



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:54 AM UTC

PDB ID : 1V7N / pdb_00001v7n
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

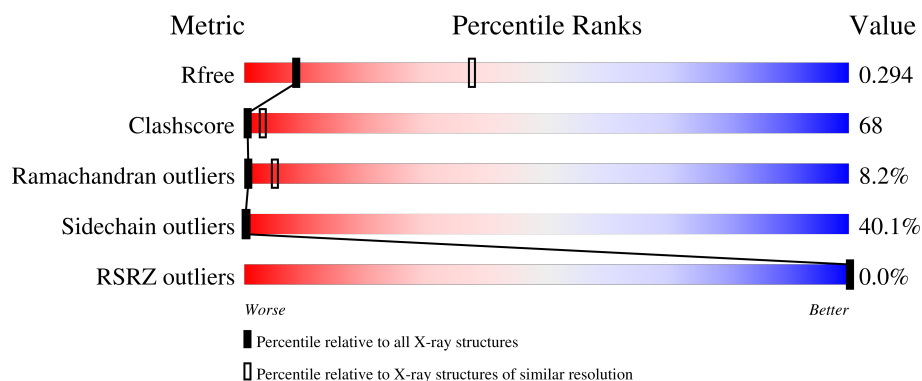
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	
2	J	217	
2	K	217	
3	V	163	
3	X	163	
3	Y	163	
3	Z	163	

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

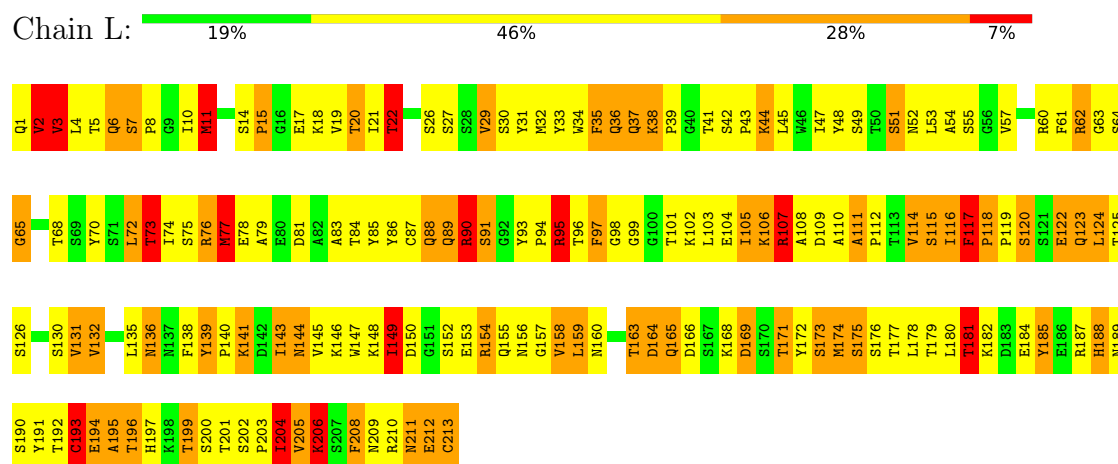
- Molecule 4 is water.

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

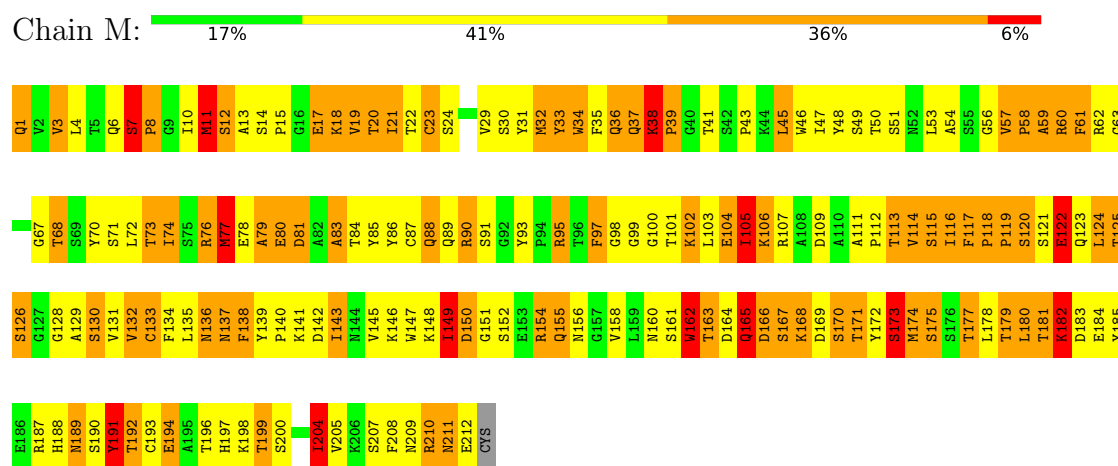
3 Residue-property plots

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

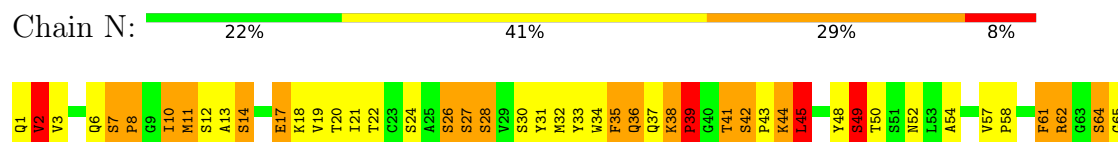
• Molecule 1: Monoclonal TN1 Fab Light Chain

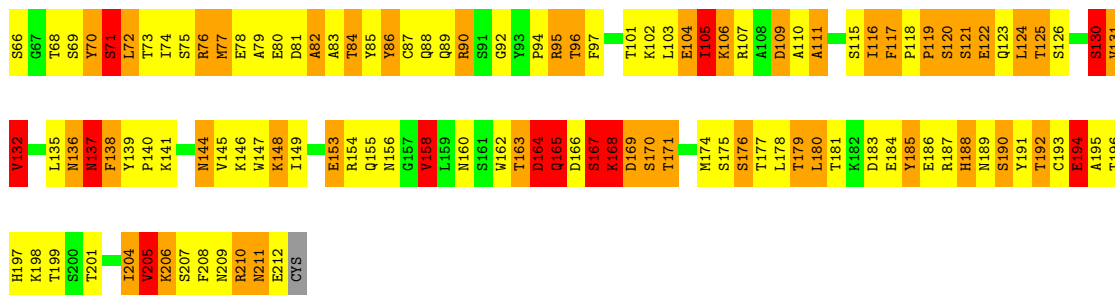


• Molecule 1: Monoclonal TN1 Fab Light Chain



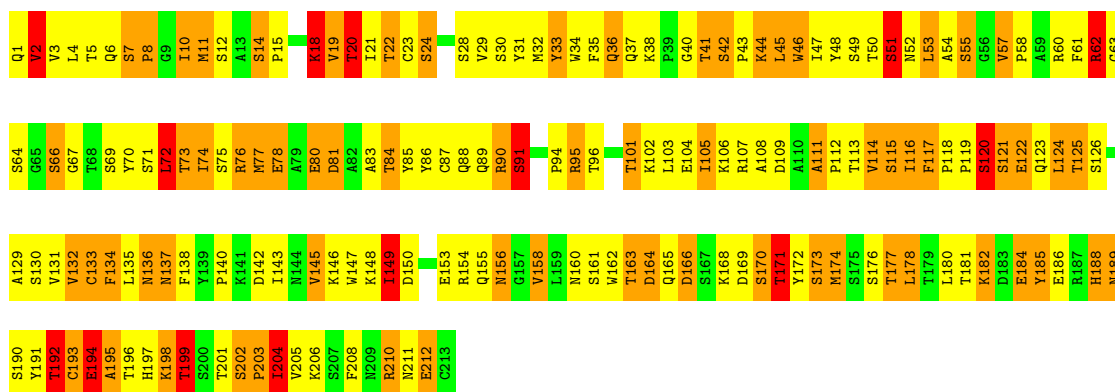
• Molecule 1: Monoclonal TN1 Fab Light Chain





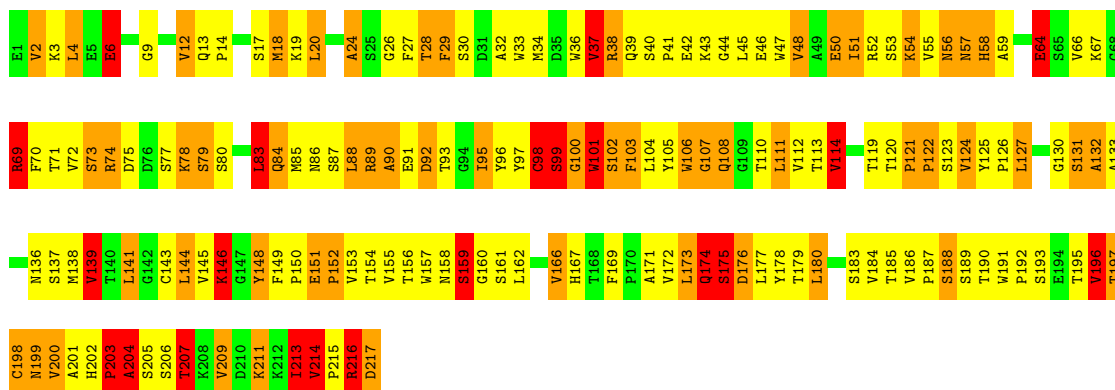
• Molecule 1: Monoclonal TN1 Fab Light Chain

Chain O: 18% 43% 32% 7%



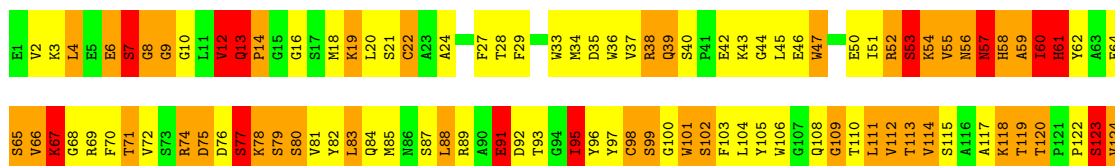
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

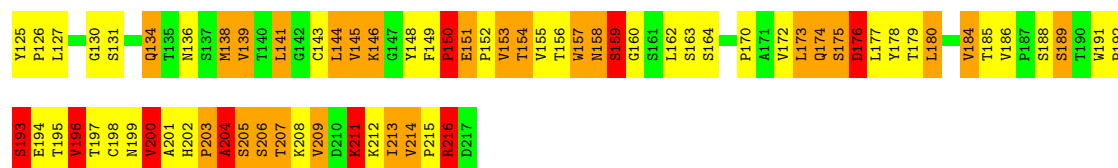
Chain H: 22% 42% 26% 10%



• Molecule 2: Monoclonal TN1 Fab Heavy Chain

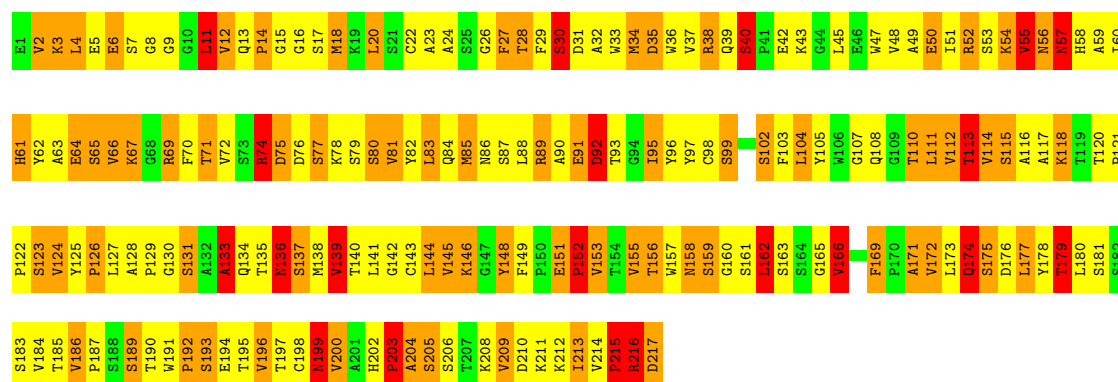
Chain I: 21% 40% 29% 10%





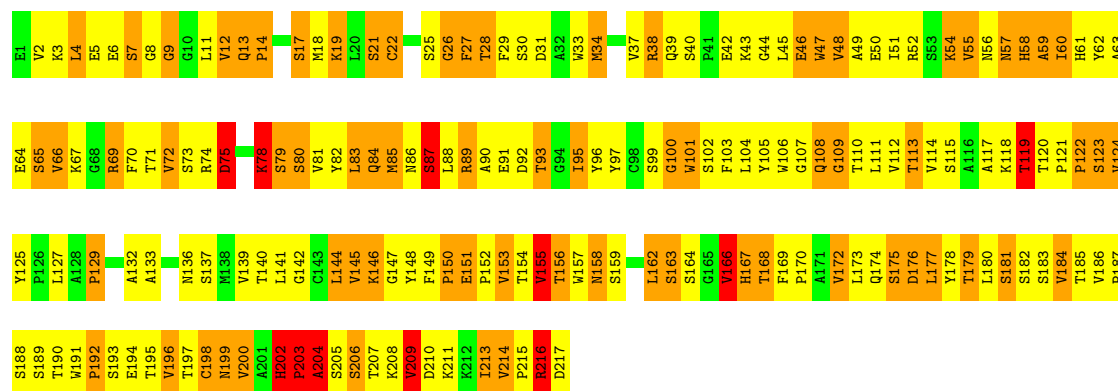
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain J: 13% 44% 34% 9%



