Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:57 AM EDT

PDB ID	:	7MK0
Title	:	Trypanosoma cruzi Nucleoside Diphosphate Kinase 1 form a quinary multi-hexameric structure
Authors	:	Gomez, J.A.; Aguilar, C.F.
Deposited on	:	2021-04-21
Resolution	:	3.50 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:

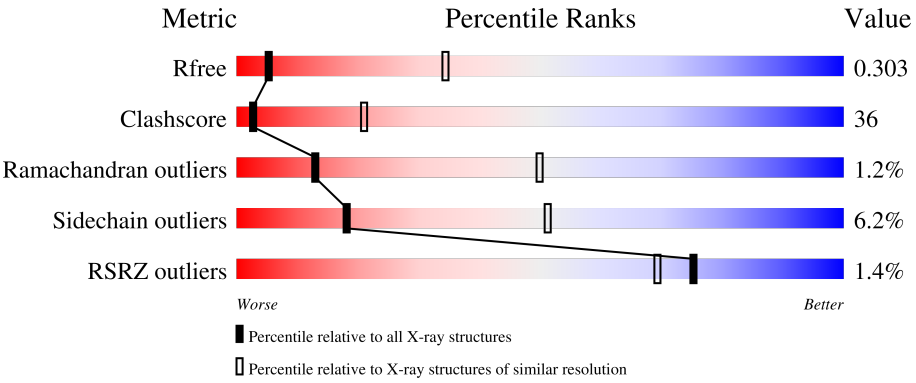
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	151	46% 50%
1	B	151	3% 46% 51%
1	C	151	5% 53% 42% 5%
1	D	151	46% 51%
1	E	151	51% 45%

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Mol	Chain	Length	Quality of chain
1	F	151	58% 38%
1	G	151	48% 49%
1	H	151	41% 55%
1	I	151	50% 47%
1	J	151	48% 50%
1	K	151	51% 43% 6%
1	L	151	50% 45% 5%
1	M	151	38% 56% 6%
1	N	151	46% 49%
1	O	151	50% 44% 6%
1	P	151	46% 50%
1	Q	151	58% 38%
1	R	151	54% 41% 5%
1	S	151	56% 42%
1	T	151	42% 56%
1	U	151	57% 41%
1	V	151	52% 45%
1	W	151	59% 36% 5%
1	X	151	46% 51%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 28296 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	B	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	C	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	D	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	E	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	F	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	G	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	H	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	I	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	J	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	K	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	L	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	M	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	N	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	O	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	P	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			

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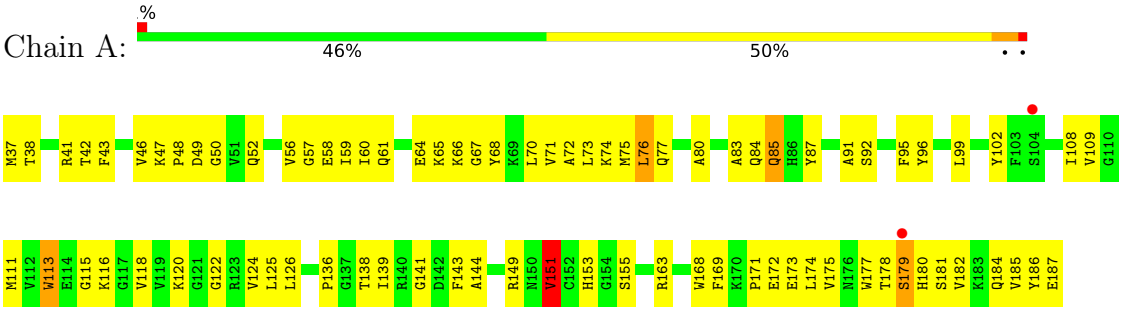
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	R	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	S	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	T	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	U	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	V	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	W	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	X	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			

3 Residue-property plots (i)

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

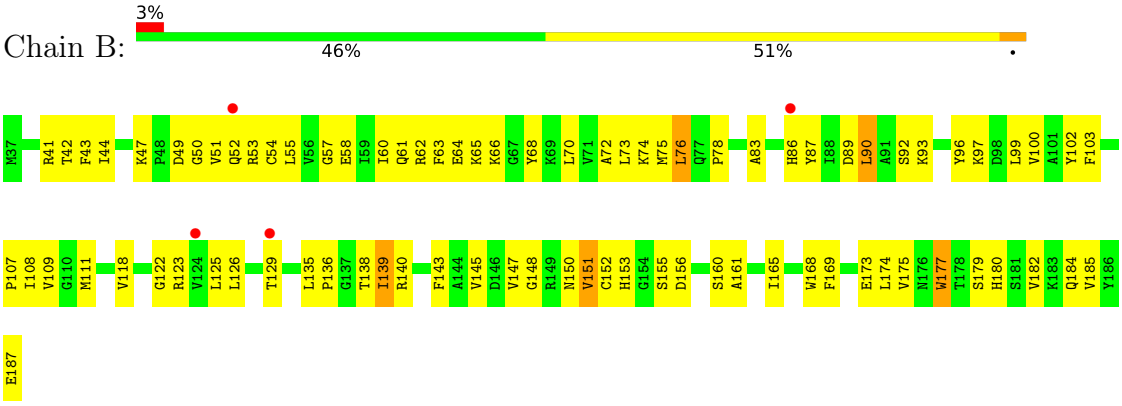
• Molecule 1: Nucleoside diphosphate kinase

Chain A:



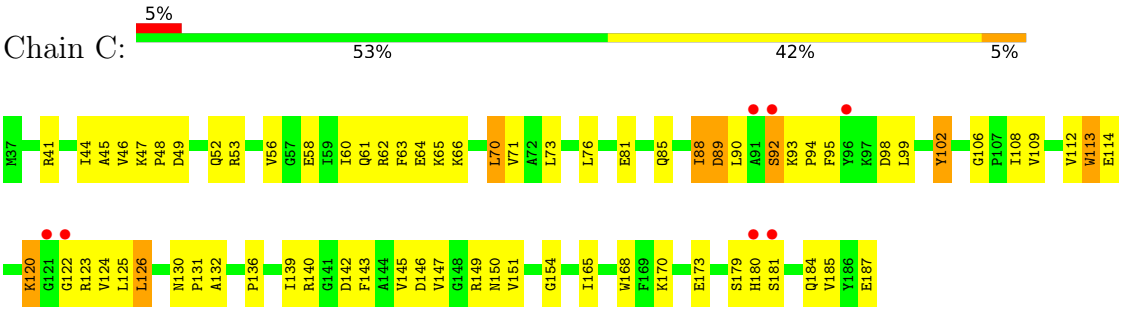
• Molecule 1: Nucleoside diphosphate kinase

Chain B:



