



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 12:16 PM EDT

PDB ID : 1V7N
Title : Human Thrombopoietin Functional Domain Complexed To Neutralizing Antibody TN1 Fab
Authors : Feese, M.D.; Tamada, T.; Kato, Y.; Maeda, Y.; Hirose, M.; Matsukura, Y.; Shigematsu, H.; Kato, T.; Miyazaki, H.; Kuroki, R.
Deposited on : 2003-12-18
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

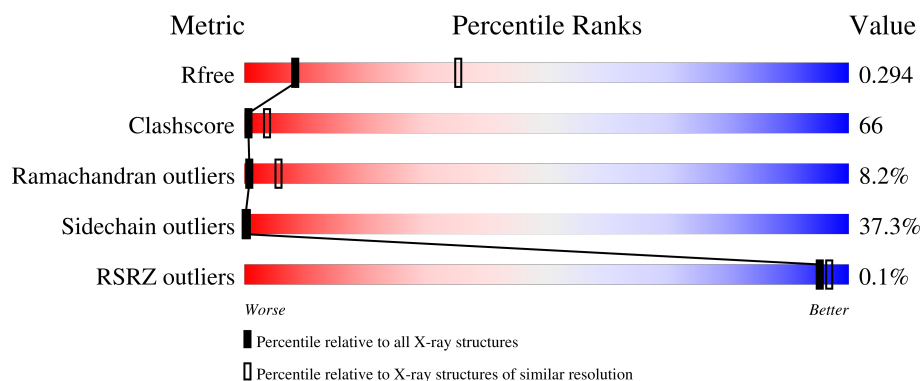
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

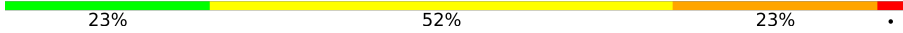

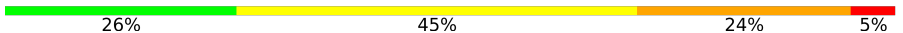

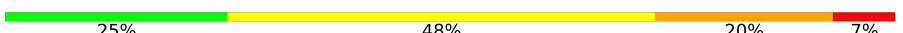
The reported resolution of this entry is 3.30 Å.

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	L	213	
1	M	213	
1	N	213	
1	O	213	
2	H	217	

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Mol	Chain	Length	Quality of chain
2	I	217	<div><div></div><div>26%41%31%. .</div></div>
2	J	217	<div><div></div><div>19%45%30%6%</div></div>
2	K	217	<div><div></div><div>19%50%29%. .</div></div>
3	V	163	<div><div></div><div>%15%40%31%. 11%</div></div>
3	X	163	<div><div></div><div>15%40%23%7%15%</div></div>
3	Y	163	<div><div></div><div>15%39%26%5%15%</div></div>
3	Z	163	<div><div></div><div>15%40%27%. 15%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17466 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 Monoclonal TN1 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1638	1018	278	333	9			
1	M	212	Total	C	N	O	S	0	0	0
			1632	1015	277	332	8			
1	N	212	Total	C	N	O	S	0	0	0
			1632	1015	277	332	8			
1	O	213	Total	C	N	O	S	0	0	0
			1638	1018	278	333	9			

- Molecule 2 is a protein called Monoclonal TN1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1630	1030	271	321	8			
2	I	217	Total	C	N	O	S	0	0	0
			1630	1030	271	321	8			
2	J	217	Total	C	N	O	S	0	0	0
			1630	1030	271	321	8			
2	K	217	Total	C	N	O	S	0	0	0
			1630	1030	271	321	8			

- Molecule 3 is a protein called Thrombopoietin.

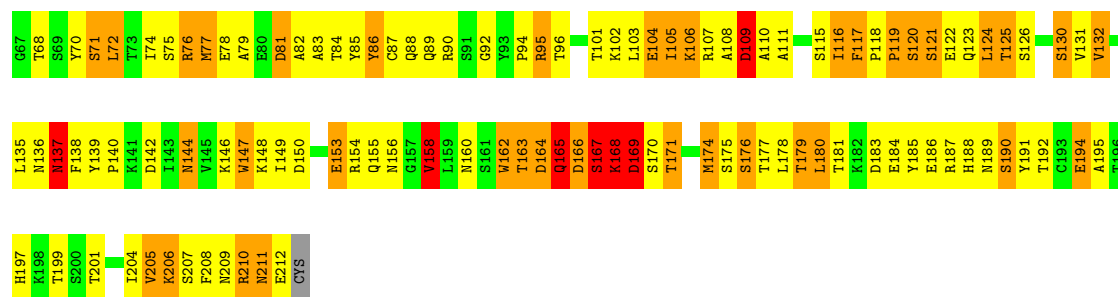
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	145	Total	C	N	O	S	0	0	0
			1090	694	194	195	7			
3	X	138	Total	C	N	O	S	0	0	0
			1049	671	187	186	5			
3	Y	139	Total	C	N	O	S	0	0	0
			1053	673	188	187	5			
3	Z	138	Total	C	N	O	S	0	0	0
			1045	669	187	184	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	115	ARG	GLN	engineered mutation	UNP P40225
X	115	ARG	GLN	engineered mutation	UNP P40225
Y	115	ARG	GLN	engineered mutation	UNP P40225
Z	115	ARG	GLN	engineered mutation	UNP P40225

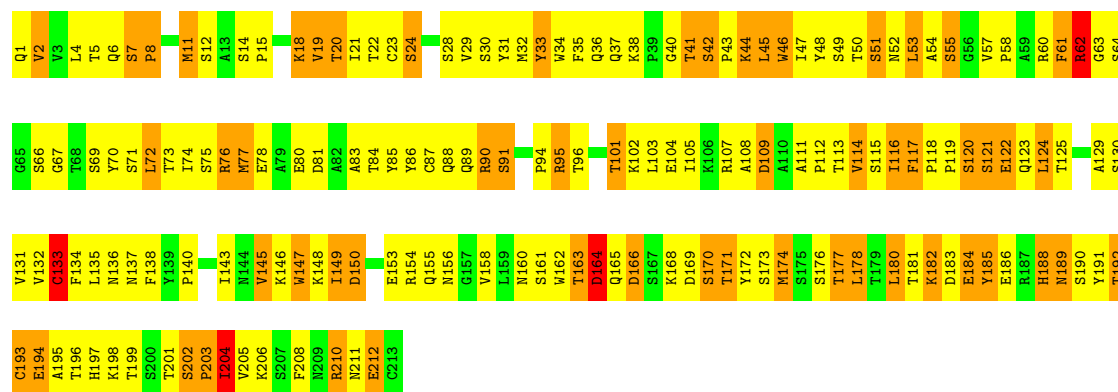
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	20	Total O 20 20	0	0
4	H	17	Total O 17 17	0	0
4	M	18	Total O 18 18	0	0
4	I	27	Total O 27 27	0	0
4	N	19	Total O 19 19	0	0
4	J	13	Total O 13 13	0	0
4	O	20	Total O 20 20	0	0
4	K	10	Total O 10 10	0	0
4	V	7	Total O 7 7	0	0
4	X	11	Total O 11 11	0	0
4	Y	3	Total O 3 3	0	0
4	Z	4	Total O 4 4	0	0



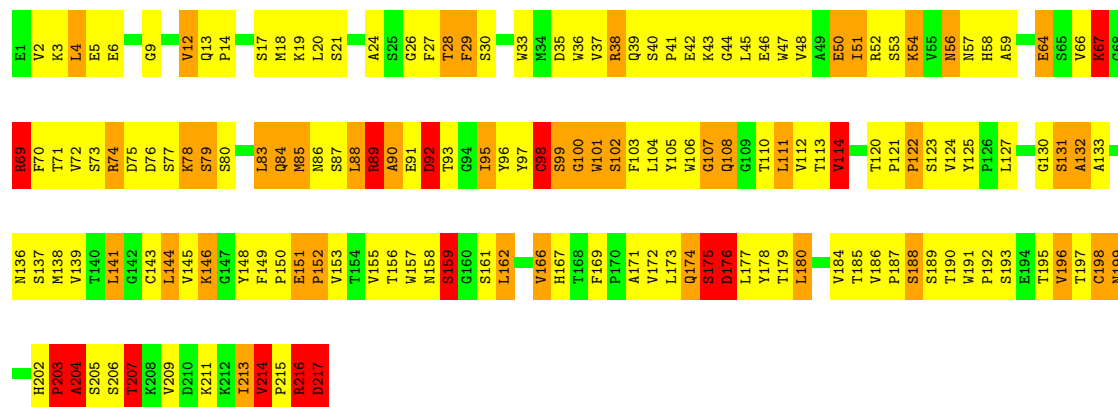
• Molecule 1: Monoclonal TN1 Fab Light Chain

Chain O: 20% 51% 27%



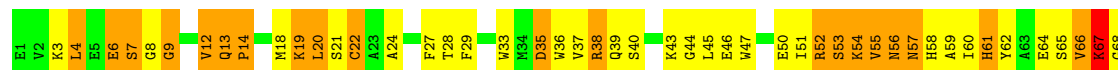
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

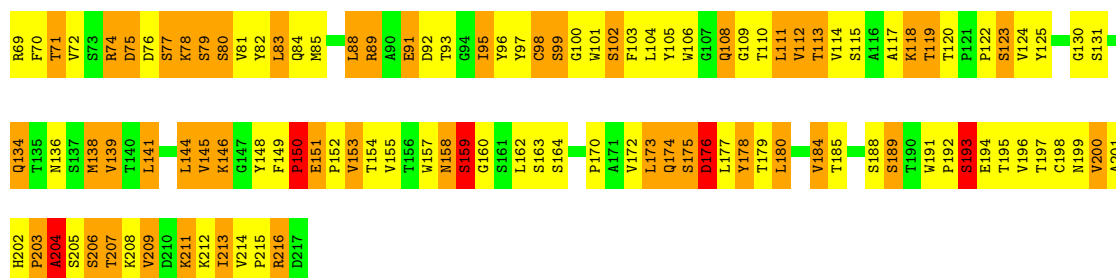
Chain H: 25% 48% 20% 7%



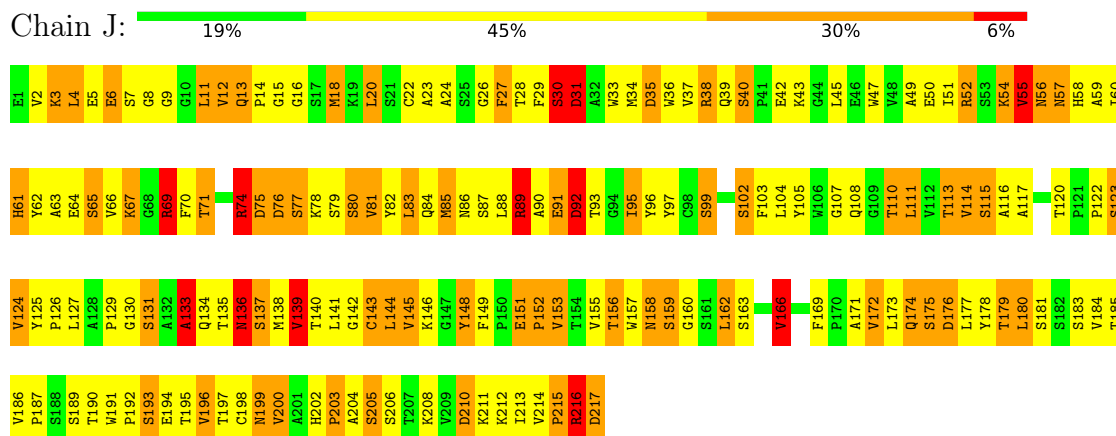
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain I: 26% 41% 31%

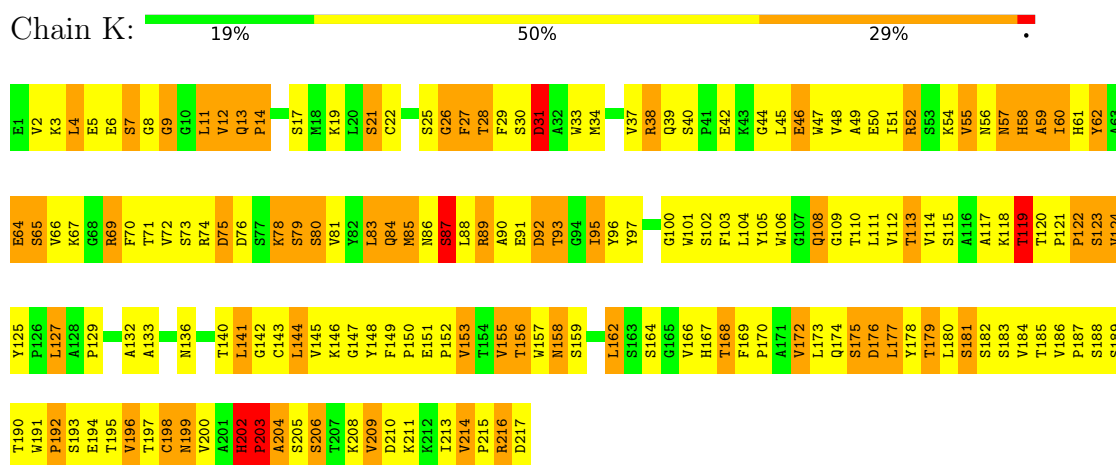




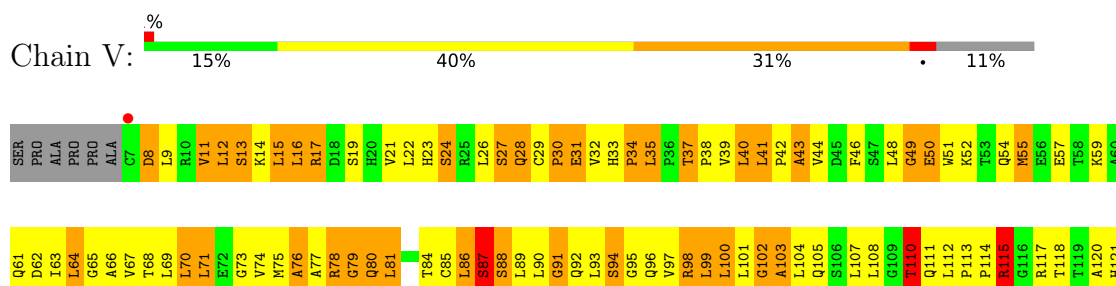
• Molecule 2: Monoclonal TN1 Fab Heavy Chain



• Molecule 2: Monoclonal TN1 Fab Heavy Chain

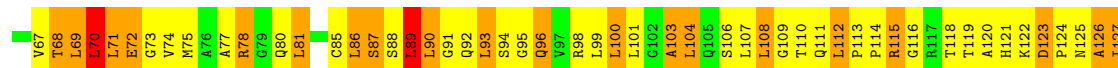


• Molecule 3: Thrombopoietin

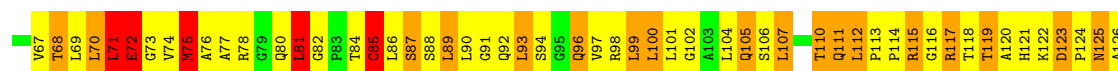
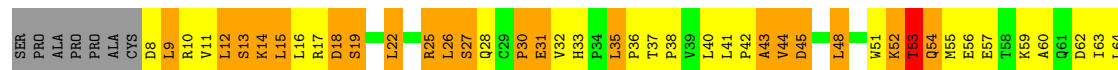




• Molecule 3: Thrombopoietin



• Molecule 3: Thrombopoietin



• Molecule 3: Thrombopoietin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.04Å 46.58Å 191.36Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	57.63 – 3.30 57.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (57.63-3.30) 98.4 (57.63-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.167 , 0.305 0.162 , 0.294	Depositor DCC
R_{free} test set	1801 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17466	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	1.31	7/1676 (0.4%)	1.35	11/2274 (0.5%)
1	M	1.33	3/1670 (0.2%)	1.42	13/2266 (0.6%)
1	N	1.28	3/1670 (0.2%)	1.39	12/2266 (0.5%)
1	O	1.26	4/1676 (0.2%)	1.39	11/2274 (0.5%)
2	H	1.37	10/1674 (0.6%)	1.40	17/2289 (0.7%)
2	I	1.23	3/1674 (0.2%)	1.39	9/2289 (0.4%)
2	J	1.25	1/1674 (0.1%)	1.45	20/2289 (0.9%)
2	K	1.21	2/1674 (0.1%)	1.40	14/2289 (0.6%)
3	V	1.23	3/1109 (0.3%)	1.38	5/1506 (0.3%)
3	X	1.14	1/1068 (0.1%)	1.37	13/1451 (0.9%)
3	Y	1.24	2/1072 (0.2%)	1.48	15/1456 (1.0%)
3	Z	1.13	2/1064 (0.2%)	1.26	6/1445 (0.4%)
All	All	1.26	41/17701 (0.2%)	1.39	146/24094 (0.6%)

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	M	0	2
1	N	0	2
2	H	0	2
2	I	0	5
2	J	0	3
2	K	0	2
3	X	0	1
3	Y	0	1
3	Z	0	2
All	All	0	20

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	139	TYR	CB-CG	-11.08	1.35	1.51
2	H	151	GLU	CD-OE2	8.63	1.35	1.25
1	L	48	TYR	CD2-CE2	-7.57	1.27	1.39
2	J	143	CYS	CB-SG	-7.46	1.69	1.82
2	H	98	CYS	CB-SG	-7.02	1.70	1.82
1	M	59	ALA	CA-CB	-6.58	1.38	1.52
1	L	139	TYR	CD2-CE2	-6.48	1.29	1.39
1	L	139	TYR	CD1-CE1	-6.15	1.30	1.39
2	H	97	TYR	CD1-CE1	-6.08	1.30	1.39
3	Y	75	MET	SD-CE	5.87	2.10	1.77
1	O	62	ARG	CB-CG	-5.87	1.36	1.52
2	K	62	TYR	CE1-CZ	-5.85	1.30	1.38
2	I	209	VAL	CA-CB	5.82	1.67	1.54
1	O	34	TRP	CB-CG	-5.68	1.40	1.50
1	N	46	TRP	CB-CG	-5.64	1.40	1.50
2	H	97	TYR	CD2-CE2	-5.63	1.30	1.39
2	K	168	THR	CA-CB	-5.57	1.38	1.53
3	Z	45	ASP	CB-CG	5.55	1.63	1.51
2	H	143	CYS	CB-SG	-5.55	1.72	1.81
1	L	62	ARG	CG-CD	5.53	1.65	1.51
1	N	147	TRP	CB-CG	-5.49	1.40	1.50
1	O	11	MET	SD-CE	5.48	2.08	1.77
1	L	162	TRP	CB-CG	-5.47	1.40	1.50
1	M	86	TYR	CE1-CZ	-5.45	1.31	1.38
3	V	21	VAL	CA-CB	-5.43	1.43	1.54
2	H	5	GLU	CD-OE1	5.43	1.31	1.25
2	H	5	GLU	CG-CD	5.36	1.59	1.51
2	H	214	VAL	CA-CB	-5.25	1.43	1.54
3	X	128	PHE	CE2-CZ	5.23	1.47	1.37
2	H	151	GLU	CD-OE1	5.22	1.31	1.25
1	N	31	TYR	CD2-CE2	-5.21	1.31	1.39
3	V	110	THR	CA-CB	-5.20	1.39	1.53
2	H	97	TYR	CB-CG	-5.14	1.44	1.51
2	I	108	GLN	CG-CD	5.14	1.62	1.51
3	Y	72	GLU	CD-OE1	5.14	1.31	1.25
3	V	141	PHE	CB-CG	5.13	1.60	1.51
1	M	184	GLU	CD-OE2	5.08	1.31	1.25
2	I	54	LYS	CD-CE	5.07	1.64	1.51
1	O	147	TRP	CB-CG	-5.04	1.41	1.50
1	L	48	TYR	CD1-CE1	-5.03	1.31	1.39
3	Z	136	ARG	CG-CD	5.02	1.64	1.51

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	53	LEU	CA-CB-CG	-11.11	89.75	115.30
1	M	169	ASP	CB-CG-OD2	10.62	127.85	118.30
3	X	140	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	N	109	ASP	CB-CG-OD2	9.86	127.17	118.30
1	N	81	ASP	CB-CG-OD2	9.80	127.12	118.30
3	X	45	ASP	CB-CG-OD2	9.74	127.07	118.30
2	H	144	LEU	CA-CB-CG	-9.38	93.72	115.30
2	I	83	LEU	CA-CB-CG	-9.36	93.77	115.30
1	N	8	PRO	N-CD-CG	-8.67	90.19	103.20
2	H	143	CYS	CA-CB-SG	-8.58	98.55	114.00
1	M	81	ASP	CB-CG-OD1	-8.52	110.63	118.30
3	Y	136	ARG	NE-CZ-NH1	8.50	124.55	120.30
2	H	176	ASP	CB-CG-OD2	8.46	125.92	118.30
2	I	203	PRO	N-CD-CG	-8.40	90.59	103.20
2	H	216	ARG	NE-CZ-NH1	8.25	124.43	120.30
2	K	175	SER	N-CA-CB	-8.22	98.17	110.50
3	V	64	LEU	CB-CG-CD2	-8.15	97.15	111.00
1	N	166	ASP	CB-CG-OD2	8.07	125.56	118.30
1	M	142	ASP	CB-CG-OD2	8.06	125.56	118.30
3	Y	71	LEU	CA-CB-CG	-8.06	96.76	115.30
2	J	89	ARG	NE-CZ-NH2	-8.02	116.29	120.30
3	Y	71	LEU	CB-CG-CD1	-7.99	97.42	111.00
1	L	95	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	M	60	ARG	NE-CZ-NH1	-7.91	116.35	120.30
2	K	203	PRO	N-CD-CG	-7.84	91.44	103.20
1	L	205	VAL	CB-CA-C	-7.76	96.66	111.40
1	N	142	ASP	CB-CG-OD2	7.75	125.27	118.30
2	I	176	ASP	CB-CG-OD2	7.64	125.17	118.30
2	J	76	ASP	CB-CG-OD2	7.61	125.15	118.30
1	N	109	ASP	CB-CG-OD1	-7.47	111.57	118.30
3	V	114	PRO	N-CD-CG	-7.45	92.03	103.20
1	M	81	ASP	CB-CG-OD2	7.40	124.96	118.30
1	O	164	ASP	CB-CG-OD2	7.36	124.92	118.30
2	H	162	LEU	CB-CG-CD1	-7.34	98.51	111.00
1	L	81	ASP	CB-CG-OD2	7.23	124.81	118.30
3	Y	136	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	O	109	ASP	CB-CG-OD2	7.03	124.63	118.30
2	J	31	ASP	CB-CG-OD2	6.96	124.56	118.30
3	X	108	LEU	CA-CB-CG	-6.95	99.32	115.30
3	Y	30	PRO	N-CD-CG	-6.90	92.85	103.20
2	K	202	HIS	N-CA-C	-6.88	92.41	111.00
2	K	192	PRO	N-CD-CG	-6.86	92.91	103.20
1	L	95	ARG	NE-CZ-NH2	6.85	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	150	ASP	CB-CG-OD2	6.85	124.46	118.30
2	J	145	VAL	N-CA-C	-6.80	92.62	111.00
2	I	35	ASP	CB-CG-OD2	6.75	124.37	118.30
3	X	104	LEU	CB-CG-CD2	-6.75	99.53	111.00
3	Y	18	ASP	CB-CG-OD2	6.73	124.36	118.30
2	K	76	ASP	CB-CG-OD2	6.66	124.30	118.30
2	J	176	ASP	CB-CG-OD2	6.60	124.24	118.30
2	H	122	PRO	N-CD-CG	-6.49	93.47	103.20
3	X	29	CYS	CA-CB-SG	6.45	125.61	114.00
1	M	150	ASP	CB-CG-OD2	6.39	124.05	118.30
1	O	183	ASP	CB-CG-OD2	6.37	124.03	118.30
2	H	204	ALA	N-CA-C	-6.34	93.88	111.00
3	Z	123	ASP	CB-CG-OD1	6.30	123.97	118.30
1	L	154	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	M	183	ASP	CB-CG-OD1	6.21	123.89	118.30
1	O	150	ASP	CB-CG-OD2	6.19	123.87	118.30
2	K	31	ASP	CB-CG-OD2	6.13	123.81	118.30
1	O	72	LEU	CB-CG-CD1	-6.10	100.62	111.00
2	H	203	PRO	C-N-CA	6.10	136.94	121.70
2	H	76	ASP	CB-CG-OD2	6.06	123.75	118.30
2	J	139	VAL	CB-CA-C	-6.04	99.92	111.40
3	X	123	ASP	CB-CG-OD2	6.03	123.73	118.30
3	Y	75	MET	CG-SD-CE	5.98	109.76	100.20
3	X	48	LEU	CA-CB-CG	5.96	129.02	115.30
2	J	74	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	J	216	ARG	N-CA-C	5.91	126.95	111.00
2	J	143	CYS	CA-CB-SG	-5.88	103.41	114.00
2	H	92	ASP	CB-CG-OD1	5.86	123.57	118.30
2	J	69	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	N	119	PRO	N-CD-CG	-5.80	94.50	103.20
3	Z	104	LEU	CB-CG-CD1	-5.80	101.14	111.00
3	Y	127	ILE	CG1-CB-CG2	-5.75	98.75	111.40
2	K	92	ASP	CB-CG-OD2	5.72	123.45	118.30
3	X	135	LEU	CA-CB-CG	-5.71	102.16	115.30
3	X	18	ASP	CB-CG-OD2	5.69	123.42	118.30
2	K	52	ARG	NE-CZ-NH2	5.66	123.13	120.30
3	Z	45	ASP	CB-CG-OD2	5.65	123.38	118.30
2	J	166	VAL	CB-CA-C	5.64	122.12	111.40
3	V	134	LEU	CB-CG-CD1	-5.64	101.42	111.00
1	L	139	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	M	191	TYR	N-CA-C	-5.61	95.85	111.00
3	X	70	LEU	CA-CB-CG	5.60	128.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	180	LEU	CB-CG-CD1	-5.60	101.48	111.00
2	I	151	GLU	CA-CB-CG	-5.60	101.09	113.40
2	J	91	GLU	N-CA-C	-5.58	95.94	111.00
2	I	44	GLY	N-CA-C	-5.53	99.27	113.10
2	J	89	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	M	118	PRO	N-CD-CG	-5.51	94.94	103.20
1	N	158	VAL	CB-CA-C	-5.50	100.94	111.40
2	J	205	SER	N-CA-C	5.47	125.77	111.00
2	J	92	ASP	CB-CG-OD1	5.46	123.22	118.30
3	X	140	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	H	67	LYS	CD-CE-NZ	5.45	124.23	111.70
3	X	16	LEU	CA-CB-CG	-5.44	102.79	115.30
1	N	169	ASP	CB-CG-OD2	5.43	123.18	118.30
2	K	141	LEU	CA-CB-CG	-5.42	102.84	115.30
2	I	54	LYS	CD-CE-NZ	5.41	124.15	111.70
3	V	144	LEU	CA-CB-CG	5.41	127.75	115.30
3	Z	70	LEU	CB-CG-CD2	5.40	120.17	111.00
1	L	144	ASN	N-CA-C	5.40	125.57	111.00
3	Y	81	LEU	CB-CG-CD2	-5.38	101.86	111.00
2	K	203	PRO	N-CA-C	5.32	125.93	112.10
2	I	89	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	Y	123	ASP	CB-CG-OD2	5.32	123.08	118.30
1	N	45	LEU	CB-CG-CD1	-5.31	101.98	111.00
3	V	115	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	L	53	LEU	CA-CB-CG	-5.30	103.11	115.30
2	K	143	CYS	CA-CB-SG	-5.29	104.48	114.00
2	J	210	ASP	CB-CG-OD2	5.27	123.05	118.30
1	O	8	PRO	N-CD-CG	-5.27	95.30	103.20
2	K	168	THR	CA-CB-CG2	-5.26	105.03	112.40
2	H	114	VAL	CB-CA-C	-5.26	101.40	111.40
1	N	144	ASN	N-CA-C	5.26	125.20	111.00
3	Y	99	LEU	CA-CB-CG	5.26	127.40	115.30
2	J	145	VAL	CB-CA-C	5.26	121.39	111.40
2	J	110	THR	N-CA-CB	5.25	120.28	110.30
3	Y	107	LEU	CA-CB-CG	5.25	127.37	115.30
3	Z	99	LEU	CB-CG-CD2	5.25	119.92	111.00
2	H	89	ARG	CG-CD-NE	5.24	122.81	111.80
3	Z	135	LEU	CA-CB-CG	-5.24	103.25	115.30
1	O	185	TYR	N-CA-C	-5.20	96.97	111.00
1	O	53	LEU	CB-CG-CD1	5.19	119.83	111.00
3	Y	25	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	L	3	VAL	CB-CA-C	5.18	121.24	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	89	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	M	53	LEU	CA-CB-CG	-5.17	103.41	115.30
3	Y	54	GLN	N-CA-C	-5.15	97.10	111.00
2	H	216	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	I	20	LEU	CB-CG-CD1	5.11	119.69	111.00
2	J	18	MET	CG-SD-CE	-5.10	92.03	100.20
2	K	11	LEU	CA-CB-CG	5.10	127.04	115.30
2	H	69	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	K	127	LEU	CB-CG-CD2	-5.08	102.37	111.00
2	H	100	GLY	N-CA-C	5.06	125.75	113.10
1	M	124	LEU	CB-CG-CD2	5.06	119.60	111.00
2	H	217	ASP	CB-CG-OD2	5.05	122.85	118.30
3	Y	136	ARG	CB-CA-C	-5.04	100.33	110.40
1	L	181	THR	OG1-CB-CG2	-5.04	98.42	110.00
1	M	102	LYS	N-CA-C	-5.02	97.45	111.00
1	L	164	ASP	CB-CG-OD2	5.01	122.81	118.30
1	M	204	ILE	N-CA-C	-5.01	97.46	111.00
1	O	101	THR	OG1-CB-CG2	-5.01	98.47	110.00
1	O	133	CYS	CA-CB-SG	-5.01	104.97	114.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	27	PHE	Peptide
2	H	99	SER	Peptide
2	I	138	MET	Peptide
2	I	175	SER	Peptide
2	I	203	PRO	Peptide
2	I	204	ALA	Peptide
2	I	7	SER	Peptide
2	J	115	SER	Peptide
2	J	133	ALA	Peptide
2	J	203	PRO	Peptide
2	K	109	GLY	Peptide
2	K	202	HIS	Peptide
1	M	61	PHE	Peptide
1	M	83	ALA	Peptide
1	N	168	LYS	Peptide
1	N	92	GLY	Peptide
3	X	49	GLY	Peptide
3	Y	53	THR	Peptide

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Mol	Chain	Res	Type	Group
3	Z	137	GLY	Peptide
3	Z	49	GLY	Peptide

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	L	1638	0	1573	218	1
1	M	1632	0	1568	247	0
1	N	1632	0	1568	213	0
1	O	1638	0	1573	216	0
2	H	1630	0	1568	220	0
2	I	1630	0	1568	194	0
2	J	1630	0	1568	231	0
2	K	1630	0	1568	240	0
3	V	1090	0	1135	153	0
3	X	1049	0	1098	157	0
3	Y	1053	0	1101	160	0
3	Z	1045	0	1097	143	0
4	H	17	0	0	9	0
4	I	27	0	0	4	0
4	J	13	0	0	2	0
4	K	10	0	0	5	0
4	L	20	0	0	3	0
4	M	18	0	0	5	0
4	N	19	0	0	2	0
4	O	20	0	0	5	0
4	V	7	0	0	0	1
4	X	11	0	0	5	0
4	Y	3	0	0	0	0
4	Z	4	0	0	0	0
All	All	17466	0	16985	2256	1

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 66.