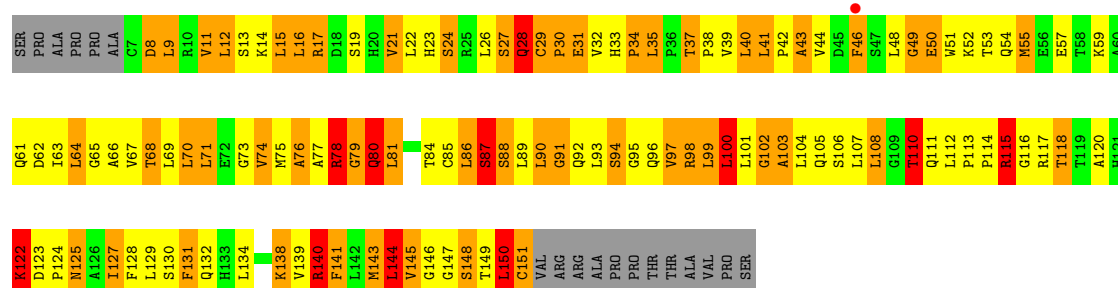
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain K: 15% 47% 33% 5%



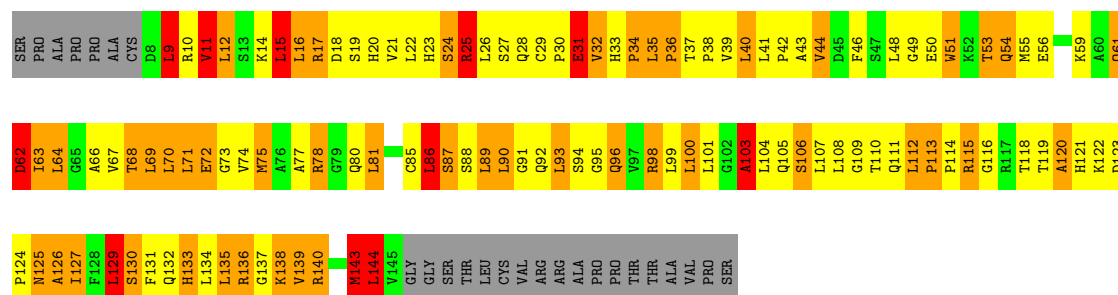
• Molecule 3: Thrombopoietin

Chain V: 14% 36% 32% 7% 11%



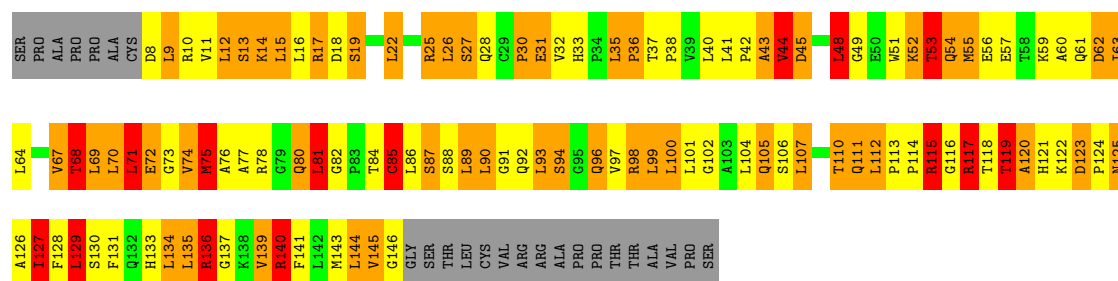
- Molecule 3: Thrombopoietin

Chain X: 



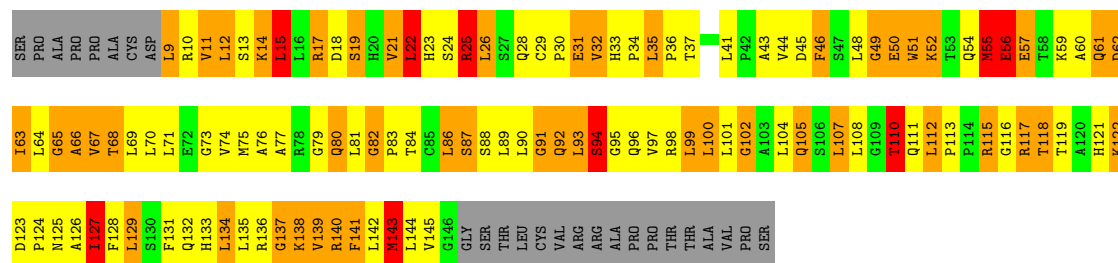
- Molecule 3: Thrombopoietin

Chain Y: 



- Molecule 3: Thrombopoietin

Chain Z: 



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 , 71.3	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	1.58	17/1676 (1.0%)	1.80	41/2274 (1.8%)
1	M	1.62	17/1670 (1.0%)	1.77	31/2266 (1.4%)
1	N	1.61	16/1670 (1.0%)	1.79	36/2266 (1.6%)
1	O	1.60	18/1676 (1.1%)	1.80	45/2274 (2.0%)
2	H	1.66	24/1674 (1.4%)	1.76	34/2289 (1.5%)
2	I	1.53	10/1674 (0.6%)	1.80	43/2289 (1.9%)
2	J	1.57	19/1674 (1.1%)	1.88	48/2289 (2.1%)
2	K	1.56	12/1674 (0.7%)	1.79	38/2289 (1.7%)
3	V	1.59	11/1109 (1.0%)	1.69	20/1506 (1.3%)
3	X	1.55	9/1068 (0.8%)	1.61	15/1451 (1.0%)
3	Y	1.66	17/1072 (1.6%)	1.79	21/1456 (1.4%)
3	Z	1.46	7/1064 (0.7%)	1.60	13/1445 (0.9%)
All	All	1.59	177/17701 (1.0%)	1.77	385/24094 (1.6%)

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 (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	75	MET	SD-CE	12.48	2.10	1.79
1	O	11	MET	SD-CE	11.60	2.08	1.79
2	I	209	VAL	CA-CB	10.50	1.67	1.53
1	L	11	MET	SD-CE	10.05	2.04	1.79
3	Z	55	MET	SD-CE	9.92	2.04	1.79
3	X	53	THR	CA-CB	9.86	1.65	1.52
1	N	11	MET	SD-CE	9.70	2.03	1.79
2	K	168	THR	CA-CB	-9.42	1.38	1.53
3	V	21	VAL	CA-CB	-9.23	1.43	1.54
2	J	34	MET	SD-CE	-9.00	1.57	1.79
1	M	59	ALA	CA-CB	-8.78	1.38	1.53
1	O	34	TRP	CA-C	-8.55	1.42	1.52
3	V	46	PHE	CA-C	8.41	1.58	1.52
2	H	48	VAL	CA-CB	-8.30	1.47	1.55
1	N	96	THR	CA-CB	-8.18	1.41	1.53
2	H	214	VAL	CA-CB	-8.10	1.43	1.54
3	V	110	THR	CA-CB	-7.95	1.39	1.53
3	X	143	MET	SD-CE	7.95	1.99	1.79
1	L	159	LEU	CA-C	7.92	1.61	1.52
1	L	205	VAL	CA-CB	-7.84	1.44	1.54
2	J	74	ARG	CA-C	-7.83	1.43	1.52
2	H	121	PRO	CA-C	-7.64	1.45	1.52
3	X	75	MET	SD-CE	7.59	1.98	1.79
1	L	139	TYR	CB-CG	-7.55	1.35	1.51
1	N	10	ILE	CA-CB	7.48	1.64	1.54
1	M	125	THR	CA-CB	7.20	1.65	1.53
2	J	203	PRO	CA-C	7.19	1.59	1.52
2	H	144	LEU	CA-C	-7.18	1.44	1.52
1	O	126	SER	CA-C	7.15	1.62	1.52
2	J	128	ALA	CA-CB	-7.13	1.45	1.54
1	O	158	VAL	CA-CB	7.10	1.62	1.54
1	M	32	MET	SD-CE	-7.06	1.61	1.79
1	N	49	SER	CA-C	-6.86	1.43	1.52
1	M	77	MET	SD-CE	-6.85	1.62	1.79
2	K	154	THR	CA-CB	6.85	1.62	1.53
1	N	20	THR	CA-C	6.83	1.60	1.52
2	I	204	ALA	CA-C	6.83	1.61	1.52
3	Y	68	THR	CA-CB	6.82	1.64	1.53
1	M	105	ILE	CA-CB	-6.81	1.46	1.54
1	L	114	VAL	CA-CB	-6.80	1.45	1.54
3	Y	80	GLN	CA-C	-6.77	1.43	1.52
1	N	69	SER	CA-C	6.75	1.61	1.53
1	L	54	ALA	CA-CB	-6.75	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	139	TYR	CA-CB	6.65	1.64	1.53
2	K	18	MET	SD-CE	6.59	1.96	1.79
2	I	7	SER	CA-C	6.48	1.60	1.52
1	O	106	LYS	CA-C	-6.48	1.44	1.53
2	J	57	ASN	CA-C	-6.47	1.44	1.53
2	J	91	GLU	CA-C	-6.38	1.44	1.52
2	K	47	TRP	CA-C	-6.37	1.44	1.52
2	H	32	ALA	CA-C	-6.33	1.45	1.52
3	Z	63	ILE	CA-CB	-6.29	1.47	1.54
2	J	139	VAL	CA-CB	-6.26	1.46	1.54
3	Y	127	ILE	CA-CB	6.24	1.62	1.54
2	K	34	MET	SD-CE	-6.24	1.64	1.79
2	K	166	VAL	CA-CB	-6.24	1.46	1.54
2	K	203	PRO	CA-C	6.22	1.61	1.52
2	K	154	THR	CA-C	6.21	1.60	1.52
1	M	162	TRP	N-CA	6.20	1.53	1.45
2	J	2	VAL	CA-CB	6.18	1.61	1.53
2	I	61	HIS	CA-C	-6.14	1.45	1.52
2	H	83	LEU	CA-C	-6.10	1.45	1.52
2	H	114	VAL	CA-CB	-6.10	1.46	1.54
2	J	72	VAL	CA-CB	-6.08	1.47	1.54
1	O	72	LEU	N-CA	6.06	1.53	1.46
2	K	175	SER	N-CA	-6.06	1.38	1.46
3	X	55	MET	SD-CE	6.02	1.94	1.79
3	X	66	ALA	CA-CB	-5.98	1.44	1.53
1	M	114	VAL	CA-CB	-5.97	1.46	1.54
1	M	11	MET	SD-CE	5.97	1.94	1.79
3	Y	120	ALA	CA-C	-5.93	1.45	1.52
3	V	80	GLN	CA-C	5.92	1.60	1.52
2	I	176	ASP	CA-C	5.91	1.60	1.52
1	N	96	THR	N-CA	-5.91	1.39	1.46
3	X	133	HIS	CA-C	5.89	1.60	1.52
3	V	106	SER	CA-C	-5.88	1.45	1.52
1	O	57	VAL	C-O	-5.88	1.17	1.24
2	H	34	MET	SD-CE	-5.87	1.64	1.79
1	O	120	SER	CA-C	-5.87	1.45	1.52
3	X	140	ARG	NE-CZ	5.86	1.39	1.33
2	K	101	TRP	CA-C	-5.86	1.46	1.53
2	J	113	THR	N-CA	5.84	1.53	1.46
1	L	204	ILE	CA-CB	5.82	1.61	1.54
1	L	2	VAL	CA-C	5.81	1.60	1.52
1	N	20	THR	CA-CB	5.80	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	128	PHE	CA-C	-5.79	1.45	1.52
2	J	199	ASN	CA-C	-5.76	1.45	1.52
1	L	41	THR	CA-C	5.76	1.59	1.52
3	Y	55	MET	SD-CE	5.76	1.94	1.79
3	V	53	THR	CA-CB	5.73	1.61	1.53
2	H	200	VAL	C-O	5.73	1.29	1.23
1	N	36	GLN	CA-C	-5.72	1.45	1.52
3	Y	135	LEU	N-CA	-5.71	1.39	1.46
3	Y	99	LEU	CA-C	5.66	1.60	1.52
2	H	37	VAL	CA-CB	-5.65	1.47	1.54
1	N	130	SER	CA-C	-5.65	1.45	1.52
3	V	115	ARG	NE-CZ	5.64	1.39	1.33
2	J	32	ALA	CA-C	-5.62	1.46	1.52
3	Z	60	ALA	CA-CB	-5.62	1.44	1.53
2	H	69	ARG	CA-C	5.59	1.58	1.52
1	O	105	ILE	CA-C	5.58	1.58	1.52
1	N	196	THR	CA-C	-5.57	1.46	1.53
1	L	95	ARG	CA-C	-5.57	1.45	1.53
1	M	133	CYS	N-CA	-5.56	1.39	1.46
1	M	34	TRP	CA-C	-5.53	1.45	1.52
2	I	39	GLN	CA-C	-5.53	1.46	1.52
2	H	183	SER	CA-C	-5.51	1.46	1.52
1	N	138	PHE	CA-C	-5.50	1.45	1.52
1	M	191	TYR	CA-C	-5.47	1.45	1.52
3	Z	21	VAL	CA-CB	5.47	1.61	1.54
1	M	93	TYR	CA-C	5.46	1.60	1.52
3	Y	62	ASP	CA-C	-5.45	1.46	1.52
2	H	196	VAL	CA-CB	5.44	1.60	1.53
2	I	214	VAL	CA-C	5.43	1.58	1.52
1	O	192	THR	CA-C	5.41	1.59	1.52
1	L	111	ALA	CA-CB	-5.40	1.43	1.52
1	O	136	ASN	CA-C	-5.40	1.46	1.52
3	X	103	ALA	CA-C	5.39	1.59	1.52
2	H	204	ALA	N-CA	5.38	1.53	1.46
3	Y	94	SER	CA-C	-5.38	1.46	1.52
2	H	18	MET	SD-CE	5.37	1.93	1.79
1	L	37	GLN	CA-C	-5.37	1.46	1.52
2	H	99	SER	N-CA	5.30	1.52	1.45
3	Y	139	VAL	CA-CB	-5.30	1.48	1.54
1	N	97	PHE	CA-C	-5.29	1.46	1.52
2	K	213	ILE	CA-CB	-5.29	1.47	1.54
3	Z	110	THR	CA-C	-5.28	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	162	LEU	C-O	-5.28	1.17	1.23
1	L	91	SER	C-O	-5.26	1.18	1.24
1	O	62	ARG	CB-CG	-5.25	1.36	1.52
3	Y	117	ARG	C-O	-5.25	1.17	1.24
2	J	110	THR	CA-C	-5.24	1.46	1.52
2	J	165	GLY	C-O	5.24	1.30	1.23
2	J	215	PRO	CA-C	5.23	1.59	1.52
3	Z	61	GLN	CA-C	5.22	1.60	1.52
3	Z	143	MET	SD-CE	5.22	1.92	1.79
3	Y	134	LEU	CA-C	-5.22	1.45	1.52
3	Y	129	LEU	N-CA	-5.21	1.40	1.46
1	M	57	VAL	CA-C	5.20	1.58	1.52
1	O	173	SER	CA-C	-5.18	1.46	1.52
1	M	29	VAL	CA-C	5.18	1.58	1.52
1	L	57	VAL	CA-C	5.18	1.57	1.53
2	J	72	VAL	CA-C	-5.17	1.46	1.52
2	H	97	TYR	CA-CB	-5.16	1.46	1.53
1	N	193	CYS	CA-C	5.16	1.58	1.52
2	H	151	GLU	CD-OE2	5.16	1.35	1.25
1	O	73	THR	N-CA	5.16	1.52	1.46
2	H	154	THR	CA-C	-5.16	1.46	1.52
2	I	120	THR	CA-CB	5.15	1.61	1.53
1	L	195	ALA	CA-CB	-5.15	1.46	1.53
1	N	105	ILE	CA-CB	5.14	1.60	1.54
1	O	195	ALA	C-O	-5.14	1.17	1.24
2	J	209	VAL	CA-CB	5.13	1.59	1.53
2	I	124	VAL	CA-CB	5.11	1.60	1.54
3	Y	90	LEU	CA-C	-5.11	1.45	1.52
1	O	57	VAL	CA-C	-5.11	1.47	1.52
1	L	22	THR	CA-C	-5.11	1.46	1.52
2	H	201	ALA	CA-C	-5.10	1.46	1.52
2	J	126	PRO	CA-C	-5.09	1.47	1.52
3	V	118	THR	CA-CB	5.09	1.60	1.53
3	X	44	VAL	CA-C	5.09	1.59	1.52
1	M	15	PRO	CA-C	-5.08	1.46	1.52
2	K	137	SER	N-CA	-5.07	1.41	1.46
1	M	119	PRO	C-O	-5.07	1.17	1.24
3	Y	81	LEU	CA-C	-5.07	1.46	1.52
2	H	24	ALA	CA-CB	-5.06	1.44	1.53
3	V	64	LEU	CG-CD1	5.05	1.69	1.52
1	N	24	SER	CA-C	-5.05	1.46	1.52
3	V	97	VAL	CA-CB	-5.05	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	98	CYS	CA-CB	-5.04	1.45	1.53
2	I	216	ARG	CA-C	5.03	1.59	1.52
1	O	105	ILE	CA-CB	5.03	1.59	1.54
3	V	97	VAL	CA-C	-5.03	1.45	1.52
1	M	173	SER	CA-C	-5.02	1.46	1.52
2	H	148	TYR	CA-C	-5.01	1.46	1.52
2	H	126	PRO	CA-C	-5.01	1.47	1.52
1	O	51	SER	C-O	-5.01	1.19	1.24

