A:434:THR:CG2	2.61	0.48
1:B:477:ASN:HD21	2:I:39:ILE:HG21	1.77	0.48
1:B:486:ASP:O	1:B:488:VAL:N	2.46	0.48
1:B:522:PRO:O	1:B:525:TYR:HB2	2.14	0.48
1:B:765:PHE:CZ	1:B:767:THR:HG23	2.48	0.48
1:B:870:ALA:O	1:B:871:PHE:C	2.55	0.48
2:G:37:MET:O	2:G:38:ILE:C	2.55	0.48
2:G:144:ARG:O	2:G:145:ARG:HB2	2.14	0.48
2:H:41:MET:O	2:H:42:ASN:C	2.56	0.48
2:I:19:VAL:HG21	2:K:128:ASN:HB3	1.94	0.48
2:J:135:TYR:OH	2:J:340:GLU:OE1	2.30	0.48
2:M:123:LYS:HG3	2:M:124:PHE:CE1	2.49	0.48
2:M:131:ASN:O	2:N:16:ASP:HB3	2.13	0.48
2:O:3:VAL:O	2:O:4:LEU:C	2.56	0.48
1:A:122:LEU:HD23	1:A:122:LEU:N	2.28	0.48
1:A:390:ARG:HE	1:A:574:GLU:HG2	1.78	0.48
1:A:416:ASN:C	1:A:418:MET:H	2.21	0.48
1:A:704:ILE:O	1:A:823:THR:HB	2.14	0.48
1:B:228:MET:HG3	1:B:228:MET:O	2.12	0.48
1:B:231:ARG:CB	1:B:240:ASN:HB2	2.42	0.48
1:B:275:PRO:HD2	1:B:278:ILE:CD1	2.43	0.48
1:B:321:ILE:O	1:B:322:THR:C	2.57	0.48
1:B:329:ALA:HB3	1:B:384:ALA:CB	2.43	0.48
1:B:422:GLU:O	1:B:425:VAL:HB	2.12	0.48
2:E:89:VAL:C	2:E:91:PHE:H	2.22	0.48
2:E:125:LYS:C	2:E:127:ILE:H	2.21	0.48
2:E:133:SER:O	2:E:136:ILE:HG22	2.13	0.48
2:J:36:GLN:OE1	2:K:23:LEU:HD21	2.13	0.48
2:L:3:VAL:O	2:L:4:LEU:C	2.56	0.48
2:L:5:TYR:HE2	2:L:130:ASP:O	1.97	0.48
2:N:151:THR:C	2:N:152:PHE:CD1	2.91	0.48
1:A:170:TYR:CE1	1:A:682:PHE:HB2	2.49	0.48
1:A:215:GLU:CD	1:A:215:GLU:H	2.21	0.48
1:A:305:GLN:OE1	1:A:564:ASN:ND2	2.44	0.48
1:A:339:LEU:O	1:A:340:VAL:C	2.55	0.48
1:A:484:VAL:CG1	1:A:485:ILE:H	2.25	0.48
1:A:486:ASP:OD2	1:A:490:ASN:HB2	2.13	0.48
1:A:545:ASP:OD1	1:A:548:ARG:NH1	2.46	0.48
1:A:810:TYR:C	1:A:812:VAL:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:LEU:O	1:A:855:LEU:C	2.56	0.48
1:A:855:LEU:O	1:A:856:ALA:C	2.56	0.48
1:B:113:PRO:CD	1:B:609:ASN:HB3	2.43	0.48
1:B:176:GLU:O	1:B:178:PRO:CD	2.61	0.48
1:B:341:SER:O	1:B:342:THR:C	2.57	0.48
1:B:392:MET:CA	1:B:573:THR:HG23	2.43	0.48
1:B:521:MET:CB	1:B:522:PRO:CD	2.90	0.48
1:B:635:GLN:C	1:B:636:LYS:O	2.50	0.48
2:D:125:LYS:O	2:D:127:ILE:N	2.46	0.48
2:E:1:MET:O	2:E:2:ASP:C	2.56	0.48
2:E:6:SER:OG	2:E:128:ASN:HA	2.13	0.48
2:H:22:THR:OG1	2:H:26:ASN:ND2	2.46	0.48
2:H:115:SER:O	2:H:119:LEU:HG	2.13	0.48
2:I:48:THR:O	2:I:56:ILE:HA	2.13	0.48
2:J:155:PRO:O	2:J:186:SER:HB3	2.14	0.48
2:M:89:VAL:C	2:M:91:PHE:H	2.21	0.48
2:O:14:ALA:O	2:O:18:ILE:CD1	2.61	0.48
2:O:42:ASN:HA	2:O:61:PHE:HB2	1.95	0.48
1:A:118:LYS:CG	1:A:119:GLN:N	2.73	0.48
1:A:296:ALA:C	1:A:297:ARG:HG2	2.38	0.48
1:A:404:LEU:CB	1:A:435:ILE:HD11	2.43	0.48
1:A:428:GLN:CB	1:A:456:PHE:HD1	2.22	0.48
1:A:659:ASP:O	1:A:660:ASP:O	2.32	0.48
1:A:822:THR:O	1:A:823:THR:OG1	2.22	0.48
1:A:865:PRO:O	1:A:867:ASN:N	2.47	0.48
1:B:104:ILE:HD12	1:B:327:ILE:CD1	2.44	0.48
1:B:782:VAL:O	1:B:785:GLN:HB2	2.14	0.48
2:C:150:PHE:N	2:C:150:PHE:CD1	2.82	0.48
2:D:24:TYR:CE1	2:D:68:THR:HG22	2.48	0.48
2:D:31:ILE:O	2:D:34:PHE:HB3	2.13	0.48
2:D:150:PHE:HB2	2:D:152:PHE:HE1	1.77	0.48
2:F:53:ASN:ND2	2:F:354:ALA:HB3	2.28	0.48
2:G:54:LEU:HD12	2:G:55:PRO:HD2	1.96	0.48
2:J:3:VAL:O	2:J:4:LEU:C	2.56	0.48
2:K:3:VAL:O	2:K:4:LEU:C	2.56	0.48
2:K:295:MET:HE3	2:K:298:PRO:HD3	1.96	0.48
2:M:128:ASN:HD22	2:N:19:VAL:HB	1.79	0.48
1:A:216:GLU:CD	1:A:216:GLU:N	2.55	0.48
1:A:458:ILE:O	1:A:462:GLN:HG2	2.13	0.48
1:A:627:ALA:O	1:A:631:LEU:HG	2.13	0.48
1:B:220:ALA:O	1:B:223:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:GLN:CG	1:B:564:ASN:HD21	2.26	0.48
1:B:312:ASP:O	1:B:312:ASP:CG	2.56	0.48
1:B:459:ALA:HB1	1:B:463:ILE:CD1	2.36	0.48
1:B:542:GLN:O	1:B:543:LEU:C	2.57	0.48
1:B:701:GLN:CD	1:B:701:GLN:N	2.72	0.48
1:B:723:ILE:O	1:B:724:ALA:CB	2.61	0.48
2:C:1:MET:O	2:C:2:ASP:C	2.56	0.48
2:C:63:PHE:CD1	2:C:63:PHE:N	2.81	0.48
2:E:23:LEU:O	2:E:26:ASN:ND2	2.47	0.48
2:F:144:ARG:O	2:F:145:ARG:HG3	2.14	0.48
2:G:23:LEU:HD23	2:G:24:TYR:N	2.28	0.48
2:H:273:TYR:C	2:H:274:GLN:HE21	2.21	0.48
2:I:89:VAL:C	2:I:91:PHE:N	2.70	0.48
2:K:150:PHE:N	2:K:150:PHE:CD1	2.82	0.48
2:N:6:SER:O	2:N:8:SER:N	2.47	0.48
2:N:153:HIS:O	2:N:154:LYS:C	2.57	0.48
2:N:295:MET:HE3	2:N:298:PRO:HD3	1.96	0.48
1:A:145:ARG:HB3	1:A:147:TYR:CE1	2.49	0.48
1:A:583:SER:O	1:A:584:LEU:C	2.56	0.48
1:B:233:GLN:HB2	1:B:238:VAL:HB	1.96	0.48
1:B:319:ASP:OD2	1:B:572:THR:N	2.46	0.48
1:B:452:PRO:O	1:B:453:GLN:OE1	2.32	0.48
1:B:594:ILE:HB	1:B:595:PRO:HD2	1.94	0.48
1:B:745:ALA:HA	1:B:748:THR:OG1	2.13	0.48
1:B:775:ILE:N	1:B:775:ILE:CD1	2.76	0.48
2:D:70:LEU:CG	2:D:71:LEU:N	2.76	0.48
2:F:3:VAL:O	2:F:4:LEU:C	2.56	0.48
2:H:1:MET:O	2:H:2:ASP:C	2.57	0.48
2:I:128:ASN:O	2:J:22:THR:HB	2.14	0.48
2:L:89:VAL:C	2:L:91:PHE:N	2.71	0.48
2:M:22:THR:HG23	2:M:73:LEU:CD1	2.39	0.48
1:A:239:VAL:HG21	1:A:845:ASN:O	2.13	0.48
1:A:298:TYR:C	1:A:298:TYR:CD1	2.91	0.48
1:A:328:LEU:HG	1:A:603:TYR:HE1	1.79	0.48
1:A:484:VAL:HG12	1:A:485:ILE:N	2.28	0.48
1:A:563:MET:O	1:A:564:ASN:C	2.56	0.48
1:A:817:TRP:CZ3	1:A:819:PRO:HA	2.49	0.48
1:B:214:ASP:O	1:B:216:GLU:N	2.47	0.48
1:B:283:ASN:O	1:B:863:VAL:HG23	2.13	0.48
1:B:466:PHE:CD1	2:H:80:THR:HG22	2.48	0.48
1:B:517:GLN:N	1:B:518:PHE:CE1	2.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LEU:N	1:B:536:LEU:CD2	2.77	0.48
1:B:712:LEU:HB3	1:B:819:PRO:HB2	1.96	0.48
1:B:811:LEU:HA	1:B:814:ASN:HD22	1.79	0.48
2:C:145:ARG:HB3	2:C:145:ARG:CZ	2.43	0.48
2:D:89:VAL:C	2:D:91:PHE:H	2.22	0.48
2:F:31:ILE:O	2:F:34:PHE:HB3	2.13	0.48
2:G:89:VAL:C	2:G:91:PHE:H	2.22	0.48
2:G:151:THR:C	2:G:152:PHE:CD1	2.92	0.48
2:J:346:VAL:CG2	2:J:385:VAL:HG13	2.44	0.48
2:K:89:VAL:C	2:K:91:PHE:H	2.21	0.48
2:K:89:VAL:C	2:K:91:PHE:N	2.71	0.48
2:L:50:GLY:HA2	2:L:56:ILE:HD11	1.95	0.48
2:L:106:ARG:HG2	2:L:107:ASN:H	1.78	0.48
2:O:295:MET:HE3	2:O:298:PRO:HD3	1.96	0.48
1:A:314:PHE:N	1:A:314:PHE:CD1	2.82	0.48
1:A:436:ILE:HD11	1:A:437:TYR:CE1	2.49	0.48
1:A:527:ARG:O	1:A:531:ARG:HG3	2.13	0.48
1:A:694:ARG:HD2	1:A:828:GLN:HG3	1.96	0.48
1:A:785:GLN:O	1:A:786:ILE:C	2.57	0.48
1:B:126:PHE:HB3	1:B:149:LYS:O	2.14	0.48
1:B:236:ARG:O	1:B:237:ASN:CB	2.61	0.48
1:B:447:TYR:OH	1:B:458:ILE:HD11	2.13	0.48
1:B:449:ASN:HD21	1:B:455:PRO:HG3	1.78	0.48
1:B:533:ILE:O	1:B:536:LEU:HB2	2.14	0.48
1:B:743:ASP:CG	1:B:744:TYR:N	2.72	0.48
1:B:770:SER:O	1:B:771:VAL:C	2.57	0.48
2:E:60:ASN:C	2:E:61:PHE:CD1	2.91	0.48
2:F:38:ILE:HG22	2:F:42:ASN:ND2	2.27	0.48
2:I:4:LEU:O	2:I:5:TYR:C	2.57	0.48
2:I:346:VAL:CG2	2:I:385:VAL:HG13	2.44	0.48
2:J:19:VAL:O	2:J:21:GLY:N	2.47	0.48
2:J:133:SER:O	2:J:136:ILE:HG22	2.13	0.48
2:K:115:SER:O	2:K:119:LEU:HG	2.14	0.48
2:L:139:TRP:HE1	2:L:143:ASN:ND2	2.11	0.48
2:O:63:PHE:CD2	2:O:84:THR:HG23	2.49	0.48
2:O:346:VAL:CG2	2:O:385:VAL:HG13	2.44	0.48
1:A:393:SER:C	1:A:394:LEU:HG	2.38	0.47
1:B:122:LEU:HD11	1:B:200:VAL:HG11	1.94	0.47
1:B:405:ILE:O	1:B:408:MET:HB2	2.14	0.47
1:B:433:ASN:C	1:B:435:ILE:H	2.22	0.47
1:B:521:MET:H	1:B:521:MET:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:ASN:N	2:C:131:ASN:ND2	2.62	0.47
2:D:66:LEU:O	2:D:67:GLY:O	2.31	0.47
2:E:131:ASN:HD22	2:E:131:ASN:N	2.11	0.47
2:H:295:MET:HE3	2:H:298:PRO:HD3	1.96	0.47
2:I:48:THR:HG21	2:I:94:ASN:HB3	1.96	0.47
2:J:48:THR:O	2:J:56:ILE:HA	2.13	0.47
2:L:346:VAL:CG2	2:L:385:VAL:HG13	2.44	0.47
2:M:74:ASP:O	2:M:75:ALA:C	2.57	0.47
2:N:3:VAL:O	2:N:4:LEU:C	2.56	0.47
2:N:42:ASN:HA	2:N:61:PHE:CB	2.44	0.47
2:N:99:GLU:OE2	2:N:112:GLN:HG2	2.13	0.47
2:N:125:LYS:C	2:N:127:ILE:H	2.22	0.47
2:N:152:PHE:CD1	2:N:152:PHE:N	2.82	0.47
2:O:12:LYS:O	2:O:14:ALA:N	2.46	0.47
1:A:540:LEU:HA	1:A:543:LEU:HB2	1.96	0.47
2:C:5:TYR:HE2	2:C:131:ASN:HA	1.80	0.47
2:C:89:VAL:C	2:C:91:PHE:N	2.72	0.47
2:D:1:MET:C	2:D:3:VAL:N	2.70	0.47
2:D:99:GLU:CD	2:D:116:LEU:CD2	2.86	0.47
2:G:3:VAL:O	2:G:4:LEU:C	2.56	0.47
2:H:22:THR:HG23	2:H:73:LEU:CD1	2.43	0.47
2:H:51:ILE:HG23	2:H:51:ILE:O	2.14	0.47
2:H:89:VAL:C	2:H:91:PHE:H	2.22	0.47
2:H:89:VAL:C	2:H:91:PHE:N	2.73	0.47
2:M:1:MET:C	2:M:3:VAL:N	2.71	0.47
2:M:115:SER:O	2:M:119:LEU:HG	2.14	0.47
2:O:89:VAL:C	2:O:91:PHE:N	2.71	0.47
1:A:306:ASP:HB3	1:A:310:LEU:HD11	1.95	0.47
1:A:437:TYR:N	1:A:438:PRO:CD	2.73	0.47
1:A:503:ILE:HG12	1:A:547:THR:HG21	1.96	0.47
1:A:539:ARG:NH2	1:A:588:ILE:O	2.47	0.47
1:A:660:ASP:O	1:A:663:TYR:N	2.47	0.47
1:A:701:GLN:HB3	1:A:826:TYR:CD2	2.46	0.47
1:B:295:THR:O	1:B:297:ARG:HG2	2.14	0.47
1:B:493:LEU:HD11	1:B:567:HIS:HB2	1.95	0.47
1:B:810:TYR:C	1:B:812:VAL:HG12	2.38	0.47
1:B:822:THR:HG22	1:B:822:THR:O	2.14	0.47
2:H:133:SER:O	2:H:136:ILE:HG22	2.14	0.47
2:I:33:GLN:HA	2:J:23:LEU:HD12	1.95	0.47
2:I:149:GLY:C	2:I:150:PHE:CD1	2.92	0.47
2:M:11:LEU:O	2:M:15:ARG:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:89:VAL:C	2:M:91:PHE:N	2.72	0.47
1:A:714:ARG:HG2	1:A:720:TYR:HD2	1.79	0.47
1:A:827:LYS:O	1:A:828:GLN:O	2.32	0.47
1:B:249:ASP:O	1:B:250:TYR:C	2.58	0.47
1:B:355:LEU:HG	1:B:356:GLU:H	1.76	0.47
1:B:369:GLY:C	1:B:371:ASN:N	2.69	0.47
1:B:460:GLU:HG3	1:B:473:HIS:CD2	2.49	0.47
1:B:513:LEU:HA	1:B:516:GLN:HE22	1.71	0.47
2:D:48:THR:O	2:D:56:ILE:HA	2.14	0.47
2:D:295:MET:HE3	2:D:298:PRO:HD3	1.96	0.47
2:F:89:VAL:C	2:F:91:PHE:N	2.72	0.47
2:G:346:VAL:CG2	2:G:385:VAL:HG13	2.45	0.47
2:K:125:LYS:C	2:K:127:ILE:H	2.22	0.47
2:L:295:MET:HE3	2:L:298:PRO:HD3	1.96	0.47
2:N:27:VAL:O	2:N:28:SER:C	2.58	0.47
1:A:148:TRP:CH2	1:A:246:HIS:HB2	2.49	0.47
1:A:311:HIS:ND1	1:A:311:HIS:N	2.63	0.47
1:A:353:LEU:C	1:A:354:GLN:HG2	2.37	0.47
1:A:587:LEU:C	1:A:587:LEU:HD22	2.39	0.47
1:A:742:GLY:CA	1:B:285:ILE:HD11	2.44	0.47
1:B:95:ILE:O	1:B:97:THR:N	2.46	0.47
1:B:413:VAL:O	1:B:414:VAL:C	2.58	0.47
1:B:481:ARG:HG2	2:I:65:LEU:CD1	2.44	0.47
1:B:513:LEU:O	1:B:516:GLN:OE1	2.32	0.47
1:B:666:ARG:HG2	1:B:667:ASP:H	1.79	0.47
1:B:735:LEU:HD21	1:B:759:LEU:CB	2.45	0.47
2:C:4:LEU:O	2:C:5:TYR:C	2.58	0.47
2:C:115:SER:O	2:C:119:LEU:HG	2.15	0.47
2:C:295:MET:HE3	2:C:298:PRO:HD3	1.96	0.47
2:D:3:VAL:O	2:D:4:LEU:C	2.57	0.47
2:F:133:SER:O	2:F:136:ILE:HG22	2.14	0.47
2:F:295:MET:HE3	2:F:298:PRO:HD3	1.96	0.47
2:I:14:ALA:C	2:I:18:ILE:HD12	2.39	0.47
2:I:295:MET:HE3	2:I:298:PRO:HD3	1.96	0.47
2:J:129:PHE:O	2:J:131:ASN:ND2	2.47	0.47
2:K:125:LYS:O	2:K:127:ILE:N	2.45	0.47
2:N:23:LEU:HD23	2:N:24:TYR:N	2.29	0.47
2:O:115:SER:O	2:O:119:LEU:HG	2.14	0.47
1:A:338:GLU:HG3	1:A:338:GLU:O	2.14	0.47
1:A:527:ARG:HH11	1:A:531:ARG:HH21	1.63	0.47
1:A:596:SER:HB3	1:A:599:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:ILE:O	1:A:824:LYS:HD2	2.14	0.47
1:A:864:GLU:CD	1:A:865:PRO:HD2	2.40	0.47
1:B:593:VAL:HG12	1:B:594:ILE:N	2.30	0.47
1:B:698:LYS:C	1:B:699:ILE:CD1	2.87	0.47
2:E:346:VAL:CG2	2:E:385:VAL:HG13	2.44	0.47
2:F:69:THR:O	2:F:70:LEU:C	2.56	0.47
2:F:78:VAL:O	2:F:81:ALA:HB3	2.14	0.47
2:F:89:VAL:C	2:F:91:PHE:H	2.22	0.47
2:I:144:ARG:O	2:I:145:ARG:HB2	2.15	0.47
2:K:100:MET:HG3	2:K:388:VAL:HG11	1.95	0.47
2:M:53:ASN:O	2:M:353:TYR:HD2	1.97	0.47
2:N:152:PHE:HD2	2:N:337:ASP:HB3	1.78	0.47
2:N:273:TYR:C	2:N:274:GLN:HE21	2.21	0.47
1:A:133:ILE:O	1:A:134:TYR:HD2	1.97	0.47
1:A:248:ILE:O	1:A:251:ALA:HB3	2.14	0.47
1:A:321:ILE:O	1:A:322:THR:C	2.58	0.47
1:A:450:GLY:O	1:A:451:ASP:CB	2.62	0.47
1:A:454:THR:HB	1:A:457:GLN:CB	2.44	0.47
1:A:508:GLU:HG2	1:A:512:GLN:HE21	1.75	0.47
1:A:699:ILE:HA	1:A:763:LEU:O	2.14	0.47
1:A:738:LEU:C	1:A:740:ARG:N	2.62	0.47
1:A:772:ILE:HA	1:A:775:ILE:CD1	2.45	0.47
1:A:775:ILE:C	1:A:777:LYS:N	2.71	0.47
1:B:122:LEU:O	1:B:253:ASN:OD1	2.32	0.47
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.73	0.47
1:B:548:ARG:O	1:B:551:ALA:HB3	2.15	0.47
1:B:557:LEU:O	1:B:558:MET:C	2.58	0.47
1:B:721:VAL:CG1	1:B:722:ASN:N	2.77	0.47
1:B:725:ARG:H	1:B:725:ARG:CD	2.22	0.47
1:B:817:TRP:CD1	1:B:818:VAL:H	2.33	0.47
1:B:852:SER:O	1:B:854:LEU:N	2.46	0.47
2:D:135:TYR:CZ	2:D:342:MET:HE3	2.49	0.47
2:E:4:LEU:O	2:E:5:TYR:C	2.57	0.47
2:E:295:MET:HE3	2:E:298:PRO:HD3	1.96	0.47
2:F:72:ASN:ND2	2:H:126:ARG:HH11	2.12	0.47
2:F:142:GLN:HE21	2:F:143:ASN:N	2.12	0.47
2:H:23:LEU:N	2:H:26:ASN:HD22	2.12	0.47
2:I:102:ARG:HG2	2:I:102:ARG:HH11	1.80	0.47
2:I:139:TRP:HE1	2:I:143:ASN:HD22	1.62	0.47
2:J:63:PHE:CD2	2:J:84:THR:HG23	2.50	0.47
2:J:89:VAL:C	2:J:91:PHE:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:128:ASN:ND2	2:M:19:VAL:HG21	2.30	0.47
2:M:3:VAL:O	2:M:4:LEU:C	2.57	0.47
2:M:27:VAL:HG21	2:M:31:ILE:HD11	1.97	0.47
2:N:11:LEU:O	2:N:15:ARG:N	2.39	0.47
2:N:115:SER:O	2:N:119:LEU:HG	2.15	0.47
2:N:124:PHE:O	2:N:127:ILE:HG13	2.15	0.47
1:A:259:HIS:O	1:A:260:GLN:C	2.56	0.47
1:A:510:LEU:HD12	1:A:513:LEU:HD12	1.96	0.47
1:A:510:LEU:CD2	1:A:540:LEU:HD13	2.29	0.47
1:A:578:LEU:HA	1:A:581:VAL:CG2	2.44	0.47
1:A:594:ILE:HG12	1:A:595:PRO:HD2	1.95	0.47
1:A:763:LEU:HD23	1:A:764:PRO:CD	2.44	0.47
1:B:195:ASP:O	1:B:196:ALA:C	2.58	0.47
1:B:443:GLN:C	1:B:445:MET:H	2.21	0.47
1:B:458:ILE:HD12	1:B:459:ALA:CA	2.45	0.47
1:B:480:PHE:CE2	1:B:493:LEU:CB	2.96	0.47
1:B:549:LEU:HD12	1:B:549:LEU:HA	1.64	0.47
2:D:115:SER:O	2:D:119:LEU:HG	2.15	0.47
2:D:346:VAL:CG2	2:D:385:VAL:HG13	2.44	0.47
2:F:46:PHE:HE2	2:F:119:LEU:HD21	1.80	0.47
2:I:115:SER:O	2:I:119:LEU:HG	2.14	0.47
2:J:74:ASP:O	2:J:75:ALA:C	2.57	0.47
2:K:103:GLU:HG3	2:K:359:PRO:HD2	1.95	0.47
2:L:100:MET:HG3	2:L:388:VAL:HG11	1.95	0.47
2:N:346:VAL:CG2	2:N:385:VAL:HG13	2.44	0.47
2:O:73:LEU:HD22	2:O:77:TYR:CD2	2.50	0.47
2:O:104:SER:O	2:O:108:GLY:HA3	2.15	0.47
1:A:211:ILE:C	1:A:213:GLN:H	2.23	0.47
1:A:217:THR:O	1:A:218:GLU:HB2	2.13	0.47
1:A:277:ARG:CD	1:A:559:ALA:HB2	2.43	0.47
1:A:663:TYR:O	1:A:666:ARG:N	2.47	0.47
1:A:803:ASN:ND2	1:A:806:SER:H	2.13	0.47
1:A:850:VAL:C	1:A:851:TYR:CD1	2.93	0.47
1:B:845:ASN:HB3	1:B:848:PHE:CE1	2.49	0.47
1:B:854:LEU:O	1:B:856:ALA:N	2.47	0.47
2:C:106:ARG:H	2:C:106:ARG:CD	2.10	0.47
2:E:5:TYR:HE2	2:E:130:ASP:O	1.98	0.47
2:F:53:ASN:HD22	2:F:354:ALA:CB	2.26	0.47
2:I:23:LEU:HD22	2:I:25:SER:OG	2.14	0.47
2:J:27:VAL:HG21	2:J:31:ILE:HD11	1.96	0.47
2:K:27:VAL:O	2:K:31:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:CD1	1:A:201:ASP:HB2	2.45	0.47
1:A:356:GLU:HB3	1:A:357:ALA:H	1.30	0.47
1:A:440:PHE:O	1:A:441:GLY:C	2.58	0.47
1:A:461:GLN:CA	2:F:32:GLN:NE2	2.75	0.47
1:B:112:LYS:N	1:B:113:PRO:CD	2.78	0.47
1:B:354:GLN:HA	1:B:354:GLN:OE1	2.15	0.47
1:B:383:ILE:HD11	1:B:550:LEU:HD23	1.97	0.47
1:B:519:PRO:O	1:B:520:THR:OG1	2.32	0.47
1:B:645:PHE:HD2	1:B:646:LEU:CD2	2.25	0.47
2:C:150:PHE:HA	2:D:397:LYS:NZ	2.30	0.47
2:E:3:VAL:O	2:E:4:LEU:C	2.57	0.47
2:F:145:ARG:C	2:F:146:GLN:HG2	2.40	0.47
2:H:11:LEU:O	2:H:15:ARG:N	2.39	0.47
2:H:346:VAL:CG2	2:H:385:VAL:HG13	2.44	0.47
2:J:295:MET:HE3	2:J:298:PRO:HD3	1.96	0.47
2:K:109:ILE:HG13	2:K:110:ALA:N	2.29	0.47
2:L:125:LYS:C	2:L:127:ILE:H	2.22	0.47
2:O:65:LEU:O	2:O:66:LEU:HD23	2.15	0.47
1:A:134:TYR:CE1	1:A:803:ASN:CG	2.93	0.46
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.62	0.46
1:A:180:TYR:CD1	1:A:181:LEU:N	2.83	0.46
1:A:286:LEU:H	1:A:286:LEU:CD2	2.10	0.46
1:B:183:LEU:O	1:B:184:LYS:C	2.57	0.46
1:B:380:LYS:O	1:B:381:THR:C	2.58	0.46
1:B:409:TRP:O	1:B:412:THR:HB	2.16	0.46
1:B:479:GLN:O	1:B:480:PHE:HB3	2.16	0.46
1:B:501:HIS:HD1	1:B:548:ARG:HG2	1.80	0.46
2:C:129:PHE:CE1	2:C:130:ASP:HB2	2.50	0.46
2:D:128:ASN:HD22	2:E:19:VAL:HG21	1.80	0.46
2:F:27:VAL:O	2:F:30:LEU:N	2.47	0.46
2:F:106:ARG:HB2	2:F:106:ARG:NH1	2.30	0.46
2:H:3:VAL:O	2:H:4:LEU:C	2.58	0.46
2:I:36:GLN:HE22	2:I:126:ARG:HD3	1.80	0.46
2:I:42:ASN:OD1	2:I:62:ASP:N	2.48	0.46
2:L:27:VAL:CG2	2:L:31:ILE:HD11	2.45	0.46
2:L:57:ARG:HB3	2:L:59:TRP:CZ2	2.49	0.46
2:N:4:LEU:O	2:N:5:TYR:C	2.58	0.46
2:N:124:PHE:O	2:N:126:ARG:N	2.49	0.46
2:O:153:HIS:C	2:O:155:PRO:N	2.71	0.46
1:A:419:PHE:N	1:A:419:PHE:CD1	2.82	0.46
1:A:746:GLN:O	1:A:750:MET:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:PHE:CD1	2:D:150:PHE:N	2.83	0.46
2:E:54:LEU:HD12	2:E:55:PRO:CD	2.42	0.46
2:I:74:ASP:O	2:I:75:ALA:C	2.57	0.46
2:I:128:ASN:HB3	2:J:19:VAL:CG2	2.44	0.46
2:I:144:ARG:O	2:I:145:ARG:CB	2.64	0.46
2:K:4:LEU:O	2:K:5:TYR:C	2.58	0.46
2:M:14:ALA:C	2:M:18:ILE:HD12	2.40	0.46
2:M:14:ALA:O	2:M:18:ILE:HD12	2.16	0.46
2:M:295:MET:HE3	2:M:298:PRO:HD3	1.96	0.46
1:A:250:TYR:HB2	1:A:840:HIS:CD2	2.50	0.46
1:A:253:ASN:O	1:A:256:PHE:HB2	2.14	0.46
1:A:499:ASN:CA	1:A:505:GLN:NE2	2.77	0.46
1:A:854:LEU:CD2	1:A:855:LEU:N	2.78	0.46
1:A:856:ALA:O	1:A:858:VAL:N	2.41	0.46
1:B:75:VAL:O	1:B:75:VAL:HG12	2.16	0.46
1:B:282:VAL:O	1:B:284:TYR:N	2.48	0.46
1:B:420:ILE:O	1:B:422:GLU:N	2.48	0.46
1:B:467:GLN:HE22	1:B:511:MET:HE3	1.80	0.46
1:B:820:THR:HG22	1:B:820:THR:O	2.15	0.46
2:C:62:ASP:H	2:C:63:PHE:HD1	1.62	0.46
2:C:110:ALA:HB1	2:C:111:PRO:HD2	1.97	0.46
2:E:73:LEU:HD22	2:E:77:TYR:CD2	2.50	0.46
2:F:100:MET:HG3	2:F:388:VAL:HG11	1.97	0.46
2:N:76:ASN:HB2	2:O:76:ASN:HB2	1.97	0.46
2:N:89:VAL:C	2:N:91:PHE:N	2.71	0.46
1:A:275:PRO:C	1:A:277:ARG:H	2.23	0.46
1:A:363:GLU:HA	1:A:366:PHE:HE1	1.80	0.46
1:A:428:GLN:HG3	1:A:456:PHE:HA	1.97	0.46
1:A:722:ASN:HB3	1:A:824:LYS:HA	1.96	0.46
1:A:848:PHE:C	1:A:849:THR:OG1	2.58	0.46
1:B:371:ASN:O	1:B:372:SER:C	2.58	0.46
1:B:383:ILE:O	1:B:384:ALA:C	2.57	0.46
1:B:500:GLY:HA3	1:B:871:PHE:HZ	1.80	0.46
1:B:818:VAL:HA	1:B:819:PRO:HD3	1.75	0.46
2:C:19:VAL:HG23	2:E:128:ASN:HB3	1.98	0.46
2:D:1:MET:O	2:D:2:ASP:C	2.56	0.46
2:D:4:LEU:O	2:D:5:TYR:C	2.58	0.46
2:D:38:ILE:HG22	2:D:42:ASN:ND2	2.30	0.46
2:D:89:VAL:C	2:D:91:PHE:N	2.72	0.46
2:F:115:SER:O	2:F:119:LEU:HG	2.14	0.46
2:G:125:LYS:C	2:G:127:ILE:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:VAL:HG21	2:H:31:ILE:HD11	1.96	0.46
2:H:150:PHE:CD1	2:H:150:PHE:N	2.84	0.46
2:I:397:LYS:HZ1	2:K:150:PHE:HA	1.79	0.46
2:K:63:PHE:CD1	2:K:63:PHE:N	2.82	0.46
2:L:153:HIS:NE2	2:M:153:HIS:CD2	2.84	0.46
2:M:128:ASN:HB3	2:N:19:VAL:HG23	1.97	0.46
2:O:4:LEU:O	2:O:5:TYR:C	2.58	0.46
1:A:145:ARG:HB3	1:A:147:TYR:HE1	1.79	0.46
1:A:151:LYS:O	1:A:152:LYS:CB	2.63	0.46
1:A:405:ILE:HG21	1:A:536:LEU:CG	2.43	0.46
1:A:633:LEU:C	1:A:635:GLN:N	2.72	0.46
1:B:360:ILE:O	1:B:361:GLN:HB2	2.15	0.46
2:D:14:ALA:O	2:D:18:ILE:HD12	2.16	0.46
2:I:6:SER:C	2:I:8:SER:N	2.73	0.46
2:J:148:THR:OG1	2:J:332:GLU:HG2	2.15	0.46
2:K:54:LEU:HD12	2:K:55:PRO:CD	2.41	0.46
2:L:6:SER:C	2:L:8:SER:N	2.73	0.46
2:L:151:THR:C	2:L:152:PHE:CD1	2.94	0.46
2:M:6:SER:C	2:M:8:SER:N	2.73	0.46
2:N:150:PHE:N	2:N:150:PHE:CD1	2.84	0.46
2:O:141:LEU:CD1	2:O:148:THR:HG21	2.46	0.46
1:A:122:LEU:CG	1:A:201:ASP:HB2	2.46	0.46
1:A:197:GLY:O	1:A:198:LYS:O	2.34	0.46
1:A:386:MET:HE3	1:A:414:VAL:HG13	1.98	0.46
1:A:414:VAL:C	1:A:416:ASN:H	2.22	0.46
1:A:454:THR:HG22	1:A:457:GLN:H	1.80	0.46
1:A:639:LYS:HE3	1:A:659:ASP:OD1	2.15	0.46
1:A:807:ASN:C	1:A:809:PHE:N	2.73	0.46
1:B:366:PHE:O	1:B:368:THR:N	2.48	0.46
1:B:490:ASN:O	1:B:492:VAL:HG23	2.15	0.46
1:B:605:ASN:ND2	1:B:855:LEU:HD12	2.30	0.46
2:D:14:ALA:C	2:D:18:ILE:HD12	2.41	0.46
2:I:61:PHE:CD1	2:I:61:PHE:N	2.83	0.46
2:O:74:ASP:O	2:O:75:ALA:C	2.58	0.46
2:O:139:TRP:NE1	2:O:143:ASN:ND2	2.63	0.46
1:A:299:ILE:O	1:A:301:PRO:HD3	2.15	0.46
1:A:314:PHE:CZ	1:A:664:ARG:HG2	2.51	0.46
1:A:329:ALA:HB3	1:A:384:ALA:CB	2.46	0.46
1:A:620:ASP:O	1:A:624:ILE:HG13	2.15	0.46
1:B:122:LEU:HD23	1:B:186:MET:HE1	1.98	0.46
1:B:413:VAL:CG1	1:B:414:VAL:H	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:ASN:C	1:B:809:PHE:H	2.23	0.46
1:B:857:PHE:N	1:B:857:PHE:CD1	2.72	0.46
2:D:61:PHE:N	2:D:61:PHE:CD1	2.84	0.46
2:D:74:ASP:O	2:D:75:ALA:C	2.59	0.46
2:D:123:LYS:HG3	2:D:124:PHE:CE1	2.50	0.46
2:F:22:THR:CG2	2:F:73:LEU:HD12	2.45	0.46
2:F:346:VAL:CG2	2:F:385:VAL:HG13	2.44	0.46
2:J:149:GLY:C	2:J:150:PHE:CD1	2.94	0.46
2:L:49:GLY:HA2	2:L:54:LEU:HD23	1.98	0.46
2:N:74:ASP:O	2:N:75:ALA:C	2.58	0.46
1:A:404:LEU:HB3	1:A:435:ILE:HD11	1.98	0.46
1:A:506:LEU:HD23	1:A:544:VAL:CA	2.29	0.46
1:A:660:ASP:HB3	1:B:539:ARG:NH1	2.20	0.46
1:A:708:ARG:HD2	1:A:708:ARG:HA	1.80	0.46
1:B:373:GLN:O	1:B:376:ASN:N	2.49	0.46
1:B:478:ASN:O	1:B:480:PHE:N	2.45	0.46
1:B:601:PHE:HB3	1:B:855:LEU:HD13	1.98	0.46
1:B:770:SER:O	1:B:773:SER:HB2	2.15	0.46
1:B:786:ILE:O	1:B:787:VAL:C	2.59	0.46
1:B:812:VAL:C	1:B:814:ASN:H	2.23	0.46
2:C:346:VAL:CG2	2:C:385:VAL:HG13	2.44	0.46
2:F:22:THR:HG23	2:F:73:LEU:HD12	1.98	0.46
2:I:3:VAL:O	2:I:4:LEU:C	2.57	0.46
2:L:153:HIS:CD2	2:N:153:HIS:NE2	2.83	0.46
2:M:346:VAL:CG2	2:M:385:VAL:HG13	2.45	0.46
2:N:61:PHE:CD1	2:N:61:PHE:N	2.84	0.46
1:A:461:GLN:CB	2:F:32:GLN:NE2	2.79	0.46
1:A:779:ASP:OD2	1:A:822:THR:O	2.34	0.46
1:A:846:LEU:HD23	1:A:846:LEU:HA	1.65	0.46
1:B:118:LYS:CG	1:B:119:GLN:N	2.73	0.46
1:B:239:VAL:CG2	1:B:845:ASN:O	2.63	0.46
1:B:252:PHE:O	1:B:253:ASN:C	2.59	0.46
1:B:314:PHE:HZ	1:B:664:ARG:HG2	1.78	0.46
1:B:345:GLN:HG3	1:B:349:MET:CE	2.46	0.46
1:B:383:ILE:HD11	1:B:550:LEU:HD22	1.97	0.46
1:B:465:ASN:O	1:B:466:PHE:C	2.58	0.46
1:B:510:LEU:HD13	1:B:540:LEU:HB2	1.98	0.46
1:B:552:TYR:O	1:B:553:ASN:C	2.58	0.46
1:B:727:LEU:HG	1:B:727:LEU:O	2.15	0.46
1:B:848:PHE:O	1:B:849:THR:OG1	2.28	0.46
1:B:856:ALA:C	1:B:858:VAL:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:72:ASN:CG	2:K:126:ARG:NH1	2.74	0.46
2:I:155:PRO:O	2:I:186:SER:HB3	2.16	0.46
2:I:382:LEU:HD22	2:I:386:PHE:CE2	2.51	0.46
2:J:27:VAL:CG2	2:J:31:ILE:HD11	2.45	0.46
2:J:142:GLN:HE21	2:J:143:ASN:N	2.13	0.46
2:L:104:SER:HB3	2:L:108:GLY:CA	2.46	0.46
2:O:22:THR:CG2	2:O:73:LEU:HD12	2.46	0.46
1:A:245:LEU:O	1:A:246:HIS:HB2	2.16	0.46
1:A:428:GLN:OE1	1:A:456:PHE:CB	2.38	0.46
1:A:509:ALA:O	1:A:513:LEU:CG	2.55	0.46
1:A:821:SER:OG	1:A:822:THR:N	2.46	0.46
1:B:94:THR:O	1:B:94:THR:HG22	2.16	0.46
1:B:489:LEU:C	1:B:489:LEU:HD23	2.41	0.46
1:B:613:ASN:O	1:B:617:ARG:HG2	2.16	0.46
1:B:706:ALA:C	1:B:708:ARG:N	2.72	0.46
1:B:776:ALA:O	1:B:777:LYS:C	2.58	0.46
2:E:74:ASP:O	2:E:75:ALA:C	2.58	0.46
2:F:239:ASN:ND2	2:F:246:THR:HG22	2.29	0.46
2:H:106:ARG:O	2:H:107:ASN:CB	2.62	0.46
2:H:239:ASN:ND2	2:H:246:THR:HG22	2.30	0.46
2:K:346:VAL:CG2	2:K:385:VAL:HG13	2.44	0.46
1:A:549:LEU:HA	1:A:549:LEU:HD12	1.65	0.45
1:B:170:TYR:CZ	1:B:682:PHE:HB2	2.52	0.45
1:B:637:LYS:HA	1:B:641:ILE:HD11	1.97	0.45
1:B:675:GLU:O	1:B:677:ARG:N	2.49	0.45
2:D:6:SER:C	2:D:8:SER:N	2.73	0.45
2:G:5:TYR:HE2	2:G:131:ASN:HA	1.80	0.45
2:H:62:ASP:H	2:H:63:PHE:HD1	1.63	0.45
2:J:27:VAL:O	2:J:28:SER:C	2.57	0.45
2:J:382:LEU:HD22	2:J:386:PHE:CE2	2.52	0.45
2:K:382:LEU:HD22	2:K:386:PHE:CE2	2.51	0.45
2:O:34:PHE:O	2:O:35:ASN:C	2.59	0.45
1:A:552:TYR:O	1:A:553:ASN:C	2.59	0.45
1:A:622:VAL:O	1:A:623:ALA:C	2.59	0.45
1:A:756:PRO:C	1:A:757:VAL:CG2	2.89	0.45
1:B:282:VAL:HG13	1:B:283:ASN:N	2.31	0.45
1:B:379:PHE:O	1:B:380:LYS:C	2.59	0.45
1:B:508:GLU:OE2	2:J:70:LEU:CD2	2.65	0.45
1:B:583:SER:OG	1:B:584:LEU:N	2.48	0.45
1:B:772:ILE:HG22	1:B:809:PHE:CE2	2.51	0.45
2:D:31:ILE:O	2:D:32:GLN:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:LYS:HE2	2:H:130:ASP:OD2	2.16	0.45
2:F:24:TYR:C	2:F:26:ASN:H	2.24	0.45
2:F:60:ASN:C	2:F:61:PHE:CD1	2.95	0.45
2:G:109:ILE:HD12	2:G:109:ILE:O	2.17	0.45
2:H:21:GLY:O	2:H:22:THR:O	2.34	0.45
2:I:36:GLN:HB2	2:J:23:LEU:HD11	1.97	0.45
2:I:136:ILE:HG23	2:I:137:GLU:N	2.31	0.45
2:L:73:LEU:HD22	2:L:77:TYR:HD2	1.77	0.45
2:L:115:SER:O	2:L:119:LEU:HG	2.15	0.45
2:M:382:LEU:HD22	2:M:386:PHE:CE2	2.52	0.45
1:A:147:TYR:HE2	1:A:717:MET:HE2	1.79	0.45
1:A:353:LEU:HD22	1:A:531:ARG:HB3	1.98	0.45
1:A:526:LYS:HG3	1:A:527:ARG:N	2.31	0.45
1:A:609:ASN:O	1:A:610:PHE:C	2.59	0.45
1:A:688:ASN:O	1:A:691:GLN:N	2.49	0.45
1:A:706:ALA:O	1:A:708:ARG:N	2.45	0.45
1:B:87:GLN:C	1:B:89:GLU:H	2.25	0.45
1:B:498:ARG:CZ	2:J:25:SER:HB3	2.47	0.45
1:B:542:GLN:N	1:B:542:GLN:OE1	2.49	0.45
1:B:594:ILE:HD12	1:B:594:ILE:O	2.17	0.45
1:B:633:LEU:O	1:B:635:GLN:N	2.48	0.45
2:C:59:TRP:N	2:C:59:TRP:CD1	2.83	0.45
2:C:124:PHE:O	2:C:127:ILE:HG13	2.16	0.45
2:D:34:PHE:O	2:D:35:ASN:C	2.59	0.45
2:E:190:VAL:HG21	2:E:210:HIS:HB2	1.99	0.45
2:F:74:ASP:O	2:F:75:ALA:C	2.59	0.45
2:H:382:LEU:HD22	2:H:386:PHE:CE2	2.51	0.45
2:J:78:VAL:O	2:J:81:ALA:N	2.40	0.45
2:J:133:SER:O	2:J:134:GLU:C	2.59	0.45
2:K:24:TYR:O	2:K:27:VAL:HG22	2.16	0.45
2:L:22:THR:CG2	2:L:73:LEU:HD12	2.24	0.45
2:L:239:ASN:ND2	2:L:246:THR:HG22	2.29	0.45
2:M:53:ASN:HD22	2:M:354:ALA:HB3	1.81	0.45
2:N:24:TYR:CE1	2:N:31:ILE:HG13	2.51	0.45
2:N:34:PHE:O	2:N:35:ASN:C	2.59	0.45
1:A:518:PHE:CB	1:A:519:PRO:CD	2.94	0.45
1:A:688:ASN:O	1:A:690:ASP:N	2.50	0.45
1:A:760:VAL:HG12	1:A:761:GLY:N	2.30	0.45
1:B:119:GLN:CG	1:B:181:LEU:HD11	2.46	0.45
1:B:159:ASP:O	1:B:162:VAL:HB	2.16	0.45
2:D:133:SER:O	2:D:134:GLU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:89:VAL:C	2:E:91:PHE:N	2.73	0.45
2:H:34:PHE:O	2:H:35:ASN:C	2.60	0.45
2:J:6:SER:C	2:J:8:SER:N	2.73	0.45
2:M:66:LEU:O	2:M:67:GLY:C	2.58	0.45
2:M:144:ARG:O	2:M:145:ARG:HB2	2.17	0.45
1:A:249:ASP:O	1:A:250:TYR:C	2.60	0.45
1:A:857:PHE:N	1:A:857:PHE:CD1	2.83	0.45
1:B:224:PHE:HE1	2:O:70:LEU:C	2.24	0.45
1:B:434:THR:O	1:B:435:ILE:CG1	2.65	0.45
1:B:543:LEU:O	1:B:544:VAL:C	2.58	0.45
1:B:854:LEU:HD22	1:B:855:LEU:H	1.82	0.45
2:C:382:LEU:HD22	2:C:386:PHE:CE2	2.51	0.45
2:D:190:VAL:HG21	2:D:210:HIS:HB2	1.99	0.45
2:D:382:LEU:HD22	2:D:386:PHE:CE2	2.52	0.45
2:E:65:LEU:C	2:E:66:LEU:HG	2.42	0.45
2:G:4:LEU:O	2:G:5:TYR:C	2.59	0.45
2:I:225:LEU:HD13	2:I:277:PHE:HD2	1.82	0.45
2:M:130:ASP:HA	2:N:17:LYS:HG2	1.98	0.45
2:N:110:ALA:HB1	2:N:111:PRO:HD2	1.99	0.45
1:A:154:THR:O	1:A:155:LEU:C	2.59	0.45
1:A:482:GLN:OE1	1:A:493:LEU:CD2	2.64	0.45
1:A:712:LEU:CG	1:A:819:PRO:HB2	2.40	0.45
1:A:804:SER:HB2	1:A:810:TYR:CA	2.47	0.45
1:A:822:THR:O	1:A:823:THR:CB	2.64	0.45
1:B:622:VAL:O	1:B:623:ALA:C	2.59	0.45
1:B:646:LEU:HD23	1:B:646:LEU:N	2.32	0.45
2:C:128:ASN:O	2:D:22:THR:HB	2.17	0.45
2:C:190:VAL:HG21	2:C:210:HIS:HB2	1.99	0.45
2:D:24:TYR:O	2:D:26:ASN:N	2.50	0.45
2:D:78:VAL:O	2:D:81:ALA:HB3	2.17	0.45
2:E:312:GLN:HB3	2:E:313:PRO:HA	1.99	0.45
2:H:107:ASN:ND2	2:H:109:ILE:HG23	2.32	0.45
2:H:190:VAL:HG21	2:H:210:HIS:HB2	1.99	0.45
2:I:16:ASP:HB3	2:K:131:ASN:C	2.42	0.45
2:I:31:ILE:O	2:I:32:GLN:C	2.59	0.45
2:L:190:VAL:HG21	2:L:210:HIS:HB2	1.99	0.45
2:M:155:PRO:HA	2:M:337:ASP:HB2	1.99	0.45
2:N:124:PHE:C	2:N:126:ARG:H	2.24	0.45
1:A:155:LEU:HA	1:A:156:PRO:HD3	1.55	0.45
1:A:319:ASP:OD2	1:A:571:LEU:N	2.49	0.45
1:A:546:LEU:HD13	1:A:584:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLN:O	1:B:374:ALA:C	2.59	0.45
1:B:477:ASN:C	1:B:479:GLN:N	2.75	0.45