All (2256) 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:N:11:MET:SD	1:N:11:MET:CE	2.03	1.46
1:L:11:MET:CE	1:L:11:MET:SD	2.04	1.45
2:J:85:MET:CE	2:J:96:TYR:HE1	1.26	1.45
2:J:148:TYR:CE1	2:J:178:TYR:HB3	1.50	1.45
3:Z:55:MET:CE	3:Z:55:MET:SD	2.04	1.44
1:O:11:MET:CE	1:O:11:MET:SD	2.08	1.41
3:Y:75:MET:CE	3:Y:75:MET:SD	2.10	1.39
2:J:85:MET:CE	2:J:96:TYR:CE1	2.09	1.36
1:O:150:ASP:OD2	1:O:188:HIS:HB3	1.33	1.28
2:J:85:MET:HE1	2:J:96:TYR:CE1	1.63	1.27
3:Z:14:LYS:O	3:Z:18:ASP:HB2	1.26	1.27
3:Z:63:ILE:O	3:Z:67:VAL:HG23	1.39	1.21
1:L:29:VAL:CG1	1:L:91:SER:HB2	1.71	1.20
1:O:90:ARG:NH2	2:K:102:SER:O	1.74	1.19
1:N:167:SER:HB2	1:N:168:LYS:NZ	1.56	1.18
2:J:122:PRO:HB3	2:J:148:TYR:HB3	1.22	1.17
1:L:185:TYR:CE1	1:L:191:TYR:HE1	1.63	1.16
1:L:197:HIS:ND1	1:L:199:THR:HB	1.60	1.16
2:J:148:TYR:CE1	2:J:178:TYR:CB	2.27	1.16
2:K:84:GLN:HE21	2:K:84:GLN:HA	1.07	1.16
1:M:197:HIS:ND1	1:M:199:THR:HB	1.61	1.15
2:J:85:MET:HE3	2:J:96:TYR:CE1	1.81	1.14
1:N:76:ARG:HG2	1:N:76:ARG:HH11	0.99	1.14
3:Z:56:GLU:HA	3:Z:56:GLU:OE2	1.46	1.14
3:X:64:LEU:O	3:X:68:THR:HG23	1.45	1.13
2:J:20:LEU:HD11	2:J:96:TYR:HD1	1.10	1.13
2:H:189:SER:CB	4:H:224:HOH:O	1.95	1.13
3:X:12:LEU:HB3	3:X:143:MET:HE1	1.20	1.12
2:K:89:ARG:HH11	2:K:89:ARG:HG3	1.06	1.12
1:M:150:ASP:OD2	1:M:188:HIS:HB3	1.50	1.11
2:K:38:ARG:HA	2:K:95:ILE:O	1.48	1.09
2:K:29:PHE:HB2	2:K:79:SER:HB3	1.33	1.09
1:L:110:ALA:O	1:L:138:PHE:HA	1.53	1.09
1:M:149:ILE:HD11	1:M:154:ARG:HD2	1.33	1.08
1:N:72:LEU:O	1:N:72:LEU:HD23	1.53	1.08
3:X:51:TRP:CZ2	3:X:138:LYS:HE2	1.88	1.08
1:L:29:VAL:HG11	1:L:91:SER:HB2	1.32	1.07
3:X:41:LEU:CD1	3:X:127:ILE:HG22	1.84	1.07
2:J:95:ILE:HG23	2:J:111:LEU:HD23	1.35	1.07
1:O:32:MET:HB2	1:O:70:TYR:HD2	1.03	1.07
2:H:78:LYS:HB2	2:H:78:LYS:NZ	1.65	1.07
3:X:17:ARG:HH11	3:X:17:ARG:HG3	1.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:189:SER:CA	4:H:224:HOH:O	2.00	1.06
2:J:29:PHE:HE1	2:J:34:MET:HE3	1.20	1.06
2:J:148:TYR:CE2	2:J:153:VAL:HB	1.88	1.06
3:X:41:LEU:HD11	3:X:127:ILE:CG2	1.84	1.06
3:Y:10:ARG:HA	3:Y:13:SER:OG	1.56	1.06
1:N:119:PRO:HD3	1:N:131:VAL:HG23	1.37	1.05
2:J:130:GLY:O	2:J:133:ALA:N	1.89	1.05
1:M:6:GLN:HG2	1:M:23:CYS:HB2	1.30	1.05
2:K:70:PHE:CD1	2:K:85:MET:HB3	1.92	1.05
2:H:78:LYS:HB2	2:H:78:LYS:HZ2	1.12	1.05
2:K:54:LYS:HE2	2:K:58:HIS:HE1	1.21	1.05
1:L:7:SER:HB3	1:L:8:PRO:HD3	1.36	1.04
3:Y:8:ASP:OD1	3:Y:11:VAL:HG13	1.57	1.04
2:J:90:ALA:HA	2:J:114:VAL:HG21	1.40	1.03
3:X:78:ARG:HH11	3:X:78:ARG:CG	1.70	1.03
1:N:185:TYR:CE1	1:N:191:TYR:HE1	1.77	1.02
2:I:153:VAL:HG23	2:I:201:ALA:O	1.57	1.02
1:N:77:MET:HE3	1:N:81:ASP:HB2	1.40	1.02
2:K:64:GLU:HA	2:K:67:LYS:HG3	1.42	1.02
1:O:32:MET:HB2	1:O:70:TYR:CD2	1.95	1.01
3:X:78:ARG:HG2	3:X:78:ARG:NH1	1.54	1.01
3:X:112:LEU:HD12	3:X:113:PRO:HD2	1.39	1.01
2:J:51:ILE:HD13	2:J:74:ARG:HG2	1.41	1.00
2:J:89:ARG:HB3	2:J:91:GLU:OE1	1.60	1.00
2:J:153:VAL:HG23	2:J:202:HIS:HB2	1.38	1.00
2:H:12:VAL:O	2:H:114:VAL:HA	1.60	1.00
2:H:199:ASN:CB	2:H:209:VAL:HG23	1.90	1.00
1:N:7:SER:CB	1:N:22:THR:HB	1.91	1.00
2:H:89:ARG:HD2	2:H:91:GLU:OE1	1.58	0.99
2:H:199:ASN:HB3	2:H:209:VAL:CG2	1.91	0.99
1:N:76:ARG:HG2	1:N:76:ARG:NH1	1.68	0.99
3:Y:136:ARG:HH22	3:Z:46:PHE:HD2	1.09	0.99
1:L:185:TYR:CE1	1:L:191:TYR:CE1	2.51	0.99
3:Y:130:SER:O	3:Y:134:LEU:HD12	1.63	0.99
1:O:37:GLN:HE22	2:K:39:GLN:HE22	1.08	0.98
2:H:189:SER:HA	4:H:224:HOH:O	1.56	0.98
1:O:197:HIS:O	1:O:199:THR:N	1.96	0.98
3:V:69:LEU:HD11	3:V:118:THR:HG21	1.42	0.98
3:X:12:LEU:HB3	3:X:143:MET:CE	1.94	0.98
2:J:124:VAL:HG11	2:J:200:VAL:HG21	1.46	0.97
1:N:7:SER:HB3	1:N:22:THR:HB	1.01	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:VAL:N	1:L:178:LEU:O	1.98	0.96
1:L:185:TYR:CD1	1:L:191:TYR:HE1	1.83	0.96
2:J:20:LEU:HD11	2:J:96:TYR:CD1	2.00	0.96
1:M:48:TYR:CE1	3:X:113:PRO:HG2	1.99	0.96
2:J:70:PHE:HA	2:J:84:GLN:O	1.65	0.96
1:N:7:SER:HB3	1:N:22:THR:CB	1.95	0.96
2:J:70:PHE:HD1	2:J:85:MET:HA	1.29	0.96
2:K:84:GLN:HE21	2:K:84:GLN:CA	1.78	0.96
2:H:203:PRO:HA	4:H:228:HOH:O	1.65	0.95
1:M:36:GLN:HB2	1:M:85:TYR:CE2	2.02	0.95
1:O:19:VAL:HG11	1:O:74:ILE:HD12	1.49	0.95
1:N:149:ILE:O	1:N:190:SER:O	1.83	0.94
2:J:51:ILE:HD13	2:J:74:ARG:CG	1.97	0.94
3:Z:64:LEU:O	3:Z:68:THR:HG22	1.65	0.94
1:N:77:MET:CE	1:N:81:ASP:HB2	1.97	0.94
2:J:29:PHE:CE1	2:J:34:MET:CE	2.49	0.94
3:Y:68:THR:HG22	3:Y:101:LEU:CD1	1.96	0.94
2:J:38:ARG:HB2	2:J:96:TYR:CE2	2.02	0.94
1:N:167:SER:HB2	1:N:168:LYS:HZ2	1.19	0.94
1:L:135:LEU:HD23	1:L:143:ILE:CD1	1.97	0.94
1:N:119:PRO:HD3	1:N:131:VAL:CG2	1.97	0.94
2:K:66:VAL:O	2:K:66:VAL:HG12	1.66	0.93
3:V:68:THR:HG22	3:V:101:LEU:HD11	1.50	0.93
1:O:116:ILE:HG13	1:O:133:CYS:SG	2.08	0.93
1:M:20:THR:HB	1:M:73:THR:OG1	1.69	0.93
3:Z:56:GLU:OE2	3:Z:56:GLU:CA	2.17	0.93
2:J:85:MET:HE1	2:J:96:TYR:HE1	0.77	0.93
1:N:72:LEU:HD23	1:N:72:LEU:C	1.89	0.93
2:K:54:LYS:HE2	2:K:58:HIS:CE1	2.03	0.93
1:N:149:ILE:HG23	1:N:191:TYR:CE2	2.04	0.92
2:J:135:THR:HG23	4:J:221:HOH:O	1.67	0.92
2:J:70:PHE:CE1	2:J:85:MET:HB3	2.04	0.92
1:O:132:VAL:HG11	2:K:127:LEU:HD13	1.52	0.92
2:H:78:LYS:HG3	2:H:78:LYS:O	1.67	0.92
2:H:145:VAL:CG1	2:H:180:LEU:HD22	1.99	0.92
3:X:17:ARG:HG3	3:X:17:ARG:NH1	1.76	0.92
1:M:32:MET:HB2	1:M:70:TYR:CD2	2.03	0.91
3:X:41:LEU:HD11	3:X:127:ILE:HG22	0.94	0.91
1:L:194:GLU:HB3	1:L:205:VAL:HG22	1.51	0.91
2:I:124:VAL:HG21	2:I:200:VAL:HG21	1.48	0.91
2:H:78:LYS:NZ	2:H:78:LYS:CB	2.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:136:ARG:NH2	3:Z:46:PHE:CD2	2.37	0.91
1:L:211:ASN:ND2	1:L:213:CYS:SG	2.44	0.90
1:O:149:ILE:HG12	1:O:191:TYR:HE2	1.34	0.90
1:N:19:VAL:HG11	1:N:103:LEU:HD22	1.52	0.90
1:M:123:GLN:NE2	1:M:130:SER:OG	2.03	0.90
2:J:29:PHE:CE1	2:J:34:MET:HE3	2.05	0.90
1:O:44:LYS:HB2	1:O:44:LYS:NZ	1.86	0.90
1:N:185:TYR:CE1	1:N:191:TYR:CE1	2.60	0.90
2:H:66:VAL:CG1	2:H:70:PHE:CD2	2.54	0.90
2:I:27:PHE:CE2	2:I:29:PHE:HA	2.07	0.90
1:N:147:TRP:CD1	1:N:158:VAL:HG11	2.07	0.90
2:J:33:TRP:H	3:Y:111:GLN:HE22	1.17	0.90
1:N:2:VAL:O	1:N:96:THR:HG21	1.72	0.89
2:I:56:ASN:HD22	2:I:56:ASN:H	1.15	0.89
3:X:112:LEU:HD12	3:X:113:PRO:CD	2.02	0.89
3:Z:64:LEU:O	3:Z:68:THR:CG2	2.21	0.89
1:N:76:ARG:HH11	1:N:76:ARG:CG	1.83	0.89
1:L:88:GLN:NE2	1:L:90:ARG:HD2	1.86	0.89
1:L:111:ALA:CB	1:L:199:THR:HG21	2.02	0.89
3:Y:11:VAL:O	3:Y:15:LEU:HB2	1.73	0.89
1:L:29:VAL:HG13	1:L:91:SER:HB2	1.53	0.88
2:J:148:TYR:HE2	2:J:153:VAL:HB	1.31	0.88
2:K:153:VAL:HG23	2:K:202:HIS:HD2	1.38	0.88
3:X:74:VAL:HG11	3:X:94:SER:HB3	1.55	0.88
3:Z:107:LEU:O	3:Z:107:LEU:HD23	1.72	0.88
1:L:2:VAL:O	1:L:96:THR:HG21	1.73	0.88
3:X:51:TRP:HZ2	3:X:138:LYS:HE2	1.32	0.88
3:Y:63:ILE:O	3:Y:67:VAL:HG23	1.73	0.88
2:I:216:ARG:HE	3:Y:122:LYS:H	1.21	0.88
1:L:84:THR:HG23	1:L:101:THR:H	1.37	0.88
1:L:88:GLN:NE2	1:L:90:ARG:HH11	1.72	0.88
2:K:29:PHE:CB	2:K:79:SER:HB3	2.04	0.88
2:J:216:ARG:HH22	3:X:123:ASP:HB3	1.39	0.88
1:M:76:ARG:HG2	1:M:76:ARG:HH11	1.39	0.88
2:I:120:THR:HG21	2:I:177:LEU:CD1	2.03	0.88
1:O:136:ASN:OD1	1:O:173:SER:HB3	1.74	0.87
1:N:186:GLU:HA	1:N:210:ARG:NH1	1.90	0.87
2:K:40:SER:O	2:K:44:GLY:HA2	1.75	0.87
1:L:185:TYR:HE1	1:L:191:TYR:CE1	1.92	0.87
1:M:120:SER:O	1:M:122:GLU:N	2.08	0.87
2:H:70:PHE:CE1	2:H:85:MET:HB3	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:105:GLN:NE2	3:Y:111:GLN:HG3	1.90	0.87
1:L:88:GLN:HE22	1:L:90:ARG:HH11	0.89	0.87
2:J:38:ARG:HB2	2:J:96:TYR:CD2	2.09	0.86
3:Y:68:THR:HG22	3:Y:101:LEU:HD11	1.57	0.86
2:J:6:GLU:OE2	2:J:97:TYR:HA	1.74	0.86
1:N:36:GLN:HE21	1:N:85:TYR:HE2	1.24	0.86
1:N:6:GLN:HE22	1:N:86:TYR:HA	1.36	0.86
3:V:69:LEU:HD11	3:V:118:THR:CG2	2.05	0.86
2:K:216:ARG:NH2	3:V:123:ASP:H	1.74	0.85
2:I:149:PHE:HB2	2:I:177:LEU:CD2	2.07	0.85
2:J:90:ALA:HA	2:J:114:VAL:CG2	2.07	0.85
1:N:19:VAL:HG11	1:N:103:LEU:CD2	2.07	0.85
1:N:189:ASN:ND2	1:N:210:ARG:H	1.75	0.85
1:N:2:VAL:HG21	1:N:89:GLN:OE1	1.77	0.85
1:O:61:PHE:CE1	1:O:74:ILE:HG12	2.11	0.85
2:J:29:PHE:HE1	2:J:34:MET:CE	1.86	0.85
3:Z:97:VAL:O	3:Z:100:LEU:HB2	1.77	0.85
2:I:56:ASN:HD22	2:I:56:ASN:N	1.74	0.84
2:J:146:LYS:HA	2:J:179:THR:OG1	1.77	0.84
3:Y:116:GLY:O	3:Y:118:THR:HG22	1.77	0.84
2:J:148:TYR:CD1	2:J:178:TYR:CB	2.60	0.84
2:K:84:GLN:HA	2:K:84:GLN:NE2	1.91	0.84
2:J:148:TYR:CD1	2:J:178:TYR:HB2	2.12	0.84
2:H:66:VAL:HG11	2:H:70:PHE:CD2	2.13	0.84
1:N:79:ALA:HA	1:N:105:ILE:HD13	1.59	0.84
3:X:51:TRP:CZ2	3:X:138:LYS:CE	2.60	0.84
1:L:88:GLN:HE22	1:L:90:ARG:NH1	1.74	0.84
3:Y:13:SER:O	3:Y:14:LYS:C	2.16	0.84
2:J:130:GLY:O	2:J:133:ALA:CA	2.25	0.84
2:J:122:PRO:CB	2:J:148:TYR:HB3	2.07	0.83
3:Z:14:LYS:O	3:Z:18:ASP:CB	2.21	0.83
2:J:216:ARG:HG3	3:X:122:LYS:HG3	1.61	0.83
3:Z:41:LEU:HD11	3:Z:127:ILE:HG22	1.59	0.83
2:H:174:GLN:O	2:H:176:ASP:N	2.11	0.83
1:M:33:TYR:CD2	1:M:33:TYR:N	2.40	0.83
2:I:158:ASN:O	2:I:160:GLY:N	2.12	0.83
2:K:39:GLN:HA	2:K:44:GLY:O	1.79	0.83
2:K:33:TRP:CE2	2:K:52:ARG:HG2	2.14	0.83
3:Y:130:SER:O	3:Y:134:LEU:CD1	2.27	0.83
1:M:188:HIS:O	1:M:210:ARG:CD	2.27	0.83
1:L:154:ARG:HG3	1:L:154:ARG:O	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:61:PHE:CE1	1:N:74:ILE:HG12	2.14	0.82
1:O:32:MET:SD	1:O:88:GLN:O	2.37	0.82
2:I:22:CYS:O	2:I:80:SER:HB3	1.80	0.82
1:N:70:TYR:O	1:N:71:SER:HB3	1.78	0.82
3:X:43:ALA:CB	3:X:119:THR:HG23	2.09	0.82
3:X:68:THR:HB	4:X:170:HOH:O	1.79	0.82
3:Y:93:LEU:O	3:Y:97:VAL:HG23	1.79	0.82
1:L:111:ALA:HB1	1:L:199:THR:HG21	1.61	0.82
1:L:185:TYR:CD1	1:L:191:TYR:CE1	2.66	0.82
2:H:85:MET:HB2	2:H:88:LEU:HD11	1.61	0.82
3:Z:41:LEU:CD1	3:Z:127:ILE:HG22	2.10	0.82
2:H:166:VAL:HB	2:H:184:VAL:HG23	1.61	0.82
1:N:3:VAL:H	1:N:26:SER:HB3	1.42	0.82
1:N:119:PRO:CD	1:N:131:VAL:CG2	2.57	0.81
1:M:107:ARG:NH2	1:N:78:GLU:OE2	2.13	0.81
3:Y:124:PRO:O	3:Y:126:ALA:N	2.13	0.81
1:M:22:THR:HG22	1:M:23:CYS:N	1.95	0.81
1:N:162:TRP:CE2	1:N:174:MET:HG3	2.15	0.81
1:O:117:PHE:N	1:O:117:PHE:HD1	1.76	0.81
2:K:33:TRP:H	3:Z:111:GLN:HE22	1.24	0.81
3:X:132:GLN:HA	3:X:135:LEU:HD12	1.62	0.81
3:Z:45:ASP:H	3:Z:133:HIS:HE1	1.26	0.81
3:Z:71:LEU:HD12	3:Z:101:LEU:HD22	1.62	0.81
1:M:138:PHE:HE2	1:M:173:SER:HA	1.46	0.81
2:I:120:THR:HG21	2:I:177:LEU:HD11	1.60	0.81
1:O:44:LYS:HB2	1:O:44:LYS:HZ3	1.43	0.81
3:X:61:GLN:O	3:X:64:LEU:N	2.12	0.81
2:H:66:VAL:HG13	2:H:70:PHE:CD2	2.14	0.81
2:H:100:GLY:HA3	2:H:105:TYR:H	1.45	0.81
1:N:45:LEU:HD12	2:J:104:LEU:HD12	1.63	0.81
3:V:81:LEU:HD12	3:V:87:SER:HB2	1.61	0.81
1:N:197:HIS:ND1	1:N:199:THR:HB	1.95	0.81
3:Z:107:LEU:O	3:Z:107:LEU:CD2	2.27	0.81
1:M:188:HIS:O	1:M:210:ARG:HD3	1.80	0.81
3:X:43:ALA:HB2	3:X:119:THR:HG23	1.62	0.81
3:Z:64:LEU:HD23	3:Z:112:LEU:HB2	1.60	0.81
1:N:89:GLN:HE21	1:N:96:THR:HB	1.46	0.81
2:K:70:PHE:CD1	2:K:85:MET:CB	2.64	0.81
3:X:63:ILE:O	3:X:67:VAL:HG23	1.79	0.81
1:L:131:VAL:O	1:L:147:TRP:CH2	2.34	0.80
1:O:6:GLN:HE22	1:O:86:TYR:HA	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:167:SER:HB2	1:N:168:LYS:HZ1	1.43	0.80
1:M:138:PHE:CE2	1:M:173:SER:HA	2.16	0.80
1:M:131:VAL:HG12	1:M:147:TRP:CH2	2.15	0.80
1:M:185:TYR:HD1	1:M:191:TYR:CZ	2.00	0.80
3:V:125:ASN:HD22	3:V:125:ASN:N	1.78	0.80
2:I:134:GLN:HE22	3:Y:117:ARG:HB3	1.47	0.80
2:J:216:ARG:NH2	3:X:123:ASP:HB3	1.96	0.80
3:V:73:GLY:O	3:V:76:ALA:HB3	1.82	0.80
2:K:146:LYS:HA	2:K:179:THR:OG1	1.80	0.80
3:Y:131:PHE:CZ	3:Y:135:LEU:HD11	2.16	0.80
1:M:37:GLN:HE22	2:I:39:GLN:HE22	1.29	0.80
2:K:100:GLY:O	2:K:104:LEU:N	2.15	0.80
3:Z:141:PHE:O	3:Z:145:VAL:HG23	1.82	0.80
1:N:185:TYR:HE1	1:N:191:TYR:CE1	1.99	0.80
1:O:107:ARG:HD2	1:O:170:SER:OG	1.80	0.80
3:V:42:PRO:HD3	3:V:70:LEU:HD23	1.61	0.80
3:X:81:LEU:HD12	3:X:87:SER:HB2	1.64	0.80
1:M:149:ILE:HD11	1:M:154:ARG:CD	2.10	0.79
2:J:70:PHE:HE1	2:J:85:MET:HB3	1.42	0.79
3:V:59:LYS:O	3:V:63:ILE:HG13	1.83	0.79
2:J:37:VAL:HG22	2:J:47:TRP:HA	1.65	0.79
1:L:72:LEU:HD23	1:L:72:LEU:O	1.83	0.79
2:I:119:THR:HA	2:I:149:PHE:O	1.83	0.79
1:O:67:GLY:N	1:O:70:TYR:HE1	1.81	0.79
2:K:51:ILE:HD11	2:K:74:ARG:HG2	1.64	0.79
1:L:93:TYR:CE1	1:L:95:ARG:NH1	2.51	0.78
2:K:213:ILE:HG23	2:K:214:VAL:N	1.96	0.78
1:M:6:GLN:HE21	1:M:98:GLY:HA3	1.47	0.78
2:K:54:LYS:CE	2:K:58:HIS:HE1	1.96	0.78
3:V:64:LEU:HD11	3:V:105:GLN:HG3	1.63	0.78
2:H:56:ASN:HB3	4:H:218:HOH:O	1.84	0.78
2:H:56:ASN:HD22	2:H:56:ASN:H	1.32	0.78
2:H:173:LEU:HD23	2:H:177:LEU:O	1.84	0.78
1:O:33:TYR:HB2	1:O:88:GLN:HB3	1.65	0.78
2:H:64:GLU:HG2	2:H:67:LYS:HZ2	1.49	0.78
2:J:148:TYR:HE1	2:J:178:TYR:HB3	0.97	0.78
1:L:89:GLN:OE1	1:L:91:SER:HB3	1.84	0.78
1:M:45:LEU:HD22	1:M:46:TRP:N	1.98	0.78
2:I:58:HIS:CD2	2:I:74:ARG:HD2	2.18	0.78
2:H:176:ASP:O	2:H:177:LEU:HD23	1.84	0.77
1:N:35:PHE:N	1:N:35:PHE:CD1	2.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:118:PRO:HB3	1:O:208:PHE:CE2	2.19	0.77
2:H:84:GLN:CA	2:H:84:GLN:HE21	1.98	0.77
1:M:149:ILE:CD1	1:M:154:ARG:HD2	2.13	0.77
1:N:48:TYR:O	1:N:52:ASN:HB2	1.84	0.77
3:X:78:ARG:HH11	3:X:78:ARG:HG2	0.75	0.77
2:J:156:THR:O	2:J:199:ASN:N	2.14	0.77
3:Z:35:LEU:N	3:Z:122:LYS:O	2.17	0.77
2:H:157:TRP:CZ3	2:H:198:CYS:HB3	2.19	0.77
2:I:76:ASP:O	2:I:79:SER:N	2.15	0.77
2:I:139:VAL:O	2:I:185:THR:HG23	1.85	0.77
1:O:119:PRO:HG2	1:O:129:ALA:HB1	1.66	0.77
2:J:29:PHE:CD2	2:J:79:SER:HA	2.20	0.77
1:L:36:GLN:HG3	1:L:85:TYR:CE2	2.19	0.77
1:L:7:SER:HB3	1:L:8:PRO:CD	2.15	0.77
2:H:91:GLU:C	2:H:93:THR:H	1.88	0.77
1:O:77:MET:HE3	1:O:78:GLU:O	1.84	0.77
1:O:33:TYR:CD1	1:O:33:TYR:N	2.52	0.77
3:Z:12:LEU:HB2	3:Z:143:MET:SD	2.24	0.77
1:N:189:ASN:ND2	1:N:210:ARG:N	2.32	0.76
1:M:189:ASN:HA	1:M:210:ARG:HG3	1.67	0.76
1:M:129:ALA:O	1:M:179:THR:HG23	1.84	0.76
2:I:75:ASP:C	2:I:75:ASP:OD1	2.23	0.76
1:N:117:PHE:N	1:N:117:PHE:CD1	2.47	0.76
2:J:70:PHE:CD1	2:J:85:MET:HA	2.17	0.76
1:L:76:ARG:HB3	1:L:76:ARG:HH11	1.50	0.76
3:Y:10:ARG:HA	3:Y:13:SER:HG	1.48	0.76
1:M:4:LEU:HD21	1:M:89:GLN:HG2	1.67	0.76
1:M:189:ASN:HA	1:M:210:ARG:CG	2.16	0.76
2:J:35:ASP:HB3	2:J:49:ALA:O	1.84	0.76
2:H:33:TRP:H	3:V:111:GLN:NE2	1.84	0.76
1:N:189:ASN:HD21	1:N:209:ASN:HB3	1.50	0.76
2:K:153:VAL:HG23	2:K:202:HIS:CD2	2.21	0.75
1:M:45:LEU:HD22	1:M:45:LEU:C	2.07	0.75
2:K:66:VAL:O	2:K:66:VAL:CG1	2.35	0.75
2:K:66:VAL:HG11	2:K:70:PHE:CD2	2.21	0.75
2:I:196:VAL:CG2	2:I:196:VAL:O	2.34	0.75
3:V:69:LEU:CD1	3:V:118:THR:HG21	2.15	0.75
2:H:202:HIS:ND1	2:H:204:ALA:HB2	2.01	0.75
1:N:13:ALA:HB1	1:N:17:GLU:CD	2.07	0.75
1:M:150:ASP:OD2	1:M:188:HIS:CB	2.33	0.75
1:N:86:TYR:CD2	2:J:45:LEU:HD12	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:64:LEU:O	3:Y:68:THR:HG23	1.86	0.75
2:H:85:MET:HE3	2:H:96:TYR:CZ	2.22	0.75
1:M:119:PRO:HA	4:M:227:HOH:O	1.87	0.75
1:N:33:TYR:CE1	1:N:90:ARG:HD3	2.22	0.75
2:J:139:VAL:O	2:J:139:VAL:HG12	1.87	0.75
1:L:111:ALA:HB2	1:L:199:THR:CG2	2.17	0.74
2:H:56:ASN:HD22	2:H:56:ASN:N	1.84	0.74
1:M:117:PHE:N	1:M:117:PHE:CD1	2.55	0.74
1:M:119:PRO:HD3	1:M:131:VAL:HG22	1.69	0.74
3:Z:101:LEU:O	3:Z:105:GLN:HB2	1.87	0.74
1:N:148:LYS:HE2	1:N:194:GLU:OE2	1.86	0.74
2:J:93:THR:HG23	2:J:113:THR:HA	1.68	0.74
1:L:120:SER:O	1:L:124:LEU:CD2	2.36	0.74
2:I:70:PHE:CD1	2:I:85:MET:HG2	2.21	0.74
2:K:156:THR:O	2:K:199:ASN:ND2	2.20	0.74
3:Y:84:THR:O	3:Y:87:SER:N	2.20	0.74
2:I:58:HIS:HD2	2:I:74:ARG:HD2	1.49	0.74
1:N:88:GLN:NE2	1:N:90:ARG:HD2	2.02	0.74
2:K:140:THR:O	2:K:141:LEU:HD23	1.86	0.74
2:K:148:TYR:O	2:K:177:LEU:HD22	1.87	0.74
1:M:162:TRP:N	1:M:162:TRP:HE3	1.84	0.74
2:K:64:GLU:O	2:K:66:VAL:N	2.20	0.74
1:M:181:THR:HA	4:M:215:HOH:O	1.87	0.74
2:J:120:THR:O	2:J:148:TYR:HA	1.87	0.74
3:Z:110:THR:O	3:Z:110:THR:HG23	1.87	0.74
2:I:216:ARG:CD	3:Y:122:LYS:HG3	2.16	0.74
1:O:77:MET:HE3	1:O:81:ASP:HB2	1.68	0.74
1:O:69:SER:C	1:O:70:TYR:HD1	1.91	0.73
3:X:17:ARG:HH11	3:X:17:ARG:CG	2.00	0.73
1:L:107:ARG:NH2	1:O:78:GLU:OE2	2.21	0.73
2:J:29:PHE:CE1	2:J:34:MET:HE2	2.24	0.73
2:H:75:ASP:OD1	2:H:77:SER:HB3	1.88	0.73
2:H:102:SER:HB2	3:V:111:GLN:HB2	1.71	0.73
1:M:7:SER:CB	1:M:8:PRO:HD3	2.19	0.73
2:I:56:ASN:N	2:I:56:ASN:ND2	2.37	0.73
1:O:147:TRP:CE3	1:O:192:THR:O	2.42	0.73
1:L:135:LEU:HD23	1:L:143:ILE:HD13	1.71	0.73
1:M:162:TRP:N	1:M:162:TRP:CE3	2.57	0.73
2:I:145:VAL:HG13	2:I:180:LEU:O	1.89	0.73
2:J:51:ILE:CD1	2:J:74:ARG:CG	2.67	0.73
2:K:89:ARG:HG3	2:K:89:ARG:NH1	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:69:LEU:CD1	3:V:118:THR:CG2	2.66	0.73
3:X:12:LEU:CB	3:X:143:MET:CE	2.67	0.73
2:I:66:VAL:HG22	2:I:70:PHE:CE2	2.24	0.72
3:X:134:LEU:O	3:X:139:VAL:HG23	1.88	0.72
3:Z:61:GLN:HG2	3:Z:112:LEU:CD2	2.19	0.72
2:I:6:GLU:OE2	2:I:109:GLY:N	2.21	0.72
1:O:117:PHE:N	1:O:117:PHE:CD1	2.49	0.72
2:K:29:PHE:CE1	2:K:34:MET:HE2	2.23	0.72
1:L:4:LEU:HB2	1:L:97:PHE:O	1.90	0.72
1:L:166:ASP:HB3	1:L:169:ASP:O	1.90	0.72
3:Z:71:LEU:HD12	3:Z:101:LEU:CD2	2.20	0.72
3:V:55:MET:H	3:V:55:MET:HE2	1.55	0.72
2:H:66:VAL:HG11	2:H:70:PHE:HD2	1.55	0.72
2:H:69:ARG:NH2	2:H:92:ASP:OD2	2.21	0.72
2:J:88:LEU:HD23	2:J:92:ASP:OD2	1.89	0.72
1:M:132:VAL:HB	1:M:177:THR:HG23	1.70	0.72
1:N:185:TYR:CD1	1:N:191:TYR:CE1	2.78	0.72
1:N:185:TYR:CD1	1:N:191:TYR:HE1	2.07	0.72
2:I:89:ARG:O	2:I:92:ASP:HB2	1.90	0.71
1:L:111:ALA:HB1	1:L:112:PRO:HD2	1.72	0.71
2:H:47:TRP:HZ2	2:H:50:GLU:HB3	1.54	0.71
2:I:145:VAL:O	2:I:145:VAL:HG22	1.90	0.71
3:Y:115:ARG:HD2	3:Y:116:GLY:N	2.06	0.71
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.72	0.71
3:V:12:LEU:HD12	3:V:139:VAL:HG12	1.71	0.71
3:V:37:THR:O	3:V:80:GLN:NE2	2.23	0.71
2:K:162:LEU:HD13	2:K:184:VAL:HG21	1.73	0.71
2:I:104:LEU:HG	2:I:105:TYR:CE1	2.24	0.71
1:L:19:VAL:HB	1:L:74:ILE:HB	1.71	0.71
2:K:13:GLN:O	2:K:14:PRO:O	2.08	0.71
2:H:85:MET:HE3	2:H:96:TYR:CE1	2.25	0.71
2:J:86:ASN:O	2:J:87:SER:C	2.27	0.71
2:J:140:THR:HG23	2:J:185:THR:OG1	1.91	0.71
3:V:71:LEU:O	3:V:75:MET:HG2	1.91	0.71
1:M:77:MET:SD	1:M:105:ILE:HD12	2.31	0.71
1:M:109:ASP:OD1	1:M:140:PRO:HD3	1.90	0.71
3:Y:10:ARG:O	3:Y:13:SER:N	2.24	0.71
3:Y:14:LYS:O	3:Y:18:ASP:HB2	1.90	0.71
1:M:192:THR:OG1	1:M:207:SER:OG	2.08	0.71
3:Z:61:GLN:HG2	3:Z:112:LEU:HD23	1.73	0.71
2:H:91:GLU:O	2:H:93:THR:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:ILE:HD13	2:H:111:LEU:HD23	1.73	0.71
1:M:169:ASP:OD2	1:M:171:THR:OG1	2.08	0.71
1:N:167:SER:CB	1:N:168:LYS:NZ	2.47	0.71
2:H:166:VAL:O	2:H:166:VAL:HG22	1.89	0.70
1:M:148:LYS:HA	1:M:152:SER:O	1.90	0.70
1:N:148:LYS:HA	1:N:153:GLU:HA	1.72	0.70
1:O:19:VAL:HG12	1:O:74:ILE:HB	1.73	0.70
3:X:51:TRP:O	3:X:54:GLN:HB2	1.92	0.70
3:Y:22:LEU:HD21	3:Y:92:GLN:HB3	1.73	0.70
1:L:6:GLN:NE2	1:L:87:CYS:H	1.90	0.70
1:M:13:ALA:HB2	1:M:19:VAL:HG21	1.71	0.70
1:O:19:VAL:CG1	1:O:74:ILE:HD12	2.19	0.70
2:H:64:GLU:HG2	2:H:67:LYS:NZ	2.06	0.70
1:O:147:TRP:CH2	1:O:193:CYS:HB2	2.26	0.70
2:K:120:THR:HG21	2:K:177:LEU:HD11	1.74	0.70
2:H:145:VAL:HG13	2:H:180:LEU:HD22	1.71	0.70
2:I:191:TRP:CD1	2:I:196:VAL:HG13	2.26	0.70
1:M:1:GLN:HG2	1:M:1:GLN:O	1.92	0.70
1:N:89:GLN:NE2	1:N:96:THR:HB	2.07	0.70
1:O:185:TYR:CD1	1:O:191:TYR:HE1	2.10	0.70
1:M:192:THR:HA	1:M:207:SER:OG	1.92	0.69
2:J:187:PRO:O	2:J:190:THR:OG1	2.09	0.69
1:O:116:ILE:C	1:O:117:PHE:HD1	1.95	0.69
3:V:86:LEU:HD22	3:V:90:LEU:HG	1.74	0.69
1:M:76:ARG:HG2	1:M:76:ARG:NH1	2.07	0.69
1:O:149:ILE:HG12	1:O:191:TYR:CE2	2.24	0.69
2:K:33:TRP:H	3:Z:111:GLN:NE2	1.90	0.69
2:H:138:MET:HE2	2:H:185:THR:HG22	1.72	0.69
1:N:106:LYS:HG3	1:N:106:LYS:O	1.91	0.69
2:K:29:PHE:HB2	2:K:79:SER:CB	2.17	0.69
2:K:29:PHE:CE1	2:K:34:MET:CE	2.74	0.69
3:Z:131:PHE:O	3:Z:134:LEU:HB2	1.91	0.69
2:J:212:LYS:O	2:J:213:ILE:HG13	1.92	0.69
1:M:60:ARG:NH1	1:M:81:ASP:OD2	2.26	0.69
3:V:100:LEU:O	3:V:103:ALA:HB3	1.92	0.69
1:L:89:GLN:HE21	1:L:96:THR:CB	2.06	0.69
2:K:66:VAL:HG21	2:K:70:PHE:CE2	2.28	0.69
3:Z:59:LYS:O	3:Z:63:ILE:HG13	1.92	0.69
2:I:191:TRP:HD1	2:I:196:VAL:HG13	1.58	0.69
1:L:37:GLN:HG2	1:L:38:LYS:N	2.07	0.69
1:L:119:PRO:HA	4:L:223:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:216:ARG:NE	3:Y:122:LYS:H	1.91	0.69
1:N:162:TRP:CH2	1:N:174:MET:HE2	2.28	0.69
3:Z:46:PHE:CE1	3:Z:133:HIS:NE2	2.60	0.69
2:H:51:ILE:HD12	2:H:74:ARG:CG	2.22	0.69
2:K:203:PRO:HB2	4:K:227:HOH:O	1.93	0.69
3:Y:110:THR:OG1	3:Y:111:GLN:N	2.26	0.69
1:N:110:ALA:HB3	1:N:139:TYR:N	2.07	0.68
2:K:202:HIS:ND1	2:K:204:ALA:HB2	2.08	0.68
3:Z:73:GLY:O	3:Z:76:ALA:HB3	1.93	0.68
1:L:154:ARG:HD2	1:L:156:ASN:O	1.92	0.68
2:J:69:ARG:NH1	2:J:89:ARG:NH2	2.40	0.68
1:L:143:ILE:HG12	1:L:197:HIS:HB2	1.74	0.68
2:H:123:SER:OG	2:H:146:LYS:HB3	1.93	0.68
1:O:132:VAL:HB	1:O:177:THR:HG23	1.74	0.68
3:V:86:LEU:CD2	3:V:90:LEU:HG	2.23	0.68
2:K:69:ARG:NH1	2:K:89:ARG:NH2	2.40	0.68
3:V:81:LEU:CD1	3:V:87:SER:HB2	2.23	0.68
1:L:48:TYR:CE1	1:L:52:ASN:HB2	2.28	0.68
2:K:22:CYS:O	2:K:80:SER:HA	1.93	0.68
3:X:12:LEU:CB	3:X:143:MET:HE1	2.12	0.68
1:M:95:ARG:HG3	2:I:47:TRP:CD2	2.28	0.68
3:X:112:LEU:CD1	3:X:113:PRO:HD2	2.22	0.68
2:H:78:LYS:CB	2:H:78:LYS:HZ3	2.06	0.68
2:J:20:LEU:HD21	2:J:85:MET:SD	2.34	0.68
1:O:67:GLY:N	1:O:70:TYR:CE1	2.61	0.68
2:I:188:SER:OG	2:I:189:SER:N	2.25	0.68
3:V:100:LEU:HD22	3:V:104:LEU:HD11	1.75	0.68
1:L:35:PHE:N	1:L:35:PHE:CD1	2.59	0.68
1:N:72:LEU:O	1:N:72:LEU:CD2	2.39	0.68
1:O:69:SER:O	1:O:70:TYR:HD1	1.75	0.68
2:K:119:THR:HG23	2:K:150:PRO:HD3	1.75	0.68
3:V:125:ASN:HD22	3:V:125:ASN:H	1.41	0.68
1:L:75:SER:OG	1:L:76:ARG:HG3	1.93	0.67
1:O:186:GLU:HB2	4:O:224:HOH:O	1.94	0.67
3:X:33:HIS:HB3	3:X:34:PRO:HD2	1.76	0.67
3:Y:13:SER:O	3:Y:15:LEU:N	2.26	0.67
3:Z:64:LEU:CD2	3:Z:112:LEU:HB2	2.23	0.67
1:L:149:ILE:O	1:L:190:SER:O	2.12	0.67
1:O:94:PRO:HB3	2:K:47:TRP:HZ3	1.59	0.67
3:X:85:CYS:O	3:X:86:LEU:C	2.32	0.67
2:H:199:ASN:HB3	2:H:209:VAL:HG23	0.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:100:GLY:HA3	2:K:105:TYR:HB2	1.75	0.67
3:X:64:LEU:O	3:X:68:THR:CG2	2.34	0.67
1:M:22:THR:HG22	1:M:23:CYS:H	1.59	0.67
1:M:109:ASP:HA	1:M:139:TYR:O	1.93	0.67
1:N:185:TYR:HE1	1:N:191:TYR:HE1	1.32	0.67
1:L:6:GLN:HE22	1:L:87:CYS:H	1.40	0.67
1:N:3:VAL:N	1:N:26:SER:HB3	2.10	0.67
1:N:119:PRO:CD	1:N:131:VAL:HG22	2.25	0.67
2:J:70:PHE:CE1	2:J:85:MET:CB	2.77	0.67
3:Z:101:LEU:HD11	3:Z:105:GLN:HE22	1.60	0.67
1:L:84:THR:HG22	1:L:85:TYR:N	2.07	0.67
1:L:120:SER:O	1:L:124:LEU:HD23	1.94	0.67
2:J:122:PRO:HB3	2:J:148:TYR:CB	2.14	0.67
1:O:116:ILE:C	1:O:117:PHE:CD1	2.68	0.67
2:K:84:GLN:CA	2:K:84:GLN:NE2	2.54	0.67
1:L:84:THR:CG2	1:L:101:THR:H	2.07	0.67
2:H:111:LEU:HD13	2:H:112:VAL:N	2.10	0.67
1:N:184:GLU:HG2	1:N:184:GLU:O	1.96	0.67
2:H:93:THR:OG1	2:H:114:VAL:HG22	1.95	0.66
2:I:69:ARG:NH2	2:I:92:ASP:OD2	2.29	0.66
2:I:93:THR:OG1	2:I:114:VAL:N	2.22	0.66
1:N:118:PRO:HB3	1:N:208:PHE:CE2	2.30	0.66
1:O:41:THR:HG23	1:O:42:SER:O	1.95	0.66
2:K:38:ARG:CA	2:K:95:ILE:O	2.35	0.66
2:K:200:VAL:O	2:K:208:LYS:N	2.23	0.66
2:H:216:ARG:NH2	3:Z:123:ASP:HB2	2.10	0.66
1:N:2:VAL:HG21	1:N:89:GLN:CD	2.16	0.66
1:N:169:ASP:CG	1:N:169:ASP:O	2.34	0.66
2:J:157:TRP:CZ3	2:J:198:CYS:HB3	2.31	0.66
3:Y:81:LEU:HD11	3:Y:86:LEU:HB3	1.76	0.66
2:H:12:VAL:O	2:H:114:VAL:CA	2.41	0.66
1:N:33:TYR:O	1:N:87:CYS:HA	1.95	0.66
3:V:61:GLN:O	3:V:65:GLY:N	2.19	0.66
2:K:202:HIS:ND1	2:K:204:ALA:CB	2.58	0.66
2:H:207:THR:O	2:H:207:THR:OG1	2.06	0.66
1:M:120:SER:O	1:M:123:GLN:N	2.27	0.66
3:Y:8:ASP:OD2	3:Y:10:ARG:CB	2.43	0.66
3:Z:97:VAL:O	3:Z:100:LEU:CB	2.43	0.66
1:L:105:ILE:HG13	1:L:106:LYS:N	2.10	0.66
2:I:174:GLN:O	2:I:176:ASP:N	2.28	0.66
2:I:214:VAL:HG11	3:Y:40:LEU:CD2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:98:ARG:HA	3:Z:101:LEU:HB2	1.77	0.66
2:I:196:VAL:O	2:I:196:VAL:HG22	1.94	0.66
1:O:185:TYR:CD1	1:O:191:TYR:CE1	2.84	0.66
2:K:26:GLY:O	2:K:27:PHE:HB3	1.95	0.66
1:L:107:ARG:HD3	1:L:139:TYR:CG	2.31	0.66
1:L:149:ILE:HG13	1:L:154:ARG:HB3	1.77	0.66
2:H:191:TRP:CH2	2:H:214:VAL:HG13	2.30	0.65
1:M:185:TYR:CD1	1:M:191:TYR:CZ	2.84	0.65
2:I:64:GLU:HA	2:I:67:LYS:HD3	1.77	0.65
1:N:194:GLU:HG2	1:N:205:VAL:HG23	1.77	0.65
2:J:133:ALA:O	2:J:134:GLN:HG2	1.96	0.65
3:V:140:ARG:O	3:V:143:MET:HE2	1.94	0.65
3:Y:75:MET:HA	3:Y:75:MET:HE3	1.79	0.65
2:H:93:THR:OG1	2:H:114:VAL:CG2	2.44	0.65
1:M:31:TYR:HA	1:M:50:THR:OG1	1.96	0.65
2:K:51:ILE:CD1	2:K:74:ARG:HD2	2.26	0.65
3:V:12:LEU:HD12	3:V:139:VAL:CG1	2.26	0.65
1:M:32:MET:HB2	1:M:70:TYR:HD2	1.56	0.65
1:N:45:LEU:HD12	2:J:104:LEU:CD1	2.27	0.65
2:K:66:VAL:CG2	2:K:70:PHE:CE2	2.79	0.65
3:V:127:ILE:HG12	3:V:128:PHE:N	2.10	0.65
1:L:157:GLY:O	1:L:179:THR:HG22	1.96	0.65
1:L:197:HIS:CE1	1:L:199:THR:HB	2.30	0.65
2:I:33:TRP:CD1	2:I:53:SER:HB2	2.30	0.65