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	91	GLU	N-CA-C	-11.46	95.94	113.02
1	L	57	VAL	N-CA-C	11.03	118.11	108.63
2	J	205	SER	N-CA-C	10.59	125.77	113.38
1	L	144	ASN	N-CA-C	10.14	125.57	108.13
3	Y	44	VAL	N-CA-C	9.79	116.68	106.21
2	K	163	SER	N-CA-C	-9.61	102.13	114.04
1	L	205	VAL	CB-CA-C	-9.36	96.66	110.33
3	Y	63	ILE	N-CA-C	-9.25	101.54	110.42
1	L	90	ARG	N-CA-C	-9.22	100.09	112.26
1	N	141	LYS	N-CA-C	9.10	122.03	111.11
2	K	192	PRO	N-CD-CG	-9.07	92.91	103.80
2	J	166	VAL	CB-CA-C	9.04	122.12	110.91
3	V	116	GLY	CA-C-O	-8.84	116.47	122.22
3	Z	127	ILE	N-CA-C	8.84	120.64	111.00
2	I	101	TRP	CA-C-N	-8.83	109.70	122.77
2	I	101	TRP	C-N-CA	-8.83	109.70	122.77
1	L	141	LYS	N-CA-C	-8.82	102.29	113.23
1	O	111	ALA	N-CA-C	8.79	123.41	110.14
3	V	46	PHE	N-CA-C	8.68	124.21	111.02
1	N	8	PRO	N-CD-CG	-8.67	90.19	103.20
2	K	202	HIS	CA-C-N	8.67	130.68	119.84
2	K	202	HIS	C-N-CA	8.67	130.68	119.84
2	I	57	ASN	N-CA-C	8.65	123.64	111.52
1	M	204	ILE	N-CA-C	-8.62	97.46	108.84
1	N	158	VAL	N-CA-C	8.62	120.12	107.37
2	I	203	PRO	N-CD-CG	-8.40	90.59	103.20
1	M	179	THR	N-CA-C	8.38	122.74	109.50
1	N	144	ASN	N-CA-C	8.37	125.20	107.70
2	J	171	ALA	N-CA-C	8.32	120.65	110.41
2	H	139	VAL	N-CA-C	8.31	120.31	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	136	ASN	N-CA-C	8.31	122.35	110.14
3	V	106	SER	N-CA-C	-8.30	102.23	111.28
2	J	139	VAL	CB-CA-C	-8.24	99.92	111.21
1	L	95	ARG	N-CA-C	-8.22	100.30	110.41
2	I	196	VAL	N-CA-C	8.20	121.01	107.24
3	X	86	LEU	N-CA-C	-8.13	97.96	111.37
2	H	203	PRO	CA-C-N	8.06	136.94	121.54
2	H	203	PRO	C-N-CA	8.06	136.94	121.54
2	J	145	VAL	N-CA-C	-8.04	92.62	109.34
2	I	44	GLY	N-CA-C	-8.03	99.27	111.24
2	J	11	LEU	CA-C-N	-7.98	110.77	122.58
2	J	11	LEU	C-N-CA	-7.98	110.77	122.58
2	K	216	ARG	N-CA-C	7.98	121.93	109.96
2	H	204	ALA	N-CA-C	-7.94	93.88	110.80
2	I	42	GLU	N-CA-C	7.91	119.53	111.07
2	K	202	HIS	N-CA-C	-7.87	92.41	109.81
2	J	165	GLY	CA-C-N	-7.86	112.23	122.37
2	J	165	GLY	C-N-CA	-7.86	112.23	122.37
2	K	203	PRO	N-CD-CG	-7.84	91.44	103.20
2	K	19	LYS	N-CA-C	7.80	122.26	107.75
3	V	29	CYS	N-CA-C	-7.76	100.23	110.40
3	Y	134	LEU	N-CA-C	-7.75	103.96	113.41
1	O	20	THR	N-CA-C	7.74	124.20	107.49
3	Y	107	LEU	N-CA-C	-7.73	102.18	111.69
2	H	174	GLN	N-CA-C	7.72	116.16	108.75
2	H	114	VAL	CB-CA-C	-7.67	101.40	110.91
2	I	12	VAL	N-CA-C	7.63	121.30	108.86
2	K	47	TRP	N-CA-C	-7.62	98.20	110.32
1	M	122	GLU	N-CA-C	-7.61	104.13	113.41
1	L	200	SER	CA-C-N	7.60	130.80	120.54
1	L	200	SER	C-N-CA	7.60	130.80	120.54
1	O	53	LEU	CA-CB-CG	-7.59	89.75	116.30
2	J	216	ARG	N-CA-C	7.58	126.95	110.80
2	I	8	GLY	N-CA-C	7.49	123.80	114.37
3	Y	54	GLN	N-CA-C	-7.47	97.10	109.80
3	V	114	PRO	N-CD-CG	-7.45	92.03	103.20
1	N	158	VAL	CB-CA-C	-7.37	100.94	111.19
3	V	150	LEU	N-CA-C	7.34	122.44	107.69
2	K	175	SER	N-CA-CB	-7.29	98.17	110.49
1	L	204	ILE	N-CA-C	-7.28	97.98	108.53
1	L	3	VAL	CB-CA-C	7.23	121.24	111.19
3	V	21	VAL	CB-CA-C	-7.22	102.59	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	77	MET	N-CA-C	7.20	120.83	110.10
2	I	211	LYS	N-CA-C	7.19	120.68	107.73
1	N	205	VAL	CA-C-N	-7.17	112.87	122.99
1	N	205	VAL	C-N-CA	-7.17	112.87	122.99
2	I	214	VAL	CB-CA-C	7.16	117.89	110.88
2	I	216	ARG	N-CA-C	7.09	120.01	109.59
1	L	159	LEU	N-CA-C	7.08	119.94	108.41
1	L	185	TYR	N-CA-C	-7.07	102.63	111.11
1	O	149	ILE	CA-C-N	-7.04	109.63	122.38
1	O	149	ILE	C-N-CA	-7.04	109.63	122.38
2	J	92	ASP	N-CA-C	-7.04	104.69	113.28
2	K	155	VAL	N-CA-C	7.04	117.99	107.51
1	O	73	THR	N-CA-C	7.03	120.38	109.07
1	O	171	THR	N-CA-C	7.03	120.38	109.07
1	M	191	TYR	N-CA-C	-7.02	95.85	110.80
2	H	98	CYS	N-CA-C	-7.00	99.15	110.20
2	J	203	PRO	N-CA-C	7.00	121.48	110.50
2	J	66	VAL	CB-CA-C	-6.99	102.58	112.22
1	M	102	LYS	N-CA-C	-6.92	97.45	108.73
3	Y	30	PRO	N-CD-CG	-6.90	92.85	103.20
3	Z	22	LEU	N-CA-C	-6.90	103.45	110.97
3	Y	94	SER	N-CA-C	-6.90	103.69	111.14
2	H	143	CYS	CA-CB-SG	-6.89	98.55	114.40
2	J	98	CYS	N-CA-C	-6.87	98.04	109.24
3	X	9	LEU	N-CA-C	-6.87	105.43	113.88
1	M	99	GLY	N-CA-C	-6.82	107.17	114.67
2	H	103	PHE	N-CA-C	6.81	121.54	113.23
3	V	122	LYS	N-CA-C	-6.81	103.31	111.69
2	H	99	SER	N-CA-C	6.74	119.18	109.14
2	K	100	GLY	N-CA-C	6.71	123.25	111.25
1	O	199	THR	N-CA-C	6.69	119.14	111.11
2	J	17	SER	N-CA-C	6.69	119.25	107.61
1	O	53	LEU	CA-C-N	-6.69	112.19	122.09
1	O	53	LEU	C-N-CA	-6.69	112.19	122.09
2	K	99	SER	N-CA-C	6.68	120.42	109.06
2	I	109	GLY	CA-C-O	-6.66	116.04	121.77
1	N	188	HIS	N-CA-C	6.65	118.23	108.86
3	X	64	LEU	N-CA-C	-6.65	104.11	111.36
3	X	113	PRO	CA-C-O	-6.64	115.48	120.73
2	I	157	TRP	N-CA-C	6.64	119.84	108.02
2	I	209	VAL	CB-CA-C	6.64	120.42	111.19
1	N	194	GLU	N-CA-C	6.64	121.67	107.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	91	SER	N-CA-C	6.63	118.17	111.07
2	K	207	THR	CA-C-N	-6.63	113.39	122.95
2	K	207	THR	C-N-CA	-6.63	113.39	122.95
3	X	63	ILE	CB-CA-C	-6.63	103.18	112.14
3	V	78	ARG	N-CA-C	-6.62	103.98	111.07
1	O	105	ILE	N-CA-C	6.58	117.53	109.30
2	K	151	GLU	N-CA-C	-6.58	101.77	109.93
1	L	206	LYS	N-CA-C	-6.56	99.48	109.85
2	H	73	SER	CA-C-N	-6.54	111.38	123.01
2	H	73	SER	C-N-CA	-6.54	111.38	123.01
2	K	203	PRO	N-CA-C	6.53	125.93	112.47
3	V	28	GLN	N-CA-C	6.53	118.49	109.54
3	Y	81	LEU	N-CA-C	-6.53	100.02	110.14
2	I	114	VAL	N-CA-CB	6.52	118.84	111.21
2	I	151	GLU	CA-CB-CG	-6.50	101.09	114.10
2	J	121	PRO	O-C-N	6.50	124.20	121.15
1	O	185	TYR	N-CA-C	-6.50	96.97	110.80
2	H	122	PRO	N-CD-CG	-6.49	93.47	103.20
2	J	213	ILE	N-CA-C	6.47	117.13	108.27
3	V	97	VAL	CB-CA-C	-6.46	102.15	112.16
2	H	144	LEU	CA-CB-CG	-6.45	93.72	116.30
2	I	83	LEU	CA-CB-CG	-6.44	93.77	116.30
3	Z	15	LEU	N-CA-C	6.43	117.97	110.97
1	L	89	GLN	CA-C-N	-6.41	113.06	122.86
1	L	89	GLN	C-N-CA	-6.41	113.06	122.86
2	I	13	GLN	N-CA-C	-6.40	100.34	109.24
1	L	136	ASN	N-CA-C	6.40	119.38	109.07
1	M	182	LYS	N-CA-C	-6.40	103.58	111.33
2	I	16	GLY	N-CA-C	-6.40	102.81	112.41
1	M	74	ILE	CB-CA-C	-6.38	102.99	110.91
1	L	208	PHE	N-CA-C	6.38	118.24	109.18
2	J	203	PRO	CB-CA-C	6.38	118.52	111.56
2	J	14	PRO	N-CA-C	-6.38	101.07	111.21
3	Y	90	LEU	N-CA-C	-6.32	105.05	112.89
1	L	73	THR	N-CA-C	6.32	118.82	108.52
3	Z	14	LYS	CA-C-N	6.31	128.98	120.65
3	Z	14	LYS	C-N-CA	6.31	128.98	120.65
3	Y	67	VAL	N-CA-C	-6.30	104.60	110.53
1	M	165	GLN	N-CA-C	-6.30	102.17	110.43
1	N	62	ARG	N-CA-C	6.29	119.15	108.90
1	L	164	ASP	CA-C-N	-6.29	110.25	120.87
1	L	164	ASP	C-N-CA	-6.29	110.25	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	17	SER	N-CA-C	6.27	118.70	108.55
2	H	58	HIS	N-CA-CB	-6.22	102.84	112.30
3	Z	66	ALA	N-CA-C	-6.22	105.34	113.12
2	K	184	VAL	N-CA-C	6.21	116.81	108.11
3	Y	136	ARG	CB-CA-C	-6.19	100.33	110.85
1	O	36	GLN	N-CA-C	-6.18	99.83	109.72
2	H	146	LYS	N-CA-C	6.17	119.45	109.40
3	Z	139	VAL	N-CA-C	6.16	117.64	110.62
2	J	145	VAL	CB-CA-C	6.16	121.39	111.29
2	H	213	ILE	N-CA-C	6.14	117.86	108.71
1	M	136	ASN	N-CA-C	6.13	118.95	109.07
1	L	188	HIS	N-CA-C	6.13	119.15	110.14
1	O	136	ASN	N-CA-C	6.13	118.89	108.90
1	O	132	VAL	N-CA-C	6.12	117.47	109.58
1	O	137	ASN	N-CA-C	6.09	118.03	110.91
2	K	63	ALA	N-CA-C	-6.09	101.47	110.48
2	K	150	PRO	N-CD-CG	-6.08	96.50	103.80
2	J	152	PRO	N-CD-CG	-6.08	96.51	103.80
2	K	75	ASP	CB-CA-C	6.08	119.49	110.62
3	Z	67	VAL	CB-CA-C	-6.08	103.94	112.14
1	O	84	THR	N-CA-C	-6.07	99.81	109.76
2	J	189	SER	N-CA-C	-6.04	104.76	111.71
2	J	174	GLN	CA-C-O	6.04	123.24	119.55
1	M	171	THR	N-CA-C	6.02	119.89	110.32
2	K	204	ALA	N-CA-C	-6.02	97.98	110.80
2	I	87	SER	N-CA-C	6.01	118.54	111.02
1	M	21	ILE	CB-CA-C	-6.01	101.67	110.62
2	K	66	VAL	CB-CA-C	-6.00	104.76	110.70
1	M	149	ILE	CA-C-N	-6.00	110.90	122.06
1	M	149	ILE	C-N-CA	-6.00	110.90	122.06
2	J	203	PRO	CA-C-O	6.00	127.94	120.92
2	H	101	TRP	CA-C-N	-5.98	112.57	122.32
2	H	101	TRP	C-N-CA	-5.98	112.57	122.32
2	H	48	VAL	N-CA-C	5.97	117.09	111.48
1	O	66	SER	N-CA-C	5.96	118.83	107.75
2	J	40	SER	N-CA-C	-5.95	98.60	108.23
1	O	115	SER	N-CA-C	-5.94	100.29	109.14