1:B:554:TYR:O	1:B:558:MET:HB2	2.17	0.45
1:B:577:GLN:O	1:B:579:THR:N	2.50	0.45
1:B:601:PHE:CD1	1:B:601:PHE:N	2.80	0.45
1:B:742:GLY:O	1:B:744:TYR:HE2	1.98	0.45
2:D:54:LEU:HD12	2:D:55:PRO:CD	2.46	0.45
2:E:11:LEU:O	2:E:15:ARG:N	2.41	0.45
2:E:382:LEU:HD22	2:E:386:PHE:CE2	2.51	0.45
2:F:190:VAL:HG21	2:F:210:HIS:HB2	1.99	0.45
2:G:150:PHE:HB2	2:G:152:PHE:CZ	2.51	0.45
2:H:6:SER:C	2:H:8:SER:N	2.74	0.45
2:H:105:GLN:O	2:H:107:ASN:N	2.50	0.45
2:H:312:GLN:HB3	2:H:313:PRO:HA	1.99	0.45
2:L:74:ASP:O	2:L:75:ALA:C	2.59	0.45
2:L:382:LEU:HD22	2:L:386:PHE:CE2	2.52	0.45
2:M:31:ILE:O	2:M:32:GLN:C	2.60	0.45
2:M:110:ALA:HB1	2:M:111:PRO:HD2	1.99	0.45
2:N:23:LEU:HD22	2:N:25:SER:OG	2.17	0.45
1:A:252:PHE:CD2	1:A:684:LEU:CD2	3.00	0.45
1:A:421:ARG:C	1:A:423:SER:H	2.25	0.45
1:A:452:PRO:O	1:A:453:GLN:OE1	2.35	0.45
1:A:454:THR:O	1:A:457:GLN:HB3	2.17	0.45
1:A:503:ILE:O	1:A:505:GLN:N	2.50	0.45
1:A:506:LEU:CD2	1:A:544:VAL:CA	2.94	0.45
1:A:649:LEU:C	1:A:650:HIS:O	2.60	0.45
1:B:400:ASN:O	1:B:404:LEU:CD1	2.65	0.45
2:D:225:LEU:HD13	2:D:277:PHE:HD2	1.82	0.45
2:E:154:LYS:N	2:E:327:GLU:O	2.42	0.45
2:F:312:GLN:HB3	2:F:313:PRO:HA	1.99	0.45
2:G:34:PHE:O	2:G:35:ASN:C	2.60	0.45
2:G:382:LEU:HD22	2:G:386:PHE:CE2	2.51	0.45
2:H:48:THR:O	2:H:56:ILE:HA	2.17	0.45
2:H:108:GLY:C	2:H:110:ALA:N	2.75	0.45
2:I:42:ASN:OD1	2:I:61:PHE:HB3	2.16	0.45
2:I:145:ARG:O	2:I:146:GLN:CG	2.65	0.45
2:J:225:LEU:HD13	2:J:277:PHE:HD2	1.82	0.45
2:M:4:LEU:O	2:M:5:TYR:C	2.58	0.45
2:M:225:LEU:HD13	2:M:277:PHE:HD2	1.82	0.45
2:O:217:VAL:HG22	2:O:286:ASP:HB3	1.99	0.45
1:A:186:MET:HG3	1:A:200:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:SER:O	1:A:342:THR:C	2.60	0.45
1:A:583:SER:OG	1:A:584:LEU:N	2.50	0.45
1:A:783:PHE:N	1:A:783:PHE:CD1	2.72	0.45
1:B:119:GLN:NE2	1:B:181:LEU:HD11	2.32	0.45
1:B:277:ARG:HB3	1:B:277:ARG:HH11	1.80	0.45
1:B:496:ASN:HB3	1:B:499:ASN:H	1.82	0.45
1:B:553:ASN:O	1:B:554:TYR:C	2.60	0.45
1:B:573:THR:CG2	1:B:574:GLU:N	2.45	0.45
1:B:771:VAL:HG21	1:B:809:PHE:O	2.17	0.45
1:B:786:ILE:HG22	1:B:792:VAL:HG12	1.98	0.45
2:C:127:ILE:HG22	2:C:127:ILE:O	2.15	0.45
2:C:136:ILE:HG23	2:C:137:GLU:N	2.32	0.45
2:D:45:GLU:C	2:D:46:PHE:CD1	2.94	0.45
2:E:225:LEU:HD13	2:E:277:PHE:HD2	1.82	0.45
2:F:225:LEU:HD13	2:F:277:PHE:HD2	1.82	0.45
2:F:382:LEU:HD22	2:F:386:PHE:CE2	2.52	0.45
2:I:217:VAL:HG22	2:I:286:ASP:HB3	1.99	0.45
2:J:70:LEU:HD22	2:J:72:ASN:O	2.16	0.45
2:K:6:SER:C	2:K:8:SER:N	2.74	0.45
2:L:4:LEU:O	2:L:5:TYR:C	2.59	0.45
2:L:133:SER:O	2:L:134:GLU:C	2.60	0.45
2:M:312:GLN:HB3	2:M:313:PRO:HA	1.99	0.45
2:O:131:ASN:N	2:O:131:ASN:HD22	2.14	0.45
2:O:190:VAL:HG21	2:O:210:HIS:HB2	1.99	0.45
2:O:225:LEU:HD13	2:O:277:PHE:HD2	1.82	0.45
1:A:269:ILE:HG21	1:A:298:TYR:CE2	2.51	0.45
1:A:380:LYS:O	1:A:381:THR:C	2.60	0.45
1:A:428:GLN:HG2	1:A:429:LEU:H	1.79	0.45
1:A:442:MET:HE3	1:A:463:ILE:HB	1.99	0.45
1:A:866:ILE:HG22	1:A:866:ILE:O	2.17	0.45
1:B:387:LEU:C	1:B:389:GLN:N	2.74	0.45
1:B:467:GLN:HE21	1:B:511:MET:HG2	1.82	0.45
1:B:772:ILE:CG2	1:B:809:PHE:HE2	2.29	0.45
1:B:846:LEU:HD12	1:B:847:THR:N	2.32	0.45
2:C:34:PHE:O	2:C:35:ASN:C	2.60	0.45
2:C:217:VAL:HG22	2:C:286:ASP:HB3	1.99	0.45
2:G:31:ILE:O	2:G:32:GLN:C	2.59	0.45
2:G:190:VAL:HG21	2:G:210:HIS:HB2	1.99	0.45
2:H:1:MET:C	2:H:3:VAL:N	2.74	0.45
2:J:217:VAL:HG22	2:J:286:ASP:HB3	1.99	0.45
2:J:312:GLN:HB3	2:J:313:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:190:VAL:HG21	2:K:210:HIS:HB2	1.99	0.45
2:M:42:ASN:HA	2:M:61:PHE:CB	2.46	0.45
2:N:382:LEU:HD22	2:N:386:PHE:CE2	2.52	0.45
1:A:118:LYS:CG	1:A:119:GLN:H	2.29	0.44
1:A:420:ILE:HD11	1:A:423:SER:HB2	1.99	0.44
1:A:587:LEU:O	1:A:587:LEU:HD22	2.17	0.44
1:A:680:ASP:HA	1:A:683:ASN:HD22	1.81	0.44
1:B:428:GLN:CB	1:B:456:PHE:CD1	2.90	0.44
1:B:763:LEU:HD22	1:B:764:PRO:HD3	1.99	0.44
2:D:8:SER:O	2:D:9:LYS:C	2.60	0.44
2:D:51:ILE:O	2:D:52:GLY:C	2.58	0.44
2:D:136:ILE:HG23	2:D:137:GLU:N	2.32	0.44
2:D:217:VAL:HG22	2:D:286:ASP:HB3	1.99	0.44
2:E:44:ASN:HB3	2:E:46:PHE:HE1	1.81	0.44
2:G:78:VAL:O	2:G:81:ALA:HB3	2.18	0.44
2:G:312:GLN:HB3	2:G:313:PRO:HA	1.99	0.44
2:I:190:VAL:HG21	2:I:210:HIS:HB2	1.99	0.44
2:J:153:HIS:NE2	2:K:153:HIS:CD2	2.84	0.44
2:K:225:LEU:HD13	2:K:277:PHE:HD2	1.82	0.44
2:L:225:LEU:HD13	2:L:277:PHE:HD2	1.82	0.44
2:L:312:GLN:HB3	2:L:313:PRO:HA	1.99	0.44
2:M:1:MET:O	2:M:2:ASP:C	2.58	0.44
1:A:270:ILE:HD11	1:A:292:LEU:CD1	2.23	0.44
1:A:286:LEU:O	1:A:287:ASN:CB	2.65	0.44
1:A:348:LYS:O	1:A:351:GLN:HB2	2.17	0.44
1:B:148:TRP:HE1	1:B:833:PHE:HD1	1.64	0.44
1:B:226:ALA:O	1:B:228:MET:N	2.50	0.44
1:B:248:ILE:O	1:B:251:ALA:HB3	2.17	0.44
1:B:374:ALA:O	1:B:580:SER:HB2	2.17	0.44
1:B:420:ILE:O	1:B:420:ILE:HG23	2.18	0.44
1:B:463:ILE:HD12	1:B:472:LEU:CD1	2.47	0.44
1:B:498:ARG:HG3	1:B:505:GLN:CD	2.42	0.44
1:B:632:ASN:C	1:B:634:TYR:H	2.23	0.44
1:B:666:ARG:O	1:B:667:ASP:C	2.60	0.44
1:B:688:ASN:O	1:B:689:MET:C	2.59	0.44
1:B:852:SER:O	1:B:853:ASP:HB3	2.16	0.44
2:C:6:SER:C	2:C:8:SER:N	2.74	0.44
2:C:22:THR:HG23	2:C:73:LEU:CD1	2.46	0.44
2:C:54:LEU:HD12	2:C:55:PRO:CD	2.44	0.44
2:D:62:ASP:C	2:D:63:PHE:CD1	2.95	0.44
2:E:8:SER:O	2:E:9:LYS:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:ILE:O	2:F:32:GLN:C	2.60	0.44
2:F:78:VAL:O	2:F:81:ALA:N	2.43	0.44
2:G:133:SER:O	2:G:134:GLU:C	2.61	0.44
2:I:140:ASN:O	2:I:143:ASN:N	2.50	0.44
2:J:4:LEU:O	2:J:5:TYR:C	2.58	0.44
2:L:397:LYS:HZ1	2:N:150:PHE:HA	1.82	0.44
2:M:239:ASN:ND2	2:M:246:THR:HG22	2.30	0.44
2:N:6:SER:C	2:N:8:SER:N	2.75	0.44
2:N:225:LEU:HD13	2:N:277:PHE:HD2	1.82	0.44
2:O:31:ILE:O	2:O:32:GLN:C	2.59	0.44
2:O:382:LEU:HD22	2:O:386:PHE:CE2	2.51	0.44
1:A:218:GLU:O	1:A:219:GLY:C	2.60	0.44
1:A:229:ARG:O	1:A:242:PRO:HG3	2.18	0.44
1:A:556:THR:O	1:A:558:MET:N	2.51	0.44
1:A:660:ASP:OD1	1:A:661:GLN:N	2.50	0.44
1:A:674:VAL:HB	1:A:679:LEU:HB2	1.99	0.44
1:A:714:ARG:O	1:A:715:ASP:C	2.59	0.44
1:B:183:LEU:HD12	1:B:844:SER:CB	2.47	0.44
1:B:368:THR:HG22	1:B:371:ASN:ND2	2.26	0.44
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.62	0.44
1:B:558:MET:O	1:B:559:ALA:C	2.60	0.44
1:B:757:VAL:HG12	1:B:758:ALA:N	2.32	0.44
1:B:870:ALA:C	1:B:872:ASP:H	2.21	0.44
2:C:27:VAL:O	2:C:30:LEU:HB3	2.17	0.44
2:C:69:THR:OG1	2:C:70:LEU:N	2.49	0.44
2:F:6:SER:C	2:F:8:SER:N	2.73	0.44
2:F:153:HIS:CD2	2:H:153:HIS:NE2	2.86	0.44
2:G:99:GLU:CD	2:G:112:GLN:H	2.25	0.44
2:J:151:THR:C	2:J:152:PHE:CD1	2.95	0.44
2:K:78:VAL:O	2:K:81:ALA:N	2.40	0.44
2:K:111:PRO:O	2:K:112:GLN:HG2	2.17	0.44
2:K:239:ASN:ND2	2:K:246:THR:HG22	2.29	0.44
2:L:136:ILE:HG23	2:L:137:GLU:N	2.32	0.44
2:M:149:GLY:C	2:M:150:PHE:CD1	2.96	0.44
1:A:589:GLY:C	1:A:591:ALA:N	2.66	0.44
1:A:597:PRO:HB3	1:A:860:ALA:HB1	1.99	0.44
1:A:758:ALA:C	1:A:759:LEU:HG	2.36	0.44
1:A:804:SER:CB	1:A:810:TYR:HA	2.48	0.44
1:B:250:TYR:HB2	1:B:840:HIS:CD2	2.53	0.44
1:B:416:ASN:CG	1:B:417:ASP:N	2.75	0.44
1:B:630:ARG:O	1:B:631:LEU:CG	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:LEU:O	1:B:754:ASN:HA	2.16	0.44
1:B:790:ARG:CG	1:B:791:LYS:N	2.71	0.44
2:C:63:PHE:CD2	2:C:84:THR:HG23	2.52	0.44
2:C:145:ARG:CB	2:C:145:ARG:HH11	2.30	0.44
2:C:152:PHE:O	2:C:328:SER:HA	2.17	0.44
2:D:125:LYS:C	2:D:127:ILE:H	2.25	0.44
2:E:66:LEU:HB3	2:E:77:TYR:OH	2.16	0.44
2:E:78:VAL:O	2:E:81:ALA:HB3	2.17	0.44
2:F:48:THR:HG22	2:F:115:SER:OG	2.18	0.44
2:J:225:LEU:HD13	2:J:277:PHE:CD2	2.53	0.44
2:K:27:VAL:CG2	2:K:31:ILE:HD11	2.48	0.44
2:L:34:PHE:O	2:L:37:MET:HB3	2.17	0.44
2:M:34:PHE:O	2:M:35:ASN:C	2.60	0.44
2:N:190:VAL:HG21	2:N:210:HIS:HB2	1.99	0.44
1:A:130:GLN:NE2	1:A:146:TRP:CZ2	2.85	0.44
1:A:305:GLN:CD	1:A:305:GLN:N	2.75	0.44
1:A:513:LEU:CA	1:A:516:GLN:NE2	2.65	0.44
1:B:277:ARG:CB	1:B:277:ARG:HH11	2.30	0.44
1:B:315:GLU:O	1:B:316:SER:C	2.59	0.44
1:B:446:HIS:O	1:B:447:TYR:CB	2.49	0.44
1:B:494:ASN:CG	1:B:495:ASP:N	2.75	0.44
1:B:498:ARG:HH11	1:B:502:VAL:HG11	1.83	0.44
1:B:707:TYR:N	1:B:707:TYR:CD1	2.85	0.44
1:B:773:SER:O	1:B:774:LEU:C	2.59	0.44
2:C:74:ASP:O	2:C:75:ALA:C	2.60	0.44
2:C:133:SER:O	2:C:134:GLU:C	2.60	0.44
2:D:75:ALA:HB3	2:L:76:ASN:HA	2.00	0.44
2:F:82:ARG:CZ	2:H:144:ARG:HD2	2.47	0.44
2:F:133:SER:O	2:F:134:GLU:C	2.60	0.44
2:G:1:MET:O	2:G:2:ASP:C	2.60	0.44
2:G:239:ASN:ND2	2:G:246:THR:HG22	2.29	0.44
2:I:101:VAL:HG11	2:I:355:ILE:HG13	1.99	0.44
2:J:31:ILE:O	2:J:32:GLN:C	2.60	0.44
2:K:136:ILE:HG23	2:K:137:GLU:N	2.32	0.44
2:K:149:GLY:C	2:K:150:PHE:CD1	2.95	0.44
2:M:136:ILE:HG23	2:M:137:GLU:N	2.33	0.44
2:M:150:PHE:O	2:M:330:VAL:HG13	2.17	0.44
2:N:38:ILE:HG22	2:N:42:ASN:ND2	2.29	0.44
2:N:78:VAL:O	2:N:81:ALA:HB3	2.17	0.44
2:O:6:SER:C	2:O:8:SER:N	2.73	0.44
1:A:426:ALA:O	1:A:427:CYS:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:O	1:A:490:ASN:N	2.51	0.44
1:A:508:GLU:C	1:A:512:GLN:NE2	2.73	0.44
1:A:516:GLN:OE1	1:A:517:GLN:N	2.50	0.44
1:A:701:GLN:CG	1:A:826:TYR:CD2	3.00	0.44
1:A:727:LEU:O	1:A:727:LEU:CD1	2.65	0.44
1:A:771:VAL:HG13	1:A:772:ILE:N	2.22	0.44
1:A:807:ASN:C	1:A:809:PHE:H	2.25	0.44
1:B:230:GLN:CD	1:B:230:GLN:H	2.25	0.44
1:B:393:SER:HA	1:B:423:SER:CB	2.47	0.44
1:B:426:ALA:O	1:B:427:CYS:C	2.61	0.44
1:B:449:ASN:ND2	1:B:455:PRO:HG3	2.33	0.44
1:B:452:PRO:C	1:B:453:GLN:CD	2.86	0.44
1:B:680:ASP:HA	1:B:683:ASN:HD22	1.82	0.44
1:B:727:LEU:HD23	1:B:826:TYR:CE1	2.53	0.44
2:E:5:TYR:O	2:E:6:SER:C	2.60	0.44
2:E:133:SER:O	2:E:134:GLU:C	2.60	0.44
2:E:225:LEU:HD13	2:E:277:PHE:CD2	2.53	0.44
2:F:11:LEU:O	2:F:15:ARG:N	2.40	0.44
2:F:153:HIS:O	2:F:154:LYS:C	2.61	0.44
2:F:249:PHE:CE2	2:F:251:PRO:HG3	2.53	0.44
2:G:33:GLN:HB2	2:H:26:ASN:OD1	2.16	0.44
2:G:89:VAL:C	2:G:91:PHE:N	2.73	0.44
2:G:104:SER:O	2:G:108:GLY:CA	2.66	0.44
2:H:31:ILE:O	2:H:32:GLN:C	2.60	0.44
2:H:67:GLY:O	2:H:69:THR:N	2.51	0.44
2:I:24:TYR:N	2:I:71:LEU:O	2.51	0.44
2:I:133:SER:O	2:I:134:GLU:C	2.60	0.44
2:J:34:PHE:O	2:J:35:ASN:C	2.60	0.44
2:K:133:SER:O	2:K:134:GLU:C	2.60	0.44
2:L:1:MET:O	2:L:2:ASP:C	2.59	0.44
2:M:225:LEU:HD13	2:M:277:PHE:CD2	2.53	0.44
2:N:63:PHE:CD1	2:N:63:PHE:N	2.85	0.44
2:O:136:ILE:HG23	2:O:137:GLU:N	2.32	0.44
1:A:312:ASP:O	1:A:313:ASN:CB	2.63	0.44
1:A:795:LEU:HD12	1:A:795:LEU:HA	1.74	0.44
1:B:102:GLU:O	1:B:103:SER:C	2.61	0.44
1:B:324:SER:O	1:B:325:ASN:C	2.61	0.44
1:B:428:GLN:HA	1:B:431:ILE:CD1	2.42	0.44
1:B:519:PRO:O	1:B:520:THR:CB	2.66	0.44
1:B:738:LEU:HD12	1:B:738:LEU:HA	1.82	0.44
1:B:786:ILE:C	1:B:788:LYS:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:LEU:O	1:B:856:ALA:C	2.60	0.44
2:D:73:LEU:HD23	2:D:73:LEU:N	2.33	0.44
2:D:249:PHE:CE2	2:D:251:PRO:HG3	2.53	0.44
2:G:6:SER:C	2:G:8:SER:N	2.72	0.44
2:H:142:GLN:NE2	2:H:143:ASN:N	2.65	0.44
2:H:217:VAL:HG22	2:H:286:ASP:HB3	2.00	0.44
2:H:249:PHE:CE2	2:H:251:PRO:HG3	2.53	0.44
2:I:46:PHE:HE2	2:I:119:LEU:HD21	1.83	0.44
2:I:225:LEU:HD13	2:I:277:PHE:CD2	2.53	0.44
2:J:78:VAL:O	2:J:81:ALA:HB3	2.17	0.44
2:K:14:ALA:O	2:K:16:ASP:N	2.51	0.44
2:K:110:ALA:HB1	2:K:111:PRO:HD2	2.00	0.44
2:K:312:GLN:HB3	2:K:313:PRO:HA	1.99	0.44
2:M:249:PHE:CE2	2:M:251:PRO:HG3	2.53	0.44
2:N:133:SER:O	2:N:134:GLU:C	2.61	0.44
2:N:217:VAL:HG22	2:N:286:ASP:HB3	2.00	0.44
2:O:153:HIS:CD2	2:O:154:LYS:N	2.86	0.44
2:O:169:SER:HA	2:O:176:LEU:HD23	2.00	0.44
2:O:225:LEU:HD13	2:O:277:PHE:CD2	2.53	0.44
1:A:216:GLU:C	1:A:218:GLU:H	2.25	0.44
1:A:625:ILE:H	1:A:625:ILE:HG13	1.62	0.44
1:B:108:LEU:N	1:B:108:LEU:CD2	2.79	0.44
1:B:155:LEU:HA	1:B:156:PRO:HD3	1.81	0.44
1:B:282:VAL:HG13	1:B:283:ASN:H	1.83	0.44
1:B:305:GLN:OE1	1:B:305:GLN:HA	2.18	0.44
1:B:406:SER:O	1:B:407:GLY:C	2.60	0.44
1:B:482:GLN:C	1:B:483:VAL:HG23	2.43	0.44
1:B:487:GLY:O	1:B:488:VAL:CB	2.66	0.44
1:B:508:GLU:O	1:B:512:GLN:NE2	2.48	0.44
2:C:249:PHE:CE2	2:C:251:PRO:HG3	2.53	0.44
2:D:66:LEU:HA	2:D:66:LEU:HD23	1.72	0.44
2:D:149:GLY:C	2:D:150:PHE:CD1	2.95	0.44
2:E:217:VAL:HG22	2:E:286:ASP:HB3	2.00	0.44
2:F:169:SER:HA	2:F:176:LEU:HD23	2.00	0.44
2:G:169:SER:HA	2:G:176:LEU:HD23	2.00	0.44
2:I:153:HIS:O	2:I:154:LYS:C	2.59	0.44
2:J:103:GLU:OE1	2:J:358:GLY:HA3	2.18	0.44
2:K:135:TYR:CZ	2:K:342:MET:HE3	2.53	0.44
2:K:227:PRO:HD3	2:K:277:PHE:CG	2.53	0.44
2:L:225:LEU:HD13	2:L:277:PHE:CD2	2.53	0.44
2:M:217:VAL:HG22	2:M:286:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:8:SER:O	2:N:9:LYS:C	2.61	0.44
2:O:312:GLN:HB3	2:O:313:PRO:HA	1.99	0.44
1:A:160:TYR:HE1	1:A:633:LEU:HA	1.83	0.44
1:A:181:LEU:H	1:A:260:GLN:HE21	1.65	0.44
1:A:226:ALA:C	1:A:228:MET:N	2.76	0.44
1:A:245:LEU:O	1:A:246:HIS:CB	2.66	0.44
1:A:456:PHE:O	1:A:457:GLN:C	2.61	0.44
1:A:521:MET:HE3	1:A:521:MET:CA	2.38	0.44
1:A:604:TYR:O	1:A:605:ASN:C	2.59	0.44
1:A:618:ILE:HD13	1:A:645:PHE:HZ	1.83	0.44
1:A:799:LEU:HD22	1:A:800:TYR:H	1.82	0.44
1:A:872:ASP:CG	1:A:874:MET:HB2	2.43	0.44
1:B:101:LYS:HB2	1:B:102:GLU:H	1.68	0.44
1:B:111:ILE:HG22	1:B:113:PRO:CD	2.48	0.44
1:B:122:LEU:HD12	1:B:124:ARG:HH22	1.82	0.44
1:B:207:ILE:O	1:B:210:ALA:HB3	2.18	0.44
1:B:218:GLU:C	1:B:220:ALA:N	2.76	0.44
1:B:353:LEU:O	1:B:353:LEU:HD23	2.18	0.44
1:B:473:HIS:HB3	2:I:126:ARG:NH1	2.26	0.44
1:B:496:ASN:HD22	1:B:498:ARG:HB2	1.83	0.44
1:B:543:LEU:O	1:B:546:LEU:HB2	2.18	0.44
1:B:675:GLU:O	1:B:678:ARG:N	2.51	0.44
1:B:790:ARG:CG	1:B:791:LYS:H	2.18	0.44
2:C:67:GLY:C	2:C:69:THR:N	2.72	0.44
2:C:397:LYS:HZ1	2:E:150:PHE:HA	1.82	0.44
2:D:5:TYR:CE2	2:D:131:ASN:HA	2.52	0.44
2:D:169:SER:HA	2:D:176:LEU:HD23	2.00	0.44
2:E:45:GLU:C	2:E:46:PHE:CD1	2.96	0.44
2:E:249:PHE:CE2	2:E:251:PRO:HG3	2.53	0.44
2:G:100:MET:HG3	2:G:388:VAL:HG11	1.99	0.44
2:G:150:PHE:N	2:G:150:PHE:CD1	2.86	0.44
2:H:78:VAL:O	2:H:81:ALA:HB3	2.17	0.44
2:I:63:PHE:CD1	2:I:63:PHE:N	2.86	0.44
2:J:8:SER:O	2:J:9:LYS:C	2.60	0.44
2:K:49:GLY:HA2	2:K:54:LEU:HD23	1.99	0.44
2:L:34:PHE:O	2:L:35:ASN:C	2.60	0.44
2:L:63:PHE:CD2	2:L:84:THR:HG23	2.53	0.44
2:M:190:VAL:HG21	2:M:210:HIS:HB2	1.99	0.44
2:N:169:SER:HA	2:N:176:LEU:HD23	2.00	0.44
2:O:65:LEU:C	2:O:66:LEU:HG	2.43	0.44
2:O:78:VAL:O	2:O:81:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:106:ARG:HG2	2:O:107:ASN:H	1.83	0.44
1:A:119:GLN:NE2	1:A:178:PRO:HG2	2.33	0.43
1:A:428:GLN:HE22	1:A:455:PRO:HB2	1.74	0.43
1:B:293:PRO:O	1:B:295:THR:N	2.50	0.43
1:B:506:LEU:CD2	1:B:544:VAL:HA	2.39	0.43
1:B:510:LEU:O	1:B:513:LEU:N	2.51	0.43
1:B:529:ILE:O	1:B:533:ILE:HG13	2.18	0.43
1:B:638:MET:HE2	1:B:666:ARG:NH1	2.32	0.43
2:C:225:LEU:HD13	2:C:277:PHE:HD2	1.82	0.43
2:D:5:TYR:O	2:D:6:SER:C	2.61	0.43
2:D:312:GLN:HB3	2:D:313:PRO:HA	1.99	0.43
2:G:8:SER:O	2:G:9:LYS:C	2.60	0.43
2:G:225:LEU:HD13	2:G:277:PHE:CD2	2.53	0.43
2:H:4:LEU:O	2:H:5:TYR:C	2.59	0.43
2:H:225:LEU:HD13	2:H:277:PHE:CD2	2.53	0.43
2:H:225:LEU:HD13	2:H:277:PHE:HD2	1.82	0.43
2:J:125:LYS:O	2:J:127:ILE:N	2.42	0.43
2:J:150:PHE:HA	2:K:397:LYS:HZ1	1.83	0.43
2:L:217:VAL:HG22	2:L:286:ASP:HB3	2.00	0.43
2:N:2:ASP:HB2	2:N:128:ASN:HD21	1.83	0.43
2:N:31:ILE:O	2:N:32:GLN:C	2.61	0.43
2:N:62:ASP:H	2:N:63:PHE:HD1	1.66	0.43
2:N:155:PRO:O	2:N:186:SER:HB3	2.17	0.43
2:O:227:PRO:HD3	2:O:277:PHE:CG	2.53	0.43
1:A:141:GLU:O	1:A:142:LEU:CB	2.65	0.43
1:A:187:ALA:O	1:A:188:VAL:CG2	2.66	0.43
1:A:333:VAL:HB	1:A:380:LYS:HG2	2.00	0.43
1:A:722:ASN:ND2	1:A:823:THR:O	2.51	0.43
1:B:138:GLY:O	1:B:804:SER:HB3	2.18	0.43
1:B:190:ASN:O	1:B:192:ASN:O	2.35	0.43
1:B:201:ASP:CG	1:B:202:SER:N	2.74	0.43
1:B:374:ALA:CB	1:B:580:SER:HB3	2.44	0.43
1:B:491:GLN:CG	1:B:564:ASN:HB3	2.48	0.43
1:B:498:ARG:CD	2:I:32:GLN:NE2	2.82	0.43
1:B:503:ILE:HG12	1:B:547:THR:HB	2.00	0.43
1:B:504:ASN:C	1:B:506:LEU:N	2.73	0.43
2:C:153:HIS:NE2	2:D:153:HIS:NE2	2.66	0.43
2:C:227:PRO:HD3	2:C:277:PHE:CG	2.53	0.43
2:C:239:ASN:ND2	2:C:246:THR:HG22	2.29	0.43
2:C:312:GLN:HB3	2:C:313:PRO:HA	1.99	0.43
2:G:61:PHE:N	2:G:61:PHE:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:36:GLN:CB	2:J:23:LEU:HD11	2.48	0.43
2:K:217:VAL:HG22	2:K:286:ASP:HB3	2.00	0.43
2:L:14:ALA:O	2:L:18:ILE:HD12	2.18	0.43
2:L:35:ASN:O	2:L:37:MET:N	2.51	0.43
2:M:22:THR:OG1	2:M:26:ASN:ND2	2.45	0.43
2:M:169:SER:HA	2:M:176:LEU:HD23	2.00	0.43
2:O:249:PHE:CE2	2:O:251:PRO:HG3	2.53	0.43
1:A:143:ARG:HG3	1:A:144:ASN:N	2.34	0.43
1:A:181:LEU:N	1:A:260:GLN:HE21	2.16	0.43
1:A:252:PHE:O	1:A:253:ASN:C	2.61	0.43
1:A:396:PHE:HD2	1:A:578:LEU:HD11	1.84	0.43
1:A:501:HIS:CA	1:A:503:ILE:HG13	2.48	0.43
1:A:520:THR:O	1:A:521:MET:HE3	2.18	0.43
1:A:591:ALA:O	1:A:877:MET:SD	2.76	0.43
1:A:751:LEU:HD21	1:A:783:PHE:O	2.18	0.43
1:A:769:SER:CB	1:A:807:ASN:OD1	2.60	0.43
1:A:772:ILE:O	1:A:774:LEU:N	2.51	0.43
1:B:306:ASP:C	1:B:308:LEU:N	2.67	0.43
1:B:309:ASN:HA	1:B:311:HIS:CE1	2.54	0.43
1:B:415:PRO:C	1:B:417:ASP:N	2.77	0.43
1:B:549:LEU:O	1:B:550:LEU:C	2.59	0.43
1:B:791:LYS:HB3	1:B:792:VAL:H	1.59	0.43
2:D:63:PHE:CD1	2:D:63:PHE:N	2.86	0.43
2:E:78:VAL:O	2:E:81:ALA:N	2.41	0.43
2:F:217:VAL:HG22	2:F:286:ASP:HB3	1.99	0.43
2:G:53:ASN:ND2	2:G:354:ALA:HB3	2.33	0.43
2:G:225:LEU:HD13	2:G:277:PHE:HD2	1.82	0.43
2:H:133:SER:O	2:H:134:GLU:C	2.60	0.43
2:H:227:PRO:HD3	2:H:277:PHE:CG	2.53	0.43
2:I:169:SER:HA	2:I:176:LEU:HD23	2.00	0.43
2:K:5:TYR:HE2	2:K:131:ASN:HA	1.79	0.43
2:K:31:ILE:O	2:K:32:GLN:C	2.60	0.43
2:M:128:ASN:HB3	2:N:19:VAL:CG2	2.48	0.43
2:M:135:TYR:OH	2:M:342:MET:HE3	2.18	0.43
2:N:136:ILE:HG23	2:N:137:GLU:N	2.33	0.43
2:N:227:PRO:HD3	2:N:277:PHE:CG	2.53	0.43
1:A:383:ILE:O	1:A:386:MET:N	2.52	0.43
1:A:750:MET:CE	1:A:757:VAL:HG21	2.48	0.43
1:A:781:THR:HG22	1:A:782:VAL:N	2.34	0.43
1:B:510:LEU:HD22	1:B:540:LEU:CD1	2.30	0.43
1:B:510:LEU:HA	1:B:513:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:PRO:HB2	1:B:600:LEU:HD11	2.00	0.43
1:B:604:TYR:O	1:B:605:ASN:C	2.61	0.43
2:E:142:GLN:HE21	2:E:143:ASN:N	2.16	0.43
2:E:227:PRO:HD3	2:E:277:PHE:CG	2.53	0.43
2:F:227:PRO:HD3	2:F:277:PHE:CG	2.53	0.43
2:G:249:PHE:CE2	2:G:251:PRO:HG3	2.53	0.43
2:H:169:SER:HA	2:H:176:LEU:HD23	2.00	0.43
2:I:146:GLN:O	2:I:148:THR:HG23	2.19	0.43
2:I:227:PRO:HD3	2:I:277:PHE:CG	2.53	0.43
2:I:312:GLN:HB3	2:I:313:PRO:HA	1.99	0.43
2:K:225:LEU:HD13	2:K:277:PHE:CD2	2.53	0.43
2:L:42:ASN:CA	2:L:61:PHE:HB2	2.30	0.43
2:M:24:TYR:N	2:M:71:LEU:O	2.49	0.43
2:N:19:VAL:O	2:N:20:GLU:C	2.60	0.43
2:N:101:VAL:HG11	2:N:355:ILE:HG13	2.01	0.43
2:N:225:LEU:HD13	2:N:277:PHE:CD2	2.53	0.43
2:O:133:SER:O	2:O:134:GLU:C	2.61	0.43
1:A:149:LYS:NZ	1:A:697:ASP:CG	2.77	0.43
1:A:243:SER:O	1:A:839:MET:HG2	2.19	0.43
1:A:408:MET:HG2	1:A:471:TRP:CH2	2.53	0.43
1:A:415:PRO:O	1:A:417:ASP:N	2.43	0.43
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.86	0.43
1:A:548:ARG:HH11	1:A:877:MET:H	1.67	0.43
1:A:714:ARG:HG2	1:A:720:TYR:CD2	2.54	0.43
1:A:799:LEU:HA	1:A:799:LEU:HD23	1.68	0.43
1:B:309:ASN:HA	1:B:311:HIS:NE2	2.33	0.43
1:B:451:ASP:H	1:B:452:PRO:CD	2.20	0.43
1:B:540:LEU:HD23	1:B:541:GLY:CA	2.48	0.43
1:B:703:VAL:CG1	1:B:704:ILE:N	2.81	0.43
1:B:772:ILE:O	1:B:775:ILE:N	2.51	0.43
2:C:8:SER:O	2:C:9:LYS:C	2.61	0.43
2:C:31:ILE:O	2:C:32:GLN:C	2.60	0.43
2:C:78:VAL:O	2:C:81:ALA:HB3	2.17	0.43
2:E:24:TYR:HE1	2:E:31:ILE:HG13	1.83	0.43
2:E:125:LYS:O	2:E:127:ILE:N	2.51	0.43
2:E:136:ILE:HG23	2:E:137:GLU:N	2.34	0.43
2:F:225:LEU:HD13	2:F:277:PHE:CD2	2.53	0.43
2:G:38:ILE:H	2:G:38:ILE:HG13	1.59	0.43
2:G:217:VAL:HG22	2:G:286:ASP:HB3	1.99	0.43
2:H:74:ASP:O	2:H:75:ALA:C	2.60	0.43
2:I:34:PHE:O	2:I:37:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:5:TYR:O	2:J:6:SER:C	2.61	0.43
2:J:124:PHE:C	2:J:126:ARG:N	2.76	0.43
2:J:125:LYS:C	2:J:127:ILE:H	2.26	0.43
2:J:169:SER:HA	2:J:176:LEU:HD23	2.00	0.43
2:K:8:SER:O	2:K:9:LYS:C	2.60	0.43
2:L:169:SER:HA	2:L:176:LEU:HD23	2.00	0.43
2:L:249:PHE:CE2	2:L:251:PRO:HG3	2.53	0.43
2:M:63:PHE:HD2	2:M:84:THR:HG23	1.81	0.43
2:M:123:LYS:HG3	2:M:124:PHE:CD1	2.53	0.43
2:M:155:PRO:HA	2:M:337:ASP:CB	2.49	0.43
2:N:24:TYR:HE1	2:N:31:ILE:HG13	1.83	0.43
2:N:63:PHE:CD2	2:N:84:THR:HG23	2.54	0.43
2:N:145:ARG:HA	2:N:145:ARG:HE	1.83	0.43
2:N:312:GLN:HB3	2:N:313:PRO:HA	1.99	0.43
2:O:72:ASN:O	2:O:73:LEU:C	2.61	0.43
2:O:105:GLN:O	2:O:106:ARG:C	2.61	0.43
1:A:501:HIS:HA	1:A:503:ILE:HG13	2.01	0.43
1:A:521:MET:CB	1:A:522:PRO:HD3	2.26	0.43
1:A:675:GLU:HB3	1:A:678:ARG:HG2	2.01	0.43
1:B:104:ILE:O	1:B:105:LEU:C	2.62	0.43
1:B:224:PHE:CD1	2:O:71:LEU:HD13	2.54	0.43
1:B:231:ARG:HD2	1:B:231:ARG:HA	1.77	0.43
1:B:383:ILE:O	1:B:386:MET:N	2.51	0.43
1:B:669:LEU:C	1:B:671:LEU:H	2.25	0.43
1:B:772:ILE:CG2	1:B:773:SER:H	2.29	0.43
2:D:153:HIS:O	2:D:154:LYS:C	2.60	0.43
2:E:6:SER:C	2:E:8:SER:N	2.73	0.43
2:E:31:ILE:O	2:E:32:GLN:C	2.60	0.43
2:E:152:PHE:O	2:E:328:SER:HA	2.19	0.43
2:F:163:SER:HB3	2:F:181:TRP:CZ2	2.54	0.43
2:L:8:SER:O	2:L:9:LYS:C	2.61	0.43
2:L:31:ILE:O	2:L:32:GLN:C	2.61	0.43
2:M:133:SER:O	2:M:134:GLU:C	2.60	0.43
2:O:62:ASP:H	2:O:63:PHE:HD1	1.66	0.43
1:A:387:LEU:HD23	1:A:554:TYR:CE1	2.54	0.43
1:A:428:GLN:O	1:A:432:VAL:HG23	2.19	0.43
1:A:693:GLU:O	1:A:695:ALA:O	2.37	0.43
1:B:447:TYR:C	1:B:448:ARG:CG	2.91	0.43
1:B:508:GLU:OE1	2:J:71:LEU:HB3	2.18	0.43
1:B:620:ASP:O	1:B:624:ILE:HG13	2.19	0.43
1:B:666:ARG:HG2	1:B:667:ASP:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:MET:HE2	2:O:69:THR:OG1	2.19	0.43
2:C:78:VAL:O	2:C:81:ALA:N	2.40	0.43
2:D:11:LEU:O	2:D:15:ARG:N	2.40	0.43
2:E:169:SER:HA	2:E:176:LEU:HD23	2.00	0.43
2:F:34:PHE:O	2:F:35:ASN:C	2.60	0.43
2:G:145:ARG:HE	2:I:142:GLN:NE2	2.17	0.43
2:H:35:ASN:O	2:H:37:MET:N	2.52	0.43
2:J:14:ALA:O	2:J:16:ASP:N	2.50	0.43
2:J:136:ILE:HG23	2:J:137:GLU:N	2.33	0.43
2:L:78:VAL:O	2:L:81:ALA:HB3	2.18	0.43
2:N:154:LYS:N	2:N:155:PRO:CD	2.82	0.43
2:O:144:ARG:C	2:O:146:GLN:H	2.26	0.43
1:A:370:ILE:O	1:A:374:ALA:HB2	2.19	0.43
1:A:571:LEU:HD22	1:A:571:LEU:HA	1.74	0.43
1:A:709:ASP:O	1:A:710:MET:HB3	2.18	0.43
1:B:252:PHE:C	1:B:254:GLU:N	2.76	0.43
1:B:387:LEU:O	1:B:388:SER:C	2.62	0.43
1:B:658:PRO:HB2	1:B:661:GLN:CG	2.39	0.43
1:B:776:ALA:O	1:B:778:LEU:N	2.52	0.43
1:B:871:PHE:CD1	1:B:872:ASP:N	2.87	0.43
2:C:53:ASN:HD22	2:C:354:ALA:HB3	1.83	0.43
2:C:126:ARG:C	2:C:127:ILE:CG1	2.92	0.43
2:E:34:PHE:O	2:E:35:ASN:C	2.60	0.43
2:I:11:LEU:O	2:I:15:ARG:N	2.38	0.43
2:J:190:VAL:HG21	2:J:210:HIS:HB2	1.99	0.43
2:N:249:PHE:CE2	2:N:251:PRO:HG3	2.53	0.43
2:O:5:TYR:O	2:O:6:SER:C	2.60	0.43
1:A:393:SER:HB2	1:A:573:THR:CG2	2.48	0.43
1:A:396:PHE:HB3	1:A:578:LEU:HG	2.00	0.43
1:A:420:ILE:HD12	1:A:422:GLU:CG	2.49	0.43
1:A:481:ARG:HH12	1:A:497:ILE:CD1	2.32	0.43
1:A:510:LEU:HD13	1:A:540:LEU:HB2	2.01	0.43
1:A:815:TYR:H	1:A:815:TYR:HD1	1.62	0.43
1:B:218:GLU:OE1	1:B:836:ARG:NH2	2.51	0.43
1:B:409:TRP:CZ3	1:B:413:VAL:HG23	2.54	0.43
1:B:475:VAL:C	1:B:477:ASN:H	2.27	0.43
1:B:625:ILE:H	1:B:625:ILE:HG13	1.60	0.43
1:B:870:ALA:O	1:B:872:ASP:N	2.52	0.43
2:C:14:ALA:O	2:C:16:ASP:N	2.52	0.43
2:C:35:ASN:O	2:C:37:MET:N	2.52	0.43
2:E:70:LEU:HB3	2:E:72:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:SER:O	2:F:9:LYS:C	2.61	0.43
2:H:8:SER:O	2:H:9:LYS:C	2.62	0.43
2:I:5:TYR:O	2:I:6:SER:C	2.60	0.43
2:I:8:SER:O	2:I:9:LYS:C	2.62	0.43
2:I:16:ASP:HB3	2:K:131:ASN:O	2.18	0.43
2:I:27:VAL:O	2:I:30:LEU:HB3	2.19	0.43
2:J:66:LEU:HA	2:J:66:LEU:HD23	1.81	0.43
2:K:163:SER:HB3	2:K:181:TRP:CZ2	2.54	0.43
2:M:23:LEU:O	2:M:24:TYR:C	2.62	0.43
2:N:24:TYR:C	2:N:26:ASN:H	2.27	0.43
2:N:50:GLY:O	2:N:51:ILE:CG2	2.61	0.43
1:A:319:ASP:OD2	1:A:572:THR:N	2.52	0.43
1:A:330:ARG:C	1:A:332:VAL:N	2.75	0.43
1:A:339:LEU:HD13	1:A:588:ILE:HG12	2.00	0.43
1:A:396:PHE:HB3	1:A:578:LEU:CG	2.47	0.43
1:A:496:ASN:O	1:A:498:ARG:N	2.51	0.43
1:A:553:ASN:O	1:A:554:TYR:C	2.62	0.43
1:A:598:GLN:H	1:A:598:GLN:HG3	1.61	0.43
1:A:656:ARG:HB3	1:B:347:GLN:NE2	2.34	0.43
1:B:89:GLU:O	1:B:91:LEU:N	2.52	0.43
1:B:97:THR:O	1:B:98:PHE:C	2.61	0.43
1:B:108:LEU:C	1:B:110:ASP:H	2.26	0.43
1:B:126:PHE:CB	1:B:149:LYS:O	2.67	0.43
1:B:134:TYR:CD1	1:B:134:TYR:N	2.86	0.43
1:B:281:ASP:O	1:B:282:VAL:C	2.61	0.43
1:B:434:THR:C	1:B:435:ILE:CG1	2.92	0.43
1:B:477:ASN:ND2	2:I:39:ILE:CG2	2.81	0.43
1:B:544:VAL:O	1:B:545:ASP:C	2.62	0.43
1:B:563:MET:C	1:B:564:ASN:O	2.60	0.43
2:D:225:LEU:HD13	2:D:277:PHE:CD2	2.53	0.43
2:E:49:GLY:HA2	2:E:54:LEU:HD23	2.01	0.43
2:G:74:ASP:O	2:G:75:ALA:C	2.61	0.43
2:J:34:PHE:O	2:J:37:MET:HB3	2.18	0.43
2:J:35:ASN:O	2:J:37:MET:N	2.52	0.43
2:K:27:VAL:O	2:K:30:LEU:N	2.52	0.43
2:K:74:ASP:O	2:K:75:ALA:C	2.61	0.43
2:M:34:PHE:O	2:M:37:MET:HB3	2.19	0.43
2:M:56:ILE:O	2:M:56:ILE:HG22	2.19	0.43
2:O:163:SER:HB3	2:O:181:TRP:CZ2	2.54	0.43
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.79	0.42
1:A:499:ASN:O	1:A:500:GLY:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LEU:C	1:A:540:LEU:CD2	2.91	0.42
1:B:99:GLU:HB3	1:B:100:PRO:CD	2.35	0.42
1:B:251:ALA:HA	2:N:69:THR:CG2	2.42	0.42
1:B:305:GLN:HG3	1:B:489:LEU:CD2	2.49	0.42
1:B:548:ARG:CD	1:B:877:MET:H	2.31	0.42
1:B:657:VAL:O	1:B:658:PRO:C	2.62	0.42
1:B:795:LEU:O	1:B:797:PRO:HD3	2.18	0.42
2:C:34:PHE:O	2:C:37:MET:HB3	2.19	0.42
2:C:38:ILE:H	2:C:38:ILE:HG13	1.58	0.42
2:D:150:PHE:HB2	2:D:152:PHE:CZ	2.53	0.42
2:D:227:PRO:HD3	2:D:277:PHE:CG	2.53	0.42
2:E:14:ALA:C	2:E:18:ILE:HD12	2.44	0.42
2:E:154:LYS:HG2	2:E:186:SER:OG	2.19	0.42
2:F:127:ILE:O	2:F:128:ASN:C	2.62	0.42
2:F:148:THR:HB	2:F:149:GLY:H	1.64	0.42
2:I:163:SER:HB3	2:I:181:TRP:CZ2	2.54	0.42
2:I:249:PHE:CE2	2:I:251:PRO:HG3	2.53	0.42
2:J:227:PRO:HD3	2:J:277:PHE:CG	2.53	0.42
2:J:249:PHE:CE2	2:J:251:PRO:HG3	2.53	0.42
2:L:38:ILE:H	2:L:38:ILE:HG13	1.55	0.42
2:M:8:SER:O	2:M:9:LYS:C	2.62	0.42
2:N:35:ASN:O	2:N:37:MET:N	2.52	0.42
2:O:23:LEU:CD2	2:O:24:TYR:N	2.82	0.42
1:A:273:TYR:O	1:A:273:TYR:HD2	2.01	0.42
1:A:613:ASN:O	1:A:617:ARG:HG2	2.19	0.42
1:B:308:LEU:HB3	1:B:310:LEU:CD2	2.49	0.42
1:B:346:ILE:HA	1:B:349:MET:HB2	2.01	0.42
1:B:393:SER:H	1:B:573:THR:CG2	2.31	0.42
1:B:491:GLN:NE2	1:B:566:GLN:CG	2.79	0.42
1:B:498:ARG:CD	2:I:32:GLN:HE21	2.32	0.42
2:C:163:SER:HB3	2:C:181:TRP:CZ2	2.54	0.42
2:C:169:SER:HA	2:C:176:LEU:HD23	2.00	0.42
2:C:225:LEU:HD13	2:C:277:PHE:CD2	2.53	0.42
2:D:14:ALA:O	2:D:16:ASP:N	2.52	0.42
2:E:150:PHE:HB2	2:E:152:PHE:HE1	1.81	0.42
2:G:5:TYR:O	2:G:6:SER:C	2.62	0.42
2:G:227:PRO:HD3	2:G:277:PHE:CG	2.54	0.42
2:I:51:ILE:O	2:I:54:LEU:HB3	2.19	0.42
2:I:61:PHE:O	2:I:62:ASP:HB3	2.19	0.42
2:J:54:LEU:HD12	2:J:55:PRO:HD2	2.00	0.42