1:O:90:ARG:HH21	2:K:102:SER:CB	2.09	0.65
1:L:194:GLU:CB	1:L:205:VAL:HG22	2.24	0.65
1:O:11:MET:HG3	1:O:103:LEU:CD1	2.27	0.65
1:N:117:PHE:N	1:N:117:PHE:HD1	1.93	0.65
1:N:169:ASP:O	1:N:169:ASP:OD2	2.15	0.65
1:O:118:PRO:HB3	1:O:208:PHE:CZ	2.31	0.65
3:Z:43:ALA:HB2	3:Z:119:THR:HG23	1.78	0.65
1:N:167:SER:CB	1:N:168:LYS:HZ2	2.01	0.65
1:N:192:THR:HG23	1:N:207:SER:HB2	1.77	0.65
1:O:192:THR:CG2	1:O:194:GLU:HG2	2.27	0.65
1:M:138:PHE:N	1:M:138:PHE:CD2	2.63	0.65
1:M:180:LEU:HD13	1:M:185:TYR:HB2	1.77	0.65
3:V:43:ALA:H	3:V:118:THR:HA	1.62	0.65
1:L:209:ASN:HB3	1:L:213:CYS:SG	2.37	0.65
1:L:111:ALA:CB	1:L:199:THR:CG2	2.73	0.65
2:K:13:GLN:O	2:K:14:PRO:C	2.35	0.65
3:Y:15:LEU:O	3:Y:19:SER:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:ILE:HG22	1:L:48:TYR:N	2.11	0.64
2:I:29:PHE:HB3	2:I:79:SER:HB3	1.79	0.64
1:N:197:HIS:CE1	1:N:199:THR:HB	2.32	0.64
2:J:54:LYS:O	2:J:57:ASN:N	2.29	0.64
2:K:152:PRO:HD2	4:K:227:HOH:O	1.98	0.64
3:X:140:ARG:O	3:X:144:LEU:HB2	1.97	0.64
1:O:15:PRO:HG3	1:O:105:ILE:HD11	1.79	0.64
2:K:57:ASN:O	2:K:59:ALA:N	2.30	0.64
2:K:122:PRO:HB3	2:K:148:TYR:HB3	1.78	0.64
3:Z:45:ASP:H	3:Z:133:HIS:CE1	2.14	0.64
2:H:198:CYS:SG	2:H:198:CYS:O	2.55	0.64
1:M:88:GLN:HE22	1:M:90:ARG:HH11	1.45	0.64
2:I:204:ALA:O	2:I:206:SER:N	2.29	0.64
1:N:31:TYR:HA	1:N:50:THR:OG1	1.98	0.64
1:N:64:SER:OG	1:N:65:GLY:N	2.28	0.64
1:O:131:VAL:N	1:O:178:LEU:O	2.26	0.64
1:O:192:THR:HG23	1:O:194:GLU:HG2	1.78	0.64
2:K:102:SER:OG	3:Z:111:GLN:HB2	1.98	0.64
2:J:191:TRP:CD1	2:J:192:PRO:HA	2.33	0.64
2:K:69:ARG:HH11	2:K:89:ARG:NH2	1.93	0.64
2:J:38:ARG:HB2	2:J:96:TYR:HE2	1.60	0.64
2:J:60:ILE:C	2:J:61:HIS:CD2	2.71	0.64
2:K:51:ILE:HD13	2:K:74:ARG:HD2	1.79	0.64
1:N:149:ILE:HG23	1:N:191:TYR:HE2	1.55	0.64
2:J:191:TRP:HA	2:J:193:SER:N	2.13	0.64
2:H:138:MET:HE3	2:H:187:PRO:HA	1.80	0.64
2:I:43:LYS:HB3	4:I:237:HOH:O	1.97	0.64
2:J:26:GLY:O	2:J:27:PHE:HB3	1.97	0.64
1:L:14:SER:HB2	1:L:17:GLU:OE1	1.98	0.64
2:H:69:ARG:O	2:H:86:ASN:HB2	1.98	0.64
1:M:147:TRP:O	1:M:154:ARG:N	2.31	0.64
2:I:93:THR:HG1	2:I:114:VAL:H	1.46	0.64
1:N:160:ASN:OD1	1:N:176:SER:OG	2.10	0.64
2:J:51:ILE:CD1	2:J:74:ARG:HG3	2.26	0.64
3:Y:124:PRO:O	3:Y:125:ASN:C	2.35	0.64
3:Z:25:ARG:HG2	3:Z:28:GLN:OE1	1.98	0.64
3:Z:31:GLU:HB3	3:Z:33:HIS:CE1	2.33	0.64
1:M:60:ARG:HH12	1:M:81:ASP:CG	2.00	0.64
1:N:19:VAL:HG21	1:N:103:LEU:HD21	1.79	0.64
2:J:51:ILE:O	2:J:52:ARG:O	2.16	0.64
2:J:144:LEU:HD12	2:J:145:VAL:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:191:TRP:CG	2:J:192:PRO:HA	2.32	0.64
1:M:22:THR:CG2	1:M:23:CYS:N	2.62	0.63
1:M:61:PHE:CE1	1:M:74:ILE:CG1	2.81	0.63
1:O:189:ASN:HA	1:O:210:ARG:HB2	1.80	0.63
3:V:41:LEU:O	3:V:118:THR:HB	1.98	0.63
2:H:70:PHE:CZ	2:H:85:MET:HE1	2.33	0.63
2:I:57:ASN:O	2:I:59:ALA:N	2.31	0.63
2:J:20:LEU:CD1	2:J:96:TYR:HD1	2.00	0.63
2:J:51:ILE:CD1	2:J:74:ARG:HG2	2.23	0.63
3:Z:132:GLN:HA	3:Z:135:LEU:HD12	1.80	0.63
1:L:89:GLN:HE21	1:L:96:THR:HB	1.62	0.63
2:I:151:GLU:CB	2:I:152:PRO:HA	2.29	0.63
1:N:14:SER:N	1:N:17:GLU:OE1	2.23	0.63
3:V:39:VAL:HG21	3:V:77:ALA:HB2	1.80	0.63
3:Y:134:LEU:O	3:Y:139:VAL:N	2.29	0.63
1:L:7:SER:HB2	1:L:22:THR:CG2	2.28	0.63
2:H:38:ARG:NH2	2:H:70:PHE:HE2	1.95	0.63
2:H:46:GLU:HG3	2:H:46:GLU:O	1.97	0.63
2:K:69:ARG:NH2	2:K:92:ASP:OD2	2.31	0.63
3:Y:116:GLY:O	3:Y:118:THR:CG2	2.44	0.63
1:L:30:SER:HB3	1:L:31:TYR:CD2	2.33	0.63
2:K:88:LEU:HB3	2:K:114:VAL:HG11	1.81	0.63
3:Y:100:LEU:O	3:Y:100:LEU:HD22	1.99	0.63
3:Z:101:LEU:CD1	3:Z:105:GLN:NE2	2.62	0.63
1:M:11:MET:CE	1:M:19:VAL:HG22	2.29	0.63
1:M:117:PHE:N	1:M:117:PHE:HD1	1.96	0.63
1:O:41:THR:HA	4:O:226:HOH:O	1.98	0.63
1:M:14:SER:O	1:M:17:GLU:HB3	1.99	0.63
2:I:173:LEU:HD22	2:I:176:ASP:HA	1.79	0.63
1:N:35:PHE:N	1:N:35:PHE:HD1	1.93	0.63
1:O:6:GLN:NE2	1:O:87:CYS:H	1.95	0.63
2:K:51:ILE:CD1	2:K:74:ARG:HG2	2.29	0.63
3:V:42:PRO:CD	3:V:70:LEU:HD23	2.29	0.63
1:L:135:LEU:HD23	1:L:143:ILE:HD12	1.80	0.63
2:H:145:VAL:HG11	2:H:180:LEU:HD22	1.79	0.63
1:N:188:HIS:O	1:N:210:ARG:NH1	2.31	0.63
2:J:124:VAL:HG11	2:J:200:VAL:CG2	2.27	0.63
3:Z:64:LEU:HD11	3:Z:105:GLN:HE21	1.63	0.63
3:Z:71:LEU:HD11	3:Z:98:ARG:HG2	1.81	0.63
3:Z:110:THR:O	3:Z:110:THR:CG2	2.47	0.63
1:M:33:TYR:N	1:M:33:TYR:HD2	1.93	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:188:HIS:O	1:M:210:ARG:HD2	1.98	0.62
3:X:69:LEU:HD22	4:X:167:HOH:O	1.98	0.62
1:L:88:GLN:HG2	1:L:89:GLN:N	2.13	0.62
2:H:153:VAL:HG23	2:H:202:HIS:HB2	1.80	0.62
1:M:190:SER:O	1:M:191:TYR:CG	2.53	0.62
1:O:150:ASP:OD2	1:O:188:HIS:CB	2.28	0.62
1:L:107:ARG:HD3	1:L:139:TYR:CB	2.29	0.62
1:L:144:ASN:HB2	1:L:196:THR:O	1.98	0.62
3:Z:71:LEU:CD1	3:Z:101:LEU:CD2	2.77	0.62
1:L:120:SER:O	1:L:124:LEU:HD22	1.99	0.62
1:M:37:GLN:HB2	1:M:43:PRO:HA	1.81	0.62
1:N:132:VAL:HG11	2:J:127:LEU:HD13	1.81	0.62
1:O:44:LYS:NZ	1:O:44:LYS:CB	2.61	0.62
1:O:203:PRO:O	1:O:205:VAL:HG23	1.99	0.62
2:I:215:PRO:O	3:Y:120:ALA:HB3	1.99	0.62
1:O:119:PRO:HG3	1:O:130:SER:N	2.14	0.62
1:O:124:LEU:O	1:O:125:THR:C	2.36	0.62
1:O:49:SER:O	1:O:51:SER:N	2.32	0.62
1:L:7:SER:HB2	1:L:22:THR:HB	1.82	0.62
2:H:176:ASP:HB3	4:H:226:HOH:O	1.97	0.62
2:J:64:GLU:HG2	2:J:67:LYS:NZ	2.15	0.62
1:O:8:PRO:O	1:O:101:THR:HG23	2.00	0.62
3:V:93:LEU:O	3:V:96:GLN:HB2	2.00	0.62
1:M:6:GLN:CG	1:M:23:CYS:HB2	2.17	0.62
1:M:78:GLU:O	1:M:79:ALA:C	2.38	0.62
2:I:120:THR:HG21	2:I:177:LEU:HD13	1.80	0.62
1:O:6:GLN:NE2	1:O:86:TYR:HA	2.13	0.62
3:V:40:LEU:N	3:V:40:LEU:HD23	2.15	0.62
1:M:132:VAL:HG23	1:M:133:CYS:N	2.14	0.62
1:M:162:TRP:HE3	1:M:162:TRP:H	1.47	0.62
2:I:202:HIS:CE1	2:I:204:ALA:HB3	2.35	0.62
1:O:120:SER:O	1:O:123:GLN:N	2.33	0.62
2:K:147:GLY:C	2:K:177:LEU:HD13	2.20	0.62
2:H:95:ILE:HD13	2:H:111:LEU:CD2	2.30	0.61
2:I:216:ARG:NH2	3:Y:121:HIS:HA	2.15	0.61
1:N:72:LEU:C	1:N:72:LEU:CD2	2.64	0.61
2:K:172:VAL:O	2:K:178:TYR:HA	1.99	0.61
3:Z:111:GLN:O	3:Z:112:LEU:HD13	2.00	0.61
2:H:38:ARG:HH21	2:H:70:PHE:HE2	1.48	0.61
1:O:149:ILE:HG23	1:O:191:TYR:CE2	2.34	0.61
2:J:51:ILE:HD13	2:J:74:ARG:HG3	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:22:LEU:HD12	3:Y:96:GLN:OE1	1.98	0.61
1:M:111:ALA:CB	1:M:199:THR:HG21	2.30	0.61
1:M:185:TYR:HA	1:M:191:TYR:OH	2.01	0.61
2:J:74:ARG:NE	2:J:76:ASP:OD1	2.29	0.61
2:K:9:GLY:HA2	2:K:112:VAL:HG22	1.83	0.61
3:Y:134:LEU:O	3:Y:139:VAL:HB	2.01	0.61
2:H:51:ILE:HD12	2:H:74:ARG:HG2	1.82	0.61
2:K:166:VAL:HG12	2:K:184:VAL:HG23	1.82	0.61
3:V:51:TRP:CZ2	3:V:138:LYS:HG2	2.36	0.61
1:L:116:ILE:HD12	1:L:193:CYS:HB3	1.83	0.61
1:L:169:ASP:OD2	1:L:171:THR:HG23	2.00	0.61
1:M:119:PRO:HD3	1:M:131:VAL:CG2	2.30	0.61
2:J:62:TYR:OH	2:J:71:THR:HA	2.00	0.61
1:O:95:ARG:HG3	2:K:47:TRP:CG	2.35	0.61
1:L:60:ARG:NH1	1:L:81:ASP:OD1	2.33	0.61
2:I:149:PHE:HB2	2:I:177:LEU:HD21	1.81	0.61
1:N:36:GLN:NE2	1:N:85:TYR:OH	2.34	0.61
1:O:19:VAL:HG12	1:O:74:ILE:CB	2.31	0.61
1:O:185:TYR:CE1	1:O:191:TYR:HE1	2.17	0.61
1:O:202:SER:O	1:O:203:PRO:C	2.39	0.61
2:K:101:TRP:CD1	3:Z:111:GLN:HB3	2.35	0.61
3:Z:43:ALA:CB	3:Z:119:THR:HG23	2.30	0.61
1:M:123:GLN:NE2	1:M:130:SER:HG	1.98	0.61
2:I:29:PHE:HE2	2:I:76:ASP:HA	1.66	0.61
1:O:33:TYR:N	1:O:33:TYR:HD1	1.97	0.61
2:K:29:PHE:CD2	2:K:79:SER:HA	2.36	0.61
3:Z:94:SER:OG	3:Z:95:GLY:N	2.32	0.61
1:L:35:PHE:N	1:L:35:PHE:HD1	1.98	0.61
2:H:151:GLU:HG2	2:H:152:PRO:HA	1.82	0.61
3:V:33:HIS:HB3	3:V:34:PRO:HD2	1.82	0.61
3:Y:10:ARG:HA	3:Y:13:SER:CB	2.31	0.61
2:J:129:PRO:HD2	2:J:191:TRP:HH2	1.64	0.60
1:M:136:ASN:HA	1:M:173:SER:HB3	1.82	0.60
1:N:211:ASN:ND2	1:N:212:GLU:H	1.98	0.60
1:L:84:THR:CG2	1:L:85:TYR:N	2.64	0.60
1:L:189:ASN:ND2	1:L:211:ASN:OD1	2.34	0.60
1:M:6:GLN:NE2	1:M:87:CYS:H	1.98	0.60
1:M:70:TYR:O	1:M:71:SER:HB3	2.02	0.60
3:V:102:GLY:O	3:V:104:LEU:N	2.35	0.60
2:H:101:TRP:HB2	2:H:104:LEU:HB3	1.83	0.60
1:M:147:TRP:CG	1:M:178:LEU:HD12	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:33:TRP:CE2	2:I:52:ARG:HG3	2.37	0.60
3:V:64:LEU:CD1	3:V:105:GLN:HG3	2.32	0.60
1:M:6:GLN:OE1	1:M:100:GLY:HA2	2.01	0.60
1:M:185:TYR:CE1	1:M:191:TYR:CE1	2.89	0.60
2:I:61:HIS:CD2	2:I:61:HIS:N	2.68	0.60
1:N:54:ALA:O	1:N:57:VAL:HG23	2.01	0.60
1:N:149:ILE:CG2	1:N:191:TYR:HE2	2.14	0.60
1:O:182:LYS:HD3	1:O:186:GLU:CD	2.22	0.60
2:H:52:ARG:O	2:H:58:HIS:HA	2.00	0.60
1:N:130:SER:HB3	1:N:179:THR:OG1	2.02	0.60
2:K:62:TYR:CE1	2:K:72:VAL:HG12	2.37	0.60
3:Z:61:GLN:HG3	3:Z:108:LEU:HD13	1.83	0.60
1:M:70:TYR:N	1:M:70:TYR:HD1	1.99	0.60
2:I:125:TYR:N	2:I:144:LEU:O	2.30	0.60
2:K:49:ALA:HA	2:K:61:HIS:O	2.02	0.60
3:Z:31:GLU:OE1	3:Z:33:HIS:HE1	1.85	0.60
3:Z:94:SER:O	3:Z:98:ARG:HG3	2.02	0.60
1:L:29:VAL:HG11	1:L:91:SER:CB	2.20	0.60
2:H:153:VAL:CG1	2:H:180:LEU:HD13	2.32	0.60
2:H:189:SER:HB3	4:H:224:HOH:O	1.78	0.60
2:I:57:ASN:O	2:I:58:HIS:C	2.38	0.60
1:M:189:ASN:O	1:M:209:ASN:HA	2.02	0.60
1:O:53:LEU:HD22	1:O:57:VAL:HG11	1.83	0.60
3:X:22:LEU:HD21	3:X:92:GLN:HE21	1.66	0.60
3:X:23:HIS:CD2	3:X:23:HIS:O	2.55	0.60
3:Y:91:GLY:O	3:Y:92:GLN:C	2.38	0.60
1:N:38:LYS:HD3	1:N:83:ALA:HB2	1.84	0.59
2:H:84:GLN:HE21	2:H:84:GLN:HA	1.66	0.59
2:H:158:ASN:ND2	2:H:197:THR:H	2.00	0.59
1:M:118:PRO:HB3	1:M:208:PHE:CZ	2.36	0.59
2:I:106:TRP:HA	4:I:235:HOH:O	2.01	0.59
2:I:202:HIS:ND1	2:I:204:ALA:HB3	2.16	0.59
2:J:124:VAL:HA	2:J:144:LEU:O	2.03	0.59
1:O:185:TYR:CE1	1:O:191:TYR:CE1	2.90	0.59
2:K:70:PHE:CD1	2:K:85:MET:HA	2.37	0.59
2:K:199:ASN:HA	2:K:208:LYS:O	2.02	0.59
1:L:106:LYS:HG3	1:L:106:LYS:O	2.02	0.59
2:H:169:PHE:O	4:H:233:HOH:O	2.17	0.59
2:K:66:VAL:CG1	2:K:70:PHE:H	2.16	0.59
3:V:100:LEU:HD22	3:V:104:LEU:CD1	2.33	0.59
3:X:12:LEU:O	3:X:12:LEU:HG	1.92	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:124:PRO:C	3:Y:126:ALA:N	2.52	0.59
1:L:175:SER:N	2:H:169:PHE:CE1	2.70	0.59
2:H:66:VAL:CG1	2:H:70:PHE:HB2	2.33	0.59
2:I:216:ARG:HE	3:Y:122:LYS:N	1.96	0.59
1:O:169:ASP:O	1:O:169:ASP:OD2	2.19	0.59
3:V:61:GLN:CD	3:V:112:LEU:HD21	2.22	0.59
3:Y:136:ARG:NH1	3:Y:136:ARG:HB2	2.16	0.59
2:I:33:TRP:HD1	2:I:53:SER:HB2	1.66	0.59
1:N:33:TYR:HD2	1:N:48:TYR:HA	1.67	0.59
2:J:57:ASN:O	2:J:59:ALA:N	2.36	0.59
3:X:95:GLY:O	3:X:98:ARG:HB2	2.02	0.59
3:Y:41:LEU:HD12	3:Y:121:HIS:CD2	2.38	0.59
2:H:29:PHE:C	2:H:29:PHE:CD2	2.75	0.59
1:N:147:TRP:CD1	1:N:158:VAL:CG1	2.85	0.59
2:K:37:VAL:HG13	2:K:46:GLU:O	2.02	0.59
2:K:66:VAL:CG1	2:K:70:PHE:CD2	2.86	0.59
2:K:148:TYR:CE1	2:K:178:TYR:HB3	2.38	0.59
2:K:202:HIS:HB3	2:K:206:SER:OG	2.03	0.59
2:K:216:ARG:HH21	3:V:123:ASP:H	1.49	0.59
3:Z:51:TRP:CH2	3:Z:138:LYS:HD3	2.37	0.59
3:Z:118:THR:O	3:Z:119:THR:CG2	2.50	0.59
1:M:20:THR:HB	1:M:73:THR:HG1	1.66	0.59
2:J:84:GLN:HE21	2:J:85:MET:N	2.00	0.59
3:Y:136:ARG:CB	3:Y:136:ARG:HH11	2.14	0.59
2:H:37:VAL:HG22	2:H:47:TRP:HA	1.83	0.59
1:M:180:LEU:N	1:M:180:LEU:HD12	2.17	0.59
2:I:158:ASN:O	2:I:159:SER:C	2.40	0.59
1:N:123:GLN:HG3	2:J:125:TYR:CE2	2.38	0.59
2:J:217:ASP:OD1	3:X:121:HIS:CE1	2.55	0.59
1:O:148:LYS:HA	1:O:153:GLU:HA	1.83	0.59
3:V:143:MET:HB2	3:V:149:THR:HG21	1.84	0.59
3:Y:100:LEU:HD22	3:Y:104:LEU:HD11	1.85	0.59
2:H:138:MET:HE2	2:H:185:THR:CG2	2.33	0.59
1:M:88:GLN:HB2	1:M:97:PHE:CD1	2.38	0.59
3:V:125:ASN:N	3:V:125:ASN:ND2	2.51	0.59
3:Y:48:LEU:HB2	3:Y:51:TRP:HB3	1.85	0.59
1:M:192:THR:CA	1:M:207:SER:OG	2.51	0.58
2:I:148:TYR:O	2:I:177:LEU:HD22	2.04	0.58
1:L:89:GLN:CG	1:L:96:THR:HB	2.33	0.58
2:H:56:ASN:N	2:H:56:ASN:ND2	2.50	0.58
2:J:56:ASN:HD22	2:J:56:ASN:N	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:48:TYR:CE2	3:Z:113:PRO:HG2	2.38	0.58
3:Y:70:LEU:HD22	3:Y:74:VAL:HG23	1.84	0.58
1:L:14:SER:O	1:L:17:GLU:HB3	2.03	0.58
2:I:148:TYR:CZ	2:I:178:TYR:HB3	2.39	0.58
1:N:78:GLU:O	1:N:81:ASP:HB2	2.03	0.58
1:O:154:ARG:NH2	1:O:184:GLU:OE1	2.35	0.58
3:X:61:GLN:O	3:X:62:ASP:C	2.42	0.58
3:X:64:LEU:HD22	3:X:108:LEU:HD12	1.85	0.58
3:Z:118:THR:O	3:Z:119:THR:HG22	2.03	0.58
1:L:93:TYR:HE1	1:L:95:ARG:NH1	2.00	0.58
2:H:102:SER:O	2:H:103:PHE:HB2	2.02	0.58
2:H:216:ARG:HH22	3:Z:123:ASP:HB2	1.68	0.58
1:M:11:MET:HE2	1:M:19:VAL:HG22	1.84	0.58
2:I:37:VAL:HG21	2:I:106:TRP:HH2	1.68	0.58
2:J:70:PHE:CD1	2:J:85:MET:CB	2.86	0.58
1:O:19:VAL:HG11	1:O:74:ILE:CD1	2.29	0.58
3:V:71:LEU:HD11	3:V:98:ARG:HG3	1.84	0.58
3:Y:100:LEU:HD12	3:Y:131:PHE:HE1	1.67	0.58
1:L:65:GLY:HA3	1:L:70:TYR:HA	1.86	0.58
1:L:153:GLU:HG2	1:L:155:GLN:HG2	1.86	0.58
2:J:61:HIS:CD2	2:J:61:HIS:N	2.70	0.58
1:O:189:ASN:O	1:O:210:ARG:N	2.32	0.58
2:H:191:TRP:CG	2:H:192:PRO:HA	2.39	0.58
1:M:70:TYR:N	1:M:70:TYR:CD1	2.70	0.58
1:M:88:GLN:HG2	1:M:89:GLN:N	2.18	0.58
2:I:139:VAL:CG1	2:I:141:LEU:HD21	2.34	0.58
2:J:216:ARG:HG3	3:X:122:LYS:CG	2.33	0.58
3:V:67:VAL:O	3:V:70:LEU:N	2.36	0.58
3:X:135:LEU:HA	3:X:139:VAL:HB	1.85	0.58
3:Y:12:LEU:HB3	3:Y:143:MET:SD	2.44	0.58
1:M:78:GLU:OE2	1:N:107:ARG:NH2	2.37	0.58
2:I:29:PHE:CD2	2:I:79:SER:HA	2.39	0.58
1:N:77:MET:CE	1:N:81:ASP:CB	2.77	0.58
1:N:147:TRP:O	1:N:154:ARG:N	2.34	0.58
2:K:64:GLU:HG2	2:K:67:LYS:HD2	1.86	0.58
3:Z:119:THR:HG1	3:Z:121:HIS:HE2	1.47	0.58
2:H:20:LEU:N	2:H:20:LEU:HD23	2.19	0.58
1:M:22:THR:CG2	1:M:23:CYS:H	2.17	0.58
2:I:214:VAL:HG11	3:Y:40:LEU:HD21	1.86	0.58
1:N:154:ARG:NH2	1:N:184:GLU:OE1	2.37	0.58
1:O:61:PHE:HZ	1:O:85:TYR:OH	1.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:185:TYR:HD1	1:O:191:TYR:CE1	2.22	0.58
3:Y:41:LEU:HD12	3:Y:121:HIS:HD2	1.69	0.58
1:L:147:TRP:CD2	1:L:178:LEU:HD12	2.39	0.58
1:L:205:VAL:HG12	1:L:206:LYS:N	2.19	0.58
2:H:88:LEU:HB3	2:H:114:VAL:HG11	1.86	0.58
2:H:120:THR:O	2:H:148:TYR:HA	2.03	0.58
1:N:139:TYR:CD2	1:N:140:PRO:HA	2.37	0.58
2:J:123:SER:N	2:J:146:LYS:O	2.37	0.58
1:O:44:LYS:HB2	1:O:44:LYS:HZ2	1.68	0.58
1:L:65:GLY:CA	1:L:70:TYR:HA	2.34	0.57
2:H:166:VAL:O	2:H:166:VAL:CG2	2.51	0.57
1:O:77:MET:CE	1:O:78:GLU:O	2.51	0.57
3:X:70:LEU:O	3:X:74:VAL:HG23	2.04	0.57
2:H:114:VAL:HG23	2:H:114:VAL:O	2.03	0.57
2:K:56:ASN:O	2:K:57:ASN:HB2	2.03	0.57
2:K:89:ARG:O	2:K:114:VAL:HG21	2.03	0.57
3:V:13:SER:O	3:V:17:ARG:HD3	2.05	0.57
1:L:131:VAL:O	1:L:147:TRP:CZ2	2.58	0.57
1:M:72:LEU:HD23	1:M:72:LEU:C	2.25	0.57
1:O:66:SER:C	1:O:70:TYR:HE1	2.07	0.57
3:V:145:VAL:HG13	3:V:145:VAL:O	2.04	0.57
1:M:84:THR:HA	1:M:101:THR:O	2.04	0.57
1:M:120:SER:C	1:M:122:GLU:H	2.07	0.57
1:N:6:GLN:NE2	1:N:86:TYR:HA	2.14	0.57
2:J:189:SER:O	2:J:193:SER:HB2	2.04	0.57
2:K:166:VAL:HG12	2:K:184:VAL:CG2	2.35	0.57
3:Z:22:LEU:HD11	3:Z:92:GLN:HB3	1.87	0.57
1:M:211:ASN:C	1:M:212:GLU:HG3	2.25	0.57
2:I:157:TRP:O	2:I:158:ASN:HB2	2.04	0.57
1:N:88:GLN:NE2	1:N:90:ARG:HH11	2.03	0.57
1:N:149:ILE:CG2	1:N:191:TYR:CE2	2.81	0.57
3:V:87:SER:O	3:V:89:LEU:N	2.37	0.57
3:V:143:MET:HB3	3:V:149:THR:HB	1.87	0.57
1:L:10:ILE:HG12	1:L:102:LYS:HB3	1.85	0.57
1:M:91:SER:HB2	4:M:228:HOH:O	2.04	0.57
2:I:92:ASP:O	2:I:96:TYR:OH	2.17	0.57
1:O:116:ILE:CG1	1:O:133:CYS:SG	2.89	0.57
1:O:132:VAL:HB	1:O:177:THR:CG2	2.34	0.57
2:H:9:GLY:HA2	2:H:112:VAL:HG22	1.86	0.57
2:H:36:TRP:CH2	2:H:98:CYS:HB2	2.40	0.57
1:M:35:PHE:N	1:M:35:PHE:CD1	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:22:CYS:O	2:I:80:SER:CB	2.51	0.57
2:I:51:ILE:CD1	2:I:74:ARG:HG3	2.35	0.57
1:N:207:SER:OG	1:N:208:PHE:N	2.35	0.57
1:O:77:MET:CE	1:O:81:ASP:HB2	2.33	0.57
3:V:41:LEU:HD11	3:V:127:ILE:HG22	1.86	0.57
3:V:41:LEU:HD22	3:V:127:ILE:HB	1.86	0.57
3:Y:12:LEU:O	3:Y:16:LEU:HB2	2.05	0.57
3:Y:75:MET:SD	3:Y:98:ARG:NH2	2.77	0.57
1:L:117:PHE:CD1	1:L:117:PHE:N	2.70	0.57
1:M:115:SER:O	1:M:133:CYS:HA	2.04	0.57
2:J:124:VAL:CG1	2:J:200:VAL:HG21	2.28	0.57
2:J:172:VAL:O	2:J:178:TYR:HA	2.04	0.57
1:O:2:VAL:O	1:O:96:THR:HG21	2.04	0.57
1:O:135:LEU:HD21	1:O:195:ALA:HB2	1.87	0.57
2:K:29:PHE:HZ	2:K:81:VAL:HB	1.69	0.57
1:L:105:ILE:HG13	1:L:106:LYS:H	1.68	0.57
1:L:173:SER:HB2	4:L:221:HOH:O	2.03	0.57
1:M:45:LEU:C	1:M:45:LEU:CD2	2.73	0.57
2:J:64:GLU:HG2	2:J:67:LYS:HZ2	1.70	0.57
2:K:22:CYS:HB3	2:K:81:VAL:HG12	1.87	0.57
3:V:12:LEU:HD21	3:V:140:ARG:HH21	1.70	0.57
3:Z:86:LEU:HD22	3:Z:90:LEU:HG	1.86	0.57
1:L:77:MET:HG3	1:L:78:GLU:N	2.20	0.57
1:M:106:LYS:HG3	1:M:106:LYS:O	2.03	0.57
2:J:129:PRO:HD2	2:J:191:TRP:CH2	2.40	0.57
3:Y:124:PRO:C	3:Y:126:ALA:H	2.08	0.57
3:Z:64:LEU:CD1	3:Z:105:GLN:HE21	2.18	0.57
2:I:139:VAL:HG11	2:I:141:LEU:HD21	1.87	0.56
2:J:130:GLY:O	2:J:133:ALA:HA	2.04	0.56
1:O:51:SER:HB3	1:O:63:GLY:O	2.05	0.56
1:O:145:VAL:HG21	1:O:174:MET:HE2	1.87	0.56
2:H:191:TRP:CD1	2:H:196:VAL:CG1	2.88	0.56
1:M:185:TYR:CD1	1:M:191:TYR:CE1	2.93	0.56
2:I:37:VAL:HG21	2:I:106:TRP:CH2	2.40	0.56
2:I:99:SER:HA	4:I:235:HOH:O	2.05	0.56
1:N:189:ASN:HD22	1:N:210:ARG:N	2.01	0.56
3:X:78:ARG:HG3	3:X:90:LEU:HB3	1.86	0.56
3:Y:85:CYS:O	3:Y:88:SER:HB3	2.05	0.56
1:L:185:TYR:O	1:L:191:TYR:OH	2.18	0.56
2:H:51:ILE:CD1	2:H:74:ARG:CG	2.83	0.56
2:H:66:VAL:HG13	2:H:70:PHE:CG	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:89:GLN:HE21	1:N:96:THR:H	1.52	0.56
2:J:70:PHE:HD1	2:J:85:MET:CA	2.11	0.56
1:O:7:SER:HB2	1:O:22:THR:HB	1.87	0.56
1:O:19:VAL:HG12	1:O:74:ILE:CG1	2.36	0.56
1:O:145:VAL:HG11	1:O:176:SER:OG	2.04	0.56
3:V:29:CYS:O	3:V:30:PRO:O	2.23	0.56
3:V:90:LEU:HD23	3:V:90:LEU:N	2.15	0.56
3:Y:144:LEU:O	3:Y:146:GLY:N	2.38	0.56
2:H:66:VAL:CG1	2:H:70:PHE:CG	2.89	0.56
1:M:116:ILE:HD13	1:M:208:PHE:CD1	2.40	0.56
2:J:125:TYR:HB2	2:J:144:LEU:HB3	1.87	0.56
2:K:213:ILE:HG12	2:K:214:VAL:H	1.70	0.56
3:X:77:ALA:O	3:X:78:ARG:C	2.38	0.56
3:Z:107:LEU:CD2	3:Z:107:LEU:C	2.73	0.56
2:H:84:GLN:HE21	2:H:84:GLN:C	2.08	0.56
2:H:191:TRP:CD1	2:H:192:PRO:HA	2.40	0.56
1:M:61:PHE:CE1	1:M:74:ILE:HG12	2.40	0.56
1:M:181:THR:O	1:M:182:LYS:C	2.42	0.56
2:I:123:SER:O	2:I:145:VAL:HA	2.06	0.56
2:I:213:ILE:O	2:I:213:ILE:HG22	2.05	0.56
1:N:149:ILE:HG23	1:N:191:TYR:CD2	2.40	0.56
2:J:191:TRP:HA	2:J:192:PRO:C	2.25	0.56
3:Y:73:GLY:HA2	3:Y:76:ALA:HB3	1.87	0.56
3:Z:23:HIS:O	3:Z:26:LEU:HB3	2.04	0.56
1:L:147:TRP:HB3	1:L:178:LEU:HD12	1.88	0.56
1:L:213:CYS:HA	3:Y:140:ARG:NH2	2.20	0.56
1:N:189:ASN:HD22	1:N:210:ARG:H	1.49	0.56
1:L:2:VAL:HG23	4:L:232:HOH:O	2.05	0.56
1:L:164:ASP:O	1:L:165:GLN:C	2.40	0.56
2:H:33:TRP:N	3:V:111:GLN:HE22	2.04	0.56
2:H:33:TRP:HD1	2:H:53:SER:HG	1.53	0.56
2:H:90:ALA:HA	2:H:114:VAL:CG2	2.36	0.56
1:N:77:MET:HE3	1:N:78:GLU:O	2.06	0.56
3:X:78:ARG:NH1	3:X:87:SER:OG	2.34	0.56
1:M:124:LEU:O	1:M:126:SER:N	2.39	0.56
1:M:48:TYR:CE1	3:X:113:PRO:CG	2.82	0.56
2:I:22:CYS:HB3	2:I:81:VAL:O	2.06	0.56
2:I:74:ARG:HG2	2:I:74:ARG:HH11	1.71	0.56
1:N:119:PRO:HD2	1:N:131:VAL:CG2	2.36	0.56
2:J:70:PHE:CD1	2:J:85:MET:CA	2.88	0.56
2:I:207:THR:O	2:I:207:THR:OG1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:101:LEU:CD1	3:Z:105:GLN:HE22	2.17	0.56
2:H:173:LEU:HD22	2:H:176:ASP:HA	1.87	0.55
1:O:132:VAL:HA	1:O:177:THR:HA	1.88	0.55
2:H:138:MET:HE3	2:H:138:MET:HA	1.86	0.55
1:M:174:MET:HG2	1:M:175:SER:N	2.21	0.55
1:N:90:ARG:O	1:N:95:ARG:NH2	2.40	0.55
1:N:162:TRP:CD2	1:N:174:MET:HG3	2.41	0.55
2:K:70:PHE:HD1	2:K:85:MET:HA	1.71	0.55
2:K:142:GLY:HA2	2:K:182:SER:O	2.06	0.55
2:J:15:GLY:N	2:J:88:LEU:O	2.34	0.55
1:O:76:ARG:NH1	1:O:76:ARG:HG2	2.20	0.55
2:K:66:VAL:HG13	2:K:70:PHE:H	1.72	0.55
2:K:70:PHE:CE1	2:K:85:MET:HB3	2.41	0.55
3:V:70:LEU:O	3:V:74:VAL:HG23	2.06	0.55
3:Y:30:PRO:O	3:Y:32:VAL:N	2.39	0.55
1:L:185:TYR:HD1	1:L:191:TYR:CE1	2.21	0.55
2:H:153:VAL:HG12	2:H:180:LEU:HD13	1.89	0.55
1:M:53:LEU:HD11	1:M:61:PHE:O	2.05	0.55
2:I:151:GLU:CG	2:I:152:PRO:HA	2.36	0.55
2:J:20:LEU:N	2:J:20:LEU:HD23	2.22	0.55
1:O:7:SER:OG	1:O:8:PRO:HD3	2.06	0.55
2:K:50:GLU:HG2	2:K:51:ILE:N	2.21	0.55
3:Z:34:PRO:HA	3:Z:124:PRO:HD2	1.89	0.55
1:L:132:VAL:HB	1:L:177:THR:HG23	1.89	0.55
1:L:154:ARG:CD	1:L:156:ASN:O	2.54	0.55
2:J:90:ALA:N	2:J:91:GLU:OE1	2.39	0.55
2:K:120:THR:O	2:K:149:PHE:N	2.35	0.55
3:V:147:GLY:O	3:V:149:THR:N	2.40	0.55
3:X:81:LEU:HD12	3:X:87:SER:CB	2.34	0.55
1:L:3:VAL:H	1:L:26:SER:CB	2.20	0.55
1:L:114:VAL:HG12	1:L:115:SER:N	2.20	0.55
2:H:148:TYR:O	2:H:178:TYR:HB2	2.06	0.55
1:M:114:VAL:HA	1:M:134:PHE:O	2.07	0.55
1:N:36:GLN:NE2	1:N:85:TYR:HE2	1.98	0.55
1:O:90:ARG:HH21	2:K:102:SER:HB3	1.71	0.55
1:O:108:ALA:O	1:O:109:ASP:C	2.43	0.55
2:H:145:VAL:CG1	2:H:180:LEU:CD2	2.80	0.55
2:H:189:SER:O	2:H:193:SER:OG	2.19	0.55
1:M:116:ILE:CD1	1:M:208:PHE:HD1	2.20	0.55
2:K:51:ILE:HD11	2:K:74:ARG:CG	2.36	0.55
3:Y:42:PRO:HD2	3:Y:130:SER:OG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:ARG:NH2	2:H:102:SER:O	2.40	0.55
1:M:116:ILE:HD13	1:M:208:PHE:HD1	1.70	0.55
2:I:12:VAL:O	2:I:114:VAL:HA	2.07	0.55
1:O:135:LEU:CD2	1:O:195:ALA:HB2	2.37	0.55
1:O:147:TRP:HA	1:O:192:THR:O	2.06	0.55
1:O:191:TYR:HB2	1:O:208:PHE:CE1	2.42	0.55
2:K:70:PHE:CZ	2:K:85:MET:HE2	2.42	0.55
2:K:125:TYR:N	2:K:144:LEU:O	2.34	0.55
3:Y:51:TRP:O	3:Y:59:LYS:HD3	2.06	0.55
1:L:143:ILE:HG13	1:L:197:HIS:HD2	1.72	0.55
2:J:91:GLU:OE1	2:J:91:GLU:N	2.40	0.55
3:X:17:ARG:O	3:X:21:VAL:HG23	2.05	0.55
3:Y:64:LEU:O	3:Y:64:LEU:HD12	2.07	0.55
1:M:160:ASN:HB3	1:M:174:MET:CE	2.37	0.55
2:J:85:MET:CE	2:J:96:TYR:CZ	2.86	0.55
2:J:162:LEU:HD13	2:J:184:VAL:HG21	1.88	0.55
2:K:175:SER:OG	2:K:177:LEU:HB2	2.07	0.55
3:Y:136:ARG:HB2	3:Y:136:ARG:HH11	1.70	0.55
2:H:4:LEU:HD12	2:H:107:GLY:H	1.72	0.54
1:M:7:SER:HB3	1:M:8:PRO:HD3	1.87	0.54
3:V:125:ASN:H	3:V:125:ASN:ND2	2.06	0.54
2:H:33:TRP:N	3:V:111:GLN:NE2	2.53	0.54
1:M:72:LEU:HD23	1:M:73:THR:N	2.22	0.54
1:M:111:ALA:HB2	1:M:199:THR:HG21	1.89	0.54
1:N:137:ASN:OD1	1:N:137:ASN:N	2.40	0.54
1:N:189:ASN:ND2	1:N:209:ASN:HB3	2.22	0.54
1:N:197:HIS:ND1	1:N:199:THR:CB	2.67	0.54
2:J:36:TRP:HE1	2:J:81:VAL:HG22	1.73	0.54
2:J:99:SER:OG	2:J:103:PHE:HA	2.06	0.54
1:O:69:SER:C	1:O:70:TYR:CD1	2.77	0.54
1:L:109:ASP:HA	1:L:139:TYR:O	2.08	0.54
2:H:138:MET:HE3	2:H:186:VAL:O	2.07	0.54
1:M:124:LEU:C	1:M:126:SER:H	2.09	0.54
2:I:148:TYR:O	2:I:178:TYR:HB2	2.05	0.54
2:K:6:GLU:HA	2:K:21:SER:O	2.06	0.54
2:K:70:PHE:CD1	2:K:85:MET:CA	2.90	0.54
3:X:125:ASN:O	3:X:127:ILE:N	2.41	0.54
3:Y:131:PHE:CE2	3:Y:135:LEU:HD11	2.42	0.54
1:M:167:SER:C	1:M:168:LYS:HE3	2.27	0.54
2:J:141:LEU:N	2:J:141:LEU:HD23	2.22	0.54
1:N:119:PRO:HG3	1:N:185:TYR:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:154:ARG:HD3	1:N:156:ASN:O	2.08	0.54
2:J:197:THR:HG23	2:J:211:LYS:HB2	1.89	0.54
2:H:6:GLU:OE2	2:H:108:GLN:OE1	2.25	0.54
2:J:145:VAL:CG1	2:J:180:LEU:O	2.56	0.54
1:O:94:PRO:HB3	2:K:47:TRP:CZ3	2.41	0.54
3:Y:51:TRP:O	3:Y:59:LYS:HE2	2.08	0.54
3:Z:116:GLY:O	3:Z:117:ARG:C	2.44	0.54
2:H:38:ARG:NH2	2:H:70:PHE:CE2	2.76	0.54
1:M:180:LEU:HB3	1:M:184:GLU:OE2	2.07	0.54
2:J:143:CYS:O	2:J:181:SER:HA	2.08	0.54
2:K:191:TRP:CD1	2:K:196:VAL:CG1	2.90	0.54
1:L:165:GLN:HA	1:L:171:THR:O	2.08	0.54
1:L:188:HIS:O	1:L:210:ARG:HD3	2.08	0.54
2:H:88:LEU:HD23	2:H:92:ASP:CB	2.37	0.54
2:H:89:ARG:HD2	2:H:91:GLU:CD	2.25	0.54
1:M:86:TYR:CD1	2:I:45:LEU:HD12	2.42	0.54
1:N:211:ASN:ND2	1:N:212:GLU:N	2.56	0.54
2:J:129:PRO:CD	2:J:191:TRP:CH2	2.91	0.54
1:O:119:PRO:HG3	1:O:130:SER:H	1.73	0.54
2:K:108:GLN:OE1	2:K:108:GLN:N	2.39	0.54
3:V:35:LEU:HD22	3:V:122:LYS:O	2.08	0.54
3:X:14:LYS:O	3:X:18:ASP:HB2	2.07	0.54
3:X:16:LEU:HD11	3:X:136:ARG:HG2	1.90	0.54
3:Y:90:LEU:HD23	3:Y:93:LEU:HD12	1.90	0.54
2:H:125:TYR:HB2	2:H:144:LEU:HB3	1.90	0.54
2:I:215:PRO:O	3:Y:120:ALA:CB	2.56	0.54
2:J:33:TRP:CG	3:Y:111:GLN:NE2	2.76	0.54
2:J:64:GLU:OE2	2:J:67:LYS:HD2	2.08	0.54
2:K:38:ARG:HB3	2:K:96:TYR:CE1	2.43	0.54
3:X:24:SER:O	3:X:26:LEU:N	2.41	0.54
2:H:51:ILE:HD12	2:H:74:ARG:HG3	1.88	0.54
1:M:174:MET:HE2	1:M:175:SER:O	2.07	0.54
1:N:79:ALA:CA	1:N:105:ILE:HD13	2.36	0.54
1:L:37:GLN:HG2	1:L:38:LYS:H	1.73	0.53
1:L:77:MET:HE3	1:L:78:GLU:O	2.07	0.53
2:H:100:GLY:HA3	2:H:105:TYR:N	2.20	0.53
2:H:149:PHE:HB2	2:H:177:LEU:CD2	2.38	0.53
1:M:118:PRO:HG3	1:M:208:PHE:CE1	2.43	0.53
1:M:123:GLN:HG3	2:I:125:TYR:CE2	2.43	0.53
1:M:132:VAL:HG11	2:I:144:LEU:HD22	1.88	0.53
1:N:41:THR:HG22	4:N:227:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:89:ARG:O	2:J:114:VAL:HG21	2.08	0.53
1:O:11:MET:CE	1:O:11:MET:HB2	2.38	0.53
3:X:67:VAL:HG21	3:X:100:LEU:HD13	1.89	0.53
1:L:20:THR:HB	1:L:73:THR:HG23	1.90	0.53
1:L:49:SER:O	1:L:51:SER:N	2.41	0.53
1:L:184:GLU:HG3	1:L:187:ARG:NH1	2.23	0.53
1:M:104:GLU:OE1	4:M:229:HOH:O	2.19	0.53
1:M:185:TYR:HD1	1:M:191:TYR:OH	1.90	0.53
1:M:185:TYR:O	1:M:191:TYR:OH	2.22	0.53
2:I:33:TRP:H	3:X:111:GLN:NE2	2.05	0.53
1:N:135:LEU:HD21	1:N:195:ALA:HB2	1.90	0.53
1:N:205:VAL:CG1	1:N:205:VAL:O	2.56	0.53