1	L	203	PRO	CA-C-O	-5.93	114.53	121.95
2	K	22	CYS	N-CA-C	5.93	119.61	107.69
2	J	179	THR	N-CA-C	5.92	118.41	109.23
3	Y	119	THR	N-CA-C	5.92	117.25	108.60
2	J	118	LYS	CA-C-N	5.91	129.15	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	118	LYS	C-N-CA	5.91	129.15	120.82
2	J	110	THR	N-CA-CB	5.89	120.28	110.85
1	N	70	TYR	N-CA-C	5.88	118.39	109.63
3	Y	74	VAL	N-CA-CB	5.85	117.00	110.62
2	I	124	VAL	N-CA-C	5.85	116.29	107.75
3	V	74	VAL	N-CA-C	5.85	116.62	110.72
2	J	192	PRO	N-CD-CG	-5.84	96.79	103.80
3	Z	141	PHE	N-CA-C	-5.82	104.77	112.34
1	L	174	MET	N-CA-C	5.81	118.95	109.59
2	J	161	SER	CA-C-N	-5.81	112.76	122.17
2	J	161	SER	C-N-CA	-5.81	112.76	122.17
1	N	119	PRO	N-CD-CG	-5.80	94.50	103.20
1	N	132	VAL	CA-C-N	-5.79	114.05	122.44
1	N	132	VAL	C-N-CA	-5.79	114.05	122.44
1	O	2	VAL	CB-CA-C	-5.78	102.83	110.98
2	J	166	VAL	N-CA-CB	5.78	117.02	110.72
1	M	194	GLU	N-CA-C	5.77	117.82	108.41
1	M	104	GLU	N-CA-C	5.76	117.80	108.41
1	N	61	PHE	CA-C-N	-5.75	114.88	122.99
1	N	61	PHE	C-N-CA	-5.75	114.88	122.99
2	I	60	ILE	CB-CA-C	-5.75	103.02	110.84
1	O	194	GLU	N-CA-C	5.74	118.00	108.13
1	N	2	VAL	CB-CA-C	-5.74	103.80	110.91
1	O	80	GLU	CA-C-N	-5.73	113.61	122.49
1	O	80	GLU	C-N-CA	-5.73	113.61	122.49
1	O	142	ASP	N-CA-C	5.72	118.01	109.25
2	H	200	VAL	CA-C-N	-5.72	112.95	122.21
2	H	200	VAL	C-N-CA	-5.72	112.95	122.21
1	M	10	ILE	N-CA-C	5.72	116.98	108.46
2	J	215	PRO	N-CA-C	5.71	124.23	112.47
1	L	97	PHE	CB-CA-C	-5.71	107.27	114.40
1	M	135	LEU	CA-C-N	-5.70	115.13	123.00
1	M	135	LEU	C-N-CA	-5.70	115.13	123.00
2	H	216	ARG	N-CA-C	5.70	118.50	110.23
1	O	192	THR	N-CA-C	5.68	118.73	109.59
1	N	145	VAL	N-CA-C	5.68	115.72	108.12
3	V	74	VAL	CB-CA-C	-5.67	104.40	112.22
2	J	18	MET	N-CA-C	5.66	118.12	108.90
2	J	169	PHE	CB-CA-C	5.66	116.85	108.87
1	N	71	SER	N-CA-C	5.65	122.83	110.80
1	O	134	PHE	N-CA-C	-5.63	100.22	109.40
3	V	9	LEU	N-CA-C	-5.63	105.62	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	20	THR	CB-CA-C	5.63	119.15	110.14
3	X	63	ILE	N-CA-C	5.62	116.35	110.62
3	X	120	ALA	CA-C-O	-5.61	115.36	121.87
2	H	124	VAL	N-CA-C	5.60	115.67	107.37
2	K	167	HIS	CA-C-N	-5.60	114.31	122.65
2	K	167	HIS	C-N-CA	-5.60	114.31	122.65
2	K	209	VAL	CB-CA-C	5.60	120.47	111.29
1	M	200	SER	CA-C-N	5.59	128.81	120.31
1	M	200	SER	C-N-CA	5.59	128.81	120.31
3	X	113	PRO	O-C-N	5.59	123.78	121.15
2	I	209	VAL	N-CA-C	-5.59	99.10	107.37
3	Y	71	LEU	CA-CB-CG	-5.58	96.76	116.30
1	N	111	ALA	CA-C-N	5.58	125.51	119.76
1	N	111	ALA	C-N-CA	5.58	125.51	119.76
1	L	117	PHE	N-CA-C	5.56	120.74	108.73
2	I	154	THR	N-CA-C	5.55	117.27	108.67
1	M	3	VAL	N-CA-C	5.54	116.08	107.99
1	N	82	ALA	N-CA-C	-5.54	101.71	109.96
2	H	64	GLU	N-CA-C	-5.53	105.40	111.82
1	L	51	SER	N-CA-C	5.52	121.88	112.99
2	I	123	SER	CA-C-N	-5.51	115.77	123.10
2	I	123	SER	C-N-CA	-5.51	115.77	123.10
2	H	119	THR	N-CA-C	5.51	117.85	110.35
1	O	156	ASN	N-CA-C	5.51	118.52	109.76
3	V	108	LEU	N-CA-C	-5.51	106.51	113.18
1	M	118	PRO	N-CD-CG	-5.51	94.94	103.20
3	Y	123	ASP	CB-CA-C	5.50	116.28	110.17
1	N	36	GLN	N-CA-C	-5.50	100.43	109.40
1	O	72	LEU	N-CA-C	5.50	118.51	109.76
1	M	58	PRO	CA-C-O	-5.50	114.88	121.48
1	O	10	ILE	N-CA-C	-5.50	100.31	108.45
2	I	156	THR	N-CA-C	5.49	116.97	109.18
2	I	143	CYS	N-CA-C	5.47	118.32	109.40
1	N	204	ILE	N-CA-CB	5.47	116.69	110.72
1	L	6	GLN	N-CA-C	-5.47	100.33	109.24
3	Y	53	THR	N-CA-C	5.46	119.99	107.48
3	V	140	ARG	N-CA-C	-5.45	104.37	111.02
1	L	181	THR	OG1-CB-CG2	-5.44	98.42	109.30
3	Y	17	ARG	N-CA-CB	5.44	118.18	110.13
1	M	38	LYS	O-C-N	5.43	126.47	121.80
2	K	66	VAL	N-CA-C	5.42	118.41	113.20
2	I	47	TRP	CA-C-N	-5.42	117.41	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	47	TRP	C-N-CA	-5.42	117.41	123.16
2	I	47	TRP	N-CA-C	-5.42	102.86	110.50
1	O	101	THR	OG1-CB-CG2	-5.42	98.47	109.30
1	M	7	SER	N-CA-C	5.42	121.78	109.81
1	N	185	TYR	N-CA-C	-5.41	104.93	112.45
1	M	68	THR	N-CA-C	5.41	120.55	113.30
1	L	65	GLY	CA-C-O	-5.40	118.43	122.37
2	K	107	GLY	N-CA-C	-5.40	102.32	112.64
3	Y	115	ARG	N-CA-C	5.40	116.74	108.42
3	X	106	SER	N-CA-C	-5.40	105.31	111.14
1	M	162	TRP	N-CA-CB	5.40	119.20	110.51
2	K	78	LYS	N-CA-C	-5.40	106.74	113.38
2	I	95	ILE	CA-C-N	-5.39	115.25	122.42
2	I	95	ILE	C-N-CA	-5.39	115.25	122.42
1	L	3	VAL	N-CA-C	5.38	115.34	107.37
1	O	22	THR	OG1-CB-CG2	-5.38	98.54	109.30
1	L	36	GLN	CA-C-N	-5.37	114.24	122.62
1	L	36	GLN	C-N-CA	-5.37	114.24	122.62
2	K	109	GLY	CA-C-O	-5.37	117.69	121.88
3	V	100	LEU	N-CA-C	-5.37	105.33	111.07
1	O	198	LYS	CA-C-N	5.36	127.78	120.54
1	O	198	LYS	C-N-CA	5.36	127.78	120.54
2	H	34	MET	N-CA-C	5.36	118.30	109.72
3	X	125	ASN	N-CA-C	-5.36	105.35	111.14
1	L	126	SER	N-CA-C	5.36	119.44	113.01
1	N	130	SER	N-CA-C	-5.35	100.18	108.90
1	M	80	GLU	N-CA-C	5.35	118.59	111.75
3	Y	49	GLY	N-CA-C	-5.35	106.30	112.50
1	O	111	ALA	CA-C-O	5.35	126.45	120.04
2	K	48	VAL	N-CA-CB	-5.34	106.28	111.57
3	X	46	PHE	N-CA-C	-5.34	105.50	112.23
1	O	74	ILE	CA-C-N	5.34	127.38	120.44
1	O	74	ILE	C-N-CA	5.34	127.38	120.44
1	O	81	ASP	N-CA-C	-5.34	106.15	113.30
2	K	146	LYS	N-CA-C	5.32	117.57	108.90
3	V	68	THR	N-CA-CB	5.31	118.53	110.14
2	H	100	GLY	N-CA-C	5.31	125.75	113.18
1	O	91	SER	CB-CA-C	-5.30	102.56	110.88
2	J	53	SER	CA-C-O	-5.28	115.02	121.67
1	N	170	SER	N-CA-C	5.28	122.04	110.80
1	N	43	PRO	CA-C-N	-5.28	115.33	122.77
1	N	43	PRO	C-N-CA	-5.28	115.33	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	164	ASP	CA-C-O	-5.28	115.87	121.94
1	O	8	PRO	N-CD-CG	-5.27	95.30	103.20
2	J	14	PRO	CA-C-O	-5.27	115.45	121.56
3	X	59	LYS	N-CA-C	-5.26	105.44	111.07
2	J	91	GLU	O-C-N	5.26	128.83	122.20
1	O	195	ALA	CA-C-N	-5.25	115.40	122.86
1	O	195	ALA	C-N-CA	-5.25	115.40	122.86
3	Z	51	TRP	N-CA-C	5.24	116.80	111.14
2	J	28	THR	CA-C-N	-5.24	113.50	120.63
2	J	28	THR	C-N-CA	-5.24	113.50	120.63
2	K	139	VAL	CA-C-N	-5.23	114.81	122.19
2	K	139	VAL	C-N-CA	-5.23	114.81	122.19
3	Y	36	PRO	N-CA-C	-5.21	106.03	113.47
2	J	48	VAL	N-CA-CB	-5.20	107.37	111.64
2	K	82	TYR	N-CA-C	5.20	117.90	108.69
1	L	158	VAL	N-CA-CB	5.20	117.23	110.99
2	I	120	THR	N-CA-C	-5.19	98.34	109.81
3	Y	48	LEU	N-CA-C	5.19	116.66	110.44
2	H	106	TRP	CB-CA-C	-5.18	105.00	111.43
2	H	209	VAL	CB-CA-C	5.18	119.78	111.29
2	J	204	ALA	N-CA-C	-5.18	99.78	110.80
3	Z	74	VAL	CA-C-N	5.18	127.64	120.29
3	Z	74	VAL	C-N-CA	5.18	127.64	120.29
2	H	160	GLY	N-CA-C	5.17	120.85	114.69
1	L	95	ARG	NE-CZ-NH1	-5.17	116.33	121.50
2	I	205	SER	N-CA-C	5.17	121.81	110.80
3	V	131	PHE	CA-C-N	5.16	127.50	120.54
3	V	131	PHE	C-N-CA	5.16	127.50	120.54
2	I	91	GLU	N-CA-C	-5.16	106.74	112.57
1	M	60	ARG	NE-CZ-NH1	-5.15	116.35	121.50
3	X	15	LEU	N-CA-C	-5.15	105.58	111.14
1	M	161	SER	CA-C-O	-5.14	114.79	120.24
2	I	53	SER	CA-CB-OG	-5.14	100.81	111.10
2	K	129	PRO	CA-C-O	-5.14	115.74	122.12
1	N	148	LYS	CA-C-O	-5.13	115.36	121.16
1	N	36	GLN	CA-C-N	-5.13	114.84	122.74
1	N	36	GLN	C-N-CA	-5.13	114.84	122.74
1	L	193	CYS	CA-C-N	-5.12	113.73	122.33
1	L	193	CYS	C-N-CA	-5.12	113.73	122.33
2	H	207	THR	OG1-CB-CG2	-5.12	99.07	109.30
2	J	112	VAL	CB-CA-C	5.11	118.29	111.19
1	L	11	MET	N-CA-C	5.11	117.44	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	62	ARG	N-CA-C	-5.11	100.20	108.52
1	O	14	SER	CA-C-O	-5.08	115.23	120.87
2	H	122	PRO	N-CA-C	-5.08	102.01	112.47
1	N	211	ASN	N-CA-C	5.07	117.46	111.33
2	J	104	LEU	N-CA-C	-5.06	107.28	113.50
2	J	34	MET	N-CA-C	-5.05	100.47	109.06
2	J	91	GLU	CA-C-O	5.05	124.84	119.34
2	I	99	SER	N-CA-C	5.05	118.30	110.17
2	H	6	GLU	N-CA-C	-5.04	103.75	110.55
1	O	18	LYS	CA-C-N	-5.04	115.83	122.98
1	O	18	LYS	C-N-CA	-5.04	115.83	122.98
3	Z	17	ARG	N-CA-C	-5.04	106.30	112.90
2	I	59	ALA	N-CA-C	5.03	116.95	109.25
1	L	95	ARG	NE-CZ-NH2	5.03	123.73	119.20
3	X	25	ARG	CA-C-N	5.03	126.97	120.44
3	X	25	ARG	C-N-CA	5.03	126.97	120.44
2	I	200	VAL	CB-CA-C	-5.01	104.02	110.84
2	I	126	PRO	CB-CA-C	-5.01	106.10	111.56
2	I	58	HIS	N-CA-CB	-5.01	104.52	112.08