2:K:145:ARG:C	2:K:146:GLN:HG2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:169:SER:HA	2:K:176:LEU:HD23	2.00	0.42
2:K:249:PHE:CE2	2:K:251:PRO:HG3	2.53	0.42
2:L:227:PRO:HD3	2:L:277:PHE:CG	2.53	0.42
2:M:227:PRO:HD3	2:M:277:PHE:CG	2.53	0.42
2:O:113:SER:O	2:O:117:ARG:HG3	2.18	0.42
1:A:265:LEU:HB3	1:A:296:ALA:HB1	2.00	0.42
1:A:370:ILE:O	1:A:374:ALA:CB	2.68	0.42
1:A:391:THR:O	1:A:573:THR:HA	2.19	0.42
1:A:510:LEU:HA	1:A:513:LEU:HD12	2.01	0.42
1:A:548:ARG:NH1	1:A:877:MET:CA	2.78	0.42
1:A:827:LYS:C	1:A:828:GLN:O	2.62	0.42
1:A:846:LEU:O	1:A:847:THR:C	2.62	0.42
1:B:177:MET:HE3	1:B:677:ARG:NE	2.34	0.42
1:B:609:ASN:O	1:B:610:PHE:C	2.62	0.42
1:B:636:LYS:O	1:B:637:LYS:CB	2.66	0.42
2:C:26:ASN:OD1	2:C:26:ASN:N	2.52	0.42
2:C:111:PRO:HB3	2:C:116:LEU:HD23	2.01	0.42
2:D:27:VAL:CG2	2:D:31:ILE:HD11	2.49	0.42
2:D:35:ASN:O	2:D:37:MET:N	2.53	0.42
2:E:19:VAL:O	2:E:20:GLU:C	2.62	0.42
2:E:63:PHE:CD1	2:E:63:PHE:N	2.87	0.42
2:G:1:MET:C	2:G:3:VAL:N	2.75	0.42
2:H:38:ILE:H	2:H:38:ILE:HG13	1.57	0.42
2:I:17:LYS:HG2	2:K:130:ASP:HA	2.01	0.42
2:I:36:GLN:NE2	2:I:126:ARG:HD3	2.34	0.42
2:L:106:ARG:H	2:L:106:ARG:CD	2.20	0.42
2:L:140:ASN:O	2:L:143:ASN:N	2.50	0.42
2:M:5:TYR:O	2:M:6:SER:C	2.62	0.42
2:N:116:LEU:O	2:N:119:LEU:N	2.48	0.42
1:A:383:ILE:HD11	1:A:550:LEU:CD2	2.49	0.42
1:A:402:MET:C	1:A:404:LEU:N	2.77	0.42
1:A:548:ARG:HH11	1:A:877:MET:N	2.17	0.42
1:A:660:ASP:CA	1:B:539:ARG:NH1	2.83	0.42
1:A:666:ARG:HA	1:A:669:LEU:HD12	2.00	0.42
1:A:714:ARG:CG	1:A:720:TYR:HD2	2.32	0.42
1:A:812:VAL:C	1:A:814:ASN:N	2.73	0.42
1:B:192:ASN:O	1:B:193:SER:HB3	2.19	0.42
1:B:239:VAL:CG2	1:B:844:SER:O	2.61	0.42
1:B:300:ARG:HA	1:B:301:PRO:HD3	1.76	0.42
1:B:478:ASN:O	1:B:478:ASN:CG	2.61	0.42
1:B:482:GLN:CA	1:B:493:LEU:HD22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:ALA:O	1:B:622:VAL:C	2.60	0.42
1:B:735:LEU:O	1:B:736:GLU:C	2.63	0.42
1:B:789:LEU:O	1:B:790:ARG:O	2.37	0.42
1:B:853:ASP:O	1:B:854:LEU:CB	2.67	0.42
1:B:879:GLU:O	1:B:880:LEU:OXT	2.37	0.42
2:C:5:TYR:O	2:C:6:SER:C	2.61	0.42
2:C:46:PHE:CE2	2:C:119:LEU:HD21	2.54	0.42
2:C:227:PRO:O	2:C:228:ASP:HB2	2.20	0.42
2:E:227:PRO:O	2:E:228:ASP:HB2	2.19	0.42
2:F:123:LYS:HG3	2:F:124:PHE:CD1	2.53	0.42
2:F:136:ILE:HG23	2:F:137:GLU:N	2.34	0.42
2:F:168:ARG:HD2	2:F:175:ASN:O	2.20	0.42
2:I:151:THR:C	2:I:152:PHE:CD1	2.97	0.42
2:J:131:ASN:N	2:J:131:ASN:ND2	2.67	0.42
2:J:163:SER:HB3	2:J:181:TRP:CZ2	2.54	0.42
2:K:5:TYR:O	2:K:6:SER:C	2.62	0.42
2:K:139:TRP:HE1	2:K:143:ASN:HD22	1.66	0.42
2:L:24:TYR:O	2:L:26:ASN:N	2.52	0.42
2:L:62:ASP:H	2:L:63:PHE:HD1	1.66	0.42
2:L:163:SER:HB3	2:L:181:TRP:CZ2	2.54	0.42
2:N:163:SER:HB3	2:N:181:TRP:CZ2	2.54	0.42
2:N:168:ARG:HD2	2:N:175:ASN:O	2.20	0.42
1:A:319:ASP:OD2	1:A:570:THR:HG22	2.19	0.42
1:A:400:ASN:O	1:A:403:SER:HB2	2.20	0.42
1:A:570:THR:CG2	1:A:571:LEU:N	2.74	0.42
1:B:113:PRO:CG	1:B:609:ASN:HB3	2.49	0.42
1:B:146:TRP:O	1:B:833:PHE:HB3	2.20	0.42
1:B:470:ASN:O	1:B:471:TRP:C	2.62	0.42
1:B:496:ASN:C	1:B:498:ARG:N	2.73	0.42
1:B:603:TYR:O	1:B:604:TYR:C	2.62	0.42
2:C:128:ASN:O	2:C:129:PHE:HB2	2.20	0.42
2:E:24:TYR:CE1	2:E:31:ILE:HG13	2.54	0.42
2:F:153:HIS:NE2	2:G:153:HIS:NE2	2.67	0.42
2:G:136:ILE:HG23	2:G:137:GLU:N	2.33	0.42
2:G:163:SER:HB3	2:G:181:TRP:CZ2	2.54	0.42
2:I:168:ARG:HD2	2:I:175:ASN:O	2.20	0.42
2:K:23:LEU:H	2:K:26:ASN:ND2	2.17	0.42
2:L:66:LEU:HB3	2:L:67:GLY:H	1.66	0.42
2:L:227:PRO:O	2:L:228:ASP:HB2	2.20	0.42
2:M:14:ALA:O	2:M:16:ASP:N	2.52	0.42
2:M:78:VAL:O	2:M:81:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:145:ARG:CB	2:M:145:ARG:HH11	2.32	0.42
2:N:21:GLY:O	2:N:22:THR:O	2.36	0.42
2:N:34:PHE:O	2:N:37:MET:HB3	2.20	0.42
2:O:8:SER:O	2:O:9:LYS:C	2.62	0.42
2:O:99:GLU:CD	2:O:112:GLN:H	2.28	0.42
2:O:227:PRO:O	2:O:228:ASP:HB2	2.20	0.42
1:A:200:VAL:CG2	1:A:241:TYR:HD2	2.32	0.42
1:A:271:PHE:HA	1:A:274:ILE:CD1	2.47	0.42
1:A:351:GLN:O	1:A:353:LEU:N	2.53	0.42
1:A:443:GLN:HE22	1:A:522:PRO:HG3	1.84	0.42
1:A:546:LEU:HD21	1:A:588:ILE:HD12	1.99	0.42
1:A:593:VAL:HG12	1:A:594:ILE:N	2.35	0.42
1:A:594:ILE:HG23	1:A:595:PRO:HD2	2.01	0.42
1:A:876:ILE:O	1:A:877:MET:CB	2.68	0.42
1:B:199:VAL:HG13	1:B:242:PRO:O	2.20	0.42
1:B:555:GLU:OE2	1:B:871:PHE:CE2	2.69	0.42
2:C:9:LYS:HE3	2:C:13:ASP:OD1	2.19	0.42
2:E:59:TRP:CD1	2:E:59:TRP:N	2.87	0.42
2:E:163:SER:HB3	2:E:181:TRP:CZ2	2.54	0.42
2:E:340:GLU:HB3	2:E:342:MET:HE2	2.02	0.42
2:G:168:ARG:HD2	2:G:175:ASN:O	2.20	0.42
2:H:83:ASN:CG	2:I:122:LEU:HB2	2.38	0.42
2:I:78:VAL:O	2:I:81:ALA:HB3	2.20	0.42
2:J:227:PRO:O	2:J:228:ASP:HB2	2.20	0.42
2:N:101:VAL:HG12	2:N:350:ARG:HG2	2.01	0.42
1:A:125:ILE:HD12	1:A:125:ILE:H	1.77	0.42
1:A:554:TYR:OH	1:A:558:MET:HE1	2.20	0.42
1:A:571:LEU:CD2	1:B:531:ARG:CZ	2.97	0.42
1:A:709:ASP:OD2	1:A:820:THR:HG21	2.20	0.42
1:A:775:ILE:HG13	1:A:775:ILE:H	1.35	0.42
1:A:810:TYR:O	1:A:811:LEU:C	2.63	0.42
1:A:839:MET:CG	1:A:840:HIS:N	2.83	0.42
1:A:853:ASP:O	1:A:854:LEU:HB2	2.18	0.42
1:A:855:LEU:C	1:A:857:PHE:N	2.77	0.42
1:B:177:MET:HE2	1:B:677:ARG:HG2	2.02	0.42
1:B:243:SER:HB3	1:B:842:LEU:HD12	2.01	0.42
1:B:390:ARG:HG3	1:B:391:THR:N	2.34	0.42
1:B:409:TRP:CZ3	1:B:413:VAL:CG2	3.02	0.42
1:B:496:ASN:HD22	1:B:498:ARG:CB	2.32	0.42
2:E:168:ARG:HD2	2:E:175:ASN:O	2.20	0.42
2:F:227:PRO:O	2:F:228:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:9:LYS:HE3	2:G:13:ASP:OD1	2.19	0.42
2:H:136:ILE:HG23	2:H:137:GLU:N	2.34	0.42
2:H:142:GLN:NE2	2:H:142:GLN:C	2.77	0.42
2:K:78:VAL:O	2:K:81:ALA:HB3	2.19	0.42
2:L:45:GLU:C	2:L:46:PHE:CD1	2.98	0.42
2:L:168:ARG:HD2	2:L:175:ASN:O	2.20	0.42
2:L:340:GLU:HB3	2:L:342:MET:HE2	2.02	0.42
2:N:5:TYR:O	2:N:6:SER:C	2.61	0.42
2:N:227:PRO:O	2:N:228:ASP:HB2	2.19	0.42
2:N:340:GLU:HB3	2:N:342:MET:HE2	2.02	0.42
1:A:517:GLN:O	1:A:517:GLN:HG3	2.20	0.42
1:A:707:TYR:N	1:A:707:TYR:CD1	2.88	0.42
1:B:218:GLU:C	1:B:220:ALA:H	2.27	0.42
1:B:482:GLN:O	1:B:483:VAL:CG2	2.68	0.42
1:B:546:LEU:HD23	1:B:546:LEU:HA	1.81	0.42
2:C:155:PRO:HA	2:C:337:ASP:HB2	2.02	0.42
2:E:9:LYS:HE3	2:E:13:ASP:OD1	2.20	0.42
2:F:4:LEU:O	2:F:5:TYR:C	2.60	0.42
2:F:5:TYR:O	2:F:6:SER:C	2.61	0.42
2:F:102:ARG:C	2:F:103:GLU:HG3	2.44	0.42
2:G:253:ILE:HG13	2:H:234:PHE:CE1	2.55	0.42
2:H:5:TYR:O	2:H:6:SER:C	2.63	0.42
2:K:34:PHE:O	2:K:35:ASN:C	2.61	0.42
2:L:42:ASN:HB3	2:L:62:ASP:N	2.35	0.42
2:L:61:PHE:CD1	2:L:61:PHE:N	2.88	0.42
2:L:116:LEU:C	2:L:118:LYS:N	2.77	0.42
2:M:153:HIS:O	2:M:154:LYS:C	2.62	0.42
2:M:163:SER:HB3	2:M:181:TRP:CZ2	2.55	0.42
2:M:355:ILE:HA	2:M:356:PRO:HD3	1.96	0.42
2:O:23:LEU:HG	2:O:24:TYR:H	1.85	0.42
2:O:124:PHE:O	2:O:127:ILE:HG13	2.19	0.42
1:A:141:GLU:O	1:A:142:LEU:HD12	2.20	0.42
1:A:201:ASP:O	1:A:202:SER:C	2.62	0.42
1:A:216:GLU:N	1:A:216:GLU:OE1	2.50	0.42
1:A:219:GLY:C	1:A:221:VAL:N	2.77	0.42
1:A:421:ARG:C	1:A:423:SER:N	2.78	0.42
1:A:487:GLY:O	1:A:488:VAL:CB	2.68	0.42
1:A:549:LEU:O	1:A:550:LEU:C	2.63	0.42
1:A:726:ASN:O	1:A:727:LEU:C	2.62	0.42
1:B:253:ASN:O	1:B:256:PHE:HB2	2.20	0.42
1:B:310:LEU:H	1:B:310:LEU:HG	1.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:THR:CG2	1:B:476:ASN:ND2	2.61	0.42
1:B:570:THR:HG22	1:B:571:LEU:N	2.34	0.42
1:B:597:PRO:O	1:B:598:GLN:C	2.62	0.42
1:B:646:LEU:HG	1:B:646:LEU:H	1.51	0.42
2:D:163:SER:HB3	2:D:181:TRP:CZ2	2.54	0.42
2:E:24:TYR:C	2:E:26:ASN:H	2.27	0.42
2:E:61:PHE:CD1	2:E:61:PHE:N	2.87	0.42
2:E:129:PHE:CE1	2:E:130:ASP:HB3	2.54	0.42
2:I:104:SER:HB3	2:I:108:GLY:HA2	2.02	0.42
2:I:340:GLU:HB3	2:I:342:MET:HE2	2.02	0.42
2:I:397:LYS:NZ	2:K:150:PHE:HA	2.34	0.42
2:J:73:LEU:HD22	2:J:77:TYR:CD2	2.54	0.42
2:J:253:ILE:HG13	2:K:234:PHE:CE1	2.55	0.42
2:K:9:LYS:HE3	2:K:13:ASP:OD1	2.20	0.42
2:K:227:PRO:O	2:K:228:ASP:HB2	2.20	0.42
2:M:7:LEU:H	2:M:7:LEU:HG	1.53	0.42
2:N:14:ALA:O	2:N:16:ASP:N	2.53	0.42
1:A:195:ASP:CG	1:A:196:ALA:N	2.73	0.42
1:A:201:ASP:O	1:A:204:THR:N	2.52	0.42
1:A:266:ASN:O	1:A:267:ASN:C	2.63	0.42
1:A:492:VAL:CG1	1:A:493:LEU:N	2.82	0.42
1:A:548:ARG:HB2	1:A:877:MET:HE2	2.01	0.42
1:A:695:ALA:O	1:A:696:SER:HB3	2.20	0.42
1:A:810:TYR:O	1:A:813:ALA:N	2.53	0.42
1:B:148:TRP:NE1	1:B:833:PHE:HD1	2.18	0.42
1:B:287:ASN:HD22	1:B:287:ASN:HA	1.60	0.42
1:B:416:ASN:C	1:B:418:MET:N	2.77	0.42
1:B:544:VAL:HG12	1:B:548:ARG:HE	1.83	0.42
1:B:746:GLN:HE22	2:D:64:GLY:HA2	1.85	0.42
1:B:756:PRO:C	1:B:757:VAL:CG2	2.93	0.42
2:C:168:ARG:HD2	2:C:175:ASN:O	2.20	0.42
2:E:14:ALA:O	2:E:16:ASP:N	2.52	0.42
2:G:23:LEU:HD23	2:G:25:SER:H	1.85	0.42
2:H:152:PHE:O	2:H:328:SER:HA	2.19	0.42
2:H:163:SER:HB3	2:H:181:TRP:CZ2	2.54	0.42
2:I:35:ASN:O	2:I:37:MET:N	2.52	0.42
2:K:35:ASN:O	2:K:37:MET:N	2.53	0.42
2:K:51:ILE:HG23	2:K:51:ILE:O	2.20	0.42
2:K:61:PHE:CD1	2:K:61:PHE:N	2.88	0.42
2:M:227:PRO:O	2:M:228:ASP:HB2	2.20	0.42
2:N:59:TRP:CD1	2:N:59:TRP:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:1:MET:HG3	2:O:2:ASP:N	2.34	0.42
2:O:239:ASN:ND2	2:O:246:THR:HG22	2.29	0.42
1:A:129:ARG:HG2	1:A:130:GLN:H	1.84	0.41
1:A:162:VAL:O	1:A:165:TYR:HB3	2.20	0.41
1:A:174:LEU:HA	1:A:177:MET:HB2	2.01	0.41
1:A:365:GLN:C	1:A:366:PHE:CD1	2.98	0.41
1:A:842:LEU:HD23	1:A:842:LEU:HA	1.76	0.41
1:A:853:ASP:OD1	1:A:854:LEU:N	2.53	0.41
1:B:224:PHE:CE1	2:O:71:LEU:N	2.87	0.41
1:B:501:HIS:O	1:B:503:ILE:N	2.53	0.41
1:B:526:LYS:O	1:B:530:GLN:HG2	2.20	0.41
1:B:549:LEU:HD22	1:B:877:MET:HE1	2.03	0.41
1:B:611:HIS:O	1:B:612:SER:C	2.63	0.41
1:B:799:LEU:HD22	1:B:799:LEU:C	2.38	0.41
2:C:235:PRO:HA	2:C:249:PHE:O	2.20	0.41
2:E:106:ARG:HB3	2:E:107:ASN:H	1.54	0.41
2:E:239:ASN:ND2	2:E:246:THR:HG22	2.30	0.41
2:F:119:LEU:C	2:F:121:GLY:N	2.78	0.41
2:H:227:PRO:O	2:H:228:ASP:HB2	2.20	0.41
2:I:27:VAL:O	2:I:31:ILE:HG12	2.19	0.41
2:I:122:LEU:C	2:I:124:PHE:N	2.78	0.41
2:L:5:TYR:O	2:L:6:SER:C	2.63	0.41
2:L:124:PHE:O	2:L:126:ARG:N	2.53	0.41
2:L:235:PRO:HA	2:L:249:PHE:O	2.20	0.41
2:M:127:ILE:O	2:M:128:ASN:C	2.62	0.41
2:N:76:ASN:HA	2:O:75:ALA:HB3	2.01	0.41
2:O:125:LYS:O	2:O:127:ILE:N	2.51	0.41
1:A:124:ARG:HD2	1:A:203:GLU:OE1	2.20	0.41
1:A:275:PRO:CG	1:A:278:ILE:HD11	2.50	0.41
1:A:314:PHE:HZ	1:A:664:ARG:HG2	1.84	0.41
1:A:379:PHE:O	1:A:380:LYS:C	2.62	0.41
1:A:404:LEU:HD22	1:A:435:ILE:HD11	2.02	0.41
1:A:493:LEU:HD11	1:A:566:GLN:O	2.20	0.41
1:A:611:HIS:O	1:A:612:SER:C	2.63	0.41
1:A:656:ARG:O	1:A:657:VAL:HG23	2.20	0.41
1:A:803:ASN:O	1:A:803:ASN:CG	2.63	0.41
1:B:406:SER:O	1:B:409:TRP:N	2.51	0.41
1:B:466:PHE:CE1	2:H:80:THR:HG22	2.55	0.41
2:C:142:GLN:OE1	2:N:145:ARG:NH1	2.48	0.41
2:C:234:PHE:CE1	2:E:253:ILE:HG13	2.55	0.41
2:C:340:GLU:HB3	2:C:342:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:LEU:CD1	2:D:71:LEU:N	2.82	0.41
2:D:116:LEU:O	2:D:119:LEU:N	2.50	0.41
2:F:27:VAL:O	2:F:31:ILE:HG12	2.20	0.41
2:F:234:PHE:CE1	2:H:253:ILE:HG13	2.55	0.41
2:H:168:ARG:HD2	2:H:175:ASN:O	2.20	0.41
2:K:168:ARG:HD2	2:K:175:ASN:O	2.20	0.41
2:L:2:ASP:O	2:L:3:VAL:C	2.63	0.41
2:M:155:PRO:O	2:M:186:SER:HB3	2.20	0.41
2:M:340:GLU:HB3	2:M:342:MET:HE2	2.02	0.41
2:N:127:ILE:O	2:N:128:ASN:C	2.63	0.41
2:O:38:ILE:HG22	2:O:42:ASN:ND2	2.33	0.41
1:A:170:TYR:CZ	1:A:682:PHE:HB2	2.55	0.41
1:A:195:ASP:O	1:A:196:ALA:C	2.63	0.41
1:A:236:ARG:HB2	1:A:238:VAL:CG2	2.47	0.41
1:A:293:PRO:C	1:A:295:THR:H	2.28	0.41
1:A:324:SER:O	1:A:325:ASN:C	2.63	0.41
1:A:382:LEU:O	1:A:385:ALA:HB3	2.20	0.41
1:A:647:LYS:HG2	1:A:654:VAL:HG21	1.99	0.41
1:B:456:PHE:O	1:B:457:GLN:O	2.38	0.41
1:B:548:ARG:O	1:B:549:LEU:C	2.63	0.41
1:B:646:LEU:O	1:B:649:LEU:HB2	2.20	0.41
1:B:721:VAL:CG1	1:B:722:ASN:H	2.30	0.41
2:C:119:LEU:C	2:C:121:GLY:N	2.78	0.41
2:D:168:ARG:HD2	2:D:175:ASN:O	2.20	0.41
2:E:35:ASN:O	2:E:37:MET:N	2.53	0.41
2:E:128:ASN:O	2:E:129:PHE:CB	2.68	0.41
2:G:144:ARG:O	2:G:145:ARG:CB	2.67	0.41
2:G:235:PRO:HA	2:G:249:PHE:O	2.21	0.41
2:I:14:ALA:O	2:I:16:ASP:N	2.53	0.41
2:I:116:LEU:C	2:I:118:LYS:N	2.77	0.41
2:J:239:ASN:ND2	2:J:246:THR:HG22	2.29	0.41
2:K:34:PHE:O	2:K:37:MET:HB3	2.20	0.41
2:K:45:GLU:C	2:K:46:PHE:CD1	2.98	0.41
2:L:48:THR:O	2:L:56:ILE:HA	2.20	0.41
2:M:153:HIS:NE2	2:N:153:HIS:CD2	2.88	0.41
2:M:253:ILE:HG13	2:N:234:PHE:CE1	2.55	0.41
2:N:91:PHE:O	2:N:92:VAL:C	2.64	0.41
2:N:148:THR:OG1	2:N:332:GLU:HG2	2.20	0.41
2:N:239:ASN:ND2	2:N:246:THR:HG22	2.29	0.41
1:A:163:ARG:NE	1:A:631:LEU:O	2.54	0.41
1:B:275:PRO:HB2	1:B:278:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:THR:HG22	1:B:390:ARG:HD3	2.02	0.41
1:B:369:GLY:C	1:B:371:ASN:H	2.28	0.41
1:B:449:ASN:ND2	1:B:455:PRO:HB3	2.36	0.41
1:B:743:ASP:OD2	1:B:745:ALA:CA	2.68	0.41
2:C:153:HIS:CD2	2:E:153:HIS:CE1	3.08	0.41
2:C:253:ILE:HG13	2:D:234:PHE:CE1	2.55	0.41
2:D:34:PHE:O	2:D:37:MET:HB3	2.20	0.41
2:G:35:ASN:O	2:G:37:MET:N	2.54	0.41
2:J:116:LEU:C	2:J:118:LYS:N	2.78	0.41
2:M:35:ASN:O	2:M:37:MET:N	2.53	0.41
2:N:78:VAL:O	2:N:81:ALA:N	2.39	0.41
2:O:61:PHE:CD1	2:O:61:PHE:N	2.87	0.41
2:O:119:LEU:C	2:O:121:GLY:N	2.79	0.41
1:A:542:GLN:N	1:A:542:GLN:OE1	2.53	0.41
1:A:810:TYR:CD1	1:A:810:TYR:C	2.97	0.41
1:B:191:LYS:HD3	1:B:191:LYS:HA	1.90	0.41
1:B:735:LEU:CG	1:B:760:VAL:O	2.59	0.41
2:D:227:PRO:O	2:D:228:ASP:HB2	2.20	0.41
2:D:253:ILE:HG13	2:E:234:PHE:CE1	2.55	0.41
2:G:11:LEU:HA	2:G:14:ALA:HB3	2.02	0.41
2:G:34:PHE:O	2:G:37:MET:HB3	2.20	0.41
2:H:9:LYS:HE3	2:H:13:ASP:OD1	2.20	0.41
2:H:34:PHE:O	2:H:37:MET:HB3	2.20	0.41
2:I:34:PHE:O	2:I:35:ASN:C	2.62	0.41
2:K:111:PRO:C	2:K:112:GLN:HG2	2.46	0.41
2:L:9:LYS:HE3	2:L:13:ASP:OD1	2.21	0.41
2:O:53:ASN:HD22	2:O:354:ALA:HB3	1.86	0.41
2:O:129:PHE:CD1	2:O:129:PHE:C	2.99	0.41
1:A:252:PHE:C	1:A:254:GLU:N	2.78	0.41
1:A:830:PRO:O	1:A:831:GLN:C	2.64	0.41
1:B:117:LYS:HB2	1:B:179:ASP:CG	2.46	0.41
1:B:190:ASN:HB2	1:B:199:VAL:CG2	2.50	0.41
1:B:206:SER:O	1:B:207:ILE:C	2.63	0.41
1:B:270:ILE:HG23	1:B:854:LEU:HD21	2.03	0.41
1:B:493:LEU:CD1	1:B:567:HIS:HB2	2.50	0.41
1:B:712:LEU:HG	1:B:721:VAL:O	2.19	0.41
2:D:239:ASN:ND2	2:D:246:THR:HG22	2.29	0.41
2:H:142:GLN:HE21	2:H:142:GLN:C	2.27	0.41
2:I:234:PHE:CE1	2:K:253:ILE:HG13	2.55	0.41
2:I:235:PRO:HA	2:I:249:PHE:O	2.21	0.41
2:I:239:ASN:ND2	2:I:246:THR:HG22	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:253:ILE:HG13	2:J:234:PHE:CE1	2.55	0.41
2:J:51:ILE:O	2:J:52:GLY:C	2.64	0.41
2:J:59:TRP:CD1	2:J:59:TRP:N	2.86	0.41
2:L:135:TYR:OH	2:L:342:MET:HE3	2.20	0.41
2:N:116:LEU:C	2:N:118:LYS:N	2.78	0.41
2:O:14:ALA:O	2:O:16:ASP:N	2.52	0.41
1:A:178:PRO:CD	1:A:256:PHE:HE2	2.32	0.41
1:A:304:LEU:H	1:A:615:ASN:ND2	2.19	0.41
1:A:345:GLN:HG3	1:A:349:MET:CE	2.51	0.41
1:A:396:PHE:CD2	1:A:578:LEU:HD11	2.56	0.41
1:A:405:ILE:O	1:A:408:MET:HB2	2.21	0.41
1:A:679:LEU:O	1:A:681:ILE:N	2.54	0.41
1:B:136:ALA:O	1:B:137:ASN:HB3	2.21	0.41
1:B:166:PHE:CE2	1:B:689:MET:CA	2.99	0.41
1:B:178:PRO:CD	1:B:256:PHE:CE2	3.04	0.41
1:B:435:ILE:C	1:B:438:PRO:HD2	2.41	0.41
1:B:515:ARG:HG3	1:B:515:ARG:O	2.21	0.41
1:B:521:MET:N	1:B:521:MET:SD	2.94	0.41
2:C:61:PHE:CD1	2:C:61:PHE:N	2.89	0.41
2:D:124:PHE:N	2:D:124:PHE:CD1	2.89	0.41
2:F:253:ILE:HG13	2:G:234:PHE:CE1	2.55	0.41
2:G:227:PRO:O	2:G:228:ASP:HB2	2.20	0.41
2:I:2:ASP:O	2:I:3:VAL:C	2.64	0.41
2:J:11:LEU:HA	2:J:14:ALA:HB3	2.03	0.41
2:J:14:ALA:O	2:J:18:ILE:HD12	2.21	0.41
2:K:110:ALA:HB1	2:K:111:PRO:CD	2.50	0.41
2:L:21:GLY:O	2:L:22:THR:O	2.38	0.41
2:M:235:PRO:HA	2:M:249:PHE:O	2.21	0.41
2:O:19:VAL:O	2:O:20:GLU:C	2.63	0.41
2:O:35:ASN:O	2:O:37:MET:N	2.53	0.41
2:O:91:PHE:O	2:O:92:VAL:C	2.64	0.41
1:A:120:THR:HB	1:A:121:LYS:H	1.66	0.41
1:A:310:LEU:HD11	1:A:614:TYR:OH	2.21	0.41
1:A:503:ILE:HG13	1:A:503:ILE:H	1.72	0.41
1:A:701:GLN:CB	1:A:826:TYR:HD2	2.33	0.41
1:B:184:LYS:C	1:B:186:MET:N	2.78	0.41
1:B:286:LEU:O	1:B:287:ASN:ND2	2.54	0.41
1:B:310:LEU:C	1:B:312:ASP:H	2.28	0.41
1:B:721:VAL:HG12	1:B:799:LEU:HD21	1.98	0.41
2:C:100:MET:HG3	2:C:388:VAL:HG11	2.01	0.41
2:C:145:ARG:NH1	2:C:145:ARG:CB	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:LYS:HE3	2:D:13:ASP:OD1	2.21	0.41
2:E:116:LEU:C	2:E:118:LYS:N	2.77	0.41
2:F:150:PHE:HA	2:G:397:LYS:HZ1	1.85	0.41
2:F:340:GLU:HB3	2:F:342:MET:HE2	2.02	0.41
2:G:14:ALA:O	2:G:16:ASP:N	2.54	0.41
2:H:235:PRO:HA	2:H:249:PHE:O	2.21	0.41
2:H:340:GLU:HB3	2:H:342:MET:HE2	2.02	0.41
2:I:153:HIS:CD2	2:K:153:HIS:CE1	3.08	0.41
2:J:136:ILE:HD12	2:J:139:TRP:HB3	2.03	0.41
2:K:2:ASP:O	2:K:3:VAL:C	2.64	0.41
2:L:23:LEU:HD22	2:L:72:ASN:OD1	2.21	0.41
2:L:35:ASN:OD1	2:L:65:LEU:HD22	2.21	0.41
2:L:150:PHE:O	2:L:330:VAL:HG13	2.20	0.41
2:L:253:ILE:HG13	2:M:234:PHE:CE1	2.55	0.41
2:M:124:PHE:CD1	2:M:124:PHE:N	2.89	0.41
2:M:168:ARG:HD2	2:M:175:ASN:O	2.20	0.41
2:N:7:LEU:H	2:N:7:LEU:HG	1.54	0.41
2:O:168:ARG:HD2	2:O:175:ASN:O	2.20	0.41
1:A:202:SER:O	1:A:205:ALA:HB3	2.21	0.41
1:A:283:ASN:HD21	1:A:869:VAL:H	1.69	0.41
1:A:287:ASN:O	1:A:858:VAL:HA	2.20	0.41
1:A:368:THR:HG23	1:A:579:THR:O	2.21	0.41
1:A:374:ALA:HB1	1:A:580:SER:HA	2.02	0.41
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.60	0.41
1:A:440:PHE:C	1:A:442:MET:N	2.78	0.41
1:A:459:ALA:C	1:A:462:GLN:HB2	2.44	0.41
1:A:472:LEU:N	1:A:472:LEU:HD23	2.36	0.41
1:A:548:ARG:O	1:A:549:LEU:C	2.63	0.41
1:A:597:PRO:O	1:A:598:GLN:C	2.62	0.41
1:A:601:PHE:CD1	1:A:601:PHE:N	2.80	0.41
1:A:621:ALA:O	1:A:622:VAL:C	2.63	0.41
1:A:706:ALA:C	1:A:708:ARG:N	2.76	0.41
1:A:710:MET:HE3	1:A:710:MET:HB2	1.91	0.41
1:A:782:VAL:CG2	1:A:798:ILE:HD11	2.51	0.41
1:A:862:THR:HG22	1:A:863:VAL:N	2.36	0.41
1:B:159:ASP:OD2	1:B:761:GLY:CA	2.69	0.41
1:B:492:VAL:O	1:B:493:LEU:O	2.38	0.41
1:B:763:LEU:HA	1:B:763:LEU:HD23	1.80	0.41
1:B:771:VAL:O	1:B:775:ILE:HD13	2.21	0.41
1:B:791:LYS:O	1:B:792:VAL:CG1	2.66	0.41
2:C:33:GLN:O	2:C:36:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:ARG:C	2:C:127:ILE:HG13	2.46	0.41
2:D:2:ASP:O	2:D:3:VAL:C	2.63	0.41
2:D:6:SER:O	2:D:7:LEU:C	2.64	0.41
2:D:128:ASN:HD22	2:E:19:VAL:CG2	2.34	0.41
2:D:235:PRO:HA	2:D:249:PHE:O	2.21	0.41
2:E:23:LEU:HD22	2:E:25:SER:OG	2.21	0.41
2:F:9:LYS:HE3	2:F:13:ASP:OD1	2.21	0.41
2:G:340:GLU:HB3	2:G:342:MET:HE2	2.02	0.41
2:H:91:PHE:O	2:H:95:VAL:HG23	2.21	0.41
2:I:9:LYS:HE3	2:I:13:ASP:OD1	2.20	0.41
2:I:106:ARG:HG2	2:I:107:ASN:H	1.84	0.41
2:I:227:PRO:O	2:I:228:ASP:HB2	2.20	0.41
2:J:9:LYS:HE3	2:J:13:ASP:OD1	2.21	0.41
2:J:168:ARG:HD2	2:J:175:ASN:O	2.20	0.41
2:J:340:GLU:HB3	2:J:342:MET:HE2	2.02	0.41
2:K:340:GLU:HB3	2:K:342:MET:HE2	2.02	0.41
2:L:14:ALA:O	2:L:16:ASP:N	2.54	0.41
2:L:26:ASN:OD1	2:N:33:GLN:HB2	2.21	0.41
2:M:119:LEU:C	2:M:121:GLY:N	2.79	0.41
2:O:5:TYR:CE2	2:O:131:ASN:HA	2.55	0.41
2:O:23:LEU:CG	2:O:24:TYR:N	2.83	0.41
2:O:136:ILE:O	2:O:137:GLU:C	2.64	0.41
2:O:147:ARG:O	2:O:148:THR:CB	2.66	0.41
2:O:152:PHE:CD1	2:O:152:PHE:N	2.89	0.41
1:A:158:GLY:O	1:A:159:ASP:C	2.63	0.41
1:A:587:LEU:C	1:A:588:ILE:CG1	2.94	0.41
1:A:726:ASN:HD22	1:A:726:ASN:HA	1.60	0.41
1:A:763:LEU:HA	1:A:764:PRO:HD3	1.68	0.41
1:A:771:VAL:HG12	1:A:809:PHE:CB	2.51	0.41
1:A:786:ILE:O	1:A:787:VAL:C	2.64	0.41
1:B:207:ILE:HG13	1:B:207:ILE:H	1.62	0.41
1:B:229:ARG:HD2	1:B:230:GLN:NE2	2.31	0.41
1:B:411:LEU:HD23	1:B:411:LEU:HA	1.83	0.41
1:B:415:PRO:HB3	1:B:480:PHE:HB2	2.01	0.41
1:B:451:ASP:N	1:B:452:PRO:CD	2.82	0.41
1:B:672:LEU:O	1:B:673:PRO:O	2.38	0.41
2:C:5:TYR:HE2	2:C:130:ASP:O	2.04	0.41
2:C:204:ASN:HB3	2:C:296:ARG:HB3	2.03	0.41
2:D:204:ASN:HB3	2:D:296:ARG:HB3	2.03	0.41
2:E:142:GLN:HE21	2:E:142:GLN:C	2.29	0.41
2:H:14:ALA:O	2:H:16:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:LYS:HG3	2:H:124:PHE:CD1	2.56	0.41
2:I:6:SER:O	2:I:7:LEU:C	2.64	0.41
2:J:27:VAL:O	2:J:31:ILE:HG12	2.20	0.41
2:J:142:GLN:NE2	2:J:142:GLN:C	2.79	0.41
2:K:235:PRO:HA	2:K:249:PHE:O	2.21	0.41
2:L:42:ASN:CB	2:L:62:ASP:HA	2.51	0.41
2:M:116:LEU:C	2:M:118:LYS:N	2.78	0.41
2:N:235:PRO:HA	2:N:249:PHE:O	2.21	0.41
1:A:594:ILE:HA	1:A:595:PRO:HD3	1.86	0.40
1:A:697:ASP:C	1:A:699:ILE:H	2.28	0.40
1:A:774:LEU:HD12	1:A:774:LEU:C	2.46	0.40
1:B:401:TYR:CD1	1:B:401:TYR:N	2.74	0.40
1:B:517:GLN:C	1:B:518:PHE:CD1	2.99	0.40
1:B:743:ASP:OD1	1:B:744:TYR:N	2.53	0.40
1:B:747:ILE:H	1:B:747:ILE:HG22	1.51	0.40
1:B:854:LEU:HD22	1:B:855:LEU:N	2.36	0.40
1:B:869:VAL:HG13	1:B:873:ASN:CA	2.51	0.40
2:D:38:ILE:H	2:D:38:ILE:HG13	1.57	0.40
2:D:122:LEU:C	2:D:124:PHE:H	2.29	0.40
2:D:144:ARG:O	2:D:145:ARG:CB	2.65	0.40
2:D:340:GLU:HB3	2:D:342:MET:HE2	2.02	0.40
2:E:2:ASP:O	2:E:3:VAL:C	2.64	0.40
2:E:235:PRO:HA	2:E:249:PHE:O	2.21	0.40
2:I:11:LEU:HA	2:I:14:ALA:HB3	2.02	0.40
2:I:116:LEU:O	2:I:119:LEU:N	2.50	0.40
2:I:144:ARG:HD2	2:J:82:ARG:CZ	2.51	0.40
2:J:110:ALA:CB	2:J:111:PRO:CD	2.96	0.40
2:J:126:ARG:NH1	2:K:72:ASN:ND2	2.69	0.40
2:J:355:ILE:HA	2:J:356:PRO:HD3	1.96	0.40
2:K:38:ILE:H	2:K:38:ILE:HG13	1.58	0.40
2:L:131:ASN:N	2:L:131:ASN:HD22	2.19	0.40
2:L:234:PHE:CE1	2:N:253:ILE:HG13	2.55	0.40
2:O:153:HIS:C	2:O:153:HIS:CD2	2.99	0.40
1:A:200:VAL:O	1:A:201:ASP:HB3	2.21	0.40
1:A:264:PRO:O	1:A:265:LEU:HB2	2.22	0.40
1:A:283:ASN:ND2	1:A:869:VAL:H	2.18	0.40
1:A:343:GLU:O	1:A:344:ALA:C	2.64	0.40
1:A:460:GLU:C	1:A:462:GLN:N	2.79	0.40
1:A:594:ILE:HG23	1:A:595:PRO:N	2.36	0.40
1:A:785:GLN:HB2	1:A:786:ILE:H	1.60	0.40
1:A:793:ASP:OD1	1:A:793:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:CD1	1:B:696:SER:HA	2.50	0.40
1:B:402:MET:C	1:B:404:LEU:N	2.77	0.40
1:B:706:ALA:C	1:B:707:TYR:HD1	2.29	0.40
1:B:839:MET:HE2	1:B:840:HIS:O	2.21	0.40
1:B:847:THR:O	1:B:847:THR:HG22	2.20	0.40
2:D:214:LEU:HD23	2:D:214:LEU:N	2.36	0.40
2:E:91:PHE:O	2:E:95:VAL:HG23	2.22	0.40
2:F:65:LEU:HB3	2:F:66:LEU:H	1.69	0.40
2:G:104:SER:O	2:G:108:GLY:HA2	2.21	0.40
2:H:65:LEU:O	2:H:66:LEU:HD23	2.22	0.40
2:H:152:PHE:HB3	2:H:337:ASP:CB	2.51	0.40
2:I:204:ASN:HB3	2:I:296:ARG:HB3	2.03	0.40
2:L:1:MET:C	2:L:3:VAL:N	2.74	0.40
2:L:153:HIS:CE1	2:M:153:HIS:CD2	3.09	0.40
2:N:124:PHE:C	2:N:126:ARG:N	2.78	0.40
2:O:21:GLY:O	2:O:22:THR:C	2.64	0.40
2:O:144:ARG:C	2:O:146:GLN:N	2.79	0.40
1:A:338:GLU:O	1:A:339:LEU:HG	2.22	0.40
1:A:362:SER:HA	1:A:365:GLN:HE21	1.87	0.40
1:A:451:ASP:O	1:A:452:PRO:O	2.39	0.40
1:A:506:LEU:HD21	1:A:544:VAL:N	2.36	0.40
1:A:542:GLN:HA	1:A:545:ASP:OD2	2.20	0.40
1:A:707:TYR:H	1:A:707:TYR:HD1	1.69	0.40
1:A:715:ASP:O	1:A:718:TYR:O	2.39	0.40
1:B:497:ILE:HG23	2:I:68:THR:CG2	2.52	0.40
1:B:743:ASP:OD2	1:B:745:ALA:N	2.54	0.40
2:C:214:LEU:HD23	2:C:214:LEU:N	2.37	0.40
2:E:136:ILE:HD12	2:E:139:TRP:HB3	2.04	0.40
2:F:14:ALA:O	2:F:16:ASP:N	2.54	0.40
2:F:155:PRO:O	2:F:186:SER:HB3	2.21	0.40
2:F:204:ASN:HB3	2:F:296:ARG:HB3	2.03	0.40
2:H:21:GLY:O	2:H:22:THR:C	2.65	0.40
2:H:23:LEU:H	2:H:26:ASN:HD21	1.67	0.40
2:H:70:LEU:O	2:H:71:LEU:C	2.64	0.40
2:I:127:ILE:O	2:I:128:ASN:C	2.64	0.40
2:I:145:ARG:NH1	2:I:145:ARG:CB	2.65	0.40
2:J:2:ASP:O	2:J:3:VAL:C	2.64	0.40
2:J:124:PHE:O	2:J:126:ARG:N	2.54	0.40
2:J:142:GLN:HE21	2:J:142:GLN:C	2.28	0.40
2:K:48:THR:O	2:K:56:ILE:HA	2.20	0.40
2:K:88:PHE:O	2:K:91:PHE:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:136:ILE:O	2:K:137:GLU:C	2.65	0.40
2:M:11:LEU:HA	2:M:14:ALA:HB3	2.04	0.40
2:M:131:ASN:N	2:M:131:ASN:ND2	2.70	0.40
2:M:204:ASN:HB3	2:M:296:ARG:HB3	2.04	0.40
2:O:9:LYS:HE3	2:O:13:ASP:OD1	2.21	0.40
2:O:204:ASN:HB3	2:O:296:ARG:HB3	2.03	0.40
1:A:163:ARG:NH2	1:A:736:GLU:OE1	2.52	0.40
1:A:293:PRO:C	1:A:295:THR:N	2.78	0.40
1:A:304:LEU:N	1:A:615:ASN:ND2	2.67	0.40
1:A:536:LEU:N	1:A:536:LEU:HD22	2.36	0.40
1:A:563:MET:HA	1:A:563:MET:HE3	1.92	0.40
1:A:653:ASP:O	1:A:654:VAL:C	2.64	0.40
1:A:657:VAL:HA	1:A:658:PRO:HD3	1.64	0.40
1:A:854:LEU:HD22	1:A:855:LEU:H	1.86	0.40
1:B:190:ASN:HB3	1:B:197:GLY:O	2.21	0.40
1:B:239:VAL:HG21	1:B:845:ASN:O	2.21	0.40
1:B:244:ILE:HG23	1:B:244:ILE:O	2.22	0.40
1:B:275:PRO:C	1:B:277:ARG:N	2.79	0.40
1:B:332:VAL:O	1:B:333:VAL:C	2.63	0.40
1:B:400:ASN:OD1	1:B:400:ASN:C	2.64	0.40
1:B:639:LYS:O	1:B:641:ILE:N	2.55	0.40
1:B:804:SER:O	1:B:805:ASP:HB2	2.22	0.40
2:C:125:LYS:C	2:C:127:ILE:H	2.30	0.40
2:D:11:LEU:HA	2:D:14:ALA:HB3	2.03	0.40
2:D:91:PHE:O	2:D:92:VAL:C	2.65	0.40
2:D:116:LEU:C	2:D:118:LYS:N	2.78	0.40
2:D:124:PHE:O	2:D:126:ARG:N	2.54	0.40
2:E:6:SER:O	2:E:7:LEU:C	2.64	0.40
2:F:11:LEU:HB2	2:F:395:LEU:HD21	2.04	0.40
2:K:11:LEU:HA	2:K:14:ALA:HB3	2.03	0.40
2:L:59:TRP:CD1	2:L:59:TRP:N	2.88	0.40
2:M:27:VAL:O	2:M:28:SER:C	2.63	0.40
2:N:91:PHE:O	2:N:95:VAL:HG23	2.21	0.40
2:O:34:PHE:O	2:O:37:MET:HB3	2.21	0.40
2:O:100:MET:HG3	2:O:388:VAL:CG1	2.51	0.40
2:O:144:ARG:O	2:O:145:ARG:CG	2.69	0.40
2:O:340:GLU:HB3	2:O:342:MET:HE2	2.02	0.40
1:A:131:LEU:HA	1:A:132:PRO:HD3	1.90	0.40
1:A:149:LYS:HZ2	1:A:697:ASP:CG	2.29	0.40
1:A:303:LEU:HA	1:A:615:ASN:HD21	1.82	0.40
1:A:359:THR:O	1:A:359:THR:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:LEU:HA	1:A:513:LEU:CD1	2.51	0.40
1:A:536:LEU:N	1:A:536:LEU:CD2	2.85	0.40
1:A:663:TYR:C	1:A:665:LEU:N	2.79	0.40
1:A:815:TYR:CD1	1:A:815:TYR:N	2.85	0.40
1:B:112:LYS:O	1:B:113:PRO:C	2.64	0.40
1:B:425:VAL:O	1:B:426:ALA:C	2.65	0.40
1:B:556:THR:HG22	1:B:557:LEU:N	2.36	0.40
1:B:746:GLN:O	1:B:750:MET:HG3	2.21	0.40
2:C:2:ASP:O	2:C:3:VAL:C	2.65	0.40
2:C:14:ALA:O	2:C:18:ILE:HD12	2.21	0.40
2:D:128:ASN:O	2:D:129:PHE:HB3	2.21	0.40
2:D:378:ARG:O	2:D:382:LEU:HB2	2.22	0.40
2:E:100:MET:HG3	2:E:388:VAL:HG11	2.04	0.40
2:F:235:PRO:HA	2:F:249:PHE:O	2.21	0.40
2:G:131:ASN:N	2:G:131:ASN:HD22	2.20	0.40
2:K:116:LEU:O	2:K:119:LEU:N	2.50	0.40
2:K:204:ASN:HB3	2:K:296:ARG:HB3	2.04	0.40
2:L:355:ILE:HA	2:L:356:PRO:HD3	1.96	0.40
2:O:101:VAL:HG23	2:O:102:ARG:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	779/880 (88%)	431 (55%)	199 (26%)	149 (19%)	0	1
1	B	808/880 (92%)	458 (57%)	204 (25%)	146 (18%)	0	2
2	C	395/397 (100%)	318 (80%)	54 (14%)	23 (6%)	1	15
2	D	395/397 (100%)	315 (80%)	50 (13%)	30 (8%)	1	11
2	E	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	395/397 (100%)	324 (82%)	47 (12%)	24 (6%)	1	14
2	G	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	1	15
2	H	395/397 (100%)	323 (82%)	50 (13%)	22 (6%)	1	15
2	I	395/397 (100%)	320 (81%)	51 (13%)	24 (6%)	1	14
2	J	395/397 (100%)	320 (81%)	53 (13%)	22 (6%)	1	15
2	K	395/397 (100%)	318 (80%)	52 (13%)	25 (6%)	1	14
2	L	395/397 (100%)	322 (82%)	47 (12%)	26 (7%)	1	13
2	M	395/397 (100%)	322 (82%)	52 (13%)	21 (5%)	1	16
2	N	395/397 (100%)	317 (80%)	50 (13%)	28 (7%)	1	12
2	O	395/397 (100%)	317 (80%)	47 (12%)	31 (8%)	1	11
All	All	6722/6921 (97%)	5051 (75%)	1054 (16%)	617 (9%)	0	8