2:H:39:GLN:O	2:H:95:ILE:HG12	2.08	0.53
2:H:84:GLN:CA	2:H:84:GLN:NE2	2.71	0.53
2:H:90:ALA:HA	2:H:114:VAL:HG23	1.90	0.53
2:I:216:ARG:HD2	3:Y:122:LYS:HG3	1.90	0.53
1:N:111:ALA:HA	1:N:199:THR:HG21	1.89	0.53
2:J:3:LYS:O	2:J:24:ALA:HA	2.08	0.53
2:J:127:LEU:HB2	2:J:142:GLY:HA3	1.90	0.53
2:K:54:LYS:O	2:K:57:ASN:N	2.41	0.53
3:Y:14:LYS:O	3:Y:18:ASP:N	2.33	0.53
3:Z:13:SER:O	3:Z:14:LYS:C	2.47	0.53
1:L:75:SER:OG	1:L:76:ARG:N	2.38	0.53
1:L:147:TRP:CE3	1:L:178:LEU:HD12	2.43	0.53
2:H:89:ARG:O	2:H:92:ASP:N	2.42	0.53
2:I:54:LYS:NZ	2:I:58:HIS:HE1	2.06	0.53
2:J:189:SER:O	2:J:193:SER:CB	2.57	0.53
1:N:120:SER:O	1:N:121:SER:C	2.46	0.53
2:K:123:SER:O	2:K:146:LYS:N	2.36	0.53
3:V:43:ALA:N	3:V:118:THR:HA	2.23	0.53
3:Z:31:GLU:OE1	3:Z:33:HIS:CE1	2.62	0.53
1:L:21:ILE:HD12	1:L:72:LEU:HD22	1.91	0.53
2:H:196:VAL:O	2:H:196:VAL:HG22	2.08	0.53
2:J:56:ASN:N	2:J:56:ASN:ND2	2.56	0.53
2:J:145:VAL:HG13	2:J:180:LEU:O	2.08	0.53
2:H:40:SER:OG	2:H:43:LYS:HB3	2.08	0.53
2:I:216:ARG:HH21	3:Y:122:LYS:N	2.05	0.53
1:N:178:LEU:HD22	1:N:180:LEU:CD2	2.39	0.53
2:K:70:PHE:CG	2:K:85:MET:HB3	2.42	0.53
3:X:9:LEU:O	3:X:11:VAL:N	2.42	0.53
3:X:56:GLU:HB3	4:X:174:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:15:LEU:HD23	3:Y:135:LEU:HD21	1.89	0.53
3:Z:15:LEU:O	3:Z:19:SER:HB3	2.08	0.53
1:M:111:ALA:HB2	1:M:199:THR:CG2	2.39	0.53
1:M:132:VAL:HG23	1:M:133:CYS:H	1.71	0.53
2:J:197:THR:HA	2:J:211:LYS:HA	1.90	0.53
2:H:138:MET:CE	2:H:185:THR:HG22	2.38	0.53
2:J:69:ARG:HH11	2:J:89:ARG:NH2	2.05	0.53
3:Y:35:LEU:N	3:Y:122:LYS:O	2.31	0.53
3:Y:133:HIS:CD2	3:Z:46:PHE:CD2	2.97	0.53
3:Z:87:SER:O	3:Z:88:SER:C	2.47	0.53
3:Z:101:LEU:HD11	3:Z:105:GLN:NE2	2.22	0.53
1:M:192:THR:OG1	1:M:207:SER:CB	2.56	0.53
2:I:158:ASN:C	2:I:160:GLY:N	2.62	0.53
1:O:84:THR:HA	1:O:101:THR:O	2.08	0.53
2:K:66:VAL:HG21	2:K:70:PHE:CD2	2.44	0.53
3:X:123:ASP:O	3:X:125:ASN:N	2.42	0.53
3:Z:93:LEU:HG	3:Z:128:PHE:CD1	2.44	0.53
1:L:7:SER:CB	1:L:22:THR:HB	2.39	0.52
2:H:72:VAL:HG22	2:H:73:SER:N	2.24	0.52
1:M:61:PHE:CE1	1:M:74:ILE:HG13	2.43	0.52
2:I:206:SER:C	2:I:207:THR:HG22	2.29	0.52
1:N:130:SER:HA	1:N:179:THR:HA	1.91	0.52
1:O:36:GLN:HG2	1:O:37:GLN:N	2.24	0.52
3:V:55:MET:O	3:V:59:LYS:HG3	2.10	0.52
3:X:90:LEU:HD11	3:X:127:ILE:HD11	1.91	0.52
1:N:121:SER:O	1:N:124:LEU:N	2.35	0.52
2:K:39:GLN:OE1	2:K:97:TYR:OH	2.24	0.52
1:L:7:SER:HB2	1:L:22:THR:CB	2.39	0.52
2:H:202:HIS:CE1	2:H:204:ALA:HB2	2.44	0.52
1:M:86:TYR:CE1	2:I:45:LEU:HD12	2.44	0.52
1:M:123:GLN:CD	1:M:130:SER:HG	2.13	0.52
1:N:70:TYR:N	1:N:70:TYR:CD1	2.75	0.52
2:K:38:ARG:NH1	2:K:46:GLU:OE1	2.30	0.52
2:K:87:SER:O	2:K:87:SER:OG	2.24	0.52
1:L:111:ALA:HB2	1:L:199:THR:OG1	2.10	0.52
1:M:35:PHE:O	1:M:85:TYR:HA	2.10	0.52
2:I:27:PHE:HE2	2:I:29:PHE:HA	1.66	0.52
1:O:107:ARG:HG3	1:O:108:ALA:N	2.24	0.52
1:O:147:TRP:CD1	1:O:158:VAL:HG12	2.45	0.52
3:Z:29:CYS:SG	3:Z:89:LEU:HD12	2.49	0.52
1:M:7:SER:OG	1:M:8:PRO:CD	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:132:VAL:CG2	1:M:133:CYS:N	2.72	0.52
2:J:70:PHE:CE1	2:J:85:MET:HG2	2.44	0.52
2:J:158:ASN:HB2	2:J:162:LEU:HB2	1.91	0.52
1:O:76:ARG:HH11	1:O:76:ARG:CG	2.23	0.52
2:K:191:TRP:CD1	2:K:192:PRO:HA	2.44	0.52
3:Y:81:LEU:CD1	3:Y:86:LEU:HB3	2.40	0.52
3:Y:100:LEU:O	3:Y:100:LEU:CD2	2.57	0.52
1:L:149:ILE:HG22	1:L:150:ASP:N	2.25	0.52
2:H:89:ARG:CD	2:H:91:GLU:OE1	2.46	0.52
2:H:91:GLU:C	2:H:93:THR:N	2.51	0.52
2:I:149:PHE:HB2	2:I:177:LEU:HD23	1.87	0.52
1:O:166:ASP:OD2	1:O:169:ASP:HB3	2.09	0.52
2:K:52:ARG:HD2	2:K:59:ALA:HB3	1.90	0.52
2:K:70:PHE:HZ	2:K:92:ASP:OD2	1.92	0.52
3:Y:72:GLU:O	3:Y:76:ALA:N	2.38	0.52
2:H:175:SER:O	2:H:175:SER:OG	2.26	0.52
1:M:160:ASN:HB3	1:M:174:MET:HE2	1.91	0.52
1:M:190:SER:O	1:M:191:TYR:CD1	2.62	0.52
1:O:88:GLN:NE2	1:O:90:ARG:HH11	2.08	0.52
2:K:216:ARG:NE	3:V:122:LYS:H	2.07	0.52
3:X:68:THR:HG22	3:X:101:LEU:CD1	2.39	0.52
3:X:86:LEU:C	3:X:86:LEU:HD22	2.30	0.52
3:X:124:PRO:O	3:X:127:ILE:HG12	2.10	0.52
3:Y:91:GLY:O	3:Y:94:SER:N	2.38	0.52
1:N:49:SER:O	1:N:50:THR:HB	2.09	0.52
1:O:28:SER:O	1:O:29:VAL:CG1	2.58	0.52
3:Z:93:LEU:HG	3:Z:128:PHE:CE1	2.44	0.52
1:M:138:PHE:N	1:M:138:PHE:HD2	2.07	0.52
2:J:213:ILE:HD13	3:X:37:THR:HG23	1.92	0.52
1:O:114:VAL:HG13	1:O:135:LEU:HG	1.92	0.52
3:X:17:ARG:NH1	3:X:17:ARG:CG	2.59	0.52
3:Z:26:LEU:CD1	3:Z:32:VAL:HG11	2.40	0.52
2:H:122:PRO:HB3	2:H:148:TYR:HB3	1.91	0.52
2:I:22:CYS:O	2:I:80:SER:HA	2.10	0.52
1:N:6:GLN:HE22	1:N:86:TYR:CA	2.17	0.52
1:N:6:GLN:NE2	1:N:87:CYS:H	2.08	0.52
3:V:16:LEU:O	3:V:19:SER:HB3	2.09	0.52
3:X:68:THR:HG22	3:X:101:LEU:HD13	1.92	0.52
2:H:70:PHE:CD1	2:H:85:MET:HA	2.44	0.51
2:H:127:LEU:HD21	2:H:144:LEU:HB2	1.91	0.51
2:I:39:GLN:HB3	2:I:95:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4:LEU:HD11	2:K:105:TYR:HB3	1.92	0.51
1:L:84:THR:HG23	1:L:101:THR:N	2.16	0.51
2:H:158:ASN:HD21	2:H:197:THR:H	1.58	0.51
1:M:179:THR:CG2	1:M:180:LEU:N	2.73	0.51
1:N:163:THR:HG23	1:N:164:ASP:O	2.10	0.51
1:O:161:SER:C	1:O:162:TRP:CE3	2.84	0.51
1:O:201:THR:O	1:O:203:PRO:HD3	2.09	0.51
3:X:20:HIS:O	3:X:24:SER:N	2.38	0.51
3:X:115:ARG:HG3	3:X:116:GLY:N	2.26	0.51
1:L:114:VAL:HG21	1:L:204:ILE:HG22	1.92	0.51
1:L:212:GLU:CG	2:H:131:SER:HB2	2.40	0.51
2:H:150:PRO:O	2:H:202:HIS:NE2	2.40	0.51
1:M:37:GLN:CG	1:M:38:LYS:N	2.73	0.51
1:N:35:PHE:HD1	1:N:35:PHE:H	1.57	0.51
1:O:19:VAL:CG1	1:O:74:ILE:CD1	2.88	0.51
1:O:109:ASP:OD1	1:O:140:PRO:HD3	2.11	0.51
2:K:93:THR:HA	2:K:112:VAL:O	2.10	0.51
3:V:44:VAL:O	3:V:44:VAL:HG12	2.10	0.51
3:Y:57:GLU:O	3:Y:60:ALA:HB3	2.11	0.51
2:H:38:ARG:HB3	2:H:48:VAL:HG21	1.93	0.51
2:I:8:GLY:C	2:I:9:GLY:O	2.49	0.51
2:J:2:VAL:HG23	2:J:27:PHE:CD1	2.45	0.51
2:J:35:ASP:OD1	2:J:50:GLU:HB2	2.11	0.51
2:J:54:LYS:NZ	2:J:58:HIS:HE1	2.08	0.51
1:O:88:GLN:NE2	1:O:90:ARG:NH1	2.59	0.51
2:K:51:ILE:CD1	2:K:74:ARG:CD	2.89	0.51
3:V:123:ASP:OD1	3:V:125:ASN:ND2	2.42	0.51
2:H:214:VAL:HG12	2:H:215:PRO:HD3	1.92	0.51
1:M:163:THR:HG23	1:M:164:ASP:O	2.11	0.51
2:I:91:GLU:H	2:I:91:GLU:CD	2.13	0.51
2:J:29:PHE:CD2	2:J:79:SER:CA	2.92	0.51
2:J:56:ASN:HD22	2:J:56:ASN:H	1.56	0.51
2:K:187:PRO:O	2:K:189:SER:N	2.44	0.51
3:V:66:ALA:O	3:V:67:VAL:C	2.49	0.51
1:L:52:ASN:ND2	3:V:115:ARG:HD3	2.26	0.51
2:I:29:PHE:CE2	2:I:76:ASP:HA	2.45	0.51
2:I:157:TRP:CZ3	2:I:184:VAL:HG11	2.46	0.51
1:N:118:PRO:HA	1:N:131:VAL:HG22	1.93	0.51
3:X:116:GLY:O	3:X:118:THR:HG22	2.10	0.51
3:Z:107:LEU:O	3:Z:107:LEU:HD22	2.09	0.51
2:H:64:GLU:OE2	2:H:67:LYS:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:ARG:HG3	1:O:62:ARG:HH11	1.76	0.51
1:O:182:LYS:HD3	1:O:186:GLU:OE1	2.11	0.51
2:K:66:VAL:HG22	2:K:70:PHE:CE2	2.46	0.51
3:V:140:ARG:HA	3:V:143:MET:HE1	1.92	0.51
1:L:77:MET:HE3	1:L:81:ASP:HB2	1.93	0.51
2:H:70:PHE:CD1	2:H:85:MET:HB3	2.44	0.51
1:M:107:ARG:HH12	1:M:169:ASP:HB2	1.74	0.51
1:M:116:ILE:CD1	1:M:208:PHE:CD1	2.93	0.51
2:I:57:ASN:C	2:I:59:ALA:N	2.63	0.51
1:N:33:TYR:CD2	1:N:48:TYR:HA	2.45	0.51
1:N:211:ASN:HD22	1:N:212:GLU:N	2.09	0.51
2:J:157:TRP:O	2:J:158:ASN:C	2.46	0.51
1:O:118:PRO:HG3	1:O:208:PHE:CD2	2.46	0.51
3:X:131:PHE:CE1	3:X:135:LEU:HD11	2.45	0.51
1:M:38:LYS:NZ	1:M:80:GLU:O	2.44	0.51
2:I:51:ILE:HD11	2:I:74:ARG:HG3	1.92	0.51
2:K:38:ARG:HB3	2:K:96:TYR:CD1	2.46	0.51
2:K:74:ARG:HB3	2:K:81:VAL:HG23	1.91	0.51
3:X:43:ALA:HB1	3:X:119:THR:HG23	1.89	0.51
3:Z:41:LEU:HD13	3:Z:127:ILE:HG22	1.89	0.51
2:H:89:ARG:O	2:H:90:ALA:C	2.48	0.51
2:I:51:ILE:HD13	2:I:74:ARG:CG	2.41	0.51
1:O:47:ILE:HG12	1:O:53:LEU:HD23	1.93	0.51
2:K:12:VAL:O	2:K:114:VAL:HA	2.11	0.51
2:K:187:PRO:HD2	2:K:190:THR:OG1	2.10	0.51
1:L:29:VAL:O	1:L:70:TYR:OH	2.28	0.50
1:M:165:GLN:HG2	1:M:172:TYR:CE1	2.46	0.50
2:I:84:GLN:HE21	2:I:84:GLN:C	2.15	0.50
2:J:2:VAL:HG11	2:J:105:TYR:CE1	2.46	0.50
1:O:48:TYR:O	1:O:52:ASN:HB2	2.11	0.50
3:Z:135:LEU:HA	3:Z:139:VAL:HB	1.92	0.50
2:H:64:GLU:CG	2:H:67:LYS:NZ	2.72	0.50
1:M:147:TRP:CZ3	1:M:193:CYS:HB3	2.46	0.50
2:I:151:GLU:CB	2:I:152:PRO:CA	2.89	0.50
1:N:14:SER:O	1:N:17:GLU:HB3	2.12	0.50
2:J:28:THR:HG22	2:J:30:SER:OG	2.11	0.50
1:O:149:ILE:CG1	1:O:191:TYR:HE2	2.17	0.50
1:L:47:ILE:CG2	1:L:48:TYR:N	2.73	0.50
1:L:106:LYS:O	1:L:106:LYS:CG	2.59	0.50
1:L:149:ILE:O	1:L:190:SER:OG	2.25	0.50
2:H:52:ARG:HD2	2:H:59:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:ILE:N	1:N:165:GLN:OE1	2.42	0.50
3:V:81:LEU:HD12	3:V:87:SER:CB	2.38	0.50
3:V:87:SER:C	3:V:89:LEU:H	2.13	0.50
3:X:67:VAL:CG2	3:X:100:LEU:HD13	2.41	0.50
3:Z:57:GLU:HG3	3:Z:108:LEU:HD21	1.93	0.50
1:L:143:ILE:HG13	1:L:197:HIS:CD2	2.46	0.50
1:L:149:ILE:HD13	1:L:191:TYR:CE2	2.47	0.50
2:H:88:LEU:HD23	2:H:92:ASP:HB2	1.93	0.50
2:J:54:LYS:HZ2	2:J:58:HIS:HE1	1.59	0.50
3:Y:36:PRO:HD2	3:Y:80:GLN:OE1	2.12	0.50
1:L:123:GLN:OE1	1:L:130:SER:N	2.44	0.50
2:H:29:PHE:HE2	2:H:74:ARG:HE	1.59	0.50
2:H:216:ARG:HD2	2:H:217:ASP:N	2.26	0.50
1:M:189:ASN:HD21	1:M:209:ASN:HB3	1.77	0.50
1:N:35:PHE:HE2	2:J:103:PHE:HB3	1.77	0.50
2:J:4:LEU:HD12	2:J:107:GLY:N	2.26	0.50
2:J:29:PHE:O	2:J:31:ASP:N	2.44	0.50
2:J:54:LYS:O	2:J:56:ASN:N	2.44	0.50
1:O:134:PHE:CE1	2:K:183:SER:HB3	2.46	0.50
3:V:93:LEU:HD23	3:V:93:LEU:C	2.32	0.50
2:H:191:TRP:CD1	2:H:196:VAL:HG13	2.47	0.50
1:M:22:THR:HG23	1:M:70:TYR:O	2.11	0.50
2:I:145:VAL:O	2:I:145:VAL:CG2	2.59	0.50
2:J:99:SER:HB2	2:J:105:TYR:O	2.12	0.50
1:O:169:ASP:O	1:O:171:THR:N	2.45	0.50
2:K:75:ASP:C	2:K:75:ASP:OD1	2.50	0.50
2:K:186:VAL:HB	2:K:187:PRO:CD	2.42	0.50
3:X:116:GLY:O	3:X:118:THR:CG2	2.60	0.50
3:Y:44:VAL:HG11	3:Z:46:PHE:CE2	2.47	0.50
3:Y:68:THR:CG2	3:Y:101:LEU:HD11	2.37	0.50
3:Z:51:TRP:CZ3	3:Z:138:LYS:HE2	2.46	0.50
1:N:2:VAL:CG2	1:N:89:GLN:CD	2.80	0.50
2:K:29:PHE:CD1	2:K:79:SER:O	2.64	0.50
2:K:29:PHE:HE1	2:K:34:MET:HE3	1.77	0.50
2:K:29:PHE:CG	2:K:79:SER:HA	2.47	0.50
3:X:42:PRO:HG2	3:X:70:LEU:HB2	1.92	0.50
3:Z:64:LEU:HD11	3:Z:105:GLN:NE2	2.25	0.50
1:M:115:SER:CB	1:M:117:PHE:HE1	2.24	0.50
2:I:206:SER:O	2:I:207:THR:HG22	2.11	0.50
1:N:82:ALA:O	1:N:83:ALA:HB2	2.11	0.50
2:J:157:TRP:C	2:J:159:SER:N	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:154:ARG:HD3	1:O:156:ASN:O	2.11	0.50
2:K:29:PHE:O	2:K:31:ASP:N	2.45	0.50
2:K:38:ARG:CB	2:K:96:TYR:CE1	2.95	0.50
3:V:22:LEU:CD1	3:V:96:GLN:NE2	2.75	0.50
3:Z:91:GLY:O	3:Z:93:LEU:N	2.44	0.50
2:H:138:MET:HA	2:H:138:MET:CE	2.41	0.50
1:M:21:ILE:O	1:M:71:SER:HB2	2.12	0.50
1:M:169:ASP:OD2	1:M:169:ASP:O	2.29	0.50
1:N:61:PHE:HE1	1:N:74:ILE:HG12	1.72	0.50
1:N:194:GLU:HG2	1:N:205:VAL:CG2	2.40	0.50
2:K:202:HIS:ND1	2:K:204:ALA:HB3	2.27	0.50
3:V:49:GLY:O	3:V:51:TRP:N	2.45	0.50
3:V:139:VAL:O	3:V:140:ARG:C	2.50	0.50
3:X:91:GLY:O	3:X:92:GLN:C	2.49	0.50
2:H:205:SER:O	2:H:207:THR:HG22	2.12	0.49
1:N:19:VAL:HB	1:N:74:ILE:HD12	1.94	0.49
1:N:42:SER:HB3	2:J:97:TYR:CE2	2.47	0.49
2:J:64:GLU:O	2:J:67:LYS:HB2	2.12	0.49
2:J:81:VAL:CG2	2:J:82:TYR:N	2.75	0.49
3:Y:52:LYS:HZ1	3:Y:145:VAL:HG23	1.76	0.49
3:Z:24:SER:O	3:Z:26:LEU:N	2.45	0.49
1:L:149:ILE:HG22	1:L:150:ASP:H	1.76	0.49
1:M:89:GLN:HA	4:M:222:HOH:O	2.11	0.49
1:M:149:ILE:HG23	1:M:191:TYR:CE2	2.46	0.49
3:Z:56:GLU:OE2	3:Z:56:GLU:N	2.45	0.49
1:L:37:GLN:O	1:L:83:ALA:HB1	2.12	0.49
2:I:69:ARG:HH22	2:I:92:ASP:CG	2.15	0.49
1:O:28:SER:O	1:O:29:VAL:HG13	2.12	0.49
3:V:127:ILE:O	3:V:128:PHE:C	2.51	0.49
3:X:9:LEU:C	3:X:11:VAL:N	2.66	0.49
3:X:134:LEU:C	3:X:139:VAL:HG23	2.32	0.49
3:Y:100:LEU:HD22	3:Y:104:LEU:CD1	2.41	0.49
2:H:137:SER:O	2:H:188:SER:HB3	2.12	0.49
1:M:117:PHE:HE2	2:I:141:LEU:HA	1.78	0.49
2:I:117:ALA:O	2:I:118:LYS:HD3	2.11	0.49
1:N:36:GLN:HB2	1:N:85:TYR:CE2	2.48	0.49
2:K:155:VAL:CG1	2:K:168:THR:HG21	2.43	0.49
1:L:77:MET:HG3	1:L:78:GLU:O	2.12	0.49
2:H:101:TRP:CB	2:H:104:LEU:HB3	2.43	0.49
1:M:7:SER:CB	1:M:8:PRO:CD	2.87	0.49
1:M:107:ARG:HH11	1:M:170:SER:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:36:GLN:NE2	1:N:85:TYR:CE2	2.60	0.49
2:J:28:THR:HB	2:J:31:ASP:HB2	1.94	0.49
1:O:161:SER:OG	2:K:170:PRO:HD2	2.12	0.49
3:X:132:GLN:OE1	3:X:136:ARG:NH2	2.45	0.49
1:L:3:VAL:H	1:L:26:SER:HB3	1.77	0.49
1:L:116:ILE:C	1:L:117:PHE:CD1	2.86	0.49
1:M:21:ILE:HG22	1:M:22:THR:O	2.12	0.49
1:N:116:ILE:C	1:N:117:PHE:CD1	2.86	0.49
1:N:205:VAL:O	1:N:205:VAL:HG12	2.12	0.49
2:J:29:PHE:C	2:J:31:ASP:H	2.15	0.49
2:J:90:ALA:H	2:J:91:GLU:CD	2.16	0.49
2:K:60:ILE:CG2	2:K:72:VAL:HG13	2.42	0.49
2:K:66:VAL:HG11	2:K:70:PHE:CG	2.48	0.49
3:Y:45:ASP:OD1	3:Y:45:ASP:N	2.45	0.49
2:I:64:GLU:O	2:I:66:VAL:N	2.38	0.49
2:I:216:ARG:NE	3:Y:122:LYS:HG3	2.27	0.49
1:N:183:ASP:O	1:N:187:ARG:HG3	2.12	0.49
2:J:214:VAL:HG11	3:X:40:LEU:HD21	1.94	0.49
1:O:5:THR:HG22	1:O:5:THR:O	2.12	0.49
3:X:95:GLY:HA2	3:X:98:ARG:HD2	1.95	0.49
3:Z:52:LYS:HG2	3:Z:141:PHE:HE1	1.78	0.49
2:J:66:VAL:HG13	2:J:70:PHE:CD2	2.48	0.49
2:K:169:PHE:HD2	2:K:181:SER:O	1.96	0.49
3:X:73:GLY:O	3:X:74:VAL:C	2.49	0.49
3:Y:77:ALA:O	3:Y:78:ARG:C	2.50	0.49
2:H:146:LYS:HG2	2:H:179:THR:OG1	2.13	0.49
1:N:110:ALA:HB3	1:N:138:PHE:C	2.33	0.49
2:J:70:PHE:CD1	2:J:85:MET:HG2	2.48	0.49
3:V:64:LEU:HD13	3:V:105:GLN:N	2.28	0.49
3:X:137:GLY:O	3:X:140:ARG:N	2.46	0.49
3:Y:133:HIS:O	3:Y:137:GLY:N	2.44	0.49
2:H:33:TRP:H	3:V:111:GLN:HE22	1.53	0.49
2:H:52:ARG:O	2:H:58:HIS:HD2	1.95	0.49
2:H:151:GLU:OE2	2:H:171:ALA:CB	2.61	0.49
1:O:47:ILE:HG12	1:O:53:LEU:CD2	2.43	0.49
2:H:101:TRP:O	2:H:103:PHE:N	2.46	0.48
2:H:149:PHE:HB2	2:H:177:LEU:HD22	1.95	0.48
2:J:38:ARG:HA	2:J:95:ILE:O	2.13	0.48
1:O:4:LEU:HD12	1:O:87:CYS:O	2.13	0.48
1:O:33:TYR:CZ	1:O:90:ARG:HD3	2.48	0.48
1:O:83:ALA:HB3	1:O:85:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:29:PHE:CE1	2:K:34:MET:HE3	2.48	0.48
2:K:89:ARG:O	2:K:114:VAL:CG2	2.61	0.48
3:V:42:PRO:HD2	3:V:130:SER:OG	2.13	0.48
1:L:174:MET:O	1:L:174:MET:HG3	2.13	0.48
2:H:70:PHE:CZ	2:H:85:MET:CE	2.96	0.48
1:M:34:TRP:HB2	1:M:47:ILE:HB	1.94	0.48
1:N:123:GLN:NE2	1:N:130:SER:OG	2.38	0.48
3:Y:133:HIS:CD2	3:Z:46:PHE:HD2	2.31	0.48
2:H:216:ARG:CD	2:H:217:ASP:N	2.76	0.48
1:M:48:TYR:CZ	3:X:113:PRO:HG2	2.46	0.48
2:I:20:LEU:HD13	2:I:96:TYR:HB2	1.95	0.48
2:I:35:ASP:OD1	2:I:50:GLU:HB2	2.12	0.48
3:Y:26:LEU:O	3:Y:28:GLN:N	2.46	0.48
1:L:61:PHE:CE1	1:L:74:ILE:HG12	2.49	0.48
1:L:160:ASN:HB3	1:L:174:MET:HE3	1.94	0.48
2:I:158:ASN:ND2	2:I:197:THR:H	2.11	0.48
1:N:37:GLN:N	1:N:84:THR:O	2.41	0.48
1:N:167:SER:CB	1:N:168:LYS:HZ1	2.20	0.48
2:K:89:ARG:O	2:K:114:VAL:HB	2.13	0.48
2:K:89:ARG:HB2	2:K:92:ASP:OD1	2.13	0.48
3:V:8:ASP:OD1	3:V:8:ASP:N	2.46	0.48
3:V:11:VAL:HG23	3:V:12:LEU:H	1.78	0.48
3:V:95:GLY:O	3:V:98:ARG:HB2	2.13	0.48
3:Y:52:LYS:NZ	3:Y:145:VAL:HG23	2.28	0.48
1:M:33:TYR:HD2	1:M:33:TYR:H	1.60	0.48
1:M:103:LEU:HD12	1:M:104:GLU:N	2.28	0.48
2:I:22:CYS:O	2:I:80:SER:CA	2.62	0.48
2:J:51:ILE:C	2:J:52:ARG:O	2.50	0.48
2:J:81:VAL:HG22	2:J:82:TYR:N	2.28	0.48
1:O:147:TRP:HD1	1:O:158:VAL:HG12	1.77	0.48
1:O:197:HIS:O	1:O:199:THR:HB	2.14	0.48
3:V:22:LEU:HG	3:V:96:GLN:HE22	1.77	0.48
1:M:113:THR:H	1:M:136:ASN:H	1.61	0.48
2:J:214:VAL:HA	2:J:215:PRO:HD3	1.72	0.48
2:K:191:TRP:CZ2	2:K:214:VAL:HG13	2.49	0.48
3:Z:82:GLY:HA3	3:Z:83:PRO:HD3	1.68	0.48
3:Z:91:GLY:O	3:Z:92:GLN:C	2.52	0.48
2:H:89:ARG:O	2:H:114:VAL:HG21	2.14	0.48
2:H:202:HIS:ND1	2:H:204:ALA:CB	2.75	0.48
1:M:179:THR:HG22	1:M:180:LEU:N	2.27	0.48
1:O:62:ARG:HG3	1:O:62:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:104:LEU:O	3:Y:105:GLN:C	2.49	0.48
1:L:147:TRP:CD1	1:L:158:VAL:HG11	2.49	0.48
2:H:180:LEU:HD23	2:H:180:LEU:C	2.34	0.48
1:M:18:LYS:HG3	1:M:19:VAL:N	2.28	0.48
2:I:206:SER:C	2:I:207:THR:CG2	2.82	0.48
1:N:139:TYR:CG	1:N:140:PRO:HA	2.49	0.48
1:O:19:VAL:CG1	1:O:74:ILE:CG1	2.92	0.48
1:O:29:VAL:O	1:O:67:GLY:HA2	2.14	0.48
2:K:29:PHE:C	2:K:31:ASP:H	2.17	0.48
3:X:126:ALA:O	3:X:130:SER:HB2	2.14	0.48
3:Z:56:GLU:OE1	3:Z:145:VAL:HB	2.13	0.48
1:L:122:GLU:CD	1:L:122:GLU:H	2.16	0.48
1:L:147:TRP:CG	1:L:178:LEU:HD12	2.49	0.48
1:L:212:GLU:HG2	2:H:131:SER:HB2	1.94	0.48
2:H:138:MET:CE	2:H:186:VAL:O	2.62	0.48
2:H:173:LEU:HA	2:H:177:LEU:O	2.14	0.48
1:N:33:TYR:CD1	1:N:90:ARG:HD3	2.49	0.48
1:N:86:TYR:CD2	2:J:45:LEU:CD1	2.94	0.48
2:K:90:ALA:HA	2:K:114:VAL:HG23	1.96	0.48
1:M:7:SER:OG	1:M:8:PRO:N	2.42	0.48
1:M:37:GLN:OE1	1:M:43:PRO:HD3	2.13	0.48
1:M:180:LEU:HD12	1:M:180:LEU:H	1.78	0.48
2:J:81:VAL:CG2	2:J:82:TYR:H	2.27	0.48
1:O:35:PHE:O	1:O:85:TYR:HA	2.13	0.48
3:X:120:ALA:O	3:X:121:HIS:CD2	2.67	0.48
3:Z:54:GLN:HB2	3:Z:59:LYS:HG3	1.96	0.48
1:L:147:TRP:CE2	1:L:178:LEU:HB2	2.49	0.47
2:H:51:ILE:CD1	2:H:74:ARG:HG3	2.44	0.47
1:M:95:ARG:HG3	2:I:47:TRP:CG	2.48	0.47
1:M:137:ASN:H	1:M:173:SER:CB	2.26	0.47
2:I:120:THR:O	2:I:149:PHE:N	2.39	0.47
2:I:216:ARG:HH21	3:Y:121:HIS:CA	2.27	0.47
1:N:119:PRO:HG3	1:N:185:TYR:CE2	2.48	0.47
2:J:157:TRP:CH2	2:J:198:CYS:HB3	2.49	0.47
2:K:17:SER:HA	2:K:88:LEU:HD12	1.95	0.47
3:X:35:LEU:HD21	3:X:77:ALA:CB	2.43	0.47
3:Z:128:PHE:O	3:Z:131:PHE:HB3	2.14	0.47
2:H:17:SER:HB3	2:H:86:ASN:OD1	2.14	0.47
1:M:6:GLN:HE22	1:M:87:CYS:H	1.61	0.47
1:M:34:TRP:CZ3	1:M:87:CYS:HB3	2.49	0.47
1:M:147:TRP:CD2	1:M:178:LEU:HD12	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:154:ARG:HG3	1:M:155:GLN:N	2.28	0.47
2:J:75:ASP:OD1	2:J:75:ASP:C	2.52	0.47
1:O:7:SER:CB	1:O:22:THR:HB	2.45	0.47
1:O:90:ARG:CZ	2:K:103:PHE:HD2	2.26	0.47
1:O:107:ARG:NE	1:O:108:ALA:O	2.42	0.47
3:V:41:LEU:CD2	3:V:127:ILE:HB	2.44	0.47
3:V:112:LEU:N	3:V:112:LEU:CD1	2.77	0.47
3:Y:90:LEU:HD23	3:Y:90:LEU:HA	1.65	0.47
3:Y:123:ASP:HA	3:Y:124:PRO:HD2	1.64	0.47
3:Y:123:ASP:O	3:Y:126:ALA:CB	2.61	0.47
1:L:48:TYR:CE1	1:L:52:ASN:CB	2.97	0.47
1:L:84:THR:HG23	1:L:101:THR:O	2.14	0.47
2:H:102:SER:HB2	3:V:111:GLN:H	1.79	0.47
1:M:111:ALA:HB1	1:M:112:PRO:HD2	1.95	0.47
2:I:102:SER:HB2	3:X:111:GLN:HB2	1.97	0.47
1:N:109:ASP:OD1	1:N:140:PRO:HD3	2.15	0.47
2:J:47:TRP:O	2:J:63:ALA:HB2	2.14	0.47
2:J:102:SER:O	2:J:103:PHE:HB2	2.14	0.47
1:O:174:MET:O	1:O:174:MET:HG2	2.11	0.47
3:Y:70:LEU:HD22	3:Y:74:VAL:CG2	2.43	0.47
3:Y:78:ARG:NH1	3:Y:87:SER:O	2.46	0.47
1:L:111:ALA:HB1	1:L:112:PRO:CD	2.44	0.47
2:H:159:SER:HA	2:H:199:ASN:HD21	1.79	0.47
1:O:58:PRO:O	1:O:61:PHE:HB2	2.13	0.47
1:O:174:MET:HA	2:K:169:PHE:HE1	1.79	0.47
3:V:24:SER:O	3:V:26:LEU:N	2.47	0.47
3:X:23:HIS:O	3:X:23:HIS:HD2	1.96	0.47
3:X:90:LEU:N	3:X:90:LEU:HD23	2.29	0.47
3:Y:30:PRO:O	3:Y:31:GLU:C	2.53	0.47
2:H:64:GLU:CG	2:H:67:LYS:HZ2	2.24	0.47
2:I:56:ASN:C	2:I:57:ASN:ND2	2.68	0.47
2:I:148:TYR:CE1	2:I:178:TYR:O	2.67	0.47
1:O:37:GLN:HE21	1:O:86:TYR:HE2	1.63	0.47
2:K:13:GLN:C	2:K:14:PRO:O	2.52	0.47
1:M:115:SER:HB2	1:M:117:PHE:HE1	1.78	0.47
1:M:185:TYR:HE1	1:M:191:TYR:CE1	2.33	0.47
2:I:8:GLY:O	2:I:9:GLY:O	2.32	0.47
2:K:17:SER:OG	2:K:86:ASN:HA	2.14	0.47
3:X:39:VAL:HG11	3:X:77:ALA:N	2.30	0.47
3:Y:43:ALA:HB2	3:Y:119:THR:OG1	2.13	0.47
3:Y:124:PRO:HA	3:Y:127:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:LEU:H	1:L:53:LEU:HG	1.60	0.47
1:L:136:ASN:ND2	2:H:167:HIS:HD2	2.12	0.47
2:H:186:VAL:HB	2:H:190:THR:OG1	2.15	0.47
1:M:36:GLN:HB2	1:M:85:TYR:HE2	1.69	0.47
1:M:88:GLN:NE2	1:M:90:ARG:HH11	2.10	0.47
2:I:216:ARG:CG	3:Y:122:LYS:HG3	2.44	0.47
1:N:34:TRP:HA	1:N:86:TYR:O	2.14	0.47
1:N:89:GLN:NE2	1:N:96:THR:H	2.13	0.47
1:N:106:LYS:HA	1:N:139:TYR:OH	2.15	0.47
2:J:124:VAL:HG21	2:J:208:LYS:CB	2.44	0.47
1:O:89:GLN:OE1	1:O:91:SER:HB3	2.14	0.47
1:O:119:PRO:HA	4:O:214:HOH:O	2.14	0.47
1:O:121:SER:HA	1:O:124:LEU:HB2	1.96	0.47
2:K:33:TRP:CZ2	2:K:52:ARG:HG2	2.48	0.47
2:K:38:ARG:HH11	2:K:46:GLU:CD	2.18	0.47
2:K:64:GLU:C	2:K:66:VAL:H	2.18	0.47
2:K:203:PRO:CB	4:K:227:HOH:O	2.58	0.47
2:K:214:VAL:O	3:V:38:PRO:HG2	2.15	0.47
3:V:52:LYS:HG3	3:V:52:LYS:O	2.14	0.47
3:Y:71:LEU:HD23	3:Y:71:LEU:O	2.15	0.47
2:H:66:VAL:O	2:H:66:VAL:HG12	2.14	0.47
1:M:84:THR:HA	1:M:102:LYS:HA	1.97	0.47
2:I:111:LEU:HD13	2:I:113:THR:OG1	2.14	0.47
2:I:216:ARG:HH21	3:Y:122:LYS:H	1.61	0.47
2:K:57:ASN:C	2:K:59:ALA:H	2.18	0.47
1:L:4:LEU:HD21	1:L:89:GLN:HB3	1.97	0.47
1:L:117:PHE:N	1:L:117:PHE:HD1	2.13	0.47
1:M:6:GLN:NE2	1:M:98:GLY:HA3	2.22	0.47
2:I:85:MET:HE2	2:I:88:LEU:HD21	1.96	0.47
2:I:211:LYS:O	2:I:212:LYS:C	2.52	0.47
2:K:8:GLY:O	2:K:9:GLY:O	2.33	0.47
2:K:89:ARG:O	2:K:114:VAL:CB	2.63	0.47
2:K:141:LEU:HD11	2:K:191:TRP:CD2	2.49	0.47
2:K:156:THR:OG1	2:K:199:ASN:ND2	2.47	0.47
3:Z:64:LEU:O	3:Z:68:THR:HG23	2.12	0.47
2:H:39:GLN:HA	2:H:44:GLY:O	2.15	0.47
2:I:51:ILE:CD1	2:I:74:ARG:CG	2.92	0.47
2:I:214:VAL:HG11	3:Y:40:LEU:HD23	1.96	0.47
1:N:132:VAL:HG11	2:J:127:LEU:CD1	2.45	0.47
2:J:148:TYR:O	2:J:178:TYR:HB2	2.15	0.47
2:K:60:ILE:HG23	2:K:72:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:93:THR:OG1	2:K:113:THR:HA	2.15	0.47
2:K:155:VAL:O	2:K:155:VAL:HG22	2.14	0.47
3:X:87:SER:O	3:X:90:LEU:HB2	2.14	0.47
1:L:88:GLN:OE1	2:H:103:PHE:CD2	2.68	0.46
1:L:107:ARG:HB2	1:L:108:ALA:H	1.43	0.46
1:M:7:SER:HB2	1:M:22:THR:HB	1.98	0.46
1:M:192:THR:HG1	1:M:207:SER:CB	2.27	0.46
1:O:76:ARG:NH1	1:O:76:ARG:CG	2.79	0.46
1:O:131:VAL:HB	1:O:178:LEU:HB3	1.96	0.46
2:K:49:ALA:HB1	2:K:72:VAL:HG11	1.97	0.46
2:K:90:ALA:O	2:K:92:ASP:N	2.48	0.46
3:X:33:HIS:HB3	3:X:34:PRO:CD	2.42	0.46
3:X:51:TRP:O	3:X:54:GLN:CB	2.63	0.46
3:Z:25:ARG:NH2	3:Z:89:LEU:HD21	2.30	0.46
2:H:36:TRP:CZ3	2:H:98:CYS:HB2	2.50	0.46
2:H:123:SER:O	2:H:145:VAL:HA	2.15	0.46
1:N:120:SER:HB3	2:J:126:PRO:HD2	1.96	0.46
2:J:83:LEU:HD22	2:J:84:GLN:N	2.30	0.46
3:V:69:LEU:HD13	3:V:118:THR:HG22	1.97	0.46
3:Z:9:LEU:C	3:Z:11:VAL:H	2.17	0.46
1:L:209:ASN:HD22	1:L:213:CYS:HB2	1.80	0.46
1:M:76:ARG:NH1	1:M:76:ARG:CG	2.78	0.46
2:J:33:TRP:CD1	3:Y:111:GLN:NE2	2.83	0.46
1:O:35:PHE:CD1	1:O:35:PHE:N	2.83	0.46
2:K:197:THR:HG23	2:K:211:LYS:HA	1.98	0.46
3:X:90:LEU:N	3:X:90:LEU:CD2	2.76	0.46
3:X:93:LEU:O	3:X:96:GLN:HB2	2.15	0.46
3:Y:52:LYS:HE2	3:Y:141:PHE:HB3	1.98	0.46
1:M:33:TYR:CD1	1:M:90:ARG:NH1	2.84	0.46
1:N:21:ILE:HB	1:N:72:LEU:HD22	1.97	0.46
1:O:43:PRO:HG2	2:K:106:TRP:CZ3	2.51	0.46
1:O:160:ASN:N	1:O:160:ASN:OD1	2.48	0.46
2:K:4:LEU:HB3	2:K:22:CYS:SG	2.55	0.46
2:K:66:VAL:CG1	2:K:70:PHE:CG	2.99	0.46
3:X:129:LEU:O	3:X:131:PHE:N	2.48	0.46
3:Y:52:LYS:HZ3	3:Y:59:LYS:NZ	2.14	0.46
3:Z:71:LEU:CD1	3:Z:101:LEU:HD23	2.44	0.46
1:N:32:MET:HG3	1:N:33:TYR:O	2.15	0.46
1:N:89:GLN:H	1:N:89:GLN:HG3	1.64	0.46
2:J:70:PHE:CA	2:J:84:GLN:O	2.49	0.46
2:J:140:THR:OG1	2:J:185:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:9:LEU:O	3:V:9:LEU:HD23	2.15	0.46
3:Z:12:LEU:CB	3:Z:143:MET:SD	3.01	0.46
1:L:124:LEU:HD11	1:L:185:TYR:CD2	2.50	0.46
2:H:89:ARG:O	2:H:91:GLU:N	2.48	0.46
1:M:8:PRO:CD	1:M:8:PRO:O	2.63	0.46
1:M:143:ILE:O	1:M:143:ILE:CG2	2.63	0.46
2:I:151:GLU:HB3	2:I:152:PRO:CA	2.45	0.46
2:J:38:ARG:HD3	2:J:43:LYS:NZ	2.30	0.46
1:O:7:SER:OG	1:O:8:PRO:CD	2.64	0.46
2:K:177:LEU:HD23	2:K:177:LEU:HA	1.66	0.46
3:X:39:VAL:HG21	3:X:77:ALA:HB2	1.98	0.46
3:X:86:LEU:HD22	3:X:86:LEU:O	2.15	0.46
3:Y:25:ARG:O	3:Y:26:LEU:C	2.54	0.46
1:L:48:TYR:CE2	3:V:113:PRO:HG3	2.51	0.46
1:L:163:THR:HG23	1:L:164:ASP:O	2.16	0.46
1:M:37:GLN:NE2	2:I:39:GLN:HE22	2.04	0.46
1:M:45:LEU:CD2	1:M:46:TRP:N	2.74	0.46
1:N:136:ASN:O	1:N:137:ASN:C	2.53	0.46
3:V:42:PRO:O	3:V:43:ALA:O	2.34	0.46
3:Y:31:GLU:HB3	3:Y:33:HIS:HE1	1.80	0.46
1:L:184:GLU:O	1:L:185:TYR:C	2.53	0.46
2:H:72:VAL:CG2	2:H:73:SER:N	2.79	0.46
2:I:43:LYS:HG3	4:I:241:HOH:O	2.15	0.46
1:N:88:GLN:HE22	1:N:90:ARG:HH11	1.64	0.46
2:J:135:THR:CG2	4:J:221:HOH:O	2.39	0.46
3:X:90:LEU:HD11	3:X:127:ILE:CD1	2.46	0.46
2:H:216:ARG:HD3	2:H:217:ASP:H	1.80	0.46
1:M:8:PRO:O	1:M:8:PRO:HD2	2.16	0.46
1:M:57:VAL:O	2:J:137:SER:OG	2.25	0.46
2:I:149:PHE:CB	2:I:177:LEU:HD21	2.44	0.46
2:K:187:PRO:O	2:K:188:SER:C	2.52	0.46
3:V:75:MET:O	3:V:76:ALA:C	2.52	0.46
3:V:86:LEU:O	3:V:89:LEU:HB2	2.16	0.46
3:X:63:ILE:O	3:X:63:ILE:HG22	2.15	0.46
1:L:47:ILE:HG12	1:L:53:LEU:HD23	1.99	0.46
1:L:175:SER:HB3	2:H:169:PHE:CD1	2.50	0.46
2:H:174:GLN:HB3	2:H:175:SER:H	1.66	0.46
2:I:13:GLN:O	2:I:14:PRO:C	2.53	0.46
1:N:79:ALA:C	1:N:81:ASP:H	2.20	0.46
1:N:131:VAL:N	1:N:178:LEU:O	2.36	0.46
1:O:33:TYR:CE2	1:O:90:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:ARG:HB3	4:O:230:HOH:O	2.16	0.46
1:O:111:ALA:HA	1:O:112:PRO:HD2	1.58	0.46
2:K:62:TYR:OH	2:K:71:THR:HA	2.15	0.46
3:V:16:LEU:HD23	3:V:16:LEU:HA	1.64	0.46
3:V:97:VAL:O	3:V:97:VAL:HG12	2.16	0.46
2:I:18:MET:SD	2:I:112:VAL:HG22	2.56	0.45
2:I:78:LYS:HE3	2:I:78:LYS:HB2	1.59	0.45
2:J:160:GLY:O	2:J:163:SER:HB3	2.15	0.45