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	225	1
1	M	1632	0	1568	258	0
1	N	1632	0	1568	218	0
1	O	1638	0	1573	219	0
2	H	1630	0	1568	229	0
2	I	1630	0	1568	203	0
2	J	1630	0	1568	234	0
2	K	1630	0	1568	246	0
3	V	1090	0	1135	158	0
3	X	1049	0	1098	163	0
3	Y	1053	0	1101	165	0
3	Z	1045	0	1097	151	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	2333	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 68.

All (2333) 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
2:J:85:MET:HE1	2:J:96:TYR:CE1	1.50	1.42
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
1:O:150:ASP:OD2	1:O:188:HIS:HB3	1.33	1.28
2:J:85:MET:CE	2:J:96:TYR:CE1	2.09	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
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
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:J:29:PHE:HE1	2:J:34:MET:HE3	1.16	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
1:N:77:MET:HE3	1:N:81:ASP:HB2	1.35	1.07
2:J:29:PHE:CE1	2:J:34:MET:HE3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:17:ARG:HH11	3:X:17:ARG:HG3	1.18	1.07
2:H:189:SER:CA	4:H:224:HOH:O	2.00	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
1:O:61:PHE:HZ	1:O:85:TYR:HH	1.05	1.04
2:J:90:ALA:HA	2:J:114:VAL:HG21	1.40	1.03
3:X:12:LEU:HB3	3:X:143:MET:HE1	1.03	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
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:J:85:MET:HE3	2:J:96:TYR:CE1	1.95	1.00
3:X:12:LEU:CB	3:X:143:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:12:LEU:HB3	3:X:143:MET:CE	1.94	0.98
1:N:72:LEU:HD23	1:N:72:LEU:C	1.89	0.97
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
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
2:H:138:MET:HE2	2:H:185:THR:HG22	1.46	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
1:O:44:LYS:HB2	1:O:44:LYS:HZ3	1.34	0.93
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:PHE:CZ	2:H:85:MET:HE2	2.06	0.91
2:H:78:LYS:NZ	2:H:78:LYS:CB	2.32	0.91
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
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:O:44:LYS:HB2	1:O:44:LYS:NZ	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
3:Y:13:SER:O	3:Y:14:LYS:C	2.16	0.89
1:L:29:VAL:HG13	1:L:91:SER:HB2	1.53	0.88
3:V:140:ARG:HA	3:V:143:MET:HE2	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:L:77:MET:HE3	1:L:81:ASP:HB2	1.61	0.81
2:H:91:GLU:C	2:H:93:THR:H	1.88	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
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
2:I:75:ASP:C	2:I:75:ASP:OD1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:M:45:LEU:HD22	1:M:45:LEU:C	2.07	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
1:O:77:MET:HE3	1:O:78:GLU:O	1.81	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:13:ALA:HB1	1:N:17:GLU:CD	2.07	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:M:22:THR:HG22	1:M:23:CYS:N	1.95	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
1:O:69:SER:C	1:O:70:TYR:HD1	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:J:85:MET:HE1	2:J:96:TYR:HE1	0.62	0.77
1:L:7:SER:HB3	1:L:8:PRO:CD	2.15	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
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
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:J:86:ASN:O	2:J:87:SER:C	2.27	0.76
2:H:33:TRP:H	3:V:111:GLN:NE2	1.84	0.76
2:H:138:MET:HA	2:H:138:MET:HE3	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:Y:64:LEU:O	3:Y:68:THR:HG23	1.86	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
1:O:116:ILE:C	1:O:117:PHE:HD1	1.95	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
3:V:55:MET:H	3:V:55:MET:HE2	1.53	0.74
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:V:69:LEU:CD1	3:V:118:THR:CG2	2.66	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
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
1:N:77:MET:HE3	1:N:81:ASP:CB	2.17	0.72
3:X:85:CYS:O	3:X:86:LEU:C	2.32	0.72
3:Z:71:LEU:HD12	3:Z:101:LEU:CD2	2.20	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:L:154:ARG:HG3	1:L:154:ARG:O	1.77	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:N:2:VAL:HG21	1:N:89:GLN:CD	2.16	0.71
1:L:19:VAL:HB	1:L:74:ILE:HB	1.71	0.71
1:N:169:ASP:CG	1:N:169:ASP:O	2.34	0.71
2:K:13:GLN:O	2:K:14:PRO:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:O:116:ILE:C	1:O:117:PHE:CD1	2.68	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
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
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
2:K:13:GLN:O	2:K:14:PRO:C	2.35	0.69
1:M:60:ARG:NH1	1:M:81:ASP:OD2	2.26	0.69
1:O:77:MET:HE3	1:O:81:ASP:HB2	1.73	0.69
3:V:100:LEU:O	3:V:103:ALA:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:138:MET:HE2	2:H:185:THR:CG2	2.21	0.69
2:I:216:ARG:NE	3:Y:122:LYS:H	1.91	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:J:60:ILE:C	2:J:61:HIS:CD2	2.71	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
3:Y:52:LYS:HZ1	3:Y:145:VAL:HG23	1.57	0.68
3:Y:124:PRO:O	3:Y:125:ASN:C	2.35	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:M:60:ARG:HH12	1:M:81:ASP:CG	2.00	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
1:M:160:ASN:HB3	1:M:174:MET:HE3	1.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:H:199:ASN:HB3	2:H:209:VAL:HG23	0.94	0.67
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
1:O:124:LEU:O	1:O:125:THR:C	2.36	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
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
3:Y:13:SER:O	3:Y:15:LEU:N	2.26	0.67
1:M:78:GLU:O	1:M:79:ALA:C	2.38	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
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
2:K:147:GLY:C	2:K:177:LEU:HD13	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:61:GLN:O	3:V:65:GLY:N	2.19	0.66
2:I:85:MET:HE2	2:I:88:LEU:HD21	1.78	0.66
2:K:202:HIS:ND1	2:K:204:ALA:CB	2.58	0.66
3:Y:75:MET:HA	3:Y:75:MET:HE3	1.78	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
1:N:72:LEU:C	1:N:72:LEU:CD2	2.64	0.66
3:Z:97:VAL:O	3:Z:100:LEU:CB	2.43	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
3:Z:98:ARG:HA	3:Z:101:LEU:HB2	1.77	0.66
1:L:105:ILE:HG13	1:L:106:LYS:N	2.10	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
1:O:202:SER:O	1:O:203:PRO:C	2.39	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
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:11:MET:HE2	1:M:19:VAL:HG22	1.77	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
2:K:70:PHE:CZ	2:K:85:MET:HE2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:182:LYS:HD3	1:O:186:GLU:CD	2.22	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
3:Y:15:LEU:O	3:Y:19:SER:HB3	1.97	0.65
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
2:I:57:ASN:O	2:I:58:HIS:C	2.38	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
3:V:61:GLN:CD	3:V:112:LEU:HD21	2.22	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
1:M:174:MET:HE2	1:M:175:SER:O	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
1:M:77:MET:HE3	1:M:103:LEU:HD21	1.79	0.64
2:J:38:ARG:HB2	2:J:96:TYR:HE2	1.60	0.64
2:K:51:ILE:HD13	2:K:74:ARG:HD2	1.79	0.64
2:I:93:THR:HG1	2:I:114:VAL:H	1.46	0.64
1:N:149:ILE:HG23	1:N:191:TYR:HE2	1.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:191:TRP:HA	2:J:193:SER:N	2.13	0.64
2:H:29:PHE:C	2:H:29:PHE:CD2	2.75	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
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: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
2:I:158:ASN:O	2:I:159:SER:C	2.40	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
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: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
2:K:29:PHE:CE1	2:K:34:MET:HE2	2.33	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:X:61:GLN:O	3:X:62:ASP:C	2.42	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:V:75:MET:HE2	3:V:98:ARG:HH22	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Y:91:GLY:O	3:Y:92:GLN:C	2.38	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
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
3:Y:124:PRO:C	3:Y:126:ALA:N	2.52	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:66:SER:C	1:O:70:TYR:HE1	2.07	0.62
1:O:119:PRO:HG3	1:O:130:SER:N	2.14	0.62
1:M:120:SER:C	1:M:122:GLU:H	2.07	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
1:M:72:LEU:HD23	1:M:72:LEU:C	2.25	0.62
1:M:211:ASN:C	1:M:212:GLU:HG3	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
2:H:138:MET:HE1	2:H:186:VAL:C	2.25	0.61
1:M:45:LEU:C	1:M:45:LEU:CD2	2.73	0.61
2:J:191:TRP:HA	2:J:192:PRO:C	2.25	0.61
1:O:149:ILE:HG23	1:O:191:TYR:CE2	2.34	0.61
1:L:88:GLN:HG2	1:L:89:GLN:N	2.13	0.61
2:J:51:ILE:HD13	2:J:74:ARG:HG3	1.79	0.61
3:Y:22:LEU:HD12	3:Y:96:GLN:OE1	1.98	0.61
3:Y:124:PRO:C	3:Y:126:ALA:H	2.08	0.61
2:H:89:ARG:HD2	2:H:91:GLU:CD	2.25	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:85:MET:HE1	2:I:96:TYR:CZ	2.35	0.61
2:I:149:PHE:HB2	2:I:177:LEU:HD21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:101:TRP:CD1	3:Z:111:GLN:HB3	2.35	0.61
3:X:77:ALA:O	3:X:78:ARG:C	2.38	0.61
3:Z:43:ALA:CB	3:Z:119:THR:HG23	2.30	0.61
3:Z:107:LEU:CD2	3:Z:107:LEU:C	2.73	0.61
2:H:84:GLN:HE21	2:H:84:GLN:C	2.08	0.61
1:M:123:GLN:NE2	1:M:130:SER:HG	1.98	0.61
1:M:181:THR:O	1:M:182:LYS:C	2.42	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:H:138:MET:HE3	2:H:138:MET:CA	2.30	0.60
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
3:X:12:LEU:CB	3:X:143:MET:CE	2.67	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:164:ASP:O	1:L:165:GLN:C	2.40	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
1:O:108:ALA:O	1:O:109:ASP:C	2.43	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
2:H:33:TRP:CD1	2:H:53:SER:HG	2.20	0.59
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:29:PHE:HE1	2:K:34:MET:HE3	1.68	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
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:Y:136:ARG:NH1	3:Y:136:ARG:HB2	2.16	0.59
1:M:167:SER:C	1:M:168:LYS:HE3	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:41:LEU:HD12	3:Y:121:HIS:CD2	2.38	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
1:M:124:LEU:C	1:M:126:SER:H	2.09	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
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
3:Z:116:GLY:O	3:Z:117:ARG:C	2.44	0.59
1:M:88:GLN:HB2	1:M:97:PHE:CD1	2.38	0.59
1:N:162:TRP:CH2	1:N:174:MET:HE2	2.38	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:J:56:ASN:HD22	2:J:56:ASN:N	2.01	0.58
1:O:48:TYR:CE2	3:Z:113:PRO:HG2	2.38	0.58
2:K:29:PHE:CE1	2:K:34:MET:HE3	2.37	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: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
2:I:37:VAL:HG21	2:I:106:TRP:HH2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:69:SER:C	1:O:70:TYR:CD1	2.77	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:I:206:SER:C	2:I:207:THR:HG22	2.29	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
3:Z:13:SER:O	3:Z:14:LYS:C	2.47	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:120:SER:O	1:N:121:SER:C	2.46	0.58
1:N:154:ARG:NH2	1:N:184:GLU:OE1	2.37	0.58
1:O:77:MET:CE	1:O:81:ASP:HB2	2.33	0.58
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
2:H:88:LEU:HB3	2:H:114:VAL:HG11	1.86	0.58
2:H:91:GLU:C	2:H:93:THR:N	2.51	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:V:145:VAL:HG13	3:V:145:VAL:O	2.04	0.57
3:Z:87:SER:O	3:Z:88:SER:C	2.47	0.57
1:M:84:THR:HA	1:M:101:THR:O	2.04	0.57
2:I:158:ASN:C	2:I:160:GLY:N	2.62	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
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
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
3:V:41:LEU:HD22	3:V:127:ILE:HB	1.86	0.57
3:V:41:LEU:HD11	3:V:127:ILE:HG22	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
1:M:123:GLN:CD	1:M:130:SER:HG	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:X:86:LEU:C	3:X:86:LEU:HD22	2.30	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:56:ASN:N	2:H:56:ASN:ND2	2.50	0.56
2:H:66:VAL:HG13	2:H:70:PHE:CG	2.39	0.56
2:H:123:SER:HG	2:H:146:LYS:HB3	1.70	0.56
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