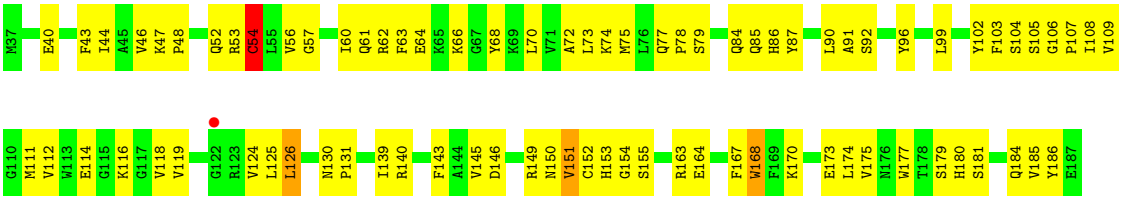
• Molecule 1: Nucleoside diphosphate kinase

Chain C:



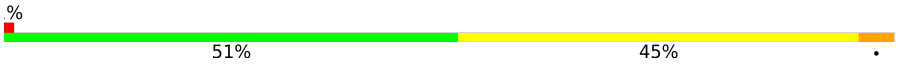
• Molecule 1: Nucleoside diphosphate kinase

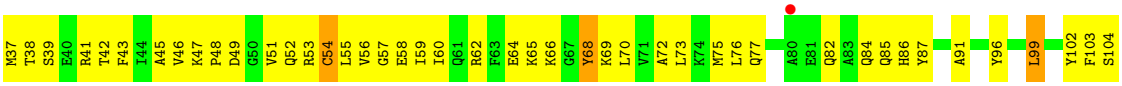
Chain D:

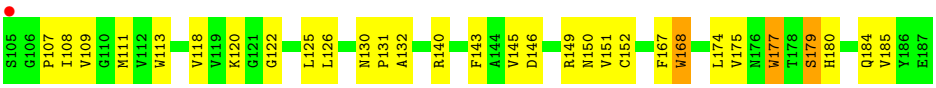


• Molecule 1: Nucleoside diphosphate kinase

Chain E:

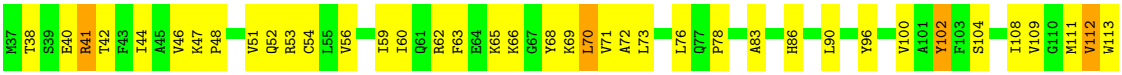


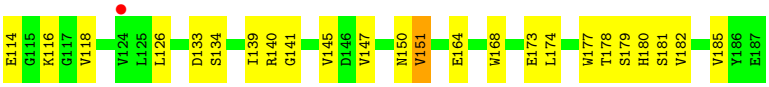




• Molecule 1: Nucleoside diphosphate kinase

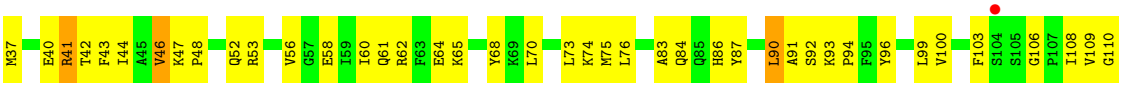
Chain F:

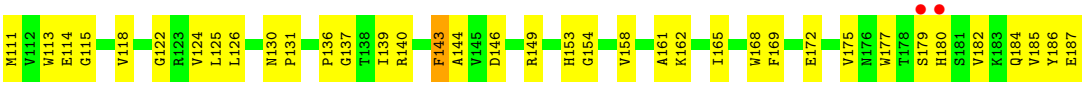




• Molecule 1: Nucleoside diphosphate kinase

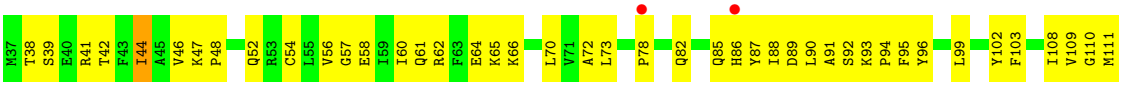
Chain G:

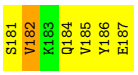




• Molecule 1: Nucleoside diphosphate kinase

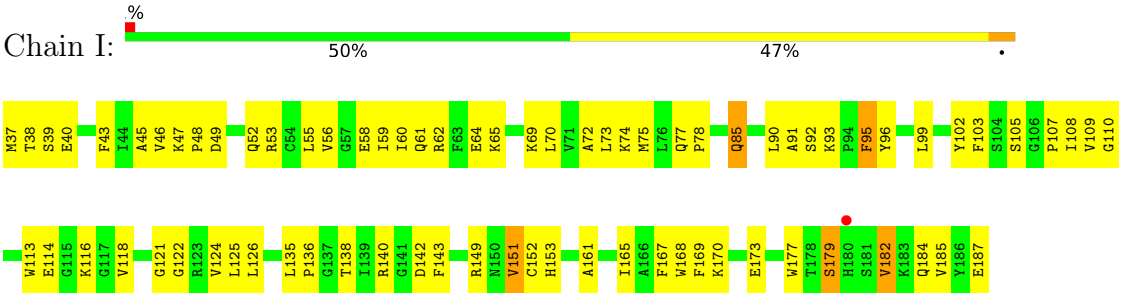
Chain H:





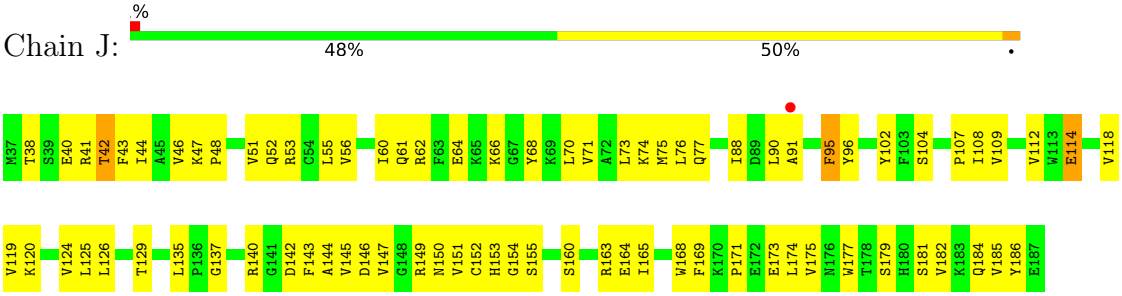
• Molecule 1: Nucleoside diphosphate kinase

Chain I:



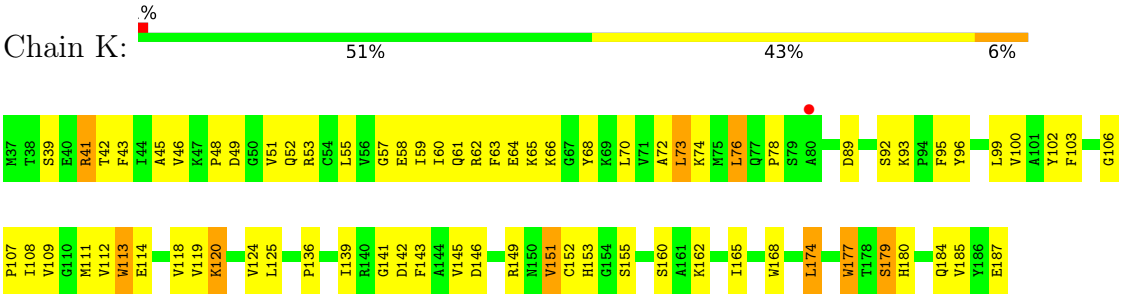
• Molecule 1: Nucleoside diphosphate kinase