3:V:144:LEU:HB3	3:V:145:VAL:H	1.47	0.45
3:Y:14:LYS:O	3:Y:18:ASP:CB	2.60	0.45
3:Z:111:GLN:O	3:Z:112:LEU:CD1	2.64	0.45
1:L:37:GLN:NE2	1:L:86:TYR:HE2	2.14	0.45
1:L:107:ARG:NE	1:L:108:ALA:O	2.36	0.45
1:M:118:PRO:HG3	1:M:208:PHE:CD1	2.50	0.45
2:I:196:VAL:O	2:I:196:VAL:HG23	2.16	0.45
2:J:22:CYS:C	2:J:80:SER:HB3	2.37	0.45
2:K:83:LEU:HD23	2:K:83:LEU:HA	1.45	0.45
3:V:38:PRO:HB3	3:V:120:ALA:HB1	1.98	0.45
3:X:15:LEU:HD23	3:X:135:LEU:CD2	2.47	0.45
1:L:191:TYR:HD1	1:L:208:PHE:CZ	2.34	0.45
1:O:103:LEU:HD12	1:O:103:LEU:HA	1.32	0.45
3:X:99:LEU:O	3:X:103:ALA:N	2.49	0.45
3:Z:100:LEU:O	3:Z:104:LEU:HD12	2.16	0.45
1:L:36:GLN:HG3	1:L:85:TYR:HE2	1.79	0.45
2:H:78:LYS:O	2:H:78:LYS:CG	2.51	0.45
1:M:36:GLN:HB2	1:M:85:TYR:CD2	2.50	0.45
1:M:164:ASP:O	1:M:165:GLN:C	2.51	0.45
2:I:191:TRP:CD1	2:I:192:PRO:HA	2.52	0.45
1:N:21:ILE:HG12	1:N:101:THR:HG21	1.98	0.45
1:N:184:GLU:O	1:N:184:GLU:CG	2.62	0.45
2:J:95:ILE:CG2	2:J:111:LEU:HD23	2.25	0.45
2:K:69:ARG:HH11	2:K:89:ARG:HH22	1.61	0.45
3:V:87:SER:C	3:V:89:LEU:N	2.70	0.45
3:Y:90:LEU:CD2	3:Y:93:LEU:HD12	2.47	0.45
2:H:111:LEU:HA	2:H:111:LEU:HD22	1.45	0.45
2:I:104:LEU:HD22	3:X:113:PRO:HB3	1.99	0.45
2:J:69:ARG:NH1	2:J:89:ARG:HH21	2.12	0.45
2:K:89:ARG:NH1	2:K:89:ARG:CG	2.67	0.45
2:K:216:ARG:NH1	3:V:121:HIS:HD1	2.14	0.45
3:V:14:LYS:HA	3:V:17:ARG:HH11	1.82	0.45
3:V:86:LEU:HD11	3:V:124:PRO:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:101:LEU:O	3:V:102:GLY:O	2.34	0.45
3:V:105:GLN:NE2	3:V:111:GLN:HG2	2.32	0.45
3:X:29:CYS:HB2	3:X:32:VAL:HG13	1.98	0.45
3:X:64:LEU:HA	3:X:104:LEU:HD13	1.98	0.45
1:M:77:MET:CE	1:M:81:ASP:HB2	2.47	0.45
1:M:124:LEU:CD1	1:M:128:GLY:O	2.65	0.45
2:I:99:SER:OG	2:I:103:PHE:HA	2.17	0.45
1:N:169:ASP:OD2	1:N:171:THR:HG23	2.17	0.45
2:K:216:ARG:HD2	2:K:217:ASP:N	2.32	0.45
3:X:17:ARG:H	3:X:17:ARG:HG2	1.34	0.45
3:Y:62:ASP:OD1	3:Y:62:ASP:N	2.49	0.45
1:O:47:ILE:HD12	1:O:72:LEU:HD12	1.98	0.45
2:K:22:CYS:O	2:K:80:SER:CA	2.64	0.45
2:K:62:TYR:CZ	2:K:72:VAL:HG12	2.52	0.45
2:K:145:VAL:HG21	2:K:153:VAL:HG11	1.98	0.45
2:K:199:ASN:HB3	2:K:209:VAL:HG23	1.98	0.45
3:V:8:ASP:H	3:V:151:CYS:CB	2.29	0.45
3:V:8:ASP:H	3:V:151:CYS:HB3	1.82	0.45
3:V:64:LEU:O	3:V:68:THR:HG23	2.16	0.45
3:V:85:CYS:O	3:V:89:LEU:HD13	2.17	0.45
3:X:78:ARG:CG	3:X:78:ARG:NH1	2.42	0.45
3:Z:62:ASP:O	3:Z:66:ALA:N	2.50	0.45
2:I:173:LEU:CD2	2:I:176:ASP:HA	2.46	0.45
1:N:147:TRP:NE1	1:N:158:VAL:CG1	2.79	0.45
2:J:51:ILE:O	2:J:52:ARG:C	2.55	0.45
1:O:53:LEU:HD23	1:O:53:LEU:HA	1.78	0.45
1:O:112:PRO:HD3	1:O:138:PHE:HB3	1.98	0.45
3:V:69:LEU:CD1	3:V:118:THR:HG22	2.47	0.45
3:X:15:LEU:HD23	3:X:135:LEU:HD21	1.99	0.45
3:Z:52:LYS:HG2	3:Z:141:PHE:CE1	2.52	0.45
1:M:160:ASN:CG	1:M:174:MET:CE	2.86	0.45
2:I:202:HIS:CE1	2:I:204:ALA:CB	3.00	0.45
1:N:65:GLY:O	1:N:66:SER:HB3	2.16	0.45
1:O:35:PHE:HE1	1:O:88:GLN:HB2	1.82	0.45
1:O:137:ASN:HA	1:O:172:TYR:O	2.17	0.45
2:K:120:THR:HA	2:K:121:PRO:HD2	1.81	0.45
3:V:78:ARG:O	3:V:79:GLY:O	2.35	0.45
3:X:70:LEU:HD22	3:X:74:VAL:HG23	1.99	0.45
1:L:103:LEU:HD12	1:L:103:LEU:HA	1.80	0.45
2:H:29:PHE:CG	2:H:79:SER:HA	2.51	0.45
2:H:120:THR:N	2:H:149:PHE:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:38:LYS:HG3	1:N:39:PRO:HD2	1.99	0.45
1:O:21:ILE:HG12	1:O:101:THR:HG21	1.98	0.45
2:K:70:PHE:HD1	2:K:85:MET:CA	2.29	0.45
3:V:89:LEU:O	3:V:92:GLN:N	2.50	0.45
3:Z:143:MET:H	3:Z:143:MET:HG2	1.59	0.45
2:I:119:THR:HG22	2:I:149:PHE:O	2.17	0.44
1:O:138:PHE:CE2	1:O:173:SER:HA	2.52	0.44
2:K:37:VAL:O	2:K:97:TYR:N	2.42	0.44
3:X:131:PHE:O	3:X:134:LEU:HB2	2.17	0.44
3:Y:16:LEU:HD23	3:Y:16:LEU:HA	1.77	0.44
1:M:7:SER:OG	1:M:8:PRO:HD3	2.17	0.44
2:I:21:SER:HA	2:I:82:TYR:CD2	2.52	0.44
2:I:151:GLU:HB3	2:I:152:PRO:HA	1.98	0.44
1:N:110:ALA:HB3	1:N:138:PHE:HA	1.98	0.44
2:J:54:LYS:NZ	2:J:58:HIS:CE1	2.86	0.44
2:K:38:ARG:CB	2:K:96:TYR:CD1	3.00	0.44
2:K:38:ARG:HD3	2:K:46:GLU:OE1	2.17	0.44
2:K:48:VAL:O	2:K:62:TYR:HA	2.17	0.44
3:X:132:GLN:O	3:X:134:LEU:N	2.50	0.44
1:L:86:TYR:CG	2:H:45:LEU:HD12	2.52	0.44
1:L:154:ARG:HE	1:L:154:ARG:HB2	1.45	0.44
2:H:19:LYS:HD3	2:H:84:GLN:HG2	2.00	0.44
1:M:12:SER:HB2	1:M:104:GLU:HB2	2.00	0.44
2:I:88:LEU:HB3	2:I:114:VAL:HG11	1.97	0.44
2:J:200:VAL:HG22	2:J:208:LYS:O	2.18	0.44
2:K:140:THR:C	2:K:141:LEU:HD23	2.37	0.44
2:K:202:HIS:CE1	2:K:204:ALA:HB2	2.52	0.44
3:X:38:PRO:HB2	3:X:120:ALA:HB1	2.00	0.44
3:X:69:LEU:CD2	4:X:167:HOH:O	2.62	0.44
3:Z:46:PHE:CE1	3:Z:133:HIS:CD2	3.05	0.44
1:L:51:SER:HB3	1:L:63:GLY:O	2.17	0.44
1:L:189:ASN:O	1:L:210:ARG:N	2.46	0.44
2:I:24:ALA:HB1	2:I:27:PHE:CE1	2.52	0.44
2:J:71:THR:O	2:J:71:THR:HG22	2.18	0.44
2:J:155:VAL:HA	2:J:199:ASN:O	2.18	0.44
1:O:120:SER:O	1:O:122:GLU:N	2.50	0.44
1:O:132:VAL:CG2	1:O:133:CYS:N	2.79	0.44
2:K:57:ASN:C	2:K:59:ALA:N	2.70	0.44
3:V:33:HIS:CB	3:V:34:PRO:HD2	2.47	0.44
3:V:61:GLN:HG2	3:V:108:LEU:HD22	2.00	0.44
3:V:75:MET:O	3:V:79:GLY:N	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:73:GLY:HA2	3:Y:76:ALA:CB	2.46	0.44
3:Y:127:ILE:HD13	3:Y:127:ILE:HG23	1.50	0.44
3:Z:63:ILE:HD12	3:Z:142:LEU:HD22	2.00	0.44
1:L:88:GLN:HE22	1:L:90:ARG:HD2	1.78	0.44
1:L:165:GLN:H	1:L:165:GLN:HG2	1.62	0.44
1:M:208:PHE:CD2	1:M:209:ASN:N	2.86	0.44
2:I:62:TYR:OH	2:I:71:THR:HA	2.18	0.44
1:N:77:MET:CE	1:N:78:GLU:O	2.65	0.44
2:J:203:PRO:HA	2:J:205:SER:H	1.83	0.44
1:O:4:LEU:HA	1:O:24:SER:O	2.18	0.44
1:O:76:ARG:HG2	1:O:76:ARG:HH11	1.81	0.44
1:O:203:PRO:O	1:O:205:VAL:N	2.51	0.44
3:V:40:LEU:N	3:V:40:LEU:CD2	2.81	0.44
3:V:52:LYS:HD2	3:V:59:LYS:NZ	2.32	0.44
3:X:16:LEU:HA	3:X:16:LEU:HD23	1.38	0.44
3:X:123:ASP:C	3:X:125:ASN:N	2.70	0.44
3:Y:8:ASP:C	3:Y:10:ARG:H	2.20	0.44
3:Y:63:ILE:HG22	3:Y:67:VAL:CG2	2.47	0.44
3:Y:114:PRO:O	3:Y:115:ARG:HB3	2.18	0.44
2:I:216:ARG:HH21	3:Y:121:HIS:HA	1.82	0.44
1:N:162:TRP:CH2	1:N:174:MET:CE	2.99	0.44
2:J:120:THR:HG21	2:J:177:LEU:HD21	1.99	0.44
1:O:163:THR:HG23	1:O:164:ASP:O	2.18	0.44
2:K:187:PRO:O	2:K:190:THR:OG1	2.30	0.44
3:X:12:LEU:HD12	3:X:135:LEU:HB3	1.99	0.44
3:Z:95:GLY:O	3:Z:99:LEU:HD23	2.17	0.44
1:L:48:TYR:CD1	1:L:52:ASN:HB2	2.52	0.44
2:H:216:ARG:CD	2:H:217:ASP:H	2.29	0.44
1:M:137:ASN:N	1:M:137:ASN:OD1	2.50	0.44
2:I:21:SER:HG	2:I:82:TYR:HE2	1.65	0.44
2:I:38:ARG:NH1	2:I:46:GLU:OE1	2.49	0.44
1:N:1:GLN:OE1	1:N:1:GLN:O	2.36	0.44
1:N:107:ARG:NH1	1:N:169:ASP:OD2	2.51	0.44
1:N:119:PRO:CD	1:N:131:VAL:HG23	2.20	0.44
2:J:40:SER:HB3	2:J:43:LYS:HE3	2.00	0.44
1:O:4:LEU:CD1	1:O:87:CYS:O	2.66	0.44
1:O:52:ASN:CG	3:Z:115:ARG:CZ	2.86	0.44
2:K:132:ALA:O	2:K:133:ALA:C	2.56	0.44
3:V:100:LEU:O	3:V:101:LEU:C	2.55	0.44
3:X:90:LEU:HD22	3:X:90:LEU:HA	1.52	0.44
1:M:47:ILE:HD13	1:M:63:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:130:GLY:C	2:J:133:ALA:H	2.18	0.44
1:O:109:ASP:OD1	1:O:140:PRO:CD	2.65	0.44
2:K:216:ARG:NH2	3:V:123:ASP:N	2.54	0.44
3:V:96:GLN:HA	3:V:99:LEU:HD12	1.99	0.44
3:V:149:THR:OG1	3:V:150:LEU:N	2.50	0.44
1:L:32:MET:HB2	1:L:70:TYR:CD2	2.53	0.44
1:L:38:LYS:HA	1:L:39:PRO:HD2	1.80	0.44
1:L:48:TYR:HE1	1:L:52:ASN:HD22	1.66	0.44
2:H:6:GLU:OE1	2:H:98:CYS:HB3	2.18	0.44
1:M:116:ILE:C	1:M:117:PHE:CD1	2.91	0.44
1:M:189:ASN:CA	1:M:210:ARG:HG3	2.42	0.44
2:I:38:ARG:HA	2:I:95:ILE:O	2.18	0.44
2:I:39:GLN:OE1	2:I:97:TYR:OH	2.23	0.44
1:N:32:MET:HB2	1:N:70:TYR:CD2	2.53	0.44
1:N:89:GLN:HE21	1:N:96:THR:CB	2.25	0.44
2:J:117:ALA:HB3	2:J:149:PHE:CE2	2.53	0.44
2:J:157:TRP:CD1	2:J:166:VAL:HG21	2.53	0.44
2:K:51:ILE:HD13	2:K:51:ILE:HG21	1.69	0.44
1:M:48:TYR:CD1	3:X:113:PRO:CG	3.00	0.43
2:I:192:PRO:O	2:I:193:SER:O	2.35	0.43
2:J:155:VAL:HB	2:J:200:VAL:HG12	2.00	0.43
3:V:19:SER:O	3:V:22:LEU:N	2.51	0.43
3:X:36:PRO:HG2	3:X:80:GLN:HB3	2.00	0.43
3:Y:63:ILE:HG22	3:Y:67:VAL:HG21	2.00	0.43
3:Z:98:ARG:HA	3:Z:101:LEU:CB	2.47	0.43
1:L:64:SER:OG	1:L:65:GLY:N	2.50	0.43
1:L:119:PRO:HB2	1:L:124:LEU:CD2	2.48	0.43
1:L:211:ASN:O	1:L:212:GLU:HB2	2.18	0.43
1:N:109:ASP:OD1	1:N:109:ASP:N	2.49	0.43
1:N:166:ASP:O	1:N:167:SER:C	2.56	0.43
2:J:22:CYS:O	2:J:80:SER:HA	2.18	0.43
1:O:90:ARG:HH21	2:K:102:SER:HB2	1.81	0.43
1:O:95:ARG:H	1:O:95:ARG:HG2	1.52	0.43
1:O:118:PRO:CB	1:O:208:PHE:CE2	2.96	0.43
1:O:191:TYR:CB	1:O:208:PHE:CE1	3.00	0.43
3:Z:26:LEU:O	3:Z:29:CYS:HB2	2.18	0.43
3:Z:26:LEU:HD11	3:Z:32:VAL:HG11	1.99	0.43
3:Z:30:PRO:O	3:Z:31:GLU:C	2.57	0.43
3:Z:46:PHE:HD1	3:Z:46:PHE:HA	1.71	0.43
3:Z:51:TRP:CD1	3:Z:51:TRP:C	2.91	0.43
3:Z:119:THR:OG1	3:Z:121:HIS:NE2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:PRO:HA	2:H:47:TRP:CZ3	2.52	0.43
1:M:11:MET:HE2	1:M:19:VAL:CG2	2.48	0.43
2:I:124:VAL:HA	2:I:144:LEU:O	2.18	0.43
2:I:152:PRO:O	2:I:152:PRO:CD	2.66	0.43
2:J:23:ALA:HA	2:J:80:SER:HA	1.99	0.43
2:J:39:GLN:HB3	2:J:95:ILE:HG12	2.00	0.43
3:Y:115:ARG:HD2	3:Y:116:GLY:CA	2.48	0.43
3:Z:127:ILE:HD13	3:Z:127:ILE:HG21	1.68	0.43
1:L:61:PHE:CD1	1:L:74:ILE:HG12	2.54	0.43
1:M:73:THR:O	1:M:73:THR:HG22	2.17	0.43
1:M:187:ARG:O	1:M:187:ARG:HG2	2.18	0.43
1:N:110:ALA:CB	1:N:138:PHE:HA	2.49	0.43
2:J:148:TYR:HD1	2:J:148:TYR:H	1.66	0.43
3:V:104:LEU:O	3:V:108:LEU:HD12	2.18	0.43
3:Y:75:MET:CE	3:Y:75:MET:HA	2.47	0.43
3:Y:115:ARG:CD	3:Y:116:GLY:N	2.79	0.43
3:Z:119:THR:HG1	3:Z:121:HIS:CD2	2.35	0.43
1:M:123:GLN:HE22	1:M:130:SER:HG	1.51	0.43
2:I:36:TRP:NE1	2:I:83:LEU:HG	2.34	0.43
2:I:158:ASN:C	2:I:160:GLY:H	2.21	0.43
1:O:46:TRP:HA	1:O:46:TRP:CE3	2.52	0.43
1:O:118:PRO:CG	1:O:208:PHE:CD2	3.01	0.43
3:X:108:LEU:HD23	3:X:108:LEU:HA	1.43	0.43
2:H:93:THR:OG1	2:H:114:VAL:HG23	2.15	0.43
1:M:7:SER:HB3	1:M:22:THR:H	1.82	0.43
1:M:97:PHE:HE2	2:I:47:TRP:N	2.15	0.43
1:M:185:TYR:CA	1:M:191:TYR:OH	2.67	0.43
2:I:51:ILE:HD13	2:I:74:ARG:HG3	2.00	0.43
3:X:100:LEU:O	3:X:100:LEU:HD22	2.18	0.43
3:X:129:LEU:O	3:X:132:GLN:N	2.51	0.43
3:Y:51:TRP:C	3:Y:53:THR:N	2.72	0.43
1:L:114:VAL:HG21	1:L:204:ILE:CG2	2.48	0.43
2:H:18:MET:O	2:H:85:MET:N	2.52	0.43
2:H:37:VAL:O	2:H:37:VAL:HG12	2.19	0.43
1:M:46:TRP:CE2	1:M:57:VAL:HG13	2.53	0.43
1:M:147:TRP:CE3	1:M:192:THR:O	2.72	0.43
2:I:9:GLY:HA2	2:I:18:MET:SD	2.58	0.43
2:J:89:ARG:O	2:J:114:VAL:HG11	2.18	0.43
2:J:174:GLN:HB3	2:J:175:SER:H	1.46	0.43
3:V:26:LEU:O	3:V:27:SER:C	2.57	0.43
3:V:123:ASP:HA	3:V:124:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:51:TRP:CZ2	3:X:138:LYS:HE3	2.51	0.43
3:X:51:TRP:CE2	3:X:138:LYS:HE3	2.53	0.43
3:X:134:LEU:HD23	3:X:134:LEU:HA	1.84	0.43
3:Y:11:VAL:O	3:Y:15:LEU:HD22	2.18	0.43
3:Y:139:VAL:O	3:Y:143:MET:HG3	2.19	0.43
1:L:79:ALA:HA	1:L:105:ILE:HD13	2.01	0.43
2:H:33:TRP:CZ3	3:V:110:THR:HA	2.53	0.43
2:I:4:LEU:HD23	2:I:24:ALA:HB2	2.01	0.43
1:N:44:LYS:HB2	1:N:44:LYS:HE3	1.53	0.43
1:O:180:LEU:C	1:O:180:LEU:HD12	2.39	0.43
3:X:132:GLN:C	3:X:134:LEU:N	2.72	0.43
3:Y:52:LYS:NZ	3:Y:145:VAL:CG2	2.82	0.43
3:Y:86:LEU:HD23	3:Y:86:LEU:HA	1.72	0.43
3:Z:75:MET:HA	3:Z:75:MET:HE3	2.00	0.43
2:H:84:GLN:HA	2:H:84:GLN:NE2	2.33	0.43
2:H:104:LEU:O	2:H:104:LEU:HG	2.18	0.43
1:M:189:ASN:HD22	1:M:210:ARG:N	2.16	0.43
2:I:54:LYS:O	2:I:55:VAL:C	2.57	0.43
2:I:177:LEU:HD23	2:I:177:LEU:HA	1.41	0.43
1:N:94:PRO:HA	2:J:47:TRP:CZ3	2.54	0.43
1:N:169:ASP:OD2	1:N:169:ASP:C	2.56	0.43
2:J:162:LEU:HA	2:J:162:LEU:HD23	1.79	0.43
2:J:186:VAL:HG23	2:J:187:PRO:O	2.18	0.43
1:O:123:GLN:HG3	2:K:125:TYR:CE2	2.54	0.43
1:O:194:GLU:HB3	1:O:205:VAL:HG13	2.00	0.43
2:K:149:PHE:HB2	2:K:177:LEU:CD2	2.49	0.43
2:K:175:SER:O	2:K:176:ASP:C	2.57	0.43
3:V:15:LEU:O	3:V:16:LEU:C	2.56	0.43
3:V:140:ARG:HA	3:V:143:MET:CE	2.48	0.43
3:X:41:LEU:HD13	3:X:127:ILE:HA	2.01	0.43
3:X:137:GLY:O	3:X:138:LYS:C	2.57	0.43
3:Z:61:GLN:O	3:Z:65:GLY:N	2.35	0.43
1:M:54:ALA:O	1:M:56:GLY:N	2.52	0.43
1:N:175:SER:HB3	2:J:169:PHE:CE1	2.54	0.43
2:K:33:TRP:CZ3	3:Z:110:THR:HA	2.53	0.43
2:K:51:ILE:HD11	2:K:74:ARG:CD	2.49	0.43
3:V:74:VAL:HG22	3:V:127:ILE:HG13	2.01	0.43
3:X:30:PRO:O	3:X:31:GLU:C	2.57	0.43
3:Y:37:THR:HG22	3:Y:38:PRO:O	2.18	0.43
3:Z:12:LEU:HD13	3:Z:143:MET:SD	2.59	0.43
3:Z:61:GLN:O	3:Z:62:ASP:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:36:TRP:CD1	2:I:83:LEU:HG	2.54	0.42
1:N:58:PRO:O	1:N:61:PHE:HB2	2.20	0.42
1:N:125:THR:O	1:N:125:THR:HG22	2.19	0.42
2:K:124:VAL:HA	2:K:144:LEU:O	2.19	0.42
3:V:70:LEU:HD23	3:V:70:LEU:HA	1.82	0.42
3:V:75:MET:O	3:V:77:ALA:N	2.52	0.42
3:X:37:THR:HA	3:X:38:PRO:HD3	1.71	0.42
3:Z:101:LEU:HD12	3:Z:105:GLN:NE2	2.34	0.42
2:I:93:THR:HG23	2:I:112:VAL:O	2.19	0.42
1:O:117:PHE:HA	1:O:118:PRO:HD3	1.66	0.42
3:X:12:LEU:HD22	3:X:143:MET:SD	2.60	0.42
3:Y:115:ARG:HD2	3:Y:115:ARG:C	2.40	0.42
3:Y:123:ASP:O	3:Y:124:PRO:C	2.57	0.42
3:Z:119:THR:O	3:Z:121:HIS:HD2	2.02	0.42
2:H:214:VAL:HG12	2:H:215:PRO:CD	2.49	0.42
1:N:18:LYS:HA	1:N:75:SER:O	2.19	0.42
1:N:27:SER:O	1:N:28:SER:C	2.58	0.42
1:N:118:PRO:HB3	1:N:208:PHE:CZ	2.54	0.42
2:J:54:LYS:O	2:J:55:VAL:C	2.54	0.42
2:J:77:SER:C	2:J:79:SER:H	2.21	0.42
2:J:111:LEU:HD22	2:J:111:LEU:HA	1.73	0.42
2:J:184:VAL:HG22	2:J:185:THR:N	2.33	0.42
1:O:185:TYR:CE1	1:O:210:ARG:HG3	2.54	0.42
1:O:185:TYR:HE1	1:O:191:TYR:CE1	2.37	0.42
2:K:9:GLY:HA2	2:K:112:VAL:CG2	2.48	0.42
2:K:25:SER:O	2:K:27:PHE:HD1	2.03	0.42
2:K:45:LEU:HD23	2:K:45:LEU:HA	1.74	0.42
2:K:122:PRO:CB	2:K:148:TYR:HB3	2.47	0.42
3:V:64:LEU:HB2	3:V:104:LEU:HB3	1.99	0.42
3:V:78:ARG:O	3:V:79:GLY:C	2.57	0.42
3:V:90:LEU:HD21	3:V:128:PHE:CE2	2.54	0.42
3:V:90:LEU:O	3:V:94:SER:HB3	2.19	0.42
3:V:97:VAL:HA	3:V:131:PHE:CZ	2.53	0.42
1:L:33:TYR:CE1	1:L:90:ARG:HD3	2.54	0.42
1:M:189:ASN:O	1:M:210:ARG:N	2.45	0.42
1:N:1:GLN:N	1:N:94:PRO:HD2	2.34	0.42
1:N:162:TRP:CZ2	1:N:174:MET:CE	3.02	0.42
2:J:11:LEU:O	2:J:12:VAL:HG13	2.19	0.42
2:J:151:GLU:HA	2:J:152:PRO:HA	1.68	0.42
1:O:104:GLU:HB3	4:O:217:HOH:O	2.19	0.42
3:Y:13:SER:O	3:Y:16:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:26:LEU:C	3:Y:28:GLN:N	2.73	0.42
1:L:6:GLN:HE22	1:L:87:CYS:N	2.13	0.42
1:L:76:ARG:HB3	1:L:76:ARG:NH1	2.27	0.42
1:M:50:THR:HG23	1:M:70:TYR:CD2	2.55	0.42
1:M:139:TYR:CG	1:M:140:PRO:HA	2.55	0.42
2:I:149:PHE:CG	2:I:150:PRO:HA	2.55	0.42
1:O:20:THR:HG23	1:O:20:THR:O	2.18	0.42
2:K:90:ALA:O	2:K:114:VAL:HG23	2.20	0.42
3:X:87:SER:O	3:X:89:LEU:N	2.52	0.42
3:Z:51:TRP:HZ2	3:Z:63:ILE:HD11	1.85	0.42
1:M:143:ILE:O	1:M:143:ILE:HG23	2.18	0.42
2:I:19:LYS:HG3	2:I:84:GLN:HB2	2.00	0.42
2:I:60:ILE:HG21	2:I:62:TYR:CE2	2.54	0.42
2:J:8:GLY:C	2:J:9:GLY:O	2.56	0.42
2:J:177:LEU:HD23	2:J:177:LEU:HA	1.82	0.42
1:O:70:TYR:CD1	1:O:70:TYR:N	2.87	0.42
1:O:124:LEU:HD12	1:O:124:LEU:HA	1.92	0.42
1:O:188:HIS:CD2	1:O:188:HIS:N	2.88	0.42
2:K:3:LYS:HD2	4:K:224:HOH:O	2.19	0.42
2:K:29:PHE:CB	2:K:79:SER:CB	2.87	0.42
2:K:38:ARG:CD	2:K:46:GLU:HG2	2.49	0.42
2:K:216:ARG:HH21	3:V:123:ASP:N	2.13	0.42
3:V:22:LEU:O	3:V:23:HIS:C	2.56	0.42
3:X:22:LEU:CD2	3:X:92:GLN:HE21	2.32	0.42
3:Y:86:LEU:O	3:Y:89:LEU:N	2.53	0.42
1:L:114:VAL:CG1	1:L:115:SER:N	2.82	0.42
2:H:151:GLU:OE2	2:H:171:ALA:HB2	2.19	0.42
1:M:132:VAL:CG1	2:I:144:LEU:HD22	2.49	0.42
2:I:98:CYS:O	2:I:98:CYS:SG	2.77	0.42
1:O:46:TRP:HB3	1:O:47:ILE:H	1.62	0.42
3:Z:75:MET:HE3	3:Z:75:MET:CA	2.49	0.42
3:Z:101:LEU:O	3:Z:102:GLY:C	2.58	0.42
1:L:14:SER:O	1:L:15:PRO:C	2.56	0.42
1:L:48:TYR:CE2	3:V:113:PRO:CG	3.03	0.42
2:I:19:LYS:HG3	2:I:84:GLN:HA	2.01	0.42
2:I:62:TYR:CZ	2:I:72:VAL:HG12	2.55	0.42
1:O:7:SER:CB	1:O:8:PRO:HD3	2.49	0.42
1:O:88:GLN:HE22	1:O:90:ARG:NH1	2.17	0.42
2:K:141:LEU:HD23	2:K:141:LEU:HA	1.55	0.42
3:V:78:ARG:HD2	3:V:91:GLY:N	2.34	0.42
3:Y:26:LEU:C	3:Y:28:GLN:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:43:ALA:H	3:Y:118:THR:HA	1.85	0.42
1:L:43:PRO:HD2	2:H:106:TRP:CE3	2.54	0.42
1:L:65:GLY:HA2	1:L:70:TYR:HA	2.01	0.42
1:L:135:LEU:HB2	1:L:174:MET:HG2	2.00	0.42
2:H:211:LYS:O	2:H:213:ILE:HG12	2.20	0.42
1:M:37:GLN:O	1:M:83:ALA:HB1	2.20	0.42
2:J:134:GLN:HB3	2:J:136:ASN:HD21	1.84	0.42
1:O:202:SER:O	1:O:204:ILE:N	2.53	0.42
2:K:129:PRO:O	2:K:215:PRO:HG3	2.19	0.42
2:K:157:TRP:CZ3	2:K:198:CYS:HB3	2.55	0.42
2:K:183:SER:O	2:K:183:SER:OG	2.37	0.42
3:X:17:ARG:O	3:X:20:HIS:HB2	2.19	0.42
3:X:123:ASP:OD2	3:X:125:ASN:HB2	2.20	0.42
3:Y:101:LEU:O	3:Y:104:LEU:N	2.53	0.42
3:Z:96:GLN:O	3:Z:97:VAL:C	2.58	0.42
3:Z:100:LEU:HD23	3:Z:100:LEU:HA	1.58	0.42
3:Z:121:HIS:ND1	3:Z:126:ALA:HB1	2.35	0.42
2:H:122:PRO:CB	2:H:148:TYR:HB3	2.50	0.42
1:M:185:TYR:CD1	1:M:191:TYR:OH	2.73	0.42
1:N:107:ARG:HG3	1:N:108:ALA:N	2.34	0.42
2:J:86:ASN:O	2:J:87:SER:O	2.36	0.42
1:O:169:ASP:O	1:O:169:ASP:CG	2.57	0.42
3:X:31:GLU:HB3	3:X:33:HIS:CE1	2.55	0.42
3:Y:125:ASN:O	3:Y:129:LEU:HB2	2.19	0.42
1:L:76:ARG:HH11	1:L:76:ARG:CB	2.27	0.41
1:L:114:VAL:CG2	1:L:204:ILE:HG21	2.50	0.41
2:H:176:ASP:CB	4:H:226:HOH:O	2.62	0.41
2:H:216:ARG:HH22	3:Z:123:ASP:CB	2.31	0.41
1:M:78:GLU:CD	1:N:107:ARG:HH22	2.24	0.41
1:M:211:ASN:O	1:M:212:GLU:HB2	2.20	0.41
2:I:200:VAL:HG23	2:I:208:LYS:O	2.19	0.41
1:N:86:TYR:CG	2:J:45:LEU:HD12	2.55	0.41
2:J:13:GLN:O	2:J:14:PRO:C	2.56	0.41
2:J:213:ILE:HG23	2:J:214:VAL:HG23	2.01	0.41
1:O:31:TYR:HA	1:O:50:THR:OG1	2.19	0.41
1:O:107:ARG:CG	1:O:108:ALA:N	2.77	0.41
2:K:123:SER:HB3	2:K:125:TYR:OH	2.19	0.41
2:K:192:PRO:O	2:K:193:SER:C	2.58	0.41
3:V:93:LEU:O	3:V:96:GLN:CB	2.67	0.41
3:X:35:LEU:HA	3:X:36:PRO:HD2	1.76	0.41
1:L:37:GLN:HE21	1:L:86:TYR:HE2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:TRP:HD1	2:H:53:SER:OG	2.02	0.41
2:H:40:SER:O	2:H:44:GLY:HA2	2.20	0.41
2:H:130:GLY:C	2:H:132:ALA:H	2.23	0.41
1:M:166:ASP:HB3	1:M:169:ASP:O	2.19	0.41
2:I:76:ASP:O	2:I:78:LYS:N	2.53	0.41
2:J:38:ARG:NH2	2:J:92:ASP:HA	2.34	0.41
3:V:26:LEU:O	3:V:28:GLN:N	2.53	0.41
3:V:66:ALA:O	3:V:69:LEU:N	2.52	0.41
3:Z:108:LEU:HD23	3:Z:108:LEU:HA	1.65	0.41
3:Z:123:ASP:C	3:Z:125:ASN:N	2.71	0.41
1:L:33:TYR:CD1	1:L:90:ARG:HD3	2.55	0.41
1:L:89:GLN:NE2	1:L:96:THR:HB	2.32	0.41
1:M:184:GLU:HG3	1:M:187:ARG:HH12	1.85	0.41
2:J:38:ARG:HB2	2:J:96:TYR:HD2	1.72	0.41
2:J:56:ASN:OD1	3:Y:105:GLN:HB3	2.20	0.41
2:J:135:THR:C	2:J:136:ASN:O	2.57	0.41
1:O:94:PRO:CB	2:K:47:TRP:CZ3	3.03	0.41
1:O:174:MET:HA	2:K:169:PHE:CE1	2.56	0.41
2:K:7:SER:O	2:K:21:SER:N	2.47	0.41
2:K:27:PHE:O	2:K:27:PHE:CG	2.73	0.41
2:K:157:TRP:O	2:K:158:ASN:C	2.57	0.41
3:V:128:PHE:O	3:V:132:GLN:HG3	2.20	0.41
3:Y:112:LEU:HA	3:Y:113:PRO:HD3	1.79	0.41
3:Z:108:LEU:O	3:Z:110:THR:HG22	2.20	0.41
1:L:147:TRP:CB	1:L:178:LEU:HD12	2.50	0.41
1:M:57:VAL:HA	1:M:58:PRO:HD3	1.83	0.41
1:M:211:ASN:O	1:M:212:GLU:CB	2.68	0.41
2:I:35:ASP:O	2:I:99:SER:N	2.39	0.41
2:I:214:VAL:HA	2:I:215:PRO:HD3	1.84	0.41
1:O:18:LYS:HG3	1:O:75:SER:O	2.20	0.41
1:O:189:ASN:ND2	1:O:210:ARG:N	2.67	0.41
3:Y:70:LEU:O	3:Y:74:VAL:HG23	2.20	0.41
1:L:110:ALA:O	1:L:138:PHE:CA	2.45	0.41
1:L:159:LEU:HA	1:L:159:LEU:HD23	1.84	0.41
1:L:169:ASP:OD2	1:L:169:ASP:C	2.58	0.41
1:L:178:LEU:HD23	1:L:179:THR:N	2.36	0.41
1:M:90:ARG:CA	1:M:95:ARG:HH21	2.33	0.41
1:N:132:VAL:HB	1:N:177:THR:HG23	2.01	0.41
1:N:135:LEU:CD2	1:N:195:ALA:HB2	2.50	0.41
2:J:29:PHE:C	2:J:31:ASP:N	2.73	0.41
2:K:40:SER:CB	2:K:42:GLU:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:52:ARG:HB3	2:K:56:ASN:HB2	2.02	0.41
2:K:158:ASN:HD22	2:K:158:ASN:HA	1.50	0.41
3:V:22:LEU:HD12	3:V:96:GLN:NE2	2.36	0.41
3:X:143:MET:H	3:X:143:MET:HG3	1.60	0.41
1:L:35:PHE:HB3	1:L:44:LYS:O	2.21	0.41
1:L:135:LEU:O	1:L:138:PHE:HE2	2.04	0.41
1:L:185:TYR:HE1	1:L:191:TYR:CD1	2.33	0.41
2:H:157:TRP:CE3	2:H:198:CYS:HB3	2.53	0.41
2:I:122:PRO:HA	2:I:146:LYS:O	2.20	0.41
2:J:216:ARG:NE	3:X:122:LYS:H	2.18	0.41
3:Y:86:LEU:O	3:Y:87:SER:C	2.59	0.41
3:Z:140:ARG:C	3:Z:142:LEU:N	2.73	0.41
1:L:52:ASN:ND2	3:V:115:ARG:HH11	2.19	0.41
1:L:114:VAL:HG23	1:L:204:ILE:HG21	2.02	0.41
2:H:70:PHE:HD1	2:H:85:MET:HA	1.85	0.41
1:M:204:ILE:HD13	1:M:204:ILE:N	2.36	0.41
1:N:125:THR:O	1:N:125:THR:CG2	2.68	0.41
1:N:184:GLU:HG3	1:N:187:ARG:NH2	2.36	0.41
2:J:89:ARG:CB	2:J:91:GLU:OE1	2.49	0.41
1:O:134:PHE:CZ	2:K:183:SER:HB3	2.56	0.41
2:K:40:SER:HB2	2:K:42:GLU:H	1.85	0.41
3:X:16:LEU:HD11	3:X:136:ARG:CG	2.50	0.41
3:X:72:GLU:OE1	3:X:114:PRO:HG3	2.21	0.41
3:Z:141:PHE:O	3:Z:142:LEU:C	2.56	0.41
1:L:141:LYS:HG3	1:L:172:TYR:CD1	2.56	0.41
2:H:2:VAL:O	2:H:2:VAL:HG22	2.20	0.41
1:M:1:GLN:O	1:M:1:GLN:CG	2.65	0.41
1:M:4:LEU:N	1:M:4:LEU:HD23	2.36	0.41
2:I:38:ARG:HB2	2:I:96:TYR:CD1	2.56	0.41
1:N:104:GLU:HB3	4:N:216:HOH:O	2.21	0.41
1:O:45:LEU:O	1:O:54:ALA:HB3	2.21	0.41
1:O:116:ILE:CA	1:O:117:PHE:HD1	2.33	0.41
2:K:174:GLN:HB3	2:K:175:SER:H	1.27	0.41
3:V:123:ASP:OD1	3:V:124:PRO:HD2	2.21	0.41
3:X:69:LEU:HD22	3:X:69:LEU:O	2.21	0.41
3:X:123:ASP:C	3:X:125:ASN:H	2.23	0.41
3:Y:63:ILE:O	3:Y:67:VAL:CG2	2.59	0.41
3:Z:59:LYS:NZ	3:Z:145:VAL:HG21	2.36	0.41
1:L:6:GLN:HE22	1:L:86:TYR:HA	1.85	0.41
1:L:34:TRP:C	1:L:35:PHE:CD1	2.94	0.41
1:L:139:TYR:CA	1:L:140:PRO:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:THR:OG1	1:L:184:GLU:HB2	2.21	0.41
2:H:2:VAL:HG21	2:H:105:TYR:CG	2.56	0.41
2:H:54:LYS:HB2	2:H:54:LYS:HE2	1.90	0.41
2:H:83:LEU:HA	2:H:83:LEU:HD23	1.48	0.41
2:H:138:MET:CE	2:H:187:PRO:HA	2.49	0.41
1:M:38:LYS:HA	1:M:39:PRO:HD2	1.68	0.41
1:M:49:SER:O	1:M:51:SER:N	2.54	0.41
1:M:137:ASN:H	1:M:173:SER:HB3	1.86	0.41
2:I:122:PRO:HB2	2:I:145:VAL:HG23	2.03	0.41
2:I:123:SER:HB2	2:I:125:TYR:CE2	2.56	0.41
2:I:148:TYR:CE2	2:I:153:VAL:HG12	2.56	0.41
2:I:176:ASP:O	2:I:177:LEU:HG	2.21	0.41
1:N:116:ILE:HD11	1:N:208:PHE:HD1	1.85	0.41
2:J:51:ILE:HD11	2:J:74:ARG:HG3	1.99	0.41
2:J:70:PHE:CE1	2:J:85:MET:CG	3.03	0.41
2:J:171:ALA:HB2	2:J:180:LEU:HD12	2.01	0.41
2:J:196:VAL:O	2:J:196:VAL:HG22	2.20	0.41
1:O:162:TRP:O	2:K:170:PRO:HG2	2.20	0.41
2:K:51:ILE:HG23	2:K:51:ILE:O	2.20	0.41
2:K:168:THR:HG22	2:K:169:PHE:N	2.36	0.41
3:V:41:LEU:HD13	3:V:127:ILE:HA	2.03	0.41
3:X:25:ARG:HH11	3:X:25:ARG:HG3	1.86	0.41
3:X:35:LEU:HD21	3:X:77:ALA:HB1	2.01	0.41
3:Y:8:ASP:O	3:Y:11:VAL:HG22	2.21	0.41
3:Y:10:ARG:O	3:Y:13:SER:CA	2.69	0.41
3:Y:22:LEU:HD21	3:Y:92:GLN:CB	2.45	0.41
3:Y:38:PRO:HG3	3:Y:122:LYS:HG2	2.01	0.41
3:Y:51:TRP:O	3:Y:52:LYS:C	2.59	0.41
3:Y:135:LEU:HA	3:Y:139:VAL:HB	2.02	0.41
1:L:29:VAL:HG12	1:L:30:SER:H	1.86	0.41
1:L:144:ASN:O	1:L:195:ALA:HA	2.21	0.41
1:L:147:TRP:CE3	1:L:178:LEU:CD1	3.04	0.41
2:J:28:THR:O	2:J:29:PHE:C	2.58	0.41
1:O:147:TRP:HE3	1:O:192:THR:O	2.01	0.41
2:K:64:GLU:C	2:K:66:VAL:N	2.71	0.41
3:V:49:GLY:C	3:V:51:TRP:H	2.25	0.41
3:Z:35:LEU:HA	3:Z:36:PRO:HD2	1.99	0.41
1:M:31:TYR:HB3	1:M:49:SER:HA	2.02	0.40
1:M:35:PHE:O	1:M:86:TYR:N	2.54	0.40
1:O:11:MET:CG	1:O:103:LEU:CD1	2.97	0.40
2:K:54:LYS:O	2:K:57:ASN:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:75:MET:CE	3:V:98:ARG:HH22	2.34	0.40
3:V:93:LEU:C	3:V:93:LEU:CD2	2.90	0.40
3:Z:116:GLY:O	3:Z:117:ARG:O	2.39	0.40
2:H:24:ALA:HB3	2:H:29:PHE:HD1	1.87	0.40
2:H:141:LEU:CD1	2:H:196:VAL:HG11	2.51	0.40
2:J:6:GLU:H	2:J:6:GLU:HG2	1.52	0.40
1:O:145:VAL:HG11	1:O:176:SER:CB	2.51	0.40
1:O:147:TRP:CZ3	1:O:193:CYS:HB2	2.56	0.40
2:K:66:VAL:CG2	2:K:70:PHE:CD2	3.03	0.40
3:X:109:GLY:O	4:X:166:HOH:O	2.22	0.40
2:H:157:TRP:CZ3	2:H:198:CYS:CB	3.00	0.40
2:I:70:PHE:CE1	2:I:85:MET:HE2	2.56	0.40
2:I:216:ARG:HE	3:Y:122:LYS:HG3	1.86	0.40
1:O:44:LYS:HZ3	1:O:44:LYS:CB	2.23	0.40
3:X:69:LEU:HD23	3:X:69:LEU:HA	1.87	0.40
3:X:100:LEU:O	3:X:103:ALA:HB3	2.22	0.40
3:Z:86:LEU:HD11	3:Z:124:PRO:HG3	2.03	0.40
2:I:216:ARG:NH2	3:Y:122:LYS:H	2.18	0.40
1:N:19:VAL:HG11	1:N:103:LEU:HD21	1.99	0.40
1:N:19:VAL:HG23	1:N:77:MET:HB2	2.03	0.40
1:N:116:ILE:HG21	1:N:206:LYS:O	2.22	0.40
1:N:124:LEU:C	1:N:126:SER:H	2.24	0.40
2:J:33:TRP:N	3:Y:111:GLN:HE22	2.00	0.40
2:K:78:LYS:HA	4:K:219:HOH:O	2.21	0.40
2:K:216:ARG:HH22	3:V:123:ASP:CB	2.34	0.40
3:X:71:LEU:HD23	3:X:71:LEU:HA	1.68	0.40
2:H:105:TYR:O	2:H:106:TRP:CD1	2.75	0.40
1:M:31:TYR:CE2	3:X:61:GLN:NE2	2.90	0.40
1:M:46:TRP:O	1:M:57:VAL:HG21	2.21	0.40
1:M:162:TRP:O	2:I:170:PRO:HD2	2.20	0.40
1:M:189:ASN:ND2	1:M:211:ASN:ND2	2.69	0.40
1:M:192:THR:OG1	1:M:207:SER:HB2	2.20	0.40
2:I:6:GLU:OE2	2:I:109:GLY:CA	2.69	0.40
2:I:66:VAL:O	2:I:68:GLY:N	2.55	0.40
1:N:185:TYR:HD1	1:N:191:TYR:CE1	2.35	0.40
2:J:214:VAL:HG23	3:X:38:PRO:HD2	2.04	0.40
1:O:19:VAL:CG1	1:O:74:ILE:HG13	2.51	0.40
1:O:134:PHE:C	1:O:135:LEU:HD12	2.42	0.40
3:V:98:ARG:O	3:V:101:LEU:HB3	2.21	0.40
3:X:120:ALA:O	3:X:121:HIS:CG	2.74	0.40
3:Z:141:PHE:HA	3:Z:144:LEU:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:ARG:NH2	4:V:165:HOH:O[1_545]	2.19	0.01