2:H:191:TRP:CD1	2:H:192:PRO:HA	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:PHE:CE1	1:M:74:ILE:HG12	2.40	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
1:O:161:SER:C	1:O:162:TRP:CE3	2.84	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
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
2:I:8:GLY:C	2:I:9:GLY:O	2.49	0.56
2:I:91:GLU:H	2:I:91:GLU:CD	2.13	0.56
3:V:66:ALA:O	3:V:67:VAL:C	2.49	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
3:Z:101:LEU:CD1	3:Z:105:GLN:HE22	2.17	0.56
2:H:138:MET:HE3	2:H:139:VAL:H	1.70	0.55
2:H:173:LEU:HD22	2:H:176:ASP:HA	1.87	0.55
2:I:57:ASN:C	2:I:59:ALA:N	2.63	0.55
2:J:157:TRP:O	2:J:158:ASN:C	2.46	0.55
1:O:132:VAL:HA	1:O:177:THR:HA	1.88	0.55
1:M:174:MET:HG2	1:M:175:SER:N	2.21	0.55
2:I:10:GLY:CA	2:I:18:MET:HE1	2.37	0.55
2:I:33:TRP:CD1	2:I:53:SER:H	2.23	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:70:PHE:CE1	2:K:85:MET:HE2	2.41	0.55
2:K:142:GLY:HA2	2:K:182:SER:O	2.06	0.55
2:H:89:ARG:O	2:H:90:ALA:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:10:GLY:N	2:I:18:MET:HE1	2.22	0.55
2:I:84:GLN:HE21	2:I:84:GLN:C	2.15	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
3:V:87:SER:C	3:V:89:LEU:H	2.13	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:V:93:LEU:HD23	3:V:93:LEU:C	2.32	0.55
3:Y:42:PRO:HD2	3:Y:130:SER:OG	2.07	0.55
1:L:90:ARG:NH2	2:H:102:SER:O	2.40	0.55
1:L:160:ASN:CG	1:L:174:MET:HE1	2.32	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:125:TYR:N	2:K:144:LEU:O	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:157:TRP:C	2:J:159:SER:N	2.63	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
3:V:139:VAL:O	3:V:140:ARG:C	2.50	0.54
1:L:109:ASP:HA	1:L:139:TYR:O	2.08	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:N:77:MET:HE2	1:N:78:GLU:O	2.07	0.54
2:J:141:LEU:N	2:J:141:LEU:HD23	2.22	0.54
2:I:69:ARG:HH22	2:I:92:ASP:CG	2.15	0.54
1:N:119:PRO:HG3	1:N:185:TYR:CZ	2.42	0.54
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
3:V:127:ILE:O	3:V:128:PHE:C	2.51	0.54
3:X:134:LEU:C	3:X:139:VAL:HG23	2.32	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:X:9:LEU:C	3:X:11:VAL:N	2.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:51:TRP:O	3:Y:59:LYS:HE2	2.08	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
1:M:86:TYR:CD1	2:I:45:LEU:HD12	2.42	0.54
1:N:116:ILE:C	1:N:117:PHE:CD1	2.86	0.54
1:N:211:ASN:ND2	1:N:212:GLU:N	2.56	0.54
2:J:29:PHE:C	2:J:31:ASP:H	2.15	0.54
2:J:90:ALA:H	2:J:91:GLU:CD	2.16	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:75:ASP:C	2:K:75:ASP:OD1	2.50	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
3:X:91:GLY:O	3:X:92:GLN:C	2.49	0.54
2:H:51:ILE:HD12	2:H:74:ARG:HG3	1.88	0.54
1:N:79:ALA:CA	1:N:105:ILE:HD13	2.36	0.54
1:N:162:TRP:CZ2	1:N:174:MET:HE3	2.43	0.54
3:X:73:GLY:O	3:X:74:VAL:C	2.49	0.54
3:Y:77:ALA:O	3:Y:78:ARG:C	2.50	0.54
1:L:37:GLN:HG2	1:L:38:LYS:H	1.73	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
1:N:110:ALA:HB3	1:N:138:PHE:C	2.33	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
2:H:39:GLN:O	2:H:95:ILE:HG12	2.08	0.53
2:H:90:ALA:HA	2:H:114:VAL:HG23	1.90	0.53
2:I:29:PHE:HE1	2:I:34:MET:HE2	1.73	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
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
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
1:L:116:ILE:C	1:L:117:PHE:CD1	2.86	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:J:51:ILE:C	2:J:52:ARG:O	2.50	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
3:Y:15:LEU:HD23	3:Y:135:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Z:91:GLY:O	3:Z:92:GLN:C	2.52	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:104:LEU:O	3:Y:105:GLN:C	2.49	0.53
3:Y:133:HIS:CD2	3:Z:46:PHE:CD2	2.97	0.53
3:Z:101:LEU:HD11	3:Z:105:GLN:NE2	2.22	0.53
2:H:180:LEU:HD23	2:H:180:LEU:C	2.34	0.53
1:M:192:THR:OG1	1:M:207:SER:CB	2.56	0.53
2:I:206:SER:C	2:I:207:THR:CG2	2.82	0.53
1:O:84:THR:HA	1:O:101:THR:O	2.08	0.53
2:K:29:PHE:C	2:K:31:ASP:H	2.17	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
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:2:VAL:CG2	1:N:89:GLN:CD	2.80	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: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
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
2:J:75:ASP:OD1	2:J:75:ASP:C	2.52	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:9:LEU:C	3:Z:11:VAL:H	2.17	0.52
3:Z:29:CYS:SG	3:Z:89:LEU:HD12	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:SER:OG	1:M:8:PRO:CD	2.58	0.52
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:122:GLU:CD	1:L:122:GLU:H	2.16	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:I:56:ASN:C	2:I:57:ASN:ND2	2.68	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:30:PRO:O	3:Y:31:GLU:C	2.53	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: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:13:GLN:C	2:K:14:PRO:O	2.52	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: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:N:205:VAL:CG1	1:N:205:VAL:O	2.56	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:L:29:VAL:O	1:L:70:TYR:OH	2.28	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
1:L:205:VAL:HG12	1:L:206:LYS:N	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:38:ARG:HH11	2:K:46:GLU:CD	2.18	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
2:K:4:LEU:HD11	2:K:105:TYR:HB3	1.92	0.51
2:K:57:ASN:C	2:K:59:ALA:H	2.18	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
2:I:211:LYS:O	2:I:212:LYS:C	2.52	0.51
1:N:163:THR:HG23	1:N:164:ASP:O	2.10	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: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: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:85:MET:HE1	2:H:96:TYR:CZ	2.46	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
1:N:136:ASN:O	1:N:137:ASN:C	2.53	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:Y:25:ARG:O	3:Y:26:LEU:C	2.54	0.51
3:Z:41:LEU:HD13	3:Z:127:ILE:HG22	1.89	0.51
1:L:184:GLU:O	1:L:185:TYR:C	2.53	0.51
1:M:23:CYS:SG	1:M:32:MET:HE3	2.51	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:64:GLU:C	2:K:66:VAL:H	2.18	0.51
2:K:187:PRO:HD2	2:K:190:THR:OG1	2.10	0.51
1:M:165:GLN:HG2	1:M:172:TYR:CE1	2.46	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:V:75:MET:O	3:V:76:ALA:C	2.52	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:13:GLN:O	2:I:14:PRO:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:187:PRO:O	2:K:188:SER:C	2.52	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
2:H:85:MET:HE3	2:H:96:TYR:CE1	2.47	0.50
1:N:79:ALA:C	1:N:81:ASP:H	2.20	0.50
1:N:105:ILE:N	1:N:165:GLN:OE1	2.42	0.50
1:O:44:LYS:HZ3	1:O:44:LYS:CB	2.14	0.50
3:V:81:LEU:HD12	3:V:87:SER:CB	2.38	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:22:CYS:C	2:J:80:SER:HB3	2.37	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
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: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:M:77:MET:HE3	1:M:103:LEU:CD2	2.41	0.50
1:M:164:ASP:O	1:M:165:GLN:C	2.51	0.50
2:K:29:PHE:CD1	2:K:79:SER:O	2.64	0.50
2:K:29:PHE:CG	2:K:79:SER:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:H:205:SER:O	2:H:207:THR:HG22	2.12	0.49
1:M:11:MET:HE2	1:M:19:VAL:CG2	2.40	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: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
2:J:51:ILE:O	2:J:52:ARG:C	2.55	0.49
3:Z:56:GLU:OE2	3:Z:56:GLU:N	2.45	0.49
3:Z:75:MET:CA	3:Z:75:MET:HE3	2.41	0.49
1:L:37:GLN:O	1:L:83:ALA:HB1	2.12	0.49
1:M:160:ASN:CG	1:M:174:MET:CE	2.86	0.49
1:O:28:SER:O	1:O:29:VAL:HG13	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:37:GLN:CG	1:M:38:LYS:N	2.73	0.49
1:M:107:ARG:HH11	1:M:170:SER:N	2.10	0.49
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:M:21:ILE:HG22	1:M:22:THR:O	2.12	0.49
1:N:205:VAL:O	1:N:205:VAL:HG12	2.12	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
2:K:140:THR:C	2:K:141:LEU:HD23	2.37	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
1:M:77:MET:HE2	1:M:81:ASP:HB2	1.95	0.49
2:J:66:VAL:HG13	2:J:70:PHE:CD2	2.48	0.49
2:K:57:ASN:C	2:K:59:ALA:N	2.70	0.49
2:K:169:PHE:HD2	2:K:181:SER:O	1.96	0.49
2:H:146:LYS:HG2	2:H:179:THR:OG1	2.13	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:123:ASP:C	3:X:125:ASN:N	2.70	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
1:L:174:MET:HE2	1:L:176:SER:HB2	1.95	0.48
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
2:J:54:LYS:O	2:J:55:VAL:C	2.54	0.48
2:J:130:GLY:C	2:J:133:ALA:H	2.18	0.48
1:O:4:LEU:HD12	1:O:87:CYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:TYR:CZ	1:O:90:ARG:HD3	2.48	0.48
1:O:52:ASN:CG	3:Z:115:ARG:CZ	2.86	0.48
1:O:83:ALA:HB3	1:O:85:TYR:CE1	2.48	0.48
2:K:89:ARG:O	2:K:114:VAL:CG2	2.61	0.48
2:K:132:ALA:O	2:K:133:ALA:C	2.56	0.48
3:V:42:PRO:HD2	3:V:130:SER:OG	2.13	0.48
3:V:100:LEU:O	3:V:101:LEU:C	2.55	0.48
3:Y:8:ASP:C	3:Y:10:ARG:H	2.20	0.48
2:H:33:TRP:CD1	2:H:53:SER:H	2.31	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
1:M:116:ILE:C	1:M:117:PHE:CD1	2.91	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
1:O:145:VAL:HG21	1:O:174:MET:HE2	1.94	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
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:166:ASP:O	1:N:167:SER:C	2.56	0.48
1:N:167:SER:CB	1:N:168:LYS:HZ1	2.20	0.48
2:K:87:SER:O	2:K:87:SER:OG	2.24	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
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: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
3:V:87:SER:C	3:V:89:LEU:N	2.70	0.48
3:Y:52:LYS:NZ	3:Y:145:VAL:HG23	2.28	0.48
3:Z:51:TRP:CD1	3:Z:51:TRP:C	2.91	0.48
1:M:113:THR:H	1:M:136:ASN:H	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:L:147:TRP:CD1	1:L:158:VAL:HG11	2.49	0.48
2:H:70:PHE:CE1	2:H:85:MET:HE2	2.47	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
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: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
2:I:158:ASN:C	2:I:160:GLY:H	2.21	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
1:O:11:MET:HB2	1:O:11:MET:HE3	1.95	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:V:26:LEU:O	3:V:27:SER:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:132:GLN:C	3:X:134:LEU:N	2.72	0.47
3:Z:30:PRO:O	3:Z:31:GLU:C	2.57	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
2:I:54:LYS:O	2:I:55:VAL:C	2.57	0.47
1:N:169:ASP:OD2	1:N:169:ASP:C	2.56	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
2:K:175:SER:O	2:K:176:ASP:C	2.57	0.47
3:V:15:LEU:O	3:V:16:LEU:C	2.56	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:X:137:GLY:O	3:X:138:LYS:C	2.57	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:X:30:PRO:O	3:X:31:GLU:C	2.57	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
3:Z:61:GLN:O	3:Z:62:ASP:C	2.58	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
2:H:64:GLU:CG	2:H:67:LYS:HZ2	2.24	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: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
3:Y:115:ARG:HD2	3:Y:115:ARG:C	2.40	0.47
3:Y:123:ASP:O	3:Y:124:PRO:C	2.57	0.47
1:M:115:SER:HB2	1:M:117:PHE:HE1	1.78	0.47
1:M:124:LEU:C	1:M:126:SER:N	2.71	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
1:N:27:SER:O	1:N:28:SER:C	2.58	0.47
2:K:17:SER:OG	2:K:86:ASN:HA	2.14	0.47
3:V:78:ARG:O	3:V:79:GLY:C	2.57	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
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:8:GLY:C	2:J:9:GLY:O	2.56	0.47
2:J:77:SER:C	2:J:79:SER:H	2.21	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: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:26:LEU:C	3:Y:28:GLN:N	2.73	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
3:V:22:LEU:O	3:V:23:HIS:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:LEU:HD21	1:L:89:GLN:HB3	1.97	0.47
1:L:14:SER:O	1:L:15:PRO:C	2.56	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:K:8:GLY:O	2:K:9:GLY:O	2.33	0.47
2:K:64:GLU:C	2:K:66:VAL:N	2.71	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