Chain J:



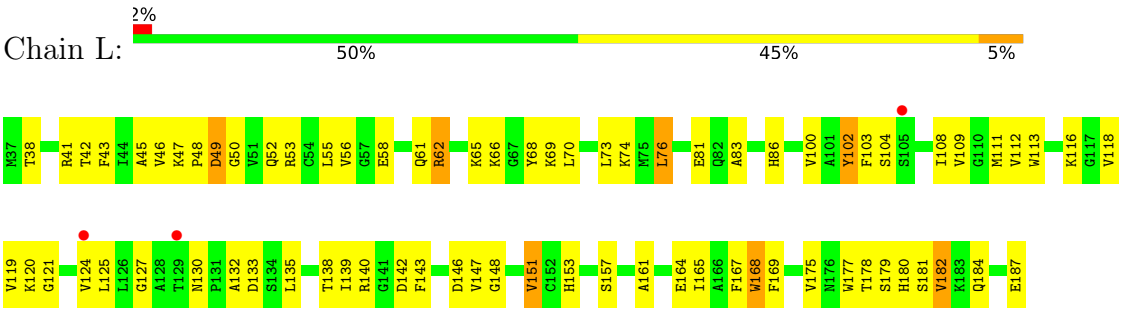
• Molecule 1: Nucleoside diphosphate kinase

Chain K:



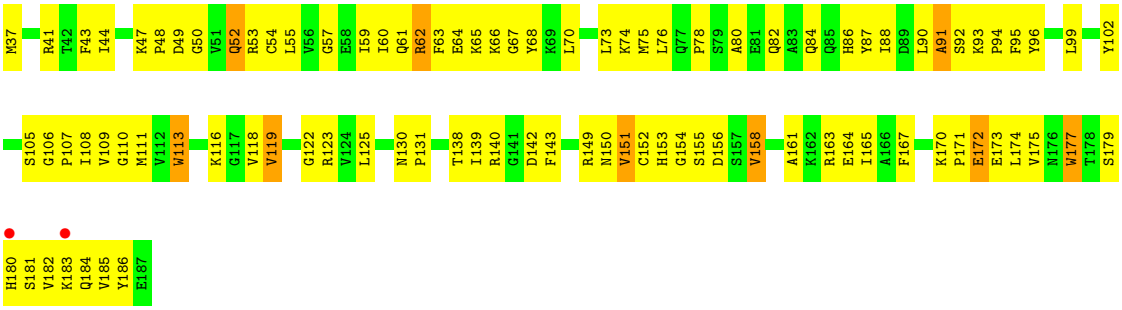
• Molecule 1: Nucleoside diphosphate kinase

Chain L:



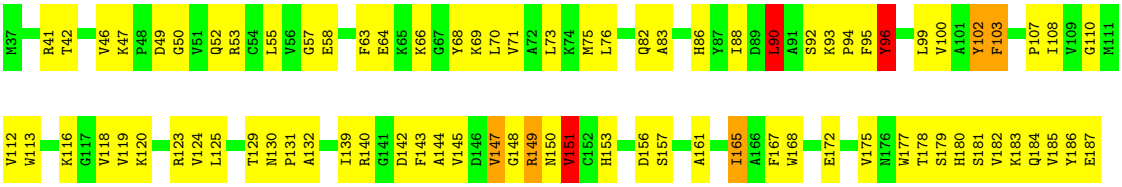
• Molecule 1: Nucleoside diphosphate kinase

Chain M:



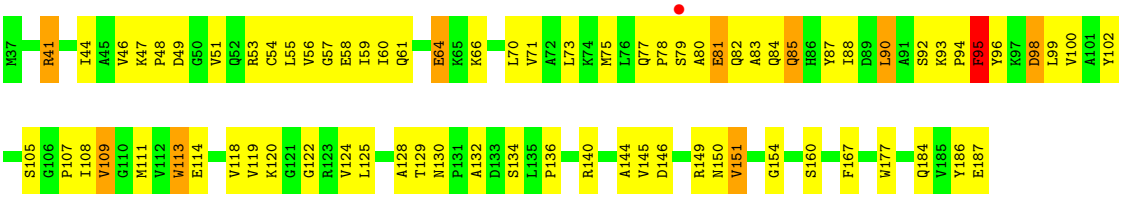
• Molecule 1: Nucleoside diphosphate kinase

Chain N:



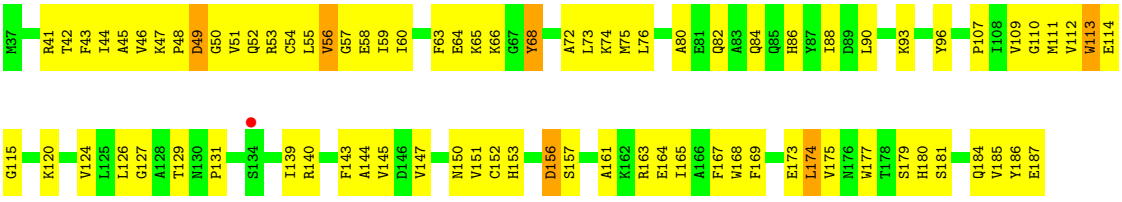
• Molecule 1: Nucleoside diphosphate kinase

Chain O:



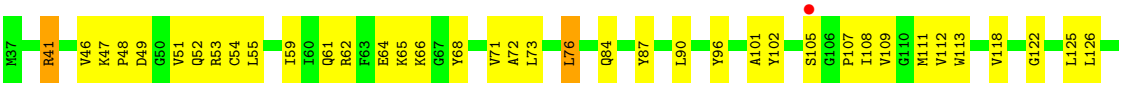
• Molecule 1: Nucleoside diphosphate kinase

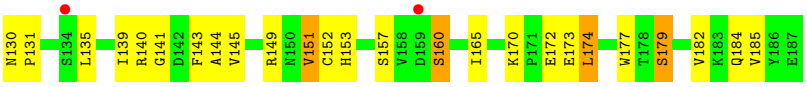
Chain P:



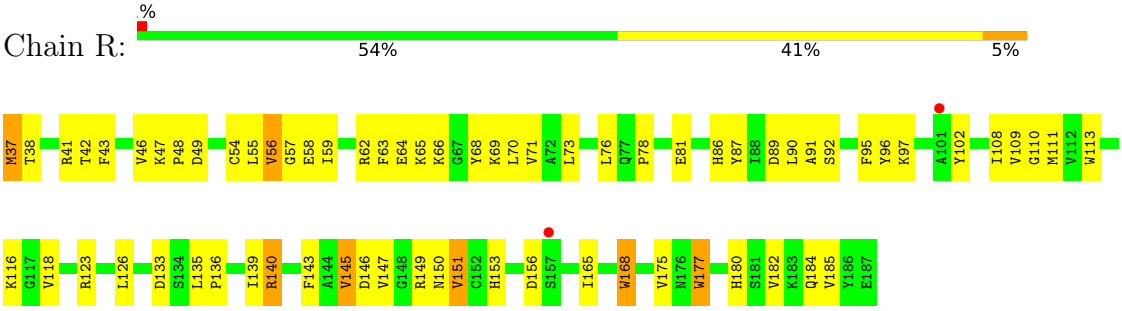
• Molecule 1: Nucleoside diphosphate kinase