All (617) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	130	GLN
1	A	193	SER
1	A	198	LYS
1	A	220	ALA
1	A	234	ALA
1	A	246	HIS
1	A	252	PHE
1	A	260	GLN
1	A	275	PRO
1	A	283	ASN
1	A	287	ASN
1	A	306	ASP
1	A	315	GLU
1	A	338	GLU
1	A	340	VAL
1	A	356	GLU
1	A	358	LEU
1	A	370	ILE
1	A	413	VAL
1	A	443	GLN
1	A	446	HIS
1	A	451	ASP

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Mol	Chain	Res	Type
1	A	452	PRO
1	A	453	GLN
1	A	484	VAL
1	A	485	ILE
1	A	488	VAL
1	A	489	LEU
1	A	501	HIS
1	A	523	VAL
1	A	558	MET
1	A	564	ASN
1	A	570	THR
1	A	573	THR
1	A	585	CYS
1	A	650	HIS
1	A	651	ILE
1	A	660	ASP
1	A	661	GLN
1	A	689	MET
1	A	701	GLN
1	A	715	ASP
1	A	743	ASP
1	A	745	ALA
1	A	770	SER
1	A	771	VAL
1	A	772	ILE
1	A	781	THR
1	A	782	VAL
1	A	785	GLN
1	A	786	ILE
1	A	808	ASP
1	A	811	LEU
1	A	814	ASN
1	A	828	GLN
1	A	854	LEU
1	A	855	LEU
1	A	856	ALA
1	A	857	PHE
1	B	191	LYS
1	B	194	ARG
1	B	195	ASP
1	B	196	ALA
1	B	200	VAL