3:Z:101:LEU:O	3:Z:102:GLY:C	2.58	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:207:THR:O	2:I:207:THR:OG1	2.24	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
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
1:O:169:ASP:O	1:O:169:ASP:CG	2.57	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
3:Z:96:GLN:O	3:Z:97:VAL:C	2.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:GLU:CD	1:N:107:ARG:HH22	2.24	0.46
2:I:29:PHE:CE1	2:I:34:MET:HE2	2.50	0.46
2:J:13:GLN:O	2:J:14:PRO:C	2.56	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:192:PRO:O	2:K:193:SER:C	2.58	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
3:Z:123:ASP:C	3:Z:125:ASN:N	2.71	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:OD1	1:O:160:ASN:N	2.48	0.46
1:O:180:LEU:C	1:O:180:LEU:HD12	2.39	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:Z:71:LEU:CD1	3:Z:101:LEU:HD23	2.44	0.46
2:H:130:GLY:C	2:H:132:ALA:H	2.23	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
2:K:157:TRP:O	2:K:158:ASN:C	2.57	0.46
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:29:PHE:C	2:J:31:ASP:N	2.73	0.46
2:J:38:ARG:HD3	2:J:43:LYS:NZ	2.30	0.46
2:J:135:THR:C	2:J:136:ASN:O	2.57	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:26:LEU:C	3:Y:28:GLN:H	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:75:MET:HE3	3:Z:75:MET:HA	1.98	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:L:169:ASP:OD2	1:L:169:ASP:C	2.58	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
2:I:70:PHE:CZ	2:I:85:MET:HE3	2.51	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
3:Y:51:TRP:C	3:Y:53:THR:N	2.72	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
3:Y:86:LEU:O	3:Y:87:SER:C	2.59	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
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
3:Z:141:PHE:O	3:Z:142:LEU:C	2.56	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
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
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
1:L:34:TRP:C	1:L:35:PHE:CD1	2.94	0.45
1:M:18:LYS:HG3	1:M:19:VAL:N	2.28	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:X:123:ASP:C	3:X:125:ASN:H	2.23	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:V:49:GLY:C	3:V:51:TRP:H	2.25	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
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: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
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
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
2:H:138:MET:HE1	2:H:187:PRO:N	2.31	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:V:93:LEU:C	3:V:93:LEU:CD2	2.90	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
2:J:28:THR:O	2:J:29:PHE:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:124:LEU:C	1:N:126:SER:H	2.24	0.45
1:N:147:TRP:NE1	1:N:158:VAL:CG1	2.79	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
1:O:134:PHE:C	1:O:135:LEU:HD12	2.42	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
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:4:LEU:HD22	1:L:32:MET:HE1	1.98	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
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:21:VAL:O	3:V:22:LEU:C	2.58	0.45
3:V:89:LEU:O	3:V:92:GLN:N	2.50	0.45
3:Z:94:SER:O	3:Z:95:GLY:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:75:MET:C	3:V:77:ALA:N	2.75	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: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
1:M:32:MET:C	1:M:33:TYR:CD2	2.95	0.44
2:I:24:ALA:HB1	2:I:27:PHE:CE1	2.52	0.44
1:N:79:ALA:C	1:N:81:ASP:N	2.76	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
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
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
2:J:203:PRO:HA	2:J:205:SER:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:174:GLN:C	2:H:176:ASP:N	2.75	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:132:VAL:CG2	1:O:133:CYS:N	2.79	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: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
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
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:105:GLN:CD	3:V:111:GLN:HG2	2.43	0.44
3:V:149:THR:OG1	3:V:150:LEU:N	2.50	0.44
3:Y:64:LEU:HD12	3:Y:64:LEU:C	2.43	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
1:L:174:MET:O	1:L:174:MET:HG3	2.13	0.44
2:H:6:GLU:OE1	2:H:98:CYS:HB3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:X:132:GLN:C	3:X:134:LEU:H	2.26	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:138:PHE:C	1:N:138:PHE:CD1	2.95	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:V:140:ARG:CA	3:V:143:MET:HE2	2.36	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:46:PHE:HD1	3:Z:46:PHE:HA	1.71	0.43
3:Z:119:THR:OG1	3:Z:121:HIS:NE2	2.42	0.43
1:L:94:PRO:HA	2:H:47:TRP:CZ3	2.52	0.43
2:H:84:GLN:CA	2:H:84:GLN:NE2	2.71	0.43
1:M:60:ARG:NH1	1:M:81:ASP:CG	2.70	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:X:23:HIS:CD2	3:X:23:HIS:C	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:187:ARG:O	1:M:187:ARG:HG2	2.18	0.43
1:N:77:MET:CE	1:N:78:GLU:O	2.65	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
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
3:Y:51:TRP:O	3:Y:52:LYS:C	2.59	0.43
3:Y:52:LYS:HZ3	3:Y:59:LYS:NZ	2.16	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
2:J:29:PHE:CE2	2:J:79:SER:C	2.97	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:8:ASP:C	3:Y:10:ARG:N	2.75	0.43
3:Z:63:ILE:C	3:Z:67:VAL:HG23	2.32	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
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:57:ASN:C	2:J:59:ALA:N	2.72	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:123:ASP:HA	3:V:124:PRO:HD3	1.81	0.43
3:X:24:SER:C	3:X:26:LEU:H	2.27	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:TRP:CZ3	3:V:110:THR:HA	2.53	0.43
2:H:56:ASN:C	2:H:57:ASN:ND2	2.76	0.43
1:M:181:THR:C	1:M:183:ASP:N	2.71	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
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
2:H:72:VAL:CG2	2:H:73:SER:N	2.79	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: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
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
3:X:41:LEU:HD13	3:X:127:ILE:HA	2.01	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
1:N:185:TYR:HD1	1:N:191:TYR:HH	1.67	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: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
2:H:138:MET:CE	2:H:187:PRO:HA	2.49	0.42
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:29:PHE:C	2:K:31:ASP:N	2.77	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
1:M:48:TYR:O	1:M:49:SER:C	2.61	0.42
1:M:72:LEU:C	1:M:72:LEU:CD2	2.92	0.42
2:I:10:GLY:C	2:I:18:MET:HE1	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:57:ASN:O	2:K:58:HIS:C	2.60	0.42
3:X:12:LEU:HD22	3:X:143:MET:SD	2.60	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:118:PRO:HB3	1:N:208:PHE:CZ	2.54	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:58:HIS:O	2:K:59:ALA:C	2.61	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:90:LEU:O	3:V:94:SER:HB3	2.19	0.42
3:V:90:LEU:HD21	3:V:128:PHE:CE2	2.54	0.42
3:V:97:VAL:HA	3:V:131:PHE:CZ	2.53	0.42
3:Z:25:ARG:HG2	3:Z:28:GLN:CD	2.45	0.42
1:L:33:TYR:CE1	1:L:90:ARG:HD3	2.54	0.42
2:H:138:MET:HE3	2:H:139:VAL:N	2.35	0.42
1:M:84:THR:HG23	1:M:101:THR:C	2.44	0.42
1:M:189:ASN:O	1:M:210:ARG:N	2.45	0.42
2:I:76:ASP:O	2:I:77:SER:C	2.62	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
3:Y:87:SER:O	3:Y:88:SER:C	2.62	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:L:160:ASN:ND2	1:L:174:MET:HE1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:85:MET:HE2	2:I:88:LEU:CD2	2.49	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:49:GLY:C	3:V:51:TRP:N	2.77	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
3:Z:140:ARG:C	3:Z:142:LEU:N	2.73	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
2:J:29:PHE:CE1	2:J:34:MET:HE2	2.48	0.42
1:O:32:MET:C	1:O:33:TYR:CD1	2.97	0.42
1:O:46:TRP:HB3	1:O:47:ILE:H	1.62	0.42
1:L:48:TYR:CE2	3:V:113:PRO:CG	3.03	0.42
1:L:98:GLY:O	1:L:99:GLY:C	2.61	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:28:SER:C	1:O:29:VAL:HG13	2.45	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:V:96:GLN:O	3:V:97:VAL:C	2.62	0.42
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:33:TRP:H	3:V:111:GLN:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:J:86:ASN:O	2:J:87:SER:O	2.36	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: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: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
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
3:Z:77:ALA:C	3:Z:79:GLY:N	2.78	0.41
1:L:37:GLN:HE21	1:L:86:TYR:HE2	1.67	0.41
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:47:TRP:HE1	2:K:49:ALA:C	2.28	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:43:LYS:HD3	2:I:46:GLU:CD	2.45	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:V:65:GLY:O	3:V:66:ALA:C	2.62	0.41
3:Y:62:ASP:O	3:Y:63:ILE:C	2.63	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:178:LEU:HD23	1:L:179:THR:N	2.36	0.41
2:H:69:ARG:HH22	2:H:92:ASP:CG	2.18	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:140:THR:C	2:J:141:LEU:HD23	2.45	0.41
2:K:40:SER:CB	2:K:42:GLU:H	2.34	0.41
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
1:N:124:LEU:C	1:N:126:SER:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:216:ARG:NE	3:X:122:LYS:H	2.18	0.41
1:O:44:LYS:HB2	1:O:44:LYS:HZ2	1.78	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:79:GLY:O	3:Z:80:GLN:C	2.63	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
2:K:175:SER:C	2:K:177:LEU:N	2.78	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: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:72:LEU:HD23	1:L:72:LEU:C	2.46	0.41
1:L:117:PHE:O	1:L:118:PRO:C	2.62	0.41
1:L:139:TYR:CA	1:L:140:PRO:O	2.69	0.41
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:89:ARG:C	2:H:114:VAL:HG21	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:TYR:C	2:K:177:LEU:HD22	2.45	0.41
3:V:41:LEU:HD13	3:V:127:ILE:HA	2.03	0.41
3:V:140:ARG:O	3:V:143:MET:HE2	2.21	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:68:THR:O	3:Y:69:LEU:C	2.64	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:81:ASP:O	1:L:85:TYR:OH	2.32	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:H:85:MET:CE	2:H:96:TYR:CE1	3.04	0.41
1:O:147:TRP:HE3	1:O:192:THR:O	2.01	0.41
3:Y:60:ALA:O	3:Y:61:GLN:C	2.64	0.41
3:Z:35:LEU:HA	3:Z:36:PRO:HD2	1.99	0.41
1:L:139:TYR:HA	1:L:140:PRO:C	2.46	0.40
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
2:K:90:ALA:C	2:K:92:ASP:N	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:89:LEU:C	3:X:91:GLY:N	2.79	0.40
3:X:109:GLY:O	4:X:166:HOH:O	2.22	0.40
3:Z:13:SER:C	3:Z:15:LEU:N	2.79	0.40
3:Z:116:GLY:O	3:Z:117:ARG:O	2.39	0.40
2:H:157:TRP:CZ3	2:H:198:CYS:CB	3.00	0.40
2:I:216:ARG:HE	3:Y:122:LYS:HG3	1.86	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:X:100:LEU:C	3:X:100:LEU:CD2	2.93	0.40
3:X:125:ASN:C	3:X:127:ILE:H	2.29	0.40
3:Z:86:LEU:HD11	3:Z:124:PRO:HG3	2.03	0.40
3:Z:93:LEU:O	3:Z:94:SER:C	2.65	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
2:J:33:TRP:N	3:Y:111:GLN:HE22	2.00	0.40
2:K:40:SER:C	2:K:42:GLU:H	2.30	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
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:137:GLY:O	3:Z:138:LYS:C	2.64	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%)	4	24
1	M	210/213 (99%)	179 (85%)	20 (10%)	11 (5%)	1	11
1	N	210/213 (99%)	177 (84%)	20 (10%)	13 (6%)	1	9
1	O	211/213 (99%)	175 (83%)	24 (11%)	12 (6%)	1	9
2	H	215/217 (99%)	175 (81%)	24 (11%)	16 (7%)	1	6
2	I	215/217 (99%)	170 (79%)	25 (12%)	20 (9%)	0	3
2	J	215/217 (99%)	166 (77%)	31 (14%)	18 (8%)	0	4
2	K	215/217 (99%)	165 (77%)	30 (14%)	20 (9%)	0	3
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%)	0	4
3	Z	136/163 (83%)	89 (65%)	31 (23%)	16 (12%)	0	1
All	All	2254/2372 (95%)	1752 (78%)	317 (14%)	185 (8%)	0	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
2	H	133	ALA
2	H	175	SER
2	H	176	ASP