Chain Q:

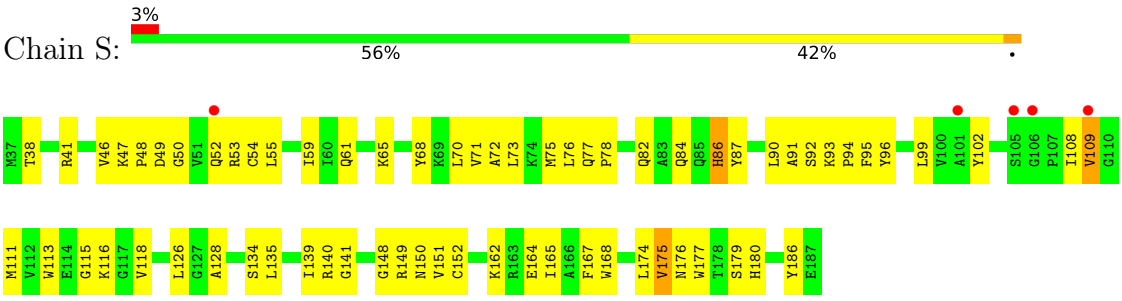




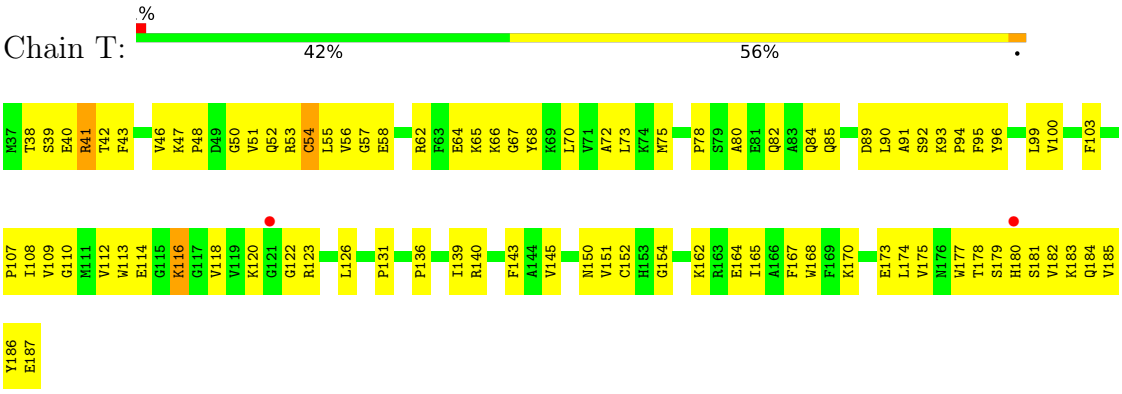
• Molecule 1: Nucleoside diphosphate kinase



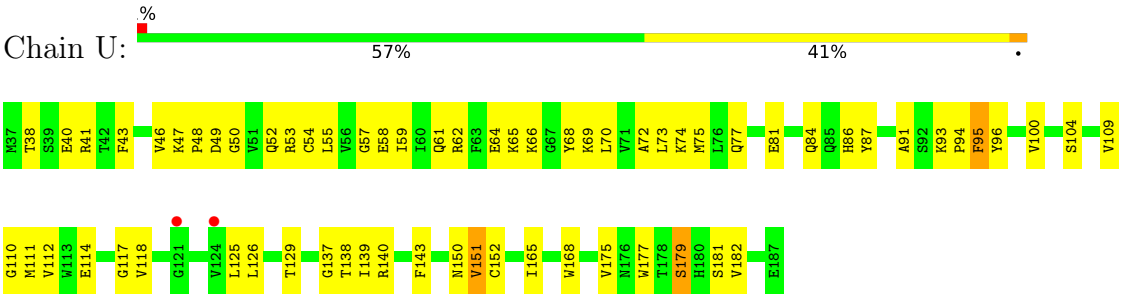
• Molecule 1: Nucleoside diphosphate kinase



• Molecule 1: Nucleoside diphosphate kinase

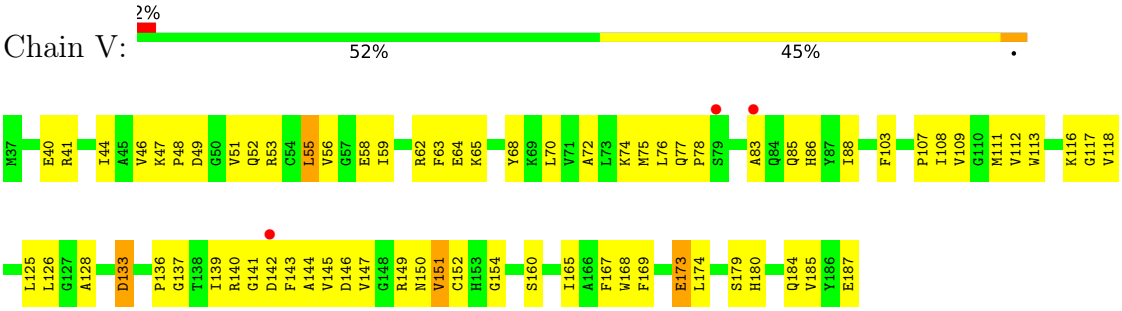


• Molecule 1: Nucleoside diphosphate kinase



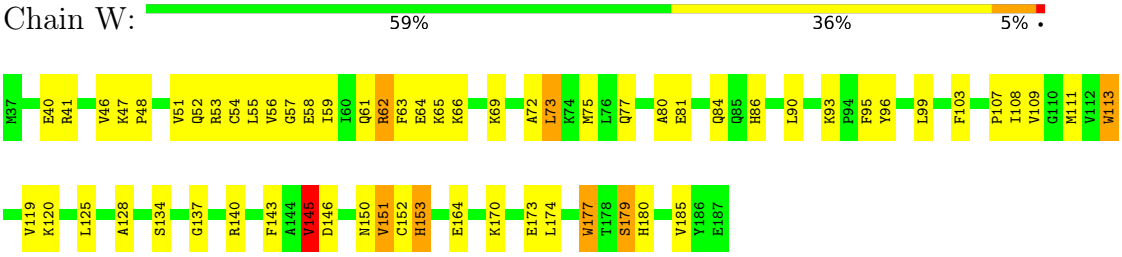
• Molecule 1: Nucleoside diphosphate kinase

Chain V:



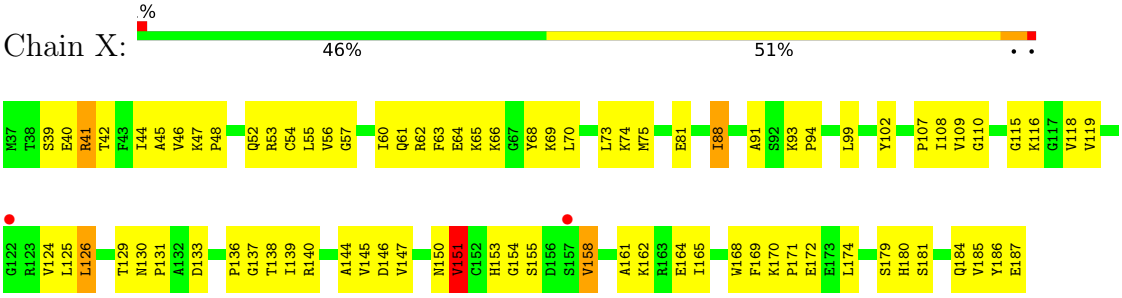
• Molecule 1: Nucleoside diphosphate kinase