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Mol	Chain	Res	Type
1	B	215	GLU
1	B	218	GLU
1	B	226	ALA
1	B	227	GLU
1	B	252	PHE
1	B	306	ASP
1	B	355	LEU
1	B	361	GLN
1	B	369	GLY
1	B	400	ASN
1	B	417	ASP
1	B	446	HIS
1	B	447	TYR
1	B	451	ASP
1	B	457	GLN
1	B	458	ILE
1	B	479	GLN
1	B	481	ARG
1	B	503	ILE
1	B	504	ASN
1	B	574	GLU
1	B	585	CYS
1	B	634	TYR
1	B	640	ALA
1	B	651	ILE
1	B	655	ALA
1	B	673	PRO
1	B	699	ILE
1	B	702	GLY
1	B	724	ALA
1	B	764	PRO
1	B	765	PHE
1	B	777	LYS
1	B	782	VAL
1	B	785	GLN
1	B	786	ILE
1	B	790	ARG
1	B	792	VAL
1	B	805	ASP
1	B	806	SER
1	B	855	LEU
1	B	856	ALA

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Mol	Chain	Res	Type
1	B	875	ARG
2	C	22	THR
2	C	70	LEU
2	C	134	GLU
2	D	25	SER
2	D	70	LEU
2	D	126	ARG
2	D	128	ASN
2	D	134	GLU
2	D	148	THR
2	E	22	THR
2	E	25	SER
2	E	106	ARG
2	E	134	GLU
2	F	22	THR
2	F	62	ASP
2	F	70	LEU
2	F	105	GLN
2	F	134	GLU
2	F	145	ARG
2	F	148	THR
2	G	20	GLU
2	G	22	THR
2	G	134	GLU
2	G	148	THR
2	H	22	THR
2	H	107	ASN
2	H	134	GLU
2	I	25	SER
2	I	62	ASP
2	I	134	GLU
2	I	148	THR
2	J	20	GLU
2	J	70	LEU
2	J	106	ARG
2	J	134	GLU
2	K	22	THR
2	K	70	LEU
2	K	126	ARG
2	K	128	ASN
2	K	134	GLU
2	K	148	THR