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Mol	Chain	Res	Type
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
3	X	11	VAL
3	X	31	GLU
3	X	88	SER

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Mol	Chain	Res	Type
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
3	V	91	GLY
3	V	102	GLY
3	V	138	LYS

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Mol	Chain	Res	Type
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
3	Y	27	SER
3	Y	140	ARG
3	Y	145	VAL

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Mol	Chain	Res	Type
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
3	Z	65	GLY
2	H	41	PRO
1	O	202	SER

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Mol	Chain	Res	Type
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 [i](#)

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%)	119 (64%)	67 (36%)	0	1
1	M	185/186 (100%)	110 (60%)	75 (40%)	0	0
1	N	185/186 (100%)	116 (63%)	69 (37%)	0	0
1	O	186/186 (100%)	112 (60%)	74 (40%)	0	0
2	H	182/185 (98%)	109 (60%)	73 (40%)	0	0
2	I	182/185 (98%)	103 (57%)	79 (43%)	0	0
2	J	182/185 (98%)	102 (56%)	80 (44%)	0	0
2	K	182/185 (98%)	110 (60%)	72 (40%)	0	0
3	V	122/138 (88%)	74 (61%)	48 (39%)	0	0
3	X	117/138 (85%)	69 (59%)	48 (41%)	0	0
3	Y	117/138 (85%)	70 (60%)	47 (40%)	0	0
3	Z	116/138 (84%)	70 (60%)	46 (40%)	0	0
All	All	1942/2036 (95%)	1164 (60%)	778 (40%)	0	0

All (778) 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	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	68	THR
1	L	72	LEU
1	L	73	THR
1	L	76	ARG
1	L	77	MET
1	L	88	GLN
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	122	GLU
1	L	123	GLN
1	L	124	LEU
1	L	125	THR
1	L	131	VAL
1	L	132	VAL
1	L	143	ILE
1	L	145	VAL
1	L	146	LYS
1	L	148	LYS

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Mol	Chain	Res	Type
1	L	149	ILE
1	L	152	SER
1	L	154	ARG
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	192	THR
1	L	193	CYS
1	L	194	GLU
1	L	196	THR
1	L	199	THR
1	L	201	THR
1	L	202	SER
1	L	204	ILE
1	L	206	LYS
1	L	211	ASN
1	L	213	CYS
2	H	2	VAL
2	H	3	LYS
2	H	4	LEU
2	H	6	GLU
2	H	12	VAL
2	H	13	GLN
2	H	20	LEU
2	H	28	THR
2	H	29	PHE
2	H	30	SER
2	H	37	VAL
2	H	38	ARG
2	H	42	GLU
2	H	50	GLU
2	H	51	ILE
2	H	54	LYS
2	H	55	VAL
2	H	56	ASN

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Mol	Chain	Res	Type
2	H	57	ASN
2	H	64	GLU
2	H	69	ARG
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	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	127	LEU
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	173	LEU
2	H	174	GLN
2	H	175	SER
2	H	180	LEU
2	H	188	SER

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Mol	Chain	Res	Type
2	H	195	THR
2	H	196	VAL
2	H	197	THR
2	H	198	CYS
2	H	199	ASN
2	H	200	VAL
2	H	206	SER
2	H	207	THR
2	H	211	LYS
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	17	GLU
1	M	18	LYS
1	M	19	VAL
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	37	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

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Mol	Chain	Res	Type
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	122	GLU
1	M	124	LEU
1	M	126	SER
1	M	130	SER
1	M	132	VAL
1	M	137	ASN
1	M	138	PHE
1	M	141	LYS
1	M	142	ASP
1	M	143	ILE
1	M	145	VAL
1	M	146	LYS
1	M	150	ASP
1	M	154	ARG
1	M	155	GLN
1	M	156	ASN
1	M	158	VAL
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	173	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

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Mol	Chain	Res	Type
1	M	204	ILE
1	M	205	VAL
1	M	210	ARG
1	M	211	ASN
2	I	2	VAL
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
2	I	52	ARG
2	I	53	SER
2	I	54	LYS
2	I	55	VAL
2	I	56	ASN
2	I	57	ASN
2	I	60	ILE
2	I	61	HIS
2	I	65	SER
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	102	SER
2	I	108	GLN
2	I	110	THR
2	I	111	LEU
2	I	112	VAL

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Mol	Chain	Res	Type
2	I	113	THR
2	I	115	SER
2	I	118	LYS
2	I	119	THR
2	I	123	SER
2	I	127	LEU
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
2	I	162	LEU
2	I	164	SER
2	I	172	VAL
2	I	173	LEU
2	I	174	GLN
2	I	179	THR
2	I	180	LEU
2	I	186	VAL
2	I	189	SER
2	I	193	SER
2	I	194	GLU
2	I	195	THR
2	I	196	VAL
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	2	VAL

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Mol	Chain	Res	Type
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	27	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
1	N	73	THR
1	N	76	ARG
1	N	77	MET
1	N	80	GLU
1	N	84	THR
1	N	86	TYR
1	N	90	ARG
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	122	GLU
1	N	124	LEU
1	N	130	SER
1	N	131	VAL
1	N	132	VAL

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Mol	Chain	Res	Type
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	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	176	SER
1	N	179	THR
1	N	180	LEU
1	N	181	THR
1	N	190	SER
1	N	192	THR
1	N	194	GLU
1	N	198	LYS
1	N	201	THR
1	N	204	ILE
1	N	205	VAL
1	N	206	LYS
1	N	210	ARG
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	18	MET
2	J	20	LEU
2	J	30	SER
2	J	35	ASP
2	J	38	ARG
2	J	40	SER
2	J	50	GLU
2	J	54	LYS
2	J	55	VAL

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Mol	Chain	Res	Type
2	J	56	ASN
2	J	57	ASN
2	J	61	HIS
2	J	64	GLU
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	112	VAL
2	J	113	THR
2	J	114	VAL
2	J	115	SER
2	J	118	LYS
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	146	LYS
2	J	148	TYR
2	J	151	GLU
2	J	153	VAL
2	J	155	VAL
2	J	156	THR

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Mol	Chain	Res	Type
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	177	LEU
2	J	179	THR
2	J	183	SER
2	J	186	VAL
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	209	VAL
2	J	210	ASP
2	J	216	ARG
2	J	217	ASP
1	O	1	GLN
1	O	2	VAL
1	O	3	VAL
1	O	10	ILE
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
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

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Mol	Chain	Res	Type
1	O	60	ARG
1	O	62	ARG
1	O	64	SER
1	O	71	SER
1	O	72	LEU
1	O	73	THR
1	O	76	ARG
1	O	77	MET
1	O	78	GLU
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	125	THR
1	O	133	CYS
1	O	143	ILE
1	O	145	VAL
1	O	146	LYS
1	O	149	ILE
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
1	O	178	LEU
1	O	181	THR
1	O	182	LYS
1	O	184	GLU
1	O	188	HIS

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Mol	Chain	Res	Type
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	199	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	38	ARG
2	K	43	LYS
2	K	46	GLU
2	K	54	LYS
2	K	55	VAL
2	K	60	ILE
2	K	65	SER
2	K	69	ARG
2	K	72	VAL
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
2	K	85	MET
2	K	87	SER
2	K	89	ARG
2	K	93	THR

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Mol	Chain	Res	Type
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	145	VAL
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	163	SER
2	K	164	SER
2	K	166	VAL
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	200	VAL
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	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	90	LEU
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	134	LEU
3	V	140	ARG

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Mol	Chain	Res	Type
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	9	LEU
3	X	11	VAL
3	X	12	LEU
3	X	15	LEU
3	X	16	LEU
3	X	17	ARG
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	35	LEU
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	98	ARG
3	X	100	LEU
3	X	105	GLN

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Mol	Chain	Res	Type
3	X	106	SER
3	X	107	LEU
3	X	110	THR
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	139	VAL
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	25	ARG
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

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Mol	Chain	Res	Type
3	Y	98	ARG
3	Y	99	LEU
3	Y	100	LEU
3	Y	105	GLN
3	Y	106	SER
3	Y	107	LEU
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	136	ARG
3	Y	140	ARG
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	21	VAL
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

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Mol	Chain	Res	Type
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
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	122	LYS
3	Z	127	ILE
3	Z	129	LEU
3	Z	134	LEU
3	Z	136	ARG
3	Z	140	ARG
3	Z	143	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) 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	209	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

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Mol	Chain	Res	Type
1	M	52	ASN
1	M	88	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
2	I	84	GLN
2	I	108	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
1	O	1	GLN
1	O	6	GLN
1	O	37	GLN
1	O	88	GLN
1	O	137	ASN
1	O	155	GLN
1	O	188	HIS
2	K	58	HIS
2	K	84	GLN
2	K	158	ASN
2	K	174	GLN
3	V	23	HIS

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Mol	Chain	Res	Type
3	V	92	GLN
3	V	105	GLN
3	V	111	GLN
3	V	125	ASN
3	X	20	HIS
3	X	23	HIS
3	X	92	GLN
3	X	96	GLN
3	Y	20	HIS
3	Y	111	GLN
3	Y	121	HIS
3	Z	33	HIS
3	Z	54	GLN
3	Z	105	GLN
3	Z	111	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	L	213/213 (100%)	-0.66	0	100	100	5, 23, 37, 46	0
1	M	212/213 (99%)	-0.62	0	100	100	5, 25, 40, 46	0
1	N	212/213 (99%)	-0.65	0	100	100	8, 26, 41, 49	0
1	O	213/213 (100%)	-0.41	0	100	100	7, 29, 50, 73	0
2	H	217/217 (100%)	-0.60	0	100	100	5, 23, 38, 63	0
2	I	217/217 (100%)	-0.51	0	100	100	10, 27, 44, 52	0
2	J	217/217 (100%)	-0.48	0	100	100	8, 24, 46, 67	0
2	K	217/217 (100%)	-0.24	0	100	100	13, 34, 54, 63	0
3	V	145/163 (88%)	-0.26	1 (0%)	84	70	8, 38, 81, 88	0
3	X	138/163 (84%)	-0.50	0	100	100	9, 32, 74, 83	0
3	Y	139/163 (85%)	-0.46	0	100	100	8, 27, 63, 70	0
3	Z	138/163 (84%)	-0.31	0	100	100	8, 41, 65, 77	0
All	All	2278/2372 (96%)	-0.49	1 (0%)	100	100	5, 27, 56, 88	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	46	PHE	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.