Chain W:



• Molecule 1: Nucleoside diphosphate kinase

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	127.84Å 127.84Å 275.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50 86.30 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-3.50) 99.3 (86.30-3.50)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.269 , 0.278 0.280 , 0.303	Depositor DCC
R_{free} test set	3152 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.27$, $< L^2 > = 0.11$	Xtriage
Estimated twinning fraction	0.309 for -h,-k,l 0.318 for h,-h-k,-l 0.317 for -k,-h,-l	Xtriage
Reported twinning fraction	0.291 for H, K, L 0.237 for -K, -H, -L 0.240 for K, H, -L 0.232 for -h,-k,l	Depositor
Outliers	0 of 63155 reflections	Xtriage
F_o,F_c correlation	0.42	EDS
Total number of atoms	28296	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	2/1206 (0.2%)	0.67	0/1628
1	B	0.57	1/1206 (0.1%)	0.68	1/1628 (0.1%)
1	C	0.57	2/1206 (0.2%)	0.69	1/1628 (0.1%)
1	D	0.57	1/1206 (0.1%)	0.69	1/1628 (0.1%)
1	E	0.56	2/1206 (0.2%)	0.67	0/1628
1	F	0.55	1/1206 (0.1%)	0.68	0/1628
1	G	0.56	0/1206	0.67	0/1628
1	H	0.56	0/1206	0.70	0/1628
1	I	0.55	1/1206 (0.1%)	0.67	0/1628
1	J	0.57	0/1206	0.68	0/1628
1	K	0.55	2/1206 (0.2%)	0.68	0/1628
1	L	0.56	2/1206 (0.2%)	0.68	0/1628
1	M	0.58	2/1206 (0.2%)	0.67	0/1628
1	N	0.57	1/1206 (0.1%)	0.67	1/1628 (0.1%)
1	O	0.57	2/1206 (0.2%)	0.70	0/1628
1	P	0.56	1/1206 (0.1%)	0.69	0/1628
1	Q	0.57	0/1206	0.66	0/1628
1	R	0.58	2/1206 (0.2%)	0.68	0/1628
1	S	0.56	1/1206 (0.1%)	0.65	0/1628
1	T	0.55	0/1206	0.67	0/1628
1	U	0.56	1/1206 (0.1%)	0.69	0/1628
1	V	0.58	1/1206 (0.1%)	0.67	1/1628 (0.1%)
1	W	0.57	2/1206 (0.2%)	0.70	1/1628 (0.1%)
1	X	0.57	0/1206	0.70	1/1628 (0.1%)
All	All	0.57	27/28944 (0.1%)	0.68	7/39072 (0.0%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	TRP	CD2-CE2	5.50	1.48	1.41
1	C	168	TRP	CD2-CE2	5.34	1.47	1.41
1	I	113	TRP	CD2-CE2	5.31	1.47	1.41
1	A	168	TRP	CD2-CE2	5.30	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	113	TRP	CD2-CE2	5.30	1.47	1.41
1	V	113	TRP	CD2-CE2	5.28	1.47	1.41
1	K	113	TRP	CD2-CE2	5.24	1.47	1.41
1	P	113	TRP	CD2-CE2	5.23	1.47	1.41
1	R	177	TRP	CD2-CE2	5.22	1.47	1.41
1	E	177	TRP	CD2-CE2	5.18	1.47	1.41
1	L	168	TRP	CD2-CE2	5.13	1.47	1.41
1	R	168	TRP	CD2-CE2	5.13	1.47	1.41
1	M	177	TRP	CD2-CE2	5.13	1.47	1.41
1	W	177	TRP	CD2-CE2	5.13	1.47	1.41
1	L	113	TRP	CD2-CE2	5.12	1.47	1.41
1	F	113	TRP	CD2-CE2	5.11	1.47	1.41
1	S	113	TRP	CD2-CE2	5.11	1.47	1.41
1	O	177	TRP	CD2-CE2	5.09	1.47	1.41
1	C	113	TRP	CD2-CE2	5.08	1.47	1.41
1	A	113	TRP	CD2-CE2	5.07	1.47	1.41
1	N	113	TRP	CD2-CE2	5.06	1.47	1.41
1	M	113	TRP	CD2-CE2	5.04	1.47	1.41
1	B	177	TRP	CD2-CE2	5.03	1.47	1.41
1	U	168	TRP	CD2-CE2	5.02	1.47	1.41
1	W	113	TRP	CD2-CE2	5.02	1.47	1.41
1	K	177	TRP	CD2-CE2	5.02	1.47	1.41
1	E	168	TRP	CD2-CE2	5.01	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	90	LEU	CA-CB-CG	5.68	128.37	115.30
1	X	126	LEU	CA-CB-CG	5.47	127.87	115.30
1	V	174	LEU	CA-CB-CG	5.31	127.52	115.30
1	D	54	CYS	CA-CB-SG	5.27	123.48	114.00
1	N	90	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	99	LEU	CA-CB-CG	5.16	127.17	115.30
1	W	73	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1179	0	1178	206	0
1	B	1179	0	1178	125	0
1	C	1179	0	1178	149	0
1	D	1179	0	1178	151	0
1	E	1179	0	1178	111	0
1	F	1179	0	1178	61	0
1	G	1179	0	1178	125	0
1	H	1179	0	1178	135	0
1	I	1179	0	1178	93	0
1	J	1179	0	1178	118	0
1	K	1179	0	1178	91	0
1	L	1179	0	1178	94	0
1	M	1179	0	1178	158	1
1	N	1179	0	1178	105	0
1	O	1179	0	1178	105	1
1	P	1179	0	1178	126	0
1	Q	1179	0	1178	86	0
1	R	1179	0	1178	80	0
1	S	1179	0	1178	118	0
1	T	1179	0	1178	169	0
1	U	1179	0	1178	86	0
1	V	1179	0	1178	119	0
1	W	1179	0	1178	94	0
1	X	1179	0	1178	114	0
All	All	28296	0	28272	2029	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 36.