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Mol	Chain	Res	Type
2	L	22	THR
2	L	62	ASP
2	L	126	ARG
2	L	134	GLU
2	L	145	ARG
2	L	148	THR
2	M	22	THR
2	M	25	SER
2	M	128	ASN
2	M	134	GLU
2	N	22	THR
2	N	25	SER
2	N	70	LEU
2	N	128	ASN
2	N	134	GLU
2	N	148	THR
2	O	65	LEU
2	O	68	THR
2	O	70	LEU
2	O	134	GLU
2	O	145	ARG
2	O	148	THR
1	A	143	ARG
1	A	202	SER
1	A	215	GLU
1	A	219	GLY
1	A	226	ALA
1	A	227	GLU
1	A	253	ASN
1	A	264	PRO
1	A	307	ARG
1	A	336	LEU
1	A	352	ASP
1	A	369	GLY
1	A	415	PRO
1	A	438	PRO
1	A	441	GLY
1	A	458	ILE
1	A	465	ASN
1	A	503	ILE
1	A	559	ALA
1	A	571	LEU

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Mol	Chain	Res	Type
1	A	590	ASN
1	A	608	VAL
1	A	630	ARG
1	A	654	VAL
1	A	680	ASP
1	A	739	MET
1	A	804	SER
1	A	815	TYR
1	A	823	THR
1	A	847	THR
1	A	866	ILE
1	B	73	LEU
1	B	141	GLU
1	B	142	LEU
1	B	212	PHE
1	B	230	GLN
1	B	253	ASN
1	B	261	LEU
1	B	264	PRO
1	B	265	LEU
1	B	278	ILE
1	B	282	VAL
1	B	283	ASN
1	B	307	ARG
1	B	313	ASN
1	B	338	GLU
1	B	388	SER
1	B	436	ILE
1	B	438	PRO
1	B	443	GLN
1	B	452	PRO
1	B	465	ASN
1	B	478	ASN
1	B	487	GLY
1	B	488	VAL
1	B	489	LEU
1	B	493	LEU
1	B	496	ASN
1	B	500	GLY
1	B	520	THR
1	B	524	ASP
1	B	608	VAL

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Mol	Chain	Res	Type
1	B	631	LEU
1	B	637	LYS
1	B	638	MET
1	B	654	VAL
1	B	674	VAL
1	B	676	VAL
1	B	787	VAL
1	B	854	LEU
2	C	7	LEU
2	C	20	GLU
2	C	25	SER
2	C	62	ASP
2	C	106	ARG
2	C	130	ASP
2	C	148	THR
2	D	7	LEU
2	D	20	GLU
2	D	42	ASN
2	D	65	LEU
2	D	67	GLY
2	D	69	THR
2	D	72	ASN
2	D	90	ASP
2	D	106	ARG
2	D	147	ARG
2	E	7	LEU
2	E	62	ASP
2	E	90	ASP
2	E	126	ARG
2	E	128	ASN
2	E	130	ASP
2	E	148	THR
2	F	7	LEU
2	F	25	SER
2	F	128	ASN
2	G	7	LEU
2	G	25	SER
2	G	125	LYS
2	G	126	ARG
2	H	7	LEU
2	H	25	SER
2	H	42	ASN

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Mol	Chain	Res	Type
2	H	51	ILE
2	H	62	ASP
2	H	68	THR
2	H	109	ILE
2	H	128	ASN
2	I	7	LEU
2	I	90	ASP
2	I	125	LYS
2	I	147	ARG
2	J	7	LEU
2	J	51	ILE
2	J	62	ASP
2	J	90	ASP
2	J	126	ARG
2	J	128	ASN
2	J	130	ASP
2	K	7	LEU
2	K	20	GLU
2	K	62	ASP
2	K	106	ARG
2	K	125	LYS
2	L	7	LEU
2	L	25	SER
2	L	69	THR
2	L	72	ASN
2	L	106	ARG
2	L	128	ASN
2	L	147	ARG
2	M	7	LEU
2	M	42	ASN
2	M	90	ASP
2	N	7	LEU
2	N	42	ASN
2	N	62	ASP
2	N	65	LEU
2	N	90	ASP
2	N	145	ARG
2	O	7	LEU
2	O	22	THR
2	O	25	SER
2	O	62	ASP
2	O	90	ASP

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Mol	Chain	Res	Type
2	O	105	GLN
1	A	137	ASN
1	A	142	LEU
1	A	218	GLU
1	A	254	GLU
1	A	265	LEU
1	A	276	GLU
1	A	496	ASN
1	A	497	ILE
1	A	521	MET
1	A	525	TYR
1	A	579	THR
1	A	597	PRO
1	A	648	ARG
1	A	658	PRO
1	A	676	VAL
1	A	687	MET
1	A	696	SER
1	A	773	SER
1	A	816	ASP
1	A	849	THR
1	B	237	ASN
1	B	254	GLU
1	B	273	TYR
1	B	359	THR
1	B	387	LEU
1	B	421	ARG
1	B	549	LEU
1	B	579	THR
1	B	581	VAL
1	B	590	ASN
1	B	635	GLN
1	B	656	ARG
1	B	670	ARG
1	B	675	GLU
1	B	794	THR
1	B	849	THR
2	C	13	ASP
2	C	42	ASN
2	C	69	THR
2	C	90	ASP
2	C	126	ARG

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Mol	Chain	Res	Type
2	D	13	ASP
2	D	32	GLN
2	D	62	ASP
2	D	68	THR
2	D	125	LYS
2	E	13	ASP
2	E	32	GLN
2	E	70	LEU
2	F	13	ASP
2	F	32	GLN
2	F	90	ASP
2	F	126	ARG
2	F	130	ASP
2	G	13	ASP
2	G	32	GLN
2	G	42	ASN
2	G	90	ASP
2	G	128	ASN
2	H	13	ASP
2	H	32	GLN
2	H	90	ASP
2	I	13	ASP
2	I	32	GLN
2	I	126	ARG
2	I	128	ASN
2	I	146	GLN
2	J	13	ASP
2	J	42	ASN
2	K	13	ASP
2	K	25	SER
2	K	32	GLN
2	K	90	ASP
2	K	111	PRO
2	L	13	ASP
2	L	20	GLU
2	L	41	MET
2	L	90	ASP
2	L	125	LYS
2	M	13	ASP
2	M	106	ARG
2	N	13	ASP
2	N	67	GLY

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Mol	Chain	Res	Type
2	N	106	ARG
2	N	125	LYS
2	N	155	PRO
2	O	20	GLU
2	O	24	TYR
2	O	32	GLN
2	O	42	ASN
2	O	73	LEU
2	O	106	ARG
2	O	126	ARG
2	O	155	PRO
1	A	131	LEU
1	A	144	ASN
1	A	155	LEU
1	A	187	ALA
1	A	195	ASP
1	A	206	SER
1	A	212	PHE
1	A	299	ILE
1	A	333	VAL
1	A	372	SER
1	A	387	LEU
1	A	457	GLN
1	A	518	PHE
1	A	524	ASP
1	A	549	LEU
1	A	552	TYR
1	A	557	LEU
1	A	581	VAL
1	A	700	ALA
1	A	730	PHE
1	A	853	ASP
1	A	877	MET
1	B	85	GLU
1	B	101	LYS
1	B	185	ASP
1	B	193	SER
1	B	206	SER
1	B	294	SER
1	B	302	ASN
1	B	372	SER
1	B	442	MET

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Mol	Chain	Res	Type
1	B	466	PHE
1	B	483	VAL
1	B	552	TYR
1	B	564	ASN
1	B	597	PRO
1	B	639	LYS
1	B	680	ASP
1	B	731	GLN
2	C	32	GLN
2	C	38	ILE
2	C	89	VAL
2	D	38	ILE
2	D	41	MET
2	D	89	VAL
2	D	123	LYS
2	D	145	ARG
2	E	38	ILE
2	F	20	GLU
2	F	38	ILE
2	F	42	ASN
2	G	38	ILE
2	G	130	ASP
2	G	145	ARG
2	H	36	GLN
2	H	38	ILE
2	H	89	VAL
2	H	106	ARG
2	I	36	GLN
2	I	38	ILE
2	I	42	ASN
2	I	89	VAL
2	I	145	ARG
2	J	32	GLN
2	J	36	GLN
2	J	38	ILE
2	J	89	VAL
2	K	9	LYS
2	K	36	GLN
2	K	38	ILE
2	K	89	VAL
2	L	32	GLN
2	L	36	GLN

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Mol	Chain	Res	Type
2	L	38	ILE
2	M	20	GLU
2	M	32	GLN
2	M	38	ILE
2	M	55	PRO
2	M	89	VAL
2	M	126	ARG
2	N	20	GLU
2	N	32	GLN
2	N	36	GLN
2	N	38	ILE
2	N	89	VAL
2	N	126	ARG
2	O	13	ASP
2	O	38	ILE
2	O	89	VAL
2	O	128	ASN
1	A	152	LYS
1	A	196	ALA
1	A	351	GLN
1	B	86	ILE
1	B	103	SER
1	B	207	ILE
1	B	277	ARG
1	B	399	THR
1	B	416	ASN
1	B	437	TYR
1	B	827	LYS
2	C	36	GLN
2	C	145	ARG
2	D	9	LYS
2	D	36	GLN
2	E	36	GLN
2	E	55	PRO
2	E	89	VAL
2	F	9	LYS
2	F	36	GLN
2	F	89	VAL
2	G	36	GLN
2	G	89	VAL
2	G	123	LYS
2	G	155	PRO

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Mol	Chain	Res	Type
2	H	9	LYS
2	H	130	ASP
2	I	9	LYS
2	I	41	MET
2	J	125	LYS
2	K	42	ASN
2	K	130	ASP
2	L	9	LYS
2	L	65	LEU
2	L	89	VAL
2	M	36	GLN
2	M	41	MET
2	M	145	ARG
2	N	9	LYS
2	N	69	THR
2	O	9	LYS
2	O	36	GLN
2	O	41	MET
1	A	207	ILE
1	A	422	GLU
1	A	622	VAL
1	A	733	ILE
1	A	819	PRO
1	B	521	MET
1	B	557	LEU
1	B	622	VAL
1	B	677	ARG
1	B	781	THR
1	B	857	PHE
2	C	3	VAL
2	E	9	LYS
2	E	20	GLU
2	E	42	ASN
2	F	55	PRO
2	G	3	VAL
2	G	9	LYS
2	I	123	LYS
2	J	3	VAL
2	J	9	LYS
2	J	69	THR
2	K	3	VAL
2	K	147	ARG

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Mol	Chain	Res	Type
2	L	3	VAL
2	N	3	VAL
2	O	3	VAL
1	A	247	PRO
1	A	334	PRO
1	B	519	PRO
1	B	723	ILE
1	B	865	PRO
2	D	3	VAL
2	E	3	VAL
2	F	3	VAL
2	H	3	VAL
2	I	3	VAL
2	M	3	VAL
1	A	502	VAL
1	A	606	VAL
1	B	415	PRO
2	E	78	VAL
2	I	78	VAL
2	I	101	VAL
2	L	78	VAL
2	N	78	VAL
1	A	405	ILE
1	A	699	ILE
1	B	128	PRO
1	B	370	ILE
1	B	405	ILE
1	B	413	VAL
2	C	78	VAL
2	F	78	VAL
2	H	78	VAL
2	J	78	VAL
2	K	78	VAL
2	M	78	VAL
2	M	101	VAL
2	N	101	VAL
2	O	51	ILE
2	O	78	VAL
2	O	101	VAL
1	A	500	GLY
1	B	435	ILE
1	B	606	VAL

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Mol	Chain	Res	Type
2	C	67	GLY
2	D	78	VAL
2	G	78	VAL
1	A	787	VAL
1	B	246	HIS
1	B	544	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	715/809 (88%)	604 (84%)	111 (16%)	2	15
1	B	744/809 (92%)	633 (85%)	111 (15%)	3	16
2	C	350/350 (100%)	326 (93%)	24 (7%)	14	40
2	D	350/350 (100%)	324 (93%)	26 (7%)	13	38
2	E	350/350 (100%)	327 (93%)	23 (7%)	15	41
2	F	350/350 (100%)	329 (94%)	21 (6%)	17	43
2	G	350/350 (100%)	329 (94%)	21 (6%)	17	43
2	H	350/350 (100%)	331 (95%)	19 (5%)	20	45
2	I	350/350 (100%)	330 (94%)	20 (6%)	18	44
2	J	350/350 (100%)	329 (94%)	21 (6%)	17	43
2	K	350/350 (100%)	330 (94%)	20 (6%)	18	44
2	L	350/350 (100%)	324 (93%)	26 (7%)	13	38
2	M	350/350 (100%)	325 (93%)	25 (7%)	13	39
2	N	350/350 (100%)	328 (94%)	22 (6%)	16	42
2	O	350/350 (100%)	329 (94%)	21 (6%)	17	43
All	All	6009/6168 (97%)	5498 (92%)	511 (8%)	10	33

All (511) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PRO
1	A	122	LEU
1	A	125	ILE
1	A	126	PHE
1	A	142	LEU
1	A	147	TYR
1	A	154	THR
1	A	157	ASP
1	A	169	LEU
1	A	193	SER
1	A	203	GLU
1	A	204	THR
1	A	215	GLU
1	A	216	GLU
1	A	227	GLU
1	A	230	GLN
1	A	239	VAL
1	A	247	PRO
1	A	259	HIS
1	A	262	VAL
1	A	273	TYR
1	A	275	PRO
1	A	276	GLU
1	A	278	ILE
1	A	280	ASN
1	A	285	ILE
1	A	286	LEU
1	A	288	MET
1	A	295	THR
1	A	298	TYR
1	A	303	LEU
1	A	305	GLN
1	A	310	LEU
1	A	311	HIS
1	A	316	SER
1	A	318	TRP
1	A	342	THR
1	A	347	GLN
1	A	348	LYS
1	A	354	GLN
1	A	366	PHE
1	A	371	ASN
1	A	382	LEU

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Mol	Chain	Res	Type
1	A	389	GLN
1	A	391	THR
1	A	392	MET
1	A	395	ASP
1	A	401	TYR
1	A	408	MET
1	A	410	LEU
1	A	414	VAL
1	A	424	LEU
1	A	428	GLN
1	A	436	ILE
1	A	443	GLN
1	A	471	TRP
1	A	473	HIS
1	A	476	ASN
1	A	495	ASP
1	A	505	GLN
1	A	506	LEU
1	A	515	ARG
1	A	516	GLN
1	A	520	THR
1	A	521	MET
1	A	534	LEU
1	A	540	LEU
1	A	542	GLN
1	A	543	LEU
1	A	563	MET
1	A	565	MET
1	A	571	LEU
1	A	587	LEU
1	A	594	ILE
1	A	601	PHE
1	A	641	ILE
1	A	646	LEU
1	A	676	VAL
1	A	680	ASP
1	A	701	GLN
1	A	704	ILE
1	A	707	TYR
1	A	712	LEU
1	A	717	MET
1	A	718	TYR

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Mol	Chain	Res	Type
1	A	720	TYR
1	A	721	VAL
1	A	723	ILE
1	A	726	ASN
1	A	730	PHE
1	A	737	GLU
1	A	743	ASP
1	A	744	TYR
1	A	747	ILE
1	A	753	ASN
1	A	759	LEU
1	A	771	VAL
1	A	775	ILE
1	A	782	VAL
1	A	793	ASP
1	A	798	ILE
1	A	799	LEU
1	A	802	ILE
1	A	816	ASP
1	A	829	VAL
1	A	837	ASN
1	A	839	MET
1	A	848	PHE
1	A	849	THR
1	A	861	ASP
1	A	864	GLU
1	B	74	GLU
1	B	126	PHE
1	B	134	TYR
1	B	135	ARG
1	B	153	ASP
1	B	157	ASP
1	B	169	LEU
1	B	177	MET
1	B	180	TYR
1	B	182	LEU
1	B	190	ASN
1	B	194	ARG
1	B	201	ASP
1	B	203	GLU
1	B	204	THR
1	B	215	GLU

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Mol	Chain	Res	Type
1	B	217	THR
1	B	239	VAL
1	B	276	GLU
1	B	286	LEU
1	B	287	ASN
1	B	298	TYR
1	B	310	LEU
1	B	311	HIS
1	B	312	ASP
1	B	314	PHE
1	B	316	SER
1	B	318	TRP
1	B	322	THR
1	B	332	VAL
1	B	336	LEU
1	B	342	THR
1	B	347	GLN
1	B	348	LYS
1	B	352	ASP
1	B	353	LEU
1	B	358	LEU
1	B	382	LEU
1	B	389	GLN
1	B	392	MET
1	B	396	PHE
1	B	397	VAL
1	B	401	TYR
1	B	408	MET
1	B	424	LEU
1	B	428	GLN
1	B	436	ILE
1	B	453	GLN
1	B	471	TRP
1	B	473	HIS
1	B	476	ASN
1	B	492	VAL
1	B	495	ASP
1	B	497	ILE
1	B	498	ARG
1	B	505	GLN
1	B	506	LEU
1	B	516	GLN