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	L	211/213 (99%)	178 (84%)	28 (13%)	5 (2%)	6	28
1	M	210/213 (99%)	179 (85%)	20 (10%)	11 (5%)	2	13
1	N	210/213 (99%)	177 (84%)	20 (10%)	13 (6%)	1	10
1	O	211/213 (99%)	175 (83%)	24 (11%)	12 (6%)	1	11
2	H	215/217 (99%)	175 (81%)	24 (11%)	16 (7%)	1	7
2	I	215/217 (99%)	170 (79%)	25 (12%)	20 (9%)	0	4
2	J	215/217 (99%)	166 (77%)	31 (14%)	18 (8%)	1	5
2	K	215/217 (99%)	165 (77%)	30 (14%)	20 (9%)	0	4
3	V	143/163 (88%)	88 (62%)	32 (22%)	23 (16%)	0	1
3	X	136/163 (83%)	98 (72%)	19 (14%)	19 (14%)	0	1
3	Y	137/163 (84%)	92 (67%)	33 (24%)	12 (9%)	1	5
3	Z	136/163 (83%)	89 (65%)	31 (23%)	16 (12%)	0	2
All	All	2254/2372 (95%)	1752 (78%)	317 (14%)	185 (8%)	1	5

All (185) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	107	ARG
1	L	212	GLU
2	H	28	THR