All (2029) 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:180:HIS:NE2	1:P:184:GLN:HG3	1.28	1.44
1:C:93:LYS:CA	1:M:92:SER:HB2	1.46	1.42
1:C:93:LYS:HA	1:M:92:SER:CB	1.54	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:SER:O	1:N:92:SER:HB3	1.29	1.32
1:G:184:GLN:HG3	1:L:180:HIS:CD2	1.65	1.31
1:S:52:GLN:CB	1:T:184:GLN:HG3	1.61	1.30
1:B:92:SER:HB3	1:N:92:SER:O	1.19	1.27
1:U:55:LEU:HD12	1:U:151:VAL:HG21	1.20	1.17
1:H:93:LYS:O	1:H:96:TYR:HD2	1.22	1.17
1:S:148:GLY:HA3	1:T:187:GLU:OE1	1.43	1.17
1:T:180:HIS:CE1	1:V:184:GLN:HG3	1.81	1.16
1:V:185:VAL:HG13	1:W:145:VAL:HG21	1.28	1.15
1:N:180:HIS:NE2	1:P:184:GLN:CG	2.11	1.14
1:A:175:VAL:CG1	1:D:107:PRO:HB3	1.78	1.13
1:A:180:HIS:NE2	1:D:53:ARG:HG2	1.63	1.13
1:H:180:HIS:CD2	1:K:52:GLN:HB3	1.83	1.13
1:C:90:LEU:HB3	1:C:93:LYS:HD2	1.13	1.12
1:H:180:HIS:CD2	1:J:184:GLN:HG3	1.85	1.12
1:B:61:GLN:HB2	1:E:57:GLY:HA3	1.27	1.11
1:S:52:GLN:HB2	1:T:184:GLN:HG3	1.23	1.11
1:V:55:LEU:HD13	1:V:151:VAL:HG21	1.26	1.11
1:A:184:GLN:NE2	1:C:52:GLN:HB2	1.65	1.11
1:O:105:SER:O	1:R:177:TRP:CE2	2.04	1.11
1:H:89:ASP:O	1:S:94:PRO:HG3	1.49	1.10
1:M:142:ASP:O	1:N:66:LYS:HA	1.49	1.10
1:T:180:HIS:NE2	1:V:184:GLN:HG3	1.63	1.10
1:M:53:ARG:HG3	1:N:184:GLN:CB	1.81	1.09
1:V:144:ALA:O	1:X:66:LYS:HE3	1.50	1.09
1:I:93:LYS:HD3	1:U:93:LYS:HD3	1.18	1.09
1:V:136:PRO:CG	1:X:124:VAL:O	2.01	1.09
1:A:67:GLY:HA3	1:C:53:ARG:NH2	1.65	1.08
1:A:184:GLN:CG	1:C:52:GLN:HB3	1.82	1.08
1:B:92:SER:CB	1:N:92:SER:O	2.01	1.08
1:C:94:PRO:CD	1:M:92:SER:HB3	1.84	1.08
1:G:184:GLN:HG3	1:L:180:HIS:NE2	1.69	1.08
1:M:49:ASP:HA	1:N:184:GLN:NE2	1.67	1.08
1:O:64:GLU:HB3	1:R:54:CYS:SG	1.95	1.07
1:J:52:GLN:HG3	1:L:184:GLN:NE2	1.68	1.07
1:B:52:GLN:OE1	1:E:179:SER:HA	1.52	1.07
1:G:92:SER:OG	1:T:94:PRO:HD3	1.54	1.06
1:A:184:GLN:HG3	1:C:52:GLN:HB3	1.30	1.06
1:P:181:SER:O	1:P:185:VAL:HG23	1.54	1.05
1:A:56:VAL:HB	1:D:64:GLU:OE2	1.56	1.05
1:A:187:GLU:HG3	1:C:149:ARG:CG	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:SER:HA	1:E:52:GLN:HE22	1.14	1.05
1:O:93:LYS:HG3	1:O:94:PRO:HD2	1.38	1.05
1:O:80:ALA:HB1	1:O:100:VAL:CG1	1.86	1.04
1:M:53:ARG:HG3	1:N:184:GLN:HB2	1.09	1.04
1:C:94:PRO:HD3	1:M:92:SER:HB3	1.05	1.04
1:S:52:GLN:HB3	1:T:184:GLN:HG3	1.39	1.04
1:D:60:ILE:O	1:D:64:GLU:HG3	1.55	1.04
1:V:185:VAL:HG13	1:W:145:VAL:CG2	1.87	1.04
1:G:175:VAL:HG11	1:J:107:PRO:HB3	1.35	1.03
1:S:149:ARG:CZ	1:T:187:GLU:HA	1.87	1.03
1:B:93:LYS:HE3	1:N:93:LYS:HE3	1.40	1.03
1:G:56:VAL:HB	1:J:64:GLU:OE1	1.58	1.02
1:N:180:HIS:O	1:P:180:HIS:HB2	1.58	1.02
1:B:92:SER:O	1:N:92:SER:CB	2.07	1.02
1:A:184:GLN:CD	1:C:52:GLN:CB	2.27	1.02
1:C:181:SER:O	1:C:185:VAL:HG23	1.58	1.02
1:H:52:GLN:HB3	1:K:180:HIS:HD2	1.23	1.01
1:T:90:LEU:HB3	1:T:93:LYS:HD2	1.39	1.01
1:L:47:LYS:HE3	1:L:153:HIS:HB2	1.39	1.01
1:B:107:PRO:HB3	1:E:175:VAL:HG11	1.04	1.01
1:U:55:LEU:CD1	1:U:151:VAL:HG21	1.90	1.01
1:C:180:HIS:NE2	1:E:184:GLN:HG3	1.75	1.01
1:G:94:PRO:HG3	1:T:89:ASP:O	1.60	1.01
1:H:145:VAL:HG21	1:I:185:VAL:CG1	1.90	1.00
1:O:105:SER:O	1:R:177:TRP:CZ2	2.15	0.99
1:B:107:PRO:CB	1:E:175:VAL:HG11	1.92	0.99
1:F:46:VAL:HG23	1:F:51:VAL:HG22	1.44	0.99
1:I:107:PRO:HB3	1:L:175:VAL:HG11	1.43	0.98
1:H:93:LYS:O	1:H:96:TYR:CD2	2.15	0.98
1:S:53:ARG:HD2	1:T:185:VAL:HG22	1.41	0.98
1:H:92:SER:O	1:S:92:SER:HB2	1.62	0.98
1:I:92:SER:HB2	1:U:94:PRO:HD3	1.43	0.98
1:C:94:PRO:HD3	1:M:92:SER:CB	1.94	0.98
1:V:136:PRO:HG3	1:X:124:VAL:O	1.65	0.97
1:C:180:HIS:CD2	1:E:184:GLN:HG3	1.98	0.97
1:H:90:LEU:HB3	1:H:93:LYS:HD2	1.44	0.97
1:V:140:ARG:O	1:X:66:LYS:NZ	1.97	0.97
1:A:120:LYS:O	1:A:124:VAL:HG23	1.63	0.97
1:H:58:GLU:HG2	1:H:143:PHE:HZ	1.26	0.96
1:T:177:TRP:CZ3	1:W:52:GLN:HA	1.99	0.96