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Mol	Chain	Res	Type
1	B	518	PHE
1	B	521	MET
1	B	522	PRO
1	B	525	TYR
1	B	534	LEU
1	B	540	LEU
1	B	542	GLN
1	B	543	LEU
1	B	560	CYS
1	B	562	THR
1	B	568	VAL
1	B	590	ASN
1	B	601	PHE
1	B	638	MET
1	B	641	ILE
1	B	646	LEU
1	B	652	PHE
1	B	660	ASP
1	B	674	VAL
1	B	676	VAL
1	B	680	ASP
1	B	697	ASP
1	B	707	TYR
1	B	710	MET
1	B	725	ARG
1	B	727	LEU
1	B	728	ASP
1	B	730	PHE
1	B	737	GLU
1	B	744	TYR
1	B	747	ILE
1	B	759	LEU
1	B	771	VAL
1	B	774	LEU
1	B	782	VAL
1	B	783	PHE
1	B	786	ILE
1	B	789	LEU
1	B	790	ARG
1	B	792	VAL
1	B	798	ILE
1	B	799	LEU

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Mol	Chain	Res	Type
1	B	808	ASP
1	B	810	TYR
1	B	811	LEU
1	B	812	VAL
1	B	818	VAL
1	B	823	THR
1	B	832	GLN
1	B	857	PHE
1	B	872	ASP
1	B	873	ASN
1	B	876	ILE
2	C	2	ASP
2	C	13	ASP
2	C	22	THR
2	C	26	ASN
2	C	59	TRP
2	C	68	THR
2	C	103	GLU
2	C	106	ARG
2	C	109	ILE
2	C	128	ASN
2	C	129	PHE
2	C	142	GLN
2	C	147	ARG
2	C	150	PHE
2	C	152	PHE
2	C	170	GLN
2	C	214	LEU
2	C	225	LEU
2	C	255	ARG
2	C	274	GLN
2	C	370	LEU
2	C	378	ARG
2	C	382	LEU
2	C	385	VAL
2	D	2	ASP
2	D	13	ASP
2	D	19	VAL
2	D	45	GLU
2	D	58	ASN
2	D	68	THR
2	D	70	LEU

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Mol	Chain	Res	Type
2	D	73	LEU
2	D	103	GLU
2	D	106	ARG
2	D	109	ILE
2	D	117	ARG
2	D	129	PHE
2	D	142	GLN
2	D	143	ASN
2	D	150	PHE
2	D	152	PHE
2	D	170	GLN
2	D	214	LEU
2	D	225	LEU
2	D	255	ARG
2	D	274	GLN
2	D	370	LEU
2	D	378	ARG
2	D	382	LEU
2	D	385	VAL
2	E	1	MET
2	E	2	ASP
2	E	13	ASP
2	E	26	ASN
2	E	58	ASN
2	E	59	TRP
2	E	69	THR
2	E	103	GLU
2	E	109	ILE
2	E	129	PHE
2	E	142	GLN
2	E	148	THR
2	E	150	PHE
2	E	152	PHE
2	E	170	GLN
2	E	214	LEU
2	E	225	LEU
2	E	255	ARG
2	E	274	GLN
2	E	370	LEU
2	E	378	ARG
2	E	382	LEU
2	E	385	VAL

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Mol	Chain	Res	Type
2	F	2	ASP
2	F	13	ASP
2	F	25	SER
2	F	60	ASN
2	F	61	PHE
2	F	109	ILE
2	F	128	ASN
2	F	129	PHE
2	F	142	GLN
2	F	148	THR
2	F	150	PHE
2	F	152	PHE
2	F	170	GLN
2	F	214	LEU
2	F	225	LEU
2	F	255	ARG
2	F	274	GLN
2	F	370	LEU
2	F	378	ARG
2	F	382	LEU
2	F	385	VAL
2	G	2	ASP
2	G	13	ASP
2	G	26	ASN
2	G	63	PHE
2	G	103	GLU
2	G	106	ARG
2	G	109	ILE
2	G	129	PHE
2	G	142	GLN
2	G	143	ASN
2	G	145	ARG
2	G	152	PHE
2	G	170	GLN
2	G	214	LEU
2	G	225	LEU
2	G	255	ARG
2	G	274	GLN
2	G	370	LEU
2	G	378	ARG
2	G	382	LEU
2	G	385	VAL

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Mol	Chain	Res	Type
2	H	2	ASP
2	H	13	ASP
2	H	103	GLU
2	H	106	ARG
2	H	109	ILE
2	H	128	ASN
2	H	129	PHE
2	H	142	GLN
2	H	150	PHE
2	H	152	PHE
2	H	170	GLN
2	H	214	LEU
2	H	225	LEU
2	H	255	ARG
2	H	274	GLN
2	H	370	LEU
2	H	378	ARG
2	H	382	LEU
2	H	385	VAL
2	I	2	ASP
2	I	13	ASP
2	I	48	THR
2	I	61	PHE
2	I	103	GLU
2	I	106	ARG
2	I	109	ILE
2	I	129	PHE
2	I	142	GLN
2	I	150	PHE
2	I	152	PHE
2	I	170	GLN
2	I	214	LEU
2	I	225	LEU
2	I	255	ARG
2	I	274	GLN
2	I	370	LEU
2	I	378	ARG
2	I	382	LEU
2	I	385	VAL
2	J	2	ASP
2	J	13	ASP
2	J	19	VAL

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Mol	Chain	Res	Type
2	J	59	TRP
2	J	71	LEU
2	J	106	ARG
2	J	109	ILE
2	J	128	ASN
2	J	129	PHE
2	J	142	GLN
2	J	150	PHE
2	J	152	PHE
2	J	170	GLN
2	J	214	LEU
2	J	225	LEU
2	J	255	ARG
2	J	274	GLN
2	J	370	LEU
2	J	378	ARG
2	J	382	LEU
2	J	385	VAL
2	K	2	ASP
2	K	13	ASP
2	K	59	TRP
2	K	62	ASP
2	K	103	GLU
2	K	109	ILE
2	K	129	PHE
2	K	142	GLN
2	K	143	ASN
2	K	150	PHE
2	K	152	PHE
2	K	170	GLN
2	K	214	LEU
2	K	225	LEU
2	K	255	ARG
2	K	274	GLN
2	K	370	LEU
2	K	378	ARG
2	K	382	LEU
2	K	385	VAL
2	L	1	MET
2	L	2	ASP
2	L	13	ASP
2	L	19	VAL

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Mol	Chain	Res	Type
2	L	22	THR
2	L	25	SER
2	L	59	TRP
2	L	62	ASP
2	L	72	ASN
2	L	103	GLU
2	L	106	ARG
2	L	109	ILE
2	L	125	LYS
2	L	129	PHE
2	L	142	GLN
2	L	150	PHE
2	L	152	PHE
2	L	170	GLN
2	L	214	LEU
2	L	225	LEU
2	L	255	ARG
2	L	274	GLN
2	L	370	LEU
2	L	378	ARG
2	L	382	LEU
2	L	385	VAL
2	M	2	ASP
2	M	13	ASP
2	M	22	THR
2	M	23	LEU
2	M	59	TRP
2	M	71	LEU
2	M	103	GLU
2	M	106	ARG
2	M	107	ASN
2	M	109	ILE
2	M	117	ARG
2	M	125	LYS
2	M	129	PHE
2	M	142	GLN
2	M	150	PHE
2	M	152	PHE
2	M	170	GLN
2	M	214	LEU
2	M	225	LEU
2	M	255	ARG

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Mol	Chain	Res	Type
2	M	274	GLN
2	M	370	LEU
2	M	378	ARG
2	M	382	LEU
2	M	385	VAL
2	N	2	ASP
2	N	13	ASP
2	N	58	ASN
2	N	66	LEU
2	N	73	LEU
2	N	103	GLU
2	N	106	ARG
2	N	107	ASN
2	N	109	ILE
2	N	129	PHE
2	N	142	GLN
2	N	145	ARG
2	N	152	PHE
2	N	170	GLN
2	N	214	LEU
2	N	225	LEU
2	N	255	ARG
2	N	274	GLN
2	N	370	LEU
2	N	378	ARG
2	N	382	LEU
2	N	385	VAL
2	O	2	ASP
2	O	13	ASP
2	O	23	LEU
2	O	25	SER
2	O	51	ILE
2	O	58	ASN
2	O	106	ARG
2	O	107	ASN
2	O	109	ILE
2	O	129	PHE
2	O	142	GLN
2	O	150	PHE
2	O	170	GLN
2	O	214	LEU
2	O	225	LEU

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Mol	Chain	Res	Type
2	O	255	ARG
2	O	274	GLN
2	O	370	LEU
2	O	378	ARG
2	O	382	LEU
2	O	385	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (261) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	137	ASN
1	A	168	ASN
1	A	230	GLN
1	A	246	HIS
1	A	260	GLN
1	A	309	ASN
1	A	347	GLN
1	A	365	GLN
1	A	371	ASN
1	A	428	GLN
1	A	443	GLN
1	A	453	GLN
1	A	467	GLN
1	A	470	ASN
1	A	473	HIS
1	A	477	ASN
1	A	490	ASN
1	A	496	ASN
1	A	553	ASN
1	A	605	ASN
1	A	607	ASN
1	A	609	ASN
1	A	613	ASN
1	A	615	ASN
1	A	661	GLN
1	A	683	ASN
1	A	701	GLN
1	A	722	ASN
1	A	726	ASN
1	A	803	ASN
1	A	807	ASN

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Mol	Chain	Res	Type
1	A	840	HIS
1	A	867	ASN
1	A	873	ASN
1	B	168	ASN
1	B	190	ASN
1	B	230	GLN
1	B	233	GLN
1	B	237	ASN
1	B	246	HIS
1	B	260	GLN
1	B	287	ASN
1	B	302	ASN
1	B	305	GLN
1	B	309	ASN
1	B	311	HIS
1	B	325	ASN
1	B	347	GLN
1	B	371	ASN
1	B	428	GLN
1	B	446	HIS
1	B	449	ASN
1	B	462	GLN
1	B	470	ASN
1	B	473	HIS
1	B	476	ASN
1	B	477	ASN
1	B	491	GLN
1	B	499	ASN
1	B	505	GLN
1	B	517	GLN
1	B	553	ASN
1	B	564	ASN
1	B	590	ASN
1	B	602	HIS
1	B	605	ASN
1	B	609	ASN
1	B	611	HIS
1	B	615	ASN
1	B	629	ASN
1	B	635	GLN
1	B	731	GLN
1	B	746	GLN

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Mol	Chain	Res	Type
1	B	749	ASN
1	B	807	ASN
1	B	814	ASN
1	B	831	GLN
1	B	840	HIS
1	B	878	ASN
2	C	26	ASN
2	C	35	ASN
2	C	53	ASN
2	C	72	ASN
2	C	107	ASN
2	C	128	ASN
2	C	131	ASN
2	C	138	ASN
2	C	143	ASN
2	C	146	GLN
2	C	167	ASN
2	C	183	ASN
2	C	239	ASN
2	C	274	GLN
2	C	284	ASN
2	D	26	ASN
2	D	36	GLN
2	D	128	ASN
2	D	131	ASN
2	D	142	GLN
2	D	143	ASN
2	D	146	GLN
2	D	167	ASN
2	D	183	ASN
2	D	239	ASN
2	D	274	GLN
2	D	284	ASN
2	E	26	ASN
2	E	53	ASN
2	E	58	ASN
2	E	94	ASN
2	E	128	ASN
2	E	131	ASN
2	E	142	GLN
2	E	167	ASN
2	E	183	ASN

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Mol	Chain	Res	Type
2	E	239	ASN
2	E	274	GLN
2	E	284	ASN
2	F	32	GLN
2	F	35	ASN
2	F	53	ASN
2	F	72	ASN
2	F	94	ASN
2	F	128	ASN
2	F	131	ASN
2	F	142	GLN
2	F	167	ASN
2	F	183	ASN
2	F	239	ASN
2	F	274	GLN
2	F	284	ASN
2	G	26	ASN
2	G	35	ASN
2	G	53	ASN
2	G	128	ASN
2	G	131	ASN
2	G	138	ASN
2	G	142	GLN
2	G	167	ASN
2	G	183	ASN
2	G	239	ASN
2	G	274	GLN
2	G	284	ASN
2	H	26	ASN
2	H	35	ASN
2	H	53	ASN
2	H	72	ASN
2	H	83	ASN
2	H	94	ASN
2	H	105	GLN
2	H	107	ASN
2	H	128	ASN
2	H	131	ASN
2	H	142	GLN
2	H	167	ASN
2	H	183	ASN
2	H	239	ASN

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Mol	Chain	Res	Type
2	H	274	GLN
2	H	284	ASN
2	I	32	GLN
2	I	33	GLN
2	I	35	ASN
2	I	47	GLN
2	I	53	ASN
2	I	76	ASN
2	I	94	ASN
2	I	128	ASN
2	I	131	ASN
2	I	143	ASN
2	I	146	GLN
2	I	167	ASN
2	I	183	ASN
2	I	239	ASN
2	I	274	GLN
2	I	284	ASN
2	J	26	ASN
2	J	35	ASN
2	J	53	ASN
2	J	94	ASN
2	J	128	ASN
2	J	131	ASN
2	J	138	ASN
2	J	142	GLN
2	J	146	GLN
2	J	167	ASN
2	J	183	ASN
2	J	239	ASN
2	J	274	GLN
2	J	284	ASN
2	K	26	ASN
2	K	33	GLN
2	K	35	ASN
2	K	53	ASN
2	K	72	ASN
2	K	94	ASN
2	K	107	ASN
2	K	131	ASN
2	K	138	ASN
2	K	143	ASN

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Mol	Chain	Res	Type
2	K	167	ASN
2	K	183	ASN
2	K	239	ASN
2	K	274	GLN
2	K	284	ASN
2	L	33	GLN
2	L	36	GLN
2	L	53	ASN
2	L	72	ASN
2	L	131	ASN
2	L	143	ASN
2	L	146	GLN
2	L	167	ASN
2	L	183	ASN
2	L	239	ASN
2	L	274	GLN
2	L	284	ASN
2	M	36	GLN
2	M	53	ASN
2	M	105	GLN
2	M	128	ASN
2	M	131	ASN
2	M	142	GLN
2	M	143	ASN
2	M	167	ASN
2	M	183	ASN
2	M	239	ASN
2	M	274	GLN
2	M	284	ASN
2	N	26	ASN
2	N	32	GLN
2	N	35	ASN
2	N	53	ASN
2	N	58	ASN
2	N	76	ASN
2	N	94	ASN
2	N	128	ASN
2	N	131	ASN
2	N	142	GLN
2	N	143	ASN
2	N	146	GLN
2	N	167	ASN

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Mol	Chain	Res	Type
2	N	183	ASN
2	N	239	ASN
2	N	274	GLN
2	N	284	ASN
2	O	26	ASN
2	O	33	GLN
2	O	35	ASN
2	O	53	ASN
2	O	131	ASN
2	O	140	ASN
2	O	142	GLN
2	O	143	ASN
2	O	146	GLN
2	O	153	HIS
2	O	167	ASN
2	O	183	ASN
2	O	239	ASN
2	O	274	GLN
2	O	284	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	781/880 (88%)	0.48	96 (12%) 8 12	62, 136, 196, 209	0
1	B	810/880 (92%)	0.35	61 (7%) 20 18	53, 131, 186, 209	0
2	C	397/397 (100%)	0.70	61 (15%) 5 8	81, 147, 203, 209	0
2	D	397/397 (100%)	0.97	83 (20%) 2 4	90, 154, 208, 209	0
2	E	397/397 (100%)	1.04	89 (22%) 2 4	72, 151, 201, 209	0
2	F	397/397 (100%)	0.82	69 (17%) 4 6	100, 182, 209, 209	0
2	G	397/397 (100%)	1.38	117 (29%) 1 2	82, 176, 209, 209	0
2	H	397/397 (100%)	0.89	69 (17%) 4 6	96, 174, 209, 209	0
2	I	397/397 (100%)	1.08	82 (20%) 2 4	83, 157, 208, 209	0
2	J	397/397 (100%)	1.14	88 (22%) 2 4	77, 155, 203, 209	0
2	K	397/397 (100%)	0.87	75 (18%) 3 5	79, 156, 208, 209	0
2	L	397/397 (100%)	1.08	92 (23%) 2 3	77, 150, 207, 209	0
2	M	397/397 (100%)	1.30	115 (28%) 1 2	81, 150, 208, 209	0
2	N	397/397 (100%)	0.71	61 (15%) 5 8	83, 150, 201, 209	0
2	O	397/397 (100%)	0.51	47 (11%) 9 12	75, 150, 200, 209	0
All	All	6752/6921 (97%)	0.83	1205 (17%) 4 6	53, 153, 208, 209	0

All (1205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	60	ASN	15.4
1	B	99	GLU	15.4
2	H	233	SER	13.1
2	G	110	ALA	12.7
2	D	55	PRO	12.3
2	L	49	GLY	11.8
2	J	221	ALA	11.6

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Mol	Chain	Res	Type	RSRZ
2	I	262	GLU	10.4
2	N	50	GLY	10.1
2	G	284	ASN	9.7
2	J	340	GLU	9.5
2	E	224	THR	9.4
2	H	68	THR	9.4
2	L	289	ARG	9.0
2	G	47	GLN	8.9
2	L	120	SER	8.9
2	G	219	THR	8.7
2	M	331	CYS	8.2
2	L	207	GLN	8.2
2	I	159	PRO	8.1
1	B	630	ARG	7.8
2	G	90	ASP	7.5
2	G	163	SER	7.5
2	J	282	ALA	7.5
2	G	203	ALA	7.4
2	G	309	PRO	7.4
2	H	72	ASN	7.4
2	D	313	PRO	7.3
2	I	193	PHE	7.3
2	L	255	ARG	7.3
2	I	184	ALA	7.3
2	G	314	PHE	7.2
2	J	318	ALA	7.2
2	I	186	SER	7.1
2	L	323	THR	7.1
2	E	288	ILE	7.0
2	L	146	GLN	7.0
2	O	50	GLY	6.9
2	J	209	GLU	6.8
2	L	262	GLU	6.8
2	M	278	GLY	6.8
2	C	108	GLY	6.8
2	L	215	ARG	6.7
2	E	50	GLY	6.7
2	G	285	PHE	6.6
2	L	212	VAL	6.6
2	D	289	ARG	6.6
2	J	192	GLY	6.6
2	J	260	GLU	6.6

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Mol	Chain	Res	Type	RSRZ
2	L	20	GLU	6.6
2	J	332	GLU	6.5
2	H	133	SER	6.5
2	M	324	LEU	6.5
2	M	133	SER	6.4
2	E	192	GLY	6.4
2	O	121	GLY	6.4
2	N	120	SER	6.4
2	M	206	GLN	6.3
2	E	320	VAL	6.3
2	E	189	GLN	6.3
2	K	161	SER	6.3
2	E	332	GLU	6.3
2	F	47	GLN	6.2
2	D	50	GLY	6.2
2	M	149	GLY	6.2
2	K	89	VAL	6.2
2	D	132	SER	6.2
2	F	292	PHE	6.2
2	C	318	ALA	6.2
2	I	50	GLY	6.1
2	H	188	ILE	6.1
2	K	102	ARG	6.1
2	M	178	GLY	6.0
2	J	313	PRO	6.0
2	J	314	PHE	6.0
2	L	287	THR	5.9
2	F	209	GLU	5.9
2	E	287	THR	5.9
2	F	208	PHE	5.9
2	H	193	PHE	5.9
2	M	205	THR	5.9
2	D	210	HIS	5.9
2	F	72	ASN	5.8
2	M	291	SER	5.8
2	L	56	ILE	5.8
2	M	216	ARG	5.8
2	J	296	ARG	5.7
2	N	233	SER	5.7
2	I	194	ASP	5.7
2	E	324	LEU	5.7
2	G	315	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
2	M	364	GLY	5.6
2	E	326	ILE	5.6
2	E	319	THR	5.6
2	G	93	ASP	5.6
2	H	336	ALA	5.6
2	J	70	LEU	5.5
2	D	188	ILE	5.5
2	J	71	LEU	5.5
2	I	333	SER	5.5
2	H	323	THR	5.5
2	J	148	THR	5.5
2	F	152	PHE	5.4
2	H	149	GLY	5.4
2	M	224	THR	5.4
2	O	148	THR	5.4
2	H	318	ALA	5.4
2	L	47	GLN	5.4
2	G	99	GLU	5.4
2	M	332	GLU	5.4
2	J	294	LEU	5.4
2	F	210	HIS	5.4
2	C	230	GLU	5.4
2	D	208	PHE	5.4
2	L	22	THR	5.3
2	M	162	ALA	5.3
1	A	300	ARG	5.3
2	C	147	ARG	5.3
2	K	19	VAL	5.3
2	G	162	ALA	5.3
2	C	234	PHE	5.3
2	I	103	GLU	5.3
2	H	50	GLY	5.3
1	B	653	ASP	5.3
2	F	291	SER	5.3
2	F	267	GLY	5.2
2	C	150	PHE	5.2
2	M	340	GLU	5.2
2	M	193	PHE	5.2
2	E	293	GLN	5.2
2	L	208	PHE	5.1
2	I	288	ILE	5.1
2	G	179	THR	5.1