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Mol	Chain	Res	Type
2	H	133	ALA
2	H	175	SER
2	H	176	ASP
2	H	204	ALA
1	M	121	SER
2	I	65	SER
2	I	67	LYS
2	I	101	TRP
2	I	159	SER
2	I	175	SER
2	I	184	VAL
2	I	193	SER
2	I	204	ALA
2	I	205	SER
1	N	28	SER
1	N	71	SER
1	N	167	SER
1	N	170	SER
2	J	30	SER
2	J	52	ARG
2	J	55	VAL
2	J	65	SER
2	J	116	ALA
2	J	131	SER
2	J	204	ALA
1	O	198	LYS
2	K	9	GLY
2	K	27	PHE
2	K	57	ASN
2	K	58	HIS
2	K	65	SER
2	K	203	PRO
3	V	11	VAL
3	V	30	PRO
3	V	43	ALA
3	V	50	GLU
3	V	54	GLN
3	V	80	GLN
3	V	103	ALA
3	V	145	VAL
3	V	148	SER
3	X	10	ARG

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Mol	Chain	Res	Type
3	X	11	VAL
3	X	31	GLU
3	X	88	SER
3	X	130	SER
3	Y	13	SER
3	Y	31	GLU
3	Y	43	ALA
3	Y	85	CYS
3	Z	50	GLU
3	Z	138	LYS
2	H	92	ASP
2	H	107	GLY
2	H	132	ALA
1	M	125	THR
1	M	167	SER
1	M	191	TYR
2	I	9	GLY
2	I	131	SER
1	N	109	ASP
1	N	125	THR
1	N	137	ASN
2	J	16	GLY
2	J	27	PHE
2	J	89	ARG
2	J	216	ARG
1	O	121	SER
1	O	170	SER
1	O	212	GLU
2	K	14	PRO
2	K	26	GLY
2	K	28	THR
2	K	55	VAL
2	K	87	SER
2	K	91	GLU
2	K	117	ALA
2	K	176	ASP
2	K	204	ALA
3	V	27	SER
3	V	31	GLU
3	V	79	GLY
3	V	87	SER
3	V	88	SER