1:M:65:LYS:HA	1:P:54:CYS:SG	2.04	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:PRO:CD	1:S:92:SER:OG	2.14	0.96
1:G:161:ALA:O	1:G:165:ILE:HG13	1.65	0.95
1:A:177:TRP:CD2	1:D:106:GLY:HA2	2.01	0.95
1:L:38:THR:HG22	1:L:116:LYS:HG2	1.47	0.95
1:V:136:PRO:HG2	1:X:138:THR:HG22	1.47	0.95
1:C:44:ILE:HD13	1:C:154:GLY:HA2	1.46	0.95
1:E:85:GLN:HB3	1:E:167:PHE:CE1	2.02	0.95
1:V:144:ALA:H	1:X:66:LYS:NZ	1.62	0.95
1:H:58:GLU:HG2	1:H:143:PHE:CZ	2.01	0.95
1:H:145:VAL:HG21	1:I:185:VAL:HG12	1.49	0.95
1:V:136:PRO:HG2	1:X:124:VAL:O	1.65	0.95
1:I:52:GLN:NE2	1:L:178:THR:O	1.99	0.94
1:N:183:LYS:HB3	1:P:180:HIS:CE1	2.02	0.94
1:T:52:GLN:HB3	1:W:180:HIS:HD2	1.32	0.94
1:G:92:SER:OG	1:T:94:PRO:CD	2.15	0.94
1:A:184:GLN:CD	1:C:52:GLN:HB3	1.85	0.93
1:I:92:SER:O	1:U:93:LYS:HA	1.66	0.93
1:M:61:GLN:HG3	1:P:57:GLY:HA3	1.50	0.93
1:A:179:SER:HA	1:D:52:GLN:OE1	1.68	0.93
1:V:144:ALA:O	1:X:66:LYS:CE	2.17	0.93
1:H:180:HIS:NE2	1:J:184:GLN:HG3	1.83	0.93
1:J:185:VAL:HG12	1:K:145:VAL:HG22	1.48	0.93
1:V:144:ALA:H	1:X:66:LYS:HZ2	1.15	0.93
1:J:52:GLN:HG3	1:L:184:GLN:HE21	1.33	0.93
1:U:50:GLY:CA	1:U:151:VAL:HG23	1.97	0.93
1:M:49:ASP:HA	1:N:184:GLN:HE21	1.28	0.93
1:B:90:LEU:HD22	1:B:93:LYS:HE2	1.49	0.92
1:A:177:TRP:CE3	1:D:105:SER:O	2.22	0.92
1:M:73:LEU:HD23	1:P:75:MET:HB2	1.51	0.92
1:O:73:LEU:HD11	1:O:109:VAL:HG12	1.51	0.92
1:S:52:GLN:HB2	1:T:184:GLN:CG	2.00	0.91
1:H:94:PRO:HD3	1:S:92:SER:OG	1.70	0.91
1:O:80:ALA:HB1	1:O:100:VAL:HG12	1.51	0.91
1:T:136:PRO:HG3	1:U:125:LEU:HD23	1.53	0.91
1:V:144:ALA:N	1:X:66:LYS:HZ2	1.68	0.91
1:M:88:ILE:HG22	1:M:163:ARG:NH2	1.86	0.90
1:A:60:ILE:HB	1:D:57:GLY:HA2	1.54	0.90
1:A:185:VAL:HG13	1:C:53:ARG:NH1	1.86	0.90
1:J:46:VAL:O	1:J:108:ILE:HG23	1.69	0.90
1:A:177:TRP:CG	1:D:106:GLY:HA2	2.07	0.89
1:N:90:LEU:HB3	1:N:93:LYS:HD2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:GLN:CG	1:L:180:HIS:NE2	2.35	0.89
1:J:185:VAL:HG12	1:K:145:VAL:CG2	2.02	0.89
1:B:107:PRO:HB3	1:E:175:VAL:CG1	1.99	0.89
1:M:53:ARG:CG	1:N:184:GLN:HB2	2.01	0.89
1:S:49:ASP:HA	1:T:184:GLN:HE21	1.38	0.89
1:T:179:SER:HB3	1:T:182:VAL:HG23	1.55	0.89
1:E:48:PRO:HD3	1:E:108:ILE:HD11	1.55	0.89
1:N:142:ASP:O	1:O:66:LYS:HA	1.73	0.89
1:A:187:GLU:HG2	1:C:149:ARG:CZ	2.03	0.88
1:T:99:LEU:HG	1:T:103:PHE:HE2	1.36	0.88
1:U:50:GLY:HA3	1:U:151:VAL:HG23	1.54	0.88
1:V:136:PRO:CG	1:X:138:THR:HG22	2.03	0.88
1:C:92:SER:O	1:M:92:SER:HA	1.74	0.88
1:X:56:VAL:O	1:X:60:ILE:HG13	1.74	0.88
1:S:149:ARG:NH2	1:T:187:GLU:HA	1.88	0.88
1:H:149:ARG:NE	1:I:184:GLN:OE1	2.07	0.88
1:M:52:GLN:HB2	1:N:184:GLN:NE2	1.87	0.88
1:M:73:LEU:HB3	1:P:75:MET:HB3	1.54	0.87
1:W:56:VAL:HG11	1:W:109:VAL:HG21	1.54	0.87
1:T:57:GLY:N	1:W:64:GLU:OE1	2.07	0.87
1:O:46:VAL:CG1	1:O:59:ILE:HD12	2.04	0.87
1:W:66:LYS:HE3	1:X:145:VAL:HG12	1.56	0.87
1:C:93:LYS:CB	1:M:92:SER:HB2	2.03	0.87
1:T:93:LYS:O	1:T:96:TYR:CD2	2.27	0.87
1:W:47:LYS:HE3	1:W:153:HIS:HB2	1.57	0.87
1:O:46:VAL:HG12	1:O:59:ILE:HD12	1.54	0.87
1:A:187:GLU:CG	1:C:149:ARG:CZ	2.53	0.87
1:B:49:ASP:HA	1:C:184:GLN:HE22	1.40	0.86
1:S:86:HIS:CE1	1:S:168:TRP:HE1	1.93	0.86
1:H:145:VAL:CG2	1:I:185:VAL:CG1	2.53	0.86
1:G:93:LYS:HG2	1:T:93:LYS:HG2	1.55	0.86
1:A:185:VAL:HG13	1:C:53:ARG:CZ	2.04	0.86
1:A:175:VAL:CB	1:D:107:PRO:HB3	2.05	0.86
1:I:46:VAL:HG12	1:I:152:CYS:SG	2.15	0.86
1:O:46:VAL:HG22	1:O:109:VAL:HG23	1.56	0.86
1:S:53:ARG:HD2	1:T:185:VAL:CG2	2.06	0.85
1:G:52:GLN:HB3	1:H:184:GLN:HG3	1.58	0.85
1:O:80:ALA:HB1	1:O:100:VAL:HG13	1.59	0.85
1:A:187:GLU:HG3	1:C:149:ARG:HG2	1.58	0.85
1:G:84:GLN:HA	1:G:96:TYR:OH	1.76	0.85
1:P:187:GLU:HA	1:Q:149:ARG:NH2	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:48:PRO:HD3	1:R:108:ILE:HD11	1.59	0.85
1:C:93:LYS:HG2	1:M:92:SER:CB	2.07	0.85