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Mol	Chain	Res	Type	RSRZ
2	D	314	PHE	5.1
2	F	332	GLU	5.1
2	H	45	GLU	5.1
2	N	149	GLY	5.1
2	O	128	ASN	5.1
2	K	389	ALA	5.1
2	K	208	PHE	5.1
2	L	233	SER	5.0
2	I	260	GLU	5.0
2	M	60	ASN	5.0
2	M	319	THR	5.0
2	D	276	ARG	5.0
2	E	255	ARG	5.0
1	B	720	TYR	5.0
2	C	2	ASP	5.0
2	G	376	PRO	5.0
2	M	210	HIS	5.0
2	G	155	PRO	5.0
2	G	259	VAL	5.0
2	I	234	PHE	5.0
2	J	2	ASP	5.0
2	N	151	THR	4.9
2	D	262	GLU	4.9
2	G	193	PHE	4.9
2	E	16	ASP	4.9
2	L	53	ASN	4.9
2	I	259	VAL	4.9
2	N	314	PHE	4.9
2	N	54	LEU	4.9
2	C	380	ASP	4.9
2	L	188	ILE	4.9
2	L	149	GLY	4.9
2	K	49	GLY	4.9
2	K	128	ASN	4.8
2	G	133	SER	4.8
2	O	334	VAL	4.8
2	G	381	ASN	4.8
2	D	99	GLU	4.8
2	F	23	LEU	4.8
2	L	21	GLY	4.8
2	L	327	GLU	4.8
2	H	102	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	186	SER	4.8
1	A	102	GLU	4.8
2	L	259	VAL	4.7
1	B	515	ARG	4.7
2	C	133	SER	4.7
2	D	375	SER	4.7
2	L	288	ILE	4.7
2	J	329	ALA	4.7
2	E	179	THR	4.7
2	O	318	ALA	4.7
2	E	159	PRO	4.7
2	C	340	GLU	4.7
1	B	334	PRO	4.7
2	E	149	GLY	4.7
2	C	60	ASN	4.7
2	N	47	GLN	4.7
2	I	379	GLU	4.6
2	J	312	GLN	4.6
2	E	325	ARG	4.6
2	H	117	ARG	4.6
2	I	320	VAL	4.6
2	D	323	THR	4.6
2	N	68	THR	4.6
2	L	256	PRO	4.6
2	G	216	ARG	4.6
2	N	102	ARG	4.6
2	I	334	VAL	4.6
1	A	828	GLN	4.6
2	M	135	TYR	4.6
2	M	225	LEU	4.5
2	M	315	GLU	4.5
2	J	280	ILE	4.5
2	H	89	VAL	4.5
2	K	278	GLY	4.5
2	J	281	ILE	4.5
1	A	611	HIS	4.5
2	E	191	ALA	4.5
2	K	165	THR	4.5
1	A	447	TYR	4.5
2	N	209	GLU	4.5
1	A	375	ALA	4.5
2	G	184	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
2	G	332	GLU	4.5
2	I	206	GLN	4.5
1	B	719	GLY	4.5
2	C	151	THR	4.5
2	L	67	GLY	4.5
2	E	379	GLU	4.5
2	J	59	TRP	4.5
2	N	110	ALA	4.5
2	G	213	GLN	4.4
2	L	116	LEU	4.4
2	K	183	ASN	4.4
2	E	212	VAL	4.4
2	L	184	ALA	4.4
2	K	316	HIS	4.4
1	B	180	TYR	4.4
2	G	218	LEU	4.4
2	N	133	SER	4.4
1	A	675	GLU	4.4
2	L	332	GLU	4.4
2	E	233	SER	4.4
2	N	108	GLY	4.4
2	G	45	GLU	4.3
2	N	207	GLN	4.3
2	E	108	GLY	4.3
2	N	93	ASP	4.3
2	H	101	VAL	4.3
2	G	20	GLU	4.3
2	C	336	ALA	4.3
2	M	310	ASN	4.3
2	K	47	GLN	4.3
2	N	334	VAL	4.3
2	E	340	GLU	4.3
2	M	189	GLN	4.3
2	D	183	ASN	4.2
2	G	261	VAL	4.2
2	I	60	ASN	4.2
2	G	164	PHE	4.2
2	J	128	ASN	4.2
2	G	123	LYS	4.2
2	N	117	ARG	4.2
2	D	310	ASN	4.2
2	J	310	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
2	G	205	THR	4.2
1	A	651	ILE	4.2
1	B	560	CYS	4.2
2	D	324	LEU	4.2
2	L	115	SER	4.2
2	I	188	ILE	4.2
2	F	262	GLU	4.1
2	J	315	GLU	4.1
2	L	161	SER	4.1
2	M	262	GLU	4.1
2	H	67	GLY	4.1
2	E	291	SER	4.1
1	A	408	MET	4.1
2	F	159	PRO	4.1
2	G	202	PRO	4.1
2	M	260	GLU	4.1
2	G	156	ASN	4.1
2	M	148	THR	4.1
2	M	288	ILE	4.1
2	L	50	GLY	4.1
2	G	310	ASN	4.1
2	D	318	ALA	4.1
2	I	336	ALA	4.1
2	D	260	GLU	4.0
2	M	20	GLU	4.0
1	A	120	THR	4.0
2	G	94	ASN	4.0
2	C	46	PHE	4.0
2	O	46	PHE	4.0
2	L	295	MET	4.0
1	A	569	GLN	4.0
1	B	808	ASP	4.0
2	M	280	ILE	4.0
2	D	234	PHE	4.0
2	L	111	PRO	4.0
2	L	397	LYS	4.0
2	I	324	LEU	4.0
2	F	114	ASP	4.0
1	B	406	SER	4.0
2	C	321	GLY	4.0
2	G	333	SER	4.0
2	H	241	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	343	GLU	4.0
2	G	148	THR	4.0
2	K	375	SER	4.0
2	L	72	ASN	4.0
2	I	15	ARG	4.0
2	G	326	ILE	4.0
2	M	86	ASP	4.0
2	L	122	LEU	3.9
2	K	217	VAL	3.9
2	G	234	PHE	3.9
2	J	151	THR	3.9
2	J	311	ALA	3.9
2	M	296	ARG	3.9
2	G	154	LYS	3.9
2	O	108	GLY	3.9
2	M	50	GLY	3.9
1	A	189	GLU	3.9
2	F	289	ARG	3.9
1	A	667	ASP	3.9
2	I	189	GLN	3.9
2	N	130	ASP	3.9
2	E	115	SER	3.9
2	E	216	ARG	3.8
1	A	304	LEU	3.8
2	J	54	LEU	3.8
2	L	324	LEU	3.8
2	F	167	ASN	3.8
2	J	58	ASN	3.8
2	J	72	ASN	3.8
1	A	487	GLY	3.8
2	M	273	TYR	3.8
2	D	53	ASN	3.8
2	D	133	SER	3.8
2	F	222	THR	3.8
2	H	301	THR	3.8
2	D	209	GLU	3.8
2	M	293	GLN	3.8
2	G	377	SER	3.8
2	G	126	ARG	3.8
2	K	126	ARG	3.8
2	O	260	GLU	3.8
2	M	309	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	347	GLN	3.8
2	G	146	GLN	3.8
1	B	276	GLU	3.8
2	E	259	VAL	3.8
2	C	119	LEU	3.8
2	K	132	SER	3.8
2	K	53	ASN	3.8
2	M	138	ASN	3.8
2	I	342	MET	3.8
2	J	46	PHE	3.8
2	M	47	GLN	3.7
2	F	20	GLU	3.7
2	F	146	GLN	3.7
1	A	283	ASN	3.7
1	A	762	ALA	3.7
2	L	114	ASP	3.7
2	M	136	ILE	3.7
2	N	331	CYS	3.7
1	B	643	GLU	3.7
2	M	230	GLU	3.7
2	G	312	GLN	3.7
2	I	106	ARG	3.7
2	C	319	THR	3.7
2	J	149	GLY	3.7
2	D	290	LEU	3.7
2	O	281	ILE	3.7
2	K	134	GLU	3.7
2	M	251	PRO	3.7
2	J	193	PHE	3.7
2	K	131	ASN	3.7
2	M	80	THR	3.7
2	G	92	VAL	3.7
2	M	97	MET	3.7
2	L	113	SER	3.7
2	H	79	GLU	3.7
2	L	380	ASP	3.7
2	K	110	ALA	3.6
2	E	21	GLY	3.6
2	M	177	MET	3.6
2	G	231	ARG	3.6
2	E	20	GLU	3.6
2	D	113	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	K	156	ASN	3.6
2	N	126	ARG	3.6
2	K	377	SER	3.6
2	K	67	GLY	3.6
2	G	101	VAL	3.6
1	A	378	CYS	3.6
2	G	159	PRO	3.6
2	N	96	CYS	3.6
2	D	329	ALA	3.6
2	G	178	GLY	3.6
2	D	217	VAL	3.6
2	G	16	ASP	3.6
2	K	62	ASP	3.6
2	K	68	THR	3.6
2	C	258	ASN	3.6
2	L	213	GLN	3.6
2	I	216	ARG	3.6
2	J	273	TYR	3.5
1	A	307	ARG	3.5
2	I	64	GLY	3.5
2	D	320	VAL	3.5
2	I	53	ASN	3.5
2	J	316	HIS	3.5
2	M	313	PRO	3.5
2	L	52	GLY	3.5
2	G	109	ILE	3.5
2	I	258	ASN	3.5
2	N	111	PRO	3.5
2	D	160	TYR	3.5
2	E	101	VAL	3.5
1	A	303	LEU	3.5
2	J	239	ASN	3.5
2	O	321	GLY	3.5
1	A	316	SER	3.5
2	F	130	ASP	3.5
2	G	125	LYS	3.5
2	C	375	SER	3.5
2	D	189	GLN	3.5
2	F	207	GLN	3.5
2	J	127	ILE	3.4
2	I	176	LEU	3.4
2	M	21	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	N	49	GLY	3.4
2	L	210	HIS	3.4
2	F	327	GLU	3.4
2	J	233	SER	3.4
2	K	149	GLY	3.4
2	M	179	THR	3.4
2	N	184	ALA	3.4
2	M	45	GLU	3.4
2	H	49	GLY	3.4
1	B	548	ARG	3.4
2	E	56	ILE	3.4
2	E	251	PRO	3.4
2	M	184	ALA	3.4
2	M	137	GLU	3.4
2	F	397	LYS	3.4
2	C	329	ALA	3.4
2	H	186	SER	3.4
2	O	210	HIS	3.4
2	I	386	PHE	3.4
2	O	49	GLY	3.4
1	A	638	MET	3.4
2	D	233	SER	3.4
2	K	6	SER	3.4
1	A	380	LYS	3.4
2	L	280	ILE	3.3
1	B	185	ASP	3.3
2	C	59	TRP	3.3
1	A	559	ALA	3.3
1	A	758	ALA	3.3
2	D	272	THR	3.3
2	I	209	GLU	3.3
2	O	105	GLN	3.3
1	A	430	ALA	3.3
2	G	256	PRO	3.3
2	K	385	VAL	3.3
2	K	396	VAL	3.3
1	A	330	ARG	3.3
2	M	326	ILE	3.3
1	B	574	GLU	3.3
2	I	315	GLU	3.3
1	A	324	SER	3.3
2	I	364	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	570	THR	3.3
1	A	281	ASP	3.3
2	E	120	SER	3.3
2	C	315	GLU	3.3
1	A	780	ALA	3.3
2	E	333	SER	3.3
2	D	128	ASN	3.3
2	N	121	GLY	3.3
2	O	67	GLY	3.3
2	G	340	GLU	3.3
2	M	146	GLN	3.3
1	A	671	LEU	3.2
2	K	191	ALA	3.2
2	N	109	ILE	3.2
2	M	261	VAL	3.2
2	D	312	GLN	3.2
2	F	129	PHE	3.2
2	L	18	ILE	3.2
2	G	375	SER	3.2
2	K	251	PRO	3.2
2	M	186	SER	3.2
2	C	128	ASN	3.2
2	L	278	GLY	3.2
2	I	222	THR	3.2
2	I	319	THR	3.2
1	A	276	GLU	3.2
1	A	329	ALA	3.2
2	F	55	PRO	3.2
2	J	247	TRP	3.2
2	D	194	ASP	3.2
2	I	67	GLY	3.2
2	M	272	THR	3.2
2	O	258	ASN	3.2
2	M	234	PHE	3.2
2	M	263	PHE	3.2
2	J	102	ARG	3.2
2	C	132	SER	3.2
2	I	101	VAL	3.2
2	J	291	SER	3.2
2	E	254	LEU	3.2
1	A	366	PHE	3.2
1	B	753	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	271	ASN	3.2
2	L	151	THR	3.2
2	O	152	PHE	3.2
2	I	102	ARG	3.2
2	J	147	ARG	3.2
2	M	132	SER	3.2
2	F	362	PRO	3.2
2	E	257	ASN	3.2
2	G	236	ARG	3.2
1	A	620	ASP	3.2
2	D	184	ALA	3.2
2	E	334	VAL	3.2
2	F	233	SER	3.2
2	O	234	PHE	3.1
2	C	15	ARG	3.1
2	E	59	TRP	3.1
1	A	659	ASP	3.1
2	C	282	ALA	3.1
2	H	3	VAL	3.1
2	M	98	ASP	3.1
2	M	226	LEU	3.1
2	M	68	THR	3.1
2	M	222	THR	3.1
1	A	477	ASN	3.1
2	G	96	CYS	3.1
2	M	110	ALA	3.1
2	O	3	VAL	3.1
2	G	174	ASP	3.1
2	M	93	ASP	3.1
2	G	263	PHE	3.1
2	M	190	VAL	3.1
1	A	315	GLU	3.1
2	I	117	ARG	3.1
2	J	117	ARG	3.1
2	I	121	GLY	3.1
2	G	237	VAL	3.1
2	K	250	ASN	3.1
2	L	261	VAL	3.1
2	N	101	VAL	3.1
2	J	326	ILE	3.1
2	D	102	ARG	3.1
2	H	90	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	100	MET	3.1
1	B	512	GLN	3.1
1	A	528	SER	3.1
2	I	104	SER	3.1
2	J	140	ASN	3.1
2	N	336	ALA	3.1
2	D	327	GLU	3.1
2	G	46	PHE	3.1
2	M	150	PHE	3.1
2	E	2	ASP	3.1
2	H	395	LEU	3.1
2	I	93	ASP	3.1
2	E	197	CYS	3.1
2	L	387	THR	3.1
2	D	110	ALA	3.0
2	C	93	ASP	3.0
2	L	358	GLY	3.0
2	J	274	GLN	3.0
2	M	316	HIS	3.0
2	H	15	ARG	3.0
2	G	111	PRO	3.0
2	E	93	ASP	3.0
2	M	194	ASP	3.0
2	I	69	THR	3.0
2	M	163	SER	3.0
2	C	241	ALA	3.0
2	K	198	ALA	3.0
2	I	289	ARG	3.0
1	B	227	GLU	3.0
2	C	209	GLU	3.0
2	L	260	GLU	3.0
2	N	99	GLU	3.0
2	J	211	ILE	3.0
1	A	377	ASP	3.0
2	E	32	GLN	3.0
2	G	186	SER	3.0
1	A	590	ASN	3.0
2	M	183	ASN	3.0
2	N	128	ASN	3.0
2	I	187	GLU	3.0
2	F	256	PRO	3.0
2	K	313	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	N	227	PRO	3.0
1	A	365	GLN	3.0
2	L	186	SER	3.0
2	L	335	LEU	3.0
1	B	656	ARG	3.0
2	M	318	ALA	3.0
2	G	59	TRP	3.0
1	A	121	LYS	3.0
1	A	775	ILE	3.0
2	K	18	ILE	3.0
1	A	829	VAL	3.0
1	A	859	SER	3.0
2	L	224	THR	3.0
2	J	255	ARG	3.0
1	B	417	ASP	3.0
2	O	380	ASP	3.0
2	E	58	ASN	2.9
1	B	658	PRO	2.9
2	H	376	PRO	2.9
2	F	197	CYS	2.9
2	I	133	SER	2.9
2	J	146	GLN	2.9
2	J	259	VAL	2.9
2	G	98	ASP	2.9
2	K	86	ASP	2.9
1	A	325	ASN	2.9
2	F	53	ASN	2.9
2	C	202	PRO	2.9
2	G	214	LEU	2.9
2	N	234	PHE	2.9
1	B	316	SER	2.9
2	H	305	ALA	2.9
1	A	327	ILE	2.9
2	I	16	ASP	2.9
2	D	103	GLU	2.9
2	E	230	GLU	2.9
2	H	187	GLU	2.9
2	M	131	ASN	2.9
2	I	132	SER	2.9
2	O	102	ARG	2.9
2	D	62	ASP	2.9
2	F	361	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	316	HIS	2.9
2	L	55	PRO	2.9
2	L	58	ASN	2.9
2	L	102	ARG	2.9
2	M	15	ARG	2.9
2	G	50	GLY	2.9
2	N	330	VAL	2.9
2	O	244	ALA	2.9
2	M	187	GLU	2.9
2	O	106	ARG	2.9
2	H	189	GLN	2.9
2	G	247	TRP	2.9
2	N	219	THR	2.9
1	B	591	ALA	2.9
2	O	51	ILE	2.9
2	L	145	ARG	2.9
1	A	722	ASN	2.9
1	B	312	ASP	2.8
2	G	228	ASP	2.8
2	H	230	GLU	2.9
2	J	330	VAL	2.8
2	H	69	THR	2.8
2	J	275	ALA	2.8
2	H	386	PHE	2.8
1	A	673	PRO	2.8
2	E	155	PRO	2.8
2	L	103	GLU	2.8
1	B	731	GLN	2.8
2	H	51	ILE	2.8
2	H	121	GLY	2.8
2	I	105	GLN	2.8
2	K	206	GLN	2.8
2	M	218	LEU	2.8
2	D	216	ARG	2.8
2	E	258	ASN	2.8
2	F	396	VAL	2.8
2	L	175	ASN	2.8
2	J	52	GLY	2.8
2	L	277	PHE	2.8
2	N	97	MET	2.8
2	D	215	ARG	2.8
2	J	57	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	488	VAL	2.8
2	G	161	SER	2.8
2	E	60	ASN	2.8
2	I	134	GLU	2.8
2	I	137	GLU	2.8
2	G	151	THR	2.8
2	D	380	ASP	2.8
2	D	261	VAL	2.8
2	K	55	PRO	2.8
2	E	262	GLU	2.8
2	G	60	ASN	2.8
2	G	222	THR	2.8
2	G	12	LYS	2.8
2	M	215	ARG	2.8
2	M	350	ARG	2.8
1	A	759	LEU	2.8
2	E	294	LEU	2.8
2	J	334	VAL	2.8
2	K	186	SER	2.8
2	C	24	TYR	2.8
2	D	60	ASN	2.8
2	D	284	ASN	2.8
2	E	128	ASN	2.8
2	F	134	GLU	2.8
2	M	379	GLU	2.8
2	G	68	THR	2.8
2	G	324	LEU	2.7
2	H	393	SER	2.7
1	A	156	PRO	2.7
2	C	123	LYS	2.7
2	J	262	GLU	2.7
2	O	332	GLU	2.7
2	C	117	ARG	2.7
2	C	296	ARG	2.7
2	L	290	LEU	2.7
2	D	211	ILE	2.7
2	G	74	ASP	2.7
1	B	388	SER	2.7
1	B	561	VAL	2.7
2	E	163	SER	2.7
2	L	390	SER	2.7
2	K	376	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	389	ALA	2.7
2	F	323	THR	2.7
2	I	182	LEU	2.7
1	A	760	VAL	2.7
2	C	334	VAL	2.7
2	E	295	MET	2.7
2	K	93	ASP	2.7
2	I	208	PHE	2.7
2	G	185	GLY	2.7
2	G	322	LEU	2.7
2	E	133	SER	2.7
2	D	130	ASP	2.7
2	K	98	ASP	2.7
1	A	145	ARG	2.7
1	A	376	ASN	2.7
2	D	156	ASN	2.7
2	I	118	LYS	2.7
1	B	739	MET	2.7
1	A	568	VAL	2.7
2	F	335	LEU	2.7
2	I	59	TRP	2.7
1	A	708	ARG	2.7
2	F	15	ARG	2.7
2	J	86	ASP	2.7
2	J	289	ARG	2.7
1	B	655	ALA	2.7
2	C	136	ILE	2.7
2	I	56	ILE	2.7
2	M	112	GLN	2.7
2	H	80	THR	2.7
2	K	138	ASN	2.7
2	M	271	ASN	2.7
2	F	161	SER	2.7
2	G	225	LEU	2.7
2	J	190	VAL	2.6
2	H	227	PRO	2.6
1	A	369	GLY	2.6
2	F	149	GLY	2.6
2	G	114	ASP	2.6
2	M	16	ASP	2.6
2	M	140	ASN	2.6
2	F	132	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	350	ARG	2.6
2	M	276	ARG	2.6
1	B	407	GLY	2.6
2	K	224	THR	2.6
1	B	418	MET	2.6
2	N	92	VAL	2.6
1	B	875	ARG	2.6
2	D	15	ARG	2.6
2	E	87	TYR	2.6
2	F	368	THR	2.6
2	M	295	MET	2.6
2	O	151	THR	2.6
2	E	150	PHE	2.6
2	I	332	GLU	2.6
1	A	523	VAL	2.6
1	A	703	VAL	2.6
2	J	157	ILE	2.6
2	L	320	VAL	2.6
2	M	325	ARG	2.6
2	F	318	ALA	2.6
2	J	189	GLN	2.6
2	G	100	MET	2.6
2	H	324	LEU	2.6
2	J	24	TYR	2.6
2	F	369	ASP	2.6
2	K	315	GLU	2.6
2	C	107	ASN	2.6
2	C	200	ASN	2.6
2	G	373	ASN	2.6
2	D	334	VAL	2.6
2	J	384	ARG	2.6
2	O	231	ARG	2.6
1	A	305	GLN	2.6
2	G	206	GLN	2.6
2	I	177	MET	2.6
2	L	189	GLN	2.6
2	K	88	PHE	2.6
2	I	287	THR	2.6
1	A	159	ASP	2.6
2	F	62	ASP	2.6
2	G	102	ARG	2.6
2	G	217	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	216	ARG	2.6
2	M	212	VAL	2.6
2	G	251	PRO	2.6
2	E	178	GLY	2.6
2	F	358	GLY	2.6
2	G	249	PHE	2.6
2	E	331	CYS	2.5
2	I	331	CYS	2.5
2	J	253	ILE	2.5
2	O	109	ILE	2.5
2	E	209	GLU	2.5
2	E	315	GLU	2.5
2	H	283	ARG	2.5
2	O	99	GLU	2.5
2	H	86	ASP	2.5
2	I	183	ASN	2.5
2	K	380	ASP	2.5
2	L	250	ASN	2.5
2	M	128	ASN	2.5
1	B	98	PHE	2.5
2	D	285	PHE	2.5
2	I	293	GLN	2.5
1	A	562	THR	2.5
2	J	272	THR	2.5
2	C	273	TYR	2.5
2	O	397	LYS	2.5
2	C	233	SER	2.5
2	F	215	ARG	2.5
2	H	25	SER	2.5
2	K	233	SER	2.5
1	A	782	VAL	2.5
2	K	330	VAL	2.5
2	J	322	LEU	2.5
2	H	394	MET	2.5
1	A	415	PRO	2.5
2	J	50	GLY	2.5
2	E	15	ARG	2.5
2	H	296	ARG	2.5
1	A	350	SER	2.5
2	F	196	SER	2.5
2	I	374	TYR	2.5
2	K	113	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	O	160	TYR	2.5
2	F	177	MET	2.5
2	M	394	MET	2.5
2	D	58	ASN	2.5
2	O	107	ASN	2.5
2	I	235	PRO	2.5
2	D	288	ILE	2.5
2	M	321	GLY	2.5
2	E	222	THR	2.5
2	I	82	ARG	2.5
2	I	135	TYR	2.5
1	A	654	VAL	2.5
2	H	346	VAL	2.5
2	C	260	GLU	2.5
2	H	20	GLU	2.5
1	A	302	ASN	2.5
2	D	131	ASN	2.5
2	I	128	ASN	2.5
2	M	152	PHE	2.5
2	N	150	PHE	2.5
2	K	326	ILE	2.5
2	F	67	GLY	2.5
1	B	300	ARG	2.5
2	D	89	VAL	2.5
2	D	295	MET	2.5
2	G	180	MET	2.5
2	M	320	VAL	2.5
2	G	91	PHE	2.5
1	A	658	PRO	2.5
1	B	865	PRO	2.5
2	G	359	PRO	2.5
2	J	362	PRO	2.5
2	J	122	LEU	2.5
2	K	225	LEU	2.5
2	O	331	CYS	2.5
1	B	398	THR	2.5
1	B	593	VAL	2.5
2	D	385	VAL	2.5
2	G	334	VAL	2.5
2	F	158	PHE	2.4
1	B	530	GLN	2.4
2	O	122	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	255	ARG	2.4
2	E	380	ASP	2.4
2	O	86	ASP	2.4
2	E	205	THR	2.4
2	E	103	GLU	2.4
1	A	155	LEU	2.4
1	A	527	ARG	2.4
2	C	146	GLN	2.4
2	D	231	ARG	2.4
2	M	284	ASN	2.4
2	K	64	GLY	2.4
2	E	279	THR	2.4
2	H	220	THR	2.4
1	B	654	VAL	2.4
2	E	234	PHE	2.4
2	H	124	PHE	2.4
2	I	249	PHE	2.4
2	K	374	TYR	2.4
2	N	122	LEU	2.4
1	B	385	ALA	2.4
2	K	221	ALA	2.4
2	C	118	LYS	2.4
2	J	279	THR	2.4
2	M	323	THR	2.4
2	D	360	VAL	2.4
2	F	234	PHE	2.4
2	C	379	GLU	2.4
2	G	317	HIS	2.4
2	H	202	PRO	2.4
2	J	159	PRO	2.4
2	J	297	PRO	2.4
2	E	341	THR	2.4
2	F	259	VAL	2.4
2	L	152	PHE	2.4
1	B	659	ASP	2.4
1	A	326	TYR	2.4
2	M	374	TYR	2.4
1	A	591	ALA	2.4
2	D	162	ALA	2.4
2	G	336	ALA	2.4
1	B	399	THR	2.4
2	I	335	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	371	ILE	2.4
2	L	222	THR	2.4
2	H	119	LEU	2.4
2	E	215	ARG	2.4
2	L	86	ASP	2.4
1	A	555	GLU	2.4
1	A	831	GLN	2.3
2	D	129	PHE	2.3
2	E	181	TRP	2.3
2	E	183	ASN	2.3
2	H	387	THR	2.3
2	J	276	ARG	2.3
2	G	97	MET	2.3
2	H	24	TYR	2.3
2	E	134	GLU	2.3
2	G	207	GLN	2.3
2	K	209	GLU	2.3
1	B	612	SER	2.3
2	C	72	ASN	2.3
2	D	149	GLY	2.3
2	H	192	GLY	2.3
2	I	108	GLY	2.3
2	M	182	LEU	2.3
2	I	300	MET	2.3
2	N	87	TYR	2.3
2	K	90	ASP	2.3
2	K	213	GLN	2.3
2	L	105	GLN	2.3
2	C	109	ILE	2.3
2	H	61	PHE	2.3
2	M	395	LEU	2.3
2	O	292	PHE	2.3
1	A	761	GLY	2.3
2	C	291	SER	2.3
2	D	278	GLY	2.3
2	K	364	GLY	2.3
2	O	52	GLY	2.3
2	G	204	ASN	2.3
2	L	357	VAL	2.3
2	K	397	LYS	2.3
2	O	117	ARG	2.3
2	C	221	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	711	GLN	2.3
2	D	214	LEU	2.3
2	E	193	PHE	2.3
2	F	351	GLN	2.3
2	G	281	ILE	2.3
2	J	47	GLN	2.3
2	M	134	GLU	2.3
2	N	20	GLU	2.3
2	O	174	ASP	2.3
2	F	359	PRO	2.3
2	N	52	GLY	2.3
2	J	53	ASN	2.3
2	J	15	ARG	2.3
2	K	365	MET	2.3
2	M	100	MET	2.3
2	N	127	ILE	2.3
2	L	312	GLN	2.3
1	B	243	SER	2.3
1	B	690	ASP	2.3
1	B	501	HIS	2.3
2	E	68	THR	2.3
2	K	289	ARG	2.3
2	L	183	ASN	2.3
2	C	152	PHE	2.3
2	E	187	GLU	2.3
2	G	390	SER	2.3
1	A	199	VAL	2.3
2	I	278	GLY	2.3
2	M	155	PRO	2.3
1	B	395	ASP	2.3
2	C	242	ASP	2.3
2	D	255	ARG	2.3
2	N	380	ASP	2.3
1	B	371	ASN	2.2
2	C	61	PHE	2.2
2	E	253	ILE	2.2
2	L	234	PHE	2.2
2	D	191	ALA	2.2
2	K	282	ALA	2.2
2	K	383	GLN	2.2
1	A	112	LYS	2.2
1	B	804	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	118	LYS	2.2
2	D	21	GLY	2.2
2	F	49	GLY	2.2
2	J	55	PRO	2.2
2	K	276	ARG	2.2
2	H	2	ASP	2.2
2	M	246	THR	2.2
2	C	386	PHE	2.2
1	B	575	LYS	2.2
1	B	696	SER	2.2
2	L	291	SER	2.2
2	M	24	TYR	2.2
1	B	315	GLU	2.2
2	D	325	ARG	2.2
2	G	57	ARG	2.2
2	K	327	GLU	2.2
2	F	343	LEU	2.2
2	L	313	PRO	2.2
1	A	823	THR	2.2
2	C	205	THR	2.2
1	B	302	ASN	2.2
2	F	93	ASP	2.2
2	H	249	PHE	2.2
2	J	98	ASP	2.2
2	L	310	ASN	2.2
2	M	391	ILE	2.2
2	G	277	PHE	2.2
1	A	501	HIS	2.2
2	D	311	ALA	2.2
2	E	318	ALA	2.2
2	H	110	ALA	2.2
1	B	815	TYR	2.2
2	G	196	SER	2.2
2	M	377	SER	2.2
2	E	52	GLY	2.2
2	F	288	ILE	2.2
2	G	84	THR	2.2
2	G	361	PHE	2.2
2	H	232	PHE	2.2
2	I	228	ASP	2.2
2	K	210	HIS	2.2
2	F	214	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	328	SER	2.2
2	F	352	GLU	2.2
2	H	359	PRO	2.2
2	J	223	ILE	2.2
2	F	22	THR	2.2
2	H	46	PHE	2.2
2	L	258	ASN	2.2
1	A	228	MET	2.2
2	K	393	SER	2.2
2	L	6	SER	2.2
1	A	674	VAL	2.2
2	C	211	ILE	2.2
1	B	216	GLU	2.2
2	I	158	PHE	2.2
2	J	298	PRO	2.2
2	M	164	PHE	2.2
1	A	822	THR	2.2
2	F	341	THR	2.2
2	M	191	ALA	2.1
2	H	236	ARG	2.1
2	I	169	SER	2.1
2	J	186	SER	2.1
2	D	374	TYR	2.1
2	G	223	ILE	2.1
2	G	280	ILE	2.1
2	M	109	ILE	2.1
1	A	797	PRO	2.1
2	M	64	GLY	2.1
2	G	209	GLU	2.1
2	N	125	LYS	2.1
1	A	391	THR	2.1
2	K	323	THR	2.1
2	E	126	ARG	2.1
2	G	378	ARG	2.1
2	E	186	SER	2.1
2	D	317	HIS	2.1
2	E	351	GLN	2.1
2	E	92	VAL	2.1
2	L	197	CYS	2.1
2	D	273	TYR	2.1
2	N	386	PHE	2.1
2	D	192	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	103	GLU	2.1
2	K	332	GLU	2.1
2	N	356	PRO	2.1
2	D	22	THR	2.1
2	K	179	THR	2.1
1	A	229	ARG	2.1
2	F	131	ASN	2.1
2	G	384	ARG	2.1
2	I	344	ALA	2.1
2	J	138	ASN	2.1
2	L	275	ALA	2.1
2	M	329	ALA	2.1
2	N	107	ASN	2.1
2	L	133	SER	2.1
1	A	704	ILE	2.1
2	L	19	VAL	2.1
1	A	289	ASP	2.1
2	C	135	TYR	2.1
2	F	135	TYR	2.1
2	M	247	TRP	2.1
2	I	21	GLY	2.1
2	N	321	GLY	2.1
2	O	111	PRO	2.1
2	C	134	GLU	2.1
2	C	148	THR	2.1
2	N	69	THR	2.1
2	H	384	ARG	2.1
2	G	229	ALA	2.1
2	G	275	ALA	2.1
2	F	366	ASN	2.1
2	I	233	SER	2.1
2	N	355	ILE	2.1
2	C	47	GLN	2.1
2	C	207	GLN	2.1
2	E	263	PHE	2.1
2	J	361	PHE	2.1
2	N	346	VAL	2.1
2	L	316	HIS	2.1
1	B	387	LEU	2.1
2	D	228	ASP	2.1
2	H	135	TYR	2.1
2	K	182	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	352	GLU	2.1
2	M	69	THR	2.1
2	N	230	GLU	2.1
2	O	103	GLU	2.1
2	C	355	ILE	2.1
2	C	154	LYS	2.1
1	A	467	GLN	2.1
2	F	128	ASN	2.1
2	I	207	GLN	2.1
2	L	314	PHE	2.1
2	M	92	VAL	2.1
2	L	73	LEU	2.1
2	J	21	GLY	2.1
2	O	87	TYR	2.1
2	G	194	ASP	2.1
2	J	380	ASP	2.1
2	D	341	THR	2.1
2	F	372	THR	2.1
1	B	733	ILE	2.1
2	N	197	CYS	2.1
2	M	161	SER	2.1
2	N	333	SER	2.1
2	G	292	PHE	2.1
2	G	72	ASN	2.1
2	H	342	MET	2.1
1	B	97	THR	2.0
2	N	84	THR	2.0
2	O	82	ARG	2.0
1	A	641	ILE	2.0
2	I	391	ILE	2.0
2	L	389	ALA	2.0
2	F	52	GLY	2.0
2	J	67	GLY	2.0
2	G	160	TYR	2.0
2	G	356	PRO	2.0
2	H	171	PRO	2.0
1	A	153	ASP	2.0
1	B	853	ASP	2.0
2	D	93	ASP	2.0
2	L	13	ASP	2.0
2	N	86	ASP	2.0
2	O	2	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	132	SER	2.0
2	H	390	SER	2.0
2	J	234	PHE	2.0
2	L	292	PHE	2.0
2	N	217	VAL	2.0
2	K	310	ASN	2.0
2	O	72	ASN	2.0
2	O	310	ASN	2.0
2	D	321	GLY	2.0
2	E	223	ILE	2.0
2	M	147	ARG	2.0
2	O	147	ARG	2.0
2	N	205	THR	2.0
1	A	123	PHE	2.0
2	E	327	GLU	2.0
2	L	187	GLU	2.0
2	M	46	PHE	2.0
2	M	294	LEU	2.0
2	I	291	SER	2.0
2	N	113	SER	2.0
2	E	3	VAL	2.0
2	N	320	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	O	398	1/1	0.70	0.27	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	I	398	1/1	0.97	0.12	51,51,51,51	0
3	ZN	F	398	1/1	0.98	0.09	51,51,51,51	0
3	ZN	L	398	1/1	0.99	0.10	51,51,51,51	0
3	ZN	C	398	1/1	0.99	0.08	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.