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Mol	Chain	Res	Type
3	V	91	GLY
3	V	102	GLY
3	V	138	LYS
3	V	144	LEU
3	V	146	GLY
3	X	25	ARG
3	X	27	SER
3	X	44	VAL
3	X	62	ASP
3	X	87	SER
3	X	103	ALA
3	X	133	HIS
3	X	138	LYS
3	Y	125	ASN
3	Z	10	ARG
3	Z	25	ARG
3	Z	92	GLN
2	H	14	PRO
2	H	90	ALA
2	H	203	PRO
1	M	39	PRO
1	M	67	GLY
2	I	14	PRO
2	I	77	SER
2	I	163	SER
2	I	176	ASP
1	N	122	GLU
2	J	136	ASN
2	J	176	ASP
1	O	7	SER
1	O	149	ILE
1	O	203	PRO
1	O	204	ILE
2	K	59	ALA
2	K	119	THR
3	V	34	PRO
3	V	49	GLY
3	V	76	ALA
3	V	141	PHE
3	X	34	PRO
3	Y	9	LEU
3	Y	14	LYS

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Mol	Chain	Res	Type
3	Y	27	SER
3	Y	140	ARG
3	Y	145	VAL
3	Z	56	GLU
3	Z	82	GLY
3	Z	91	GLY
3	Z	94	SER
3	Z	129	LEU
1	L	15	PRO
1	M	8	PRO
1	M	59	ALA
1	M	149	ILE
2	I	66	VAL
2	I	150	PRO
1	N	45	LEU
1	N	49	SER
2	J	42	GLU
2	J	215	PRO
1	O	23	CYS
1	O	55	SER
2	K	30	SER
3	X	126	ALA
3	X	129	LEU
3	X	144	LEU
3	Y	82	GLY
3	Z	31	GLU
3	Z	110	THR
3	Z	117	ARG
1	L	149	ILE
2	H	131	SER
1	M	79	ALA
2	I	158	ASN
1	N	165	GLN
2	J	133	ALA
2	J	193	SER
2	K	159	SER
2	H	159	SER
2	H	207	THR
2	I	100	GLY
1	N	39	PRO
3	X	36	PRO
3	X	61	GLN

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Mol	Chain	Res	Type
3	Z	65	GLY
2	H	41	PRO
1	O	202	SER
1	M	151	GLY
1	N	8	PRO
2	K	122	PRO
3	Y	102	GLY
3	Z	49	GLY
3	Z	102	GLY
2	J	152	PRO
1	O	40	GLY
2	I	130	GLY
2	H	152	PRO

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	L	186/186 (100%)	121 (65%)	65 (35%)	0	1
1	M	185/186 (100%)	118 (64%)	67 (36%)	0	0
1	N	185/186 (100%)	121 (65%)	64 (35%)	0	1
1	O	186/186 (100%)	117 (63%)	69 (37%)	0	0
2	H	182/185 (98%)	115 (63%)	67 (37%)	0	0
2	I	182/185 (98%)	108 (59%)	74 (41%)	0	0
2	J	182/185 (98%)	109 (60%)	73 (40%)	0	0
2	K	182/185 (98%)	115 (63%)	67 (37%)	0	0
3	V	122/138 (88%)	73 (60%)	49 (40%)	0	0
3	X	117/138 (85%)	74 (63%)	43 (37%)	0	0
3	Y	117/138 (85%)	72 (62%)	45 (38%)	0	0
3	Z	116/138 (84%)	74 (64%)	42 (36%)	0	0
All	All	1942/2036 (95%)	1217 (63%)	725 (37%)	0	0

All (725) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	2	VAL
1	L	3	VAL
1	L	5	THR
1	L	11	MET
1	L	12	SER
1	L	18	LYS
1	L	20	THR
1	L	22	THR
1	L	27	SER
1	L	29	VAL
1	L	35	PHE
1	L	38	LYS
1	L	42	SER
1	L	44	LYS
1	L	45	LEU
1	L	55	SER
1	L	60	ARG
1	L	68	THR
1	L	72	LEU
1	L	73	THR
1	L	76	ARG
1	L	77	MET
1	L	90	ARG
1	L	95	ARG
1	L	104	GLU
1	L	105	ILE
1	L	106	LYS
1	L	107	ARG
1	L	115	SER
1	L	116	ILE
1	L	117	PHE
1	L	118	PRO
1	L	120	SER
1	L	123	GLN
1	L	124	LEU
1	L	132	VAL
1	L	133	CYS
1	L	143	ILE
1	L	145	VAL
1	L	146	LYS
1	L	149	ILE

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Mol	Chain	Res	Type
1	L	152	SER
1	L	154	ARG
1	L	162	TRP
1	L	163	THR
1	L	165	GLN
1	L	168	LYS
1	L	169	ASP
1	L	171	THR
1	L	173	SER
1	L	175	SER
1	L	180	LEU
1	L	181	THR
1	L	182	LYS
1	L	190	SER
1	L	192	THR
1	L	193	CYS
1	L	194	GLU
1	L	199	THR
1	L	201	THR
1	L	202	SER
1	L	204	ILE
1	L	211	ASN
1	L	213	CYS
2	H	3	LYS
2	H	4	LEU
2	H	12	VAL
2	H	13	GLN
2	H	21	SER
2	H	28	THR
2	H	29	PHE
2	H	30	SER
2	H	35	ASP
2	H	38	ARG
2	H	42	GLU
2	H	50	GLU
2	H	51	ILE
2	H	54	LYS
2	H	56	ASN
2	H	57	ASN
2	H	64	GLU
2	H	67	LYS
2	H	69	ARG

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Mol	Chain	Res	Type
2	H	71	THR
2	H	74	ARG
2	H	78	LYS
2	H	79	SER
2	H	80	SER
2	H	83	LEU
2	H	84	GLN
2	H	85	MET
2	H	87	SER
2	H	88	LEU
2	H	89	ARG
2	H	95	ILE
2	H	98	CYS
2	H	99	SER
2	H	101	TRP
2	H	102	SER
2	H	108	GLN
2	H	110	THR
2	H	111	LEU
2	H	113	THR
2	H	114	VAL
2	H	121	PRO
2	H	124	VAL
2	H	136	ASN
2	H	139	VAL
2	H	141	LEU
2	H	146	LYS
2	H	155	VAL
2	H	156	THR
2	H	159	SER
2	H	161	SER
2	H	162	LEU
2	H	166	VAL
2	H	172	VAL
2	H	174	GLN
2	H	175	SER
2	H	180	LEU
2	H	188	SER
2	H	195	THR
2	H	196	VAL
2	H	198	CYS
2	H	199	ASN

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Mol	Chain	Res	Type
2	H	206	SER
2	H	207	THR
2	H	213	ILE
2	H	214	VAL
2	H	216	ARG
2	H	217	ASP
1	M	1	GLN
1	M	3	VAL
1	M	7	SER
1	M	11	MET
1	M	12	SER
1	M	18	LYS
1	M	20	THR
1	M	23	CYS
1	M	24	SER
1	M	30	SER
1	M	33	TYR
1	M	36	GLN
1	M	38	LYS
1	M	41	THR
1	M	45	LEU
1	M	62	ARG
1	M	68	THR
1	M	73	THR
1	M	76	ARG
1	M	77	MET
1	M	81	ASP
1	M	88	GLN
1	M	90	ARG
1	M	95	ARG
1	M	97	PHE
1	M	105	ILE
1	M	106	LYS
1	M	113	THR
1	M	115	SER
1	M	116	ILE
1	M	117	PHE
1	M	120	SER
1	M	124	LEU
1	M	126	SER
1	M	130	SER
1	M	132	VAL

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Mol	Chain	Res	Type
1	M	137	ASN
1	M	138	PHE
1	M	142	ASP
1	M	143	ILE
1	M	146	LYS
1	M	150	ASP
1	M	153	GLU
1	M	154	ARG
1	M	155	GLN
1	M	156	ASN
1	M	162	TRP
1	M	163	THR
1	M	165	GLN
1	M	166	ASP
1	M	168	LYS
1	M	170	SER
1	M	174	MET
1	M	175	SER
1	M	177	THR
1	M	180	LEU
1	M	181	THR
1	M	182	LYS
1	M	189	ASN
1	M	192	THR
1	M	194	GLU
1	M	196	THR
1	M	198	LYS
1	M	199	THR
1	M	208	PHE
1	M	210	ARG
1	M	211	ASN
2	I	3	LYS
2	I	4	LEU
2	I	6	GLU
2	I	7	SER
2	I	12	VAL
2	I	13	GLN
2	I	19	LYS
2	I	22	CYS
2	I	28	THR
2	I	38	ARG
2	I	40	SER

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Mol	Chain	Res	Type
2	I	52	ARG
2	I	53	SER
2	I	55	VAL
2	I	56	ASN
2	I	57	ASN
2	I	61	HIS
2	I	67	LYS
2	I	71	THR
2	I	74	ARG
2	I	75	ASP
2	I	77	SER
2	I	78	LYS
2	I	79	SER
2	I	80	SER
2	I	88	LEU
2	I	91	GLU
2	I	95	ILE
2	I	98	CYS
2	I	99	SER
2	I	102	SER
2	I	108	GLN
2	I	110	THR
2	I	111	LEU
2	I	112	VAL
2	I	113	THR
2	I	115	SER
2	I	118	LYS
2	I	119	THR
2	I	123	SER
2	I	134	GLN
2	I	136	ASN
2	I	138	MET
2	I	139	VAL
2	I	141	LEU
2	I	144	LEU
2	I	145	VAL
2	I	146	LYS
2	I	150	PRO
2	I	153	VAL
2	I	154	THR
2	I	155	VAL
2	I	159	SER

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Mol	Chain	Res	Type
2	I	162	LEU
2	I	164	SER
2	I	172	VAL
2	I	173	LEU
2	I	174	GLN
2	I	178	TYR
2	I	179	THR
2	I	180	LEU
2	I	189	SER
2	I	193	SER
2	I	194	GLU
2	I	195	THR
2	I	198	CYS
2	I	199	ASN
2	I	200	VAL
2	I	206	SER
2	I	207	THR
2	I	209	VAL
2	I	211	LYS
2	I	213	ILE
2	I	216	ARG
1	N	1	GLN
1	N	2	VAL
1	N	7	SER
1	N	10	ILE
1	N	12	SER
1	N	14	SER
1	N	17	GLU
1	N	26	SER
1	N	30	SER
1	N	35	PHE
1	N	38	LYS
1	N	39	PRO
1	N	41	THR
1	N	42	SER
1	N	44	LYS
1	N	45	LEU
1	N	49	SER
1	N	62	ARG
1	N	64	SER
1	N	68	THR
1	N	72	LEU

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Mol	Chain	Res	Type
1	N	76	ARG
1	N	77	MET
1	N	86	TYR
1	N	95	ARG
1	N	102	LYS
1	N	104	GLU
1	N	105	ILE
1	N	106	LYS
1	N	115	SER
1	N	116	ILE
1	N	117	PHE
1	N	120	SER
1	N	121	SER
1	N	124	LEU
1	N	130	SER
1	N	132	VAL
1	N	137	ASN
1	N	144	ASN
1	N	146	LYS
1	N	153	GLU
1	N	155	GLN
1	N	158	VAL
1	N	162	TRP
1	N	163	THR
1	N	164	ASP
1	N	165	GLN
1	N	167	SER
1	N	168	LYS
1	N	169	ASP
1	N	171	THR
1	N	174	MET
1	N	176	SER
1	N	179	THR
1	N	180	LEU
1	N	181	THR
1	N	190	SER
1	N	194	GLU
1	N	201	THR
1	N	204	ILE
1	N	205	VAL
1	N	206	LYS
1	N	210	ARG

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Mol	Chain	Res	Type
1	N	211	ASN
2	J	3	LYS
2	J	4	LEU
2	J	5	GLU
2	J	6	GLU
2	J	7	SER
2	J	11	LEU
2	J	12	VAL
2	J	13	GLN
2	J	18	MET
2	J	20	LEU
2	J	30	SER
2	J	31	ASP
2	J	35	ASP
2	J	38	ARG
2	J	40	SER
2	J	54	LYS
2	J	55	VAL
2	J	56	ASN
2	J	57	ASN
2	J	61	HIS
2	J	65	SER
2	J	67	LYS
2	J	69	ARG
2	J	71	THR
2	J	74	ARG
2	J	75	ASP
2	J	77	SER
2	J	78	LYS
2	J	80	SER
2	J	81	VAL
2	J	83	LEU
2	J	85	MET
2	J	92	ASP
2	J	95	ILE
2	J	99	SER
2	J	102	SER
2	J	108	GLN
2	J	110	THR
2	J	111	LEU
2	J	113	THR
2	J	114	VAL

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Mol	Chain	Res	Type
2	J	115	SER
2	J	123	SER
2	J	124	VAL
2	J	131	SER
2	J	136	ASN
2	J	137	SER
2	J	138	MET
2	J	139	VAL
2	J	144	LEU
2	J	148	TYR
2	J	151	GLU
2	J	153	VAL
2	J	156	THR
2	J	158	ASN
2	J	159	SER
2	J	162	LEU
2	J	166	VAL
2	J	172	VAL
2	J	173	LEU
2	J	174	GLN
2	J	175	SER
2	J	179	THR
2	J	183	SER
2	J	194	GLU
2	J	195	THR
2	J	196	VAL
2	J	199	ASN
2	J	200	VAL
2	J	206	SER
2	J	210	ASP
2	J	216	ARG
2	J	217	ASP
1	O	1	GLN
1	O	2	VAL
1	O	12	SER
1	O	14	SER
1	O	18	LYS
1	O	19	VAL
1	O	20	THR
1	O	24	SER
1	O	30	SER
1	O	33	TYR

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Mol	Chain	Res	Type
1	O	38	LYS
1	O	41	THR
1	O	42	SER
1	O	44	LYS
1	O	45	LEU
1	O	46	TRP
1	O	51	SER
1	O	55	SER
1	O	60	ARG
1	O	61	PHE
1	O	62	ARG
1	O	64	SER
1	O	71	SER
1	O	73	THR
1	O	76	ARG
1	O	77	MET
1	O	80	GLU
1	O	90	ARG
1	O	91	SER
1	O	95	ARG
1	O	102	LYS
1	O	113	THR
1	O	114	VAL
1	O	115	SER
1	O	116	ILE
1	O	117	PHE
1	O	120	SER
1	O	122	GLU
1	O	124	LEU
1	O	133	CYS
1	O	143	ILE
1	O	145	VAL
1	O	146	LYS
1	O	155	GLN
1	O	163	THR
1	O	164	ASP
1	O	165	GLN
1	O	166	ASP
1	O	168	LYS
1	O	171	THR
1	O	174	MET
1	O	177	THR

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Mol	Chain	Res	Type
1	O	178	LEU
1	O	180	LEU
1	O	181	THR
1	O	182	LYS
1	O	184	GLU
1	O	188	HIS
1	O	189	ASN
1	O	190	SER
1	O	192	THR
1	O	193	CYS
1	O	194	GLU
1	O	196	THR
1	O	204	ILE
1	O	206	LYS
1	O	210	ARG
1	O	211	ASN
1	O	212	GLU
2	K	2	VAL
2	K	4	LEU
2	K	5	GLU
2	K	7	SER
2	K	11	LEU
2	K	12	VAL
2	K	13	GLN
2	K	19	LYS
2	K	21	SER
2	K	28	THR
2	K	31	ASP
2	K	38	ARG
2	K	46	GLU
2	K	55	VAL
2	K	60	ILE
2	K	64	GLU
2	K	65	SER
2	K	69	ARG
2	K	73	SER
2	K	75	ASP
2	K	78	LYS
2	K	79	SER
2	K	80	SER
2	K	83	LEU
2	K	84	GLN

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Mol	Chain	Res	Type
2	K	85	MET
2	K	87	SER
2	K	89	ARG
2	K	93	THR
2	K	95	ILE
2	K	108	GLN
2	K	110	THR
2	K	111	LEU
2	K	113	THR
2	K	115	SER
2	K	118	LYS
2	K	119	THR
2	K	123	SER
2	K	124	VAL
2	K	136	ASN
2	K	144	LEU
2	K	151	GLU
2	K	153	VAL
2	K	155	VAL
2	K	156	THR
2	K	158	ASN
2	K	162	LEU
2	K	164	SER
2	K	167	HIS
2	K	172	VAL
2	K	173	LEU
2	K	177	LEU
2	K	179	THR
2	K	180	LEU
2	K	181	SER
2	K	185	THR
2	K	194	GLU
2	K	195	THR
2	K	196	VAL
2	K	198	CYS
2	K	199	ASN
2	K	205	SER
2	K	206	SER
2	K	209	VAL
2	K	210	ASP
2	K	214	VAL
2	K	216	ARG

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Mol	Chain	Res	Type
3	V	8	ASP
3	V	12	LEU
3	V	13	SER
3	V	15	LEU
3	V	16	LEU
3	V	17	ARG
3	V	24	SER
3	V	28	GLN
3	V	31	GLU
3	V	32	VAL
3	V	35	LEU
3	V	37	THR
3	V	40	LEU
3	V	41	LEU
3	V	46	PHE
3	V	48	LEU
3	V	50	GLU
3	V	55	MET
3	V	57	GLU
3	V	62	ASP
3	V	70	LEU
3	V	71	LEU
3	V	78	ARG
3	V	81	LEU
3	V	84	THR
3	V	86	LEU
3	V	87	SER
3	V	88	SER
3	V	94	SER
3	V	98	ARG
3	V	99	LEU
3	V	100	LEU
3	V	107	LEU
3	V	110	THR
3	V	115	ARG
3	V	117	ARG
3	V	122	LYS
3	V	125	ASN
3	V	127	ILE
3	V	129	LEU
3	V	130	SER
3	V	134	LEU

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Mol	Chain	Res	Type
3	V	140	ARG
3	V	141	PHE
3	V	143	MET
3	V	144	LEU
3	V	148	SER
3	V	150	LEU
3	V	151	CYS
3	X	11	VAL
3	X	12	LEU
3	X	16	LEU
3	X	17	ARG
3	X	18	ASP
3	X	19	SER
3	X	24	SER
3	X	25	ARG
3	X	28	GLN
3	X	31	GLU
3	X	32	VAL
3	X	40	LEU
3	X	48	LEU
3	X	50	GLU
3	X	51	TRP
3	X	53	THR
3	X	54	GLN
3	X	62	ASP
3	X	68	THR
3	X	69	LEU
3	X	70	LEU
3	X	71	LEU
3	X	72	GLU
3	X	75	MET
3	X	78	ARG
3	X	81	LEU
3	X	86	LEU
3	X	89	LEU
3	X	90	LEU
3	X	93	LEU
3	X	96	GLN
3	X	100	LEU
3	X	106	SER
3	X	107	LEU
3	X	110	THR

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Mol	Chain	Res	Type
3	X	112	LEU
3	X	115	ARG
3	X	127	ILE
3	X	129	LEU
3	X	135	LEU
3	X	136	ARG
3	X	143	MET
3	X	144	LEU
3	Y	9	LEU
3	Y	12	LEU
3	Y	15	LEU
3	Y	17	ARG
3	Y	19	SER
3	Y	22	LEU
3	Y	26	LEU
3	Y	27	SER
3	Y	35	LEU
3	Y	44	VAL
3	Y	45	ASP
3	Y	48	LEU
3	Y	52	LYS
3	Y	53	THR
3	Y	54	GLN
3	Y	55	MET
3	Y	56	GLU
3	Y	68	THR
3	Y	69	LEU
3	Y	70	LEU
3	Y	71	LEU
3	Y	72	GLU
3	Y	75	MET
3	Y	81	LEU
3	Y	85	CYS
3	Y	87	SER
3	Y	89	LEU
3	Y	93	LEU
3	Y	96	GLN
3	Y	99	LEU
3	Y	100	LEU
3	Y	105	GLN
3	Y	106	SER
3	Y	107	LEU

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Mol	Chain	Res	Type
3	Y	110	THR
3	Y	111	GLN
3	Y	112	LEU
3	Y	115	ARG
3	Y	117	ARG
3	Y	119	THR
3	Y	127	ILE
3	Y	129	LEU
3	Y	140	ARG
3	Y	143	MET
3	Y	144	LEU
3	Z	9	LEU
3	Z	11	VAL
3	Z	12	LEU
3	Z	15	LEU
3	Z	17	ARG
3	Z	19	SER
3	Z	22	LEU
3	Z	25	ARG
3	Z	26	LEU
3	Z	32	VAL
3	Z	35	LEU
3	Z	37	THR
3	Z	44	VAL
3	Z	46	PHE
3	Z	48	LEU
3	Z	50	GLU
3	Z	52	LYS
3	Z	55	MET
3	Z	56	GLU
3	Z	57	GLU
3	Z	62	ASP
3	Z	68	THR
3	Z	69	LEU
3	Z	70	LEU
3	Z	80	GLN
3	Z	81	LEU
3	Z	84	THR
3	Z	86	LEU
3	Z	87	SER
3	Z	93	LEU
3	Z	94	SER

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Mol	Chain	Res	Type
3	Z	99	LEU
3	Z	100	LEU
3	Z	105	GLN
3	Z	107	LEU
3	Z	112	LEU
3	Z	115	ARG
3	Z	118	THR
3	Z	127	ILE
3	Z	129	LEU
3	Z	140	ARG
3	Z	143	MET

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

Mol	Chain	Res	Type
1	L	1	GLN
1	L	6	GLN
1	L	37	GLN
1	L	88	GLN
1	L	189	ASN
1	L	211	ASN
2	H	13	GLN
2	H	56	ASN
2	H	57	ASN
2	H	84	GLN
2	H	158	ASN
2	H	174	GLN
2	H	199	ASN
1	M	1	GLN
1	M	6	GLN
1	M	37	GLN
1	M	88	GLN
1	M	155	GLN
1	M	165	GLN
1	M	188	HIS
1	M	189	ASN
1	M	211	ASN
2	I	13	GLN
2	I	56	ASN
2	I	57	ASN
2	I	58	HIS
2	I	61	HIS

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Mol	Chain	Res	Type
2	I	84	GLN
2	I	134	GLN
2	I	158	ASN
2	I	199	ASN
1	N	6	GLN
1	N	36	GLN
1	N	37	GLN
1	N	88	GLN
1	N	89	GLN
1	N	155	GLN
1	N	189	ASN
1	N	211	ASN
2	J	58	HIS
2	J	61	HIS
2	J	84	GLN
2	J	134	GLN
2	J	136	ASN
2	J	158	ASN
2	J	199	ASN
1	O	6	GLN
1	O	37	GLN
1	O	88	GLN
1	O	155	GLN
1	O	188	HIS
1	O	189	ASN
2	K	58	HIS
2	K	84	GLN
2	K	158	ASN
3	V	23	HIS
3	V	111	GLN
3	V	125	ASN
3	X	20	HIS
3	X	23	HIS
3	X	28	GLN
3	X	92	GLN
3	Y	111	GLN
3	Y	121	HIS
3	Y	133	HIS
3	Z	20	HIS
3	Z	33	HIS
3	Z	61	GLN
3	Z	105	GLN

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Mol	Chain	Res	Type
3	Z	111	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	L	213/213 (100%)	-0.83	0 100 100	5, 23, 37, 46	0
1	M	212/213 (99%)	-0.74	0 100 100	5, 25, 40, 46	0
1	N	212/213 (99%)	-0.74	0 100 100	8, 26, 41, 49	0
1	O	213/213 (100%)	-0.69	0 100 100	7, 29, 50, 73	0
2	H	217/217 (100%)	-0.83	0 100 100	5, 23, 38, 63	0
2	I	217/217 (100%)	-0.78	0 100 100	10, 27, 44, 52	0
2	J	217/217 (100%)	-0.79	0 100 100	8, 24, 46, 67	0
2	K	217/217 (100%)	-0.60	0 100 100	13, 34, 54, 63	0
3	V	145/163 (88%)	-0.47	2 (1%) 75 75	8, 38, 81, 88	0
3	X	138/163 (84%)	-0.59	0 100 100	9, 32, 74, 83	0
3	Y	139/163 (85%)	-0.67	0 100 100	8, 27, 63, 70	0
3	Z	138/163 (84%)	-0.48	0 100 100	8, 41, 65, 77	0
All	All	2278/2372 (96%)	-0.70	2 (0%) 95 97	5, 27, 56, 88	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	7	CYS	4.3
3	V	151	CYS	2.7

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.