1:J:171:PRO:HA	1:J:174:LEU:HD23	1.59	0.85
1:B:54:CYS:SG	1:E:64:GLU:HB3	2.17	0.84
1:N:64:GLU:HB3	1:Q:54:CYS:SG	2.17	0.84
1:C:47:LYS:HB3	1:C:48:PRO:CD	2.07	0.84
1:B:179:SER:HA	1:E:52:GLN:NE2	1.93	0.84
1:P:47:LYS:HB3	1:P:48:PRO:CD	2.07	0.84
1:A:74:LYS:HA	1:D:73:LEU:HG	1.59	0.84
1:A:185:VAL:HG22	1:C:53:ARG:NE	1.93	0.84
1:B:92:SER:HB2	1:N:94:PRO:HD3	1.58	0.84
1:J:66:LYS:HA	1:K:142:ASP:O	1.78	0.84
1:A:184:GLN:HG3	1:C:52:GLN:CB	2.08	0.84
1:A:184:GLN:CD	1:C:52:GLN:HB2	1.92	0.83
1:T:93:LYS:O	1:T:96:TYR:HD2	1.58	0.83
1:A:175:VAL:HG11	1:D:107:PRO:HB3	1.59	0.83
1:M:52:GLN:HB3	1:N:184:GLN:CD	1.99	0.83
1:V:55:LEU:HD13	1:V:151:VAL:CG2	2.06	0.83
1:B:61:GLN:CB	1:E:57:GLY:HA3	2.08	0.83
1:I:56:VAL:HG21	1:L:70:LEU:HD23	1.60	0.83
1:E:85:GLN:HB3	1:E:167:PHE:HE1	1.41	0.83
1:D:145:VAL:HG13	1:F:66:LYS:O	1.79	0.83
1:S:149:ARG:NH1	1:T:187:GLU:HG2	1.94	0.83
1:N:93:LYS:O	1:N:96:TYR:CD1	2.31	0.82
1:R:47:LYS:HA	1:R:108:ILE:CD1	2.08	0.82
1:G:92:SER:O	1:T:92:SER:O	1.97	0.82
1:I:52:GLN:HB3	1:L:180:HIS:CD2	2.13	0.82
1:K:120:LYS:O	1:K:124:VAL:HG23	1.78	0.82
1:V:144:ALA:N	1:X:66:LYS:NZ	2.26	0.82
1:P:68:TYR:HE1	1:Q:145:VAL:HG12	1.44	0.82
1:M:47:LYS:HB3	1:M:48:PRO:HD2	1.62	0.82
1:G:46:VAL:HG22	1:G:109:VAL:HB	1.62	0.82
1:M:140:ARG:HD3	1:M:150:ASN:HB2	1.62	0.82
1:A:185:VAL:HA	1:C:53:ARG:HD2	1.60	0.82
1:K:187:GLU:OE2	1:L:148:GLY:HA3	1.78	0.82
1:X:62:ARG:HA	1:X:65:LYS:HE3	1.61	0.82
1:M:73:LEU:HD11	1:M:109:VAL:HG12	1.63	0.81
1:H:99:LEU:HG	1:H:103:PHE:CE2	2.16	0.81
1:T:175:VAL:HG11	1:W:107:PRO:HB3	1.61	0.81
1:H:94:PRO:N	1:S:92:SER:OG	2.14	0.81
1:M:49:ASP:O	1:M:53:ARG:HB2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ALA:HB2	1:K:174:LEU:HA	1.62	0.81
1:A:56:VAL:HB	1:D:64:GLU:CD	2.02	0.81
1:A:58:GLU:N	1:D:61:GLN:OE1	2.14	0.81
1:G:149:ARG:NH2	1:H:186:TYR:O	2.13	0.80
1:G:149:ARG:NH2	1:H:187:GLU:HA	1.96	0.80
1:N:180:HIS:CD2	1:Q:52:GLN:HB3	2.17	0.80
1:A:184:GLN:CG	1:C:52:GLN:CB	2.58	0.80
1:B:60:ILE:HD12	1:E:60:ILE:HD12	1.62	0.80
1:C:94:PRO:CD	1:M:92:SER:CB	2.53	0.80
1:M:47:LYS:HB3	1:M:48:PRO:CD	2.11	0.80
1:S:48:PRO:HD3	1:S:108:ILE:HG12	1.64	0.80
1:Q:41:ARG:HH12	1:Q:174:LEU:HD13	1.47	0.80
1:J:181:SER:OG	1:K:53:ARG:HG2	1.82	0.80
1:A:67:GLY:HA3	1:C:53:ARG:HH21	1.46	0.79
1:U:58:GLU:OE1	1:X:61:GLN:NE2	2.14	0.79
1:E:84:GLN:HA	1:E:96:TYR:OH	1.81	0.79
1:T:180:HIS:O	1:V:180:HIS:HB3	1.82	0.79
1:C:46:VAL:HG22	1:C:109:VAL:HB	1.62	0.79
1:J:55:LEU:HD13	1:J:151:VAL:HG21	1.61	0.79
1:X:140:ARG:HD3	1:X:150:ASN:HB2	1.64	0.79
1:A:37:MET:HG3	1:A:116:LYS:HG2	1.63	0.79
1:G:61:GLN:O	1:G:65:LYS:HG3	1.81	0.79
1:A:116:LYS:HB3	1:C:145:VAL:HB	1.64	0.79
1:C:93:LYS:HG2	1:M:92:SER:OG	1.82	0.79
1:J:179:SER:HB2	1:J:182:VAL:HG23	1.65	0.79
1:P:65:LYS:HD2	1:Q:143:PHE:HE1	1.48	0.79
1:I:43:PHE:CE2	1:I:45:ALA:HB2	2.18	0.79
1:S:50:GLY:HA2	1:S:55:LEU:HD12	1.65	0.79
1:M:54:CYS:SG	1:P:64:GLU:HB3	2.22	0.79
1:S:53:ARG:CD	1:T:185:VAL:HG22	2.12	0.79
1:S:93:LYS:HD3	1:S:95:PHE:CZ	2.17	0.79
1:D:44:ILE:O	1:D:111:MET:HB2	1.83	0.79
1:G:184:GLN:CG	1:L:180:HIS:CD2	2.57	0.79
1:N:139:ILE:O	1:N:143:PHE:HD2	1.65	0.79
1:M:90:LEU:C	1:M:92:SER:H	1.87	0.79
1:T:180:HIS:CE1	1:V:184:GLN:CG	2.64	0.79
1:A:67:GLY:HA3	1:C:53:ARG:HH22	1.45	0.78
1:H:93:LYS:HG2	1:S:93:LYS:HG2	1.64	0.78
1:I:93:LYS:CD	1:U:93:LYS:HD3	2.09	0.78
1:N:178:THR:O	1:Q:52:GLN:NE2	2.14	0.78
1:P:75:MET:HE2	1:P:109:VAL:HG22	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HA	1:C:142:ASP:O	1.84	0.78
1:K:59:ILE:HG23	1:K:139:ILE:HD13	1.64	0.78
1:C:93:LYS:CE	1:M:93:LYS:HG2	2.12	0.78
1:H:52:GLN:NE2	1:K:177:TRP:HE1	1.82	0.78
1:U:55:LEU:HD12	1:U:151:VAL:CG2	2.09	0.78
1:M:66:LYS:HE3	1:O:144:ALA:O	1.83	0.78
1:U:64:GLU:HB3	1:X:54:CYS:SG	2.24	0.78
1:B:52:GLN:NE2	1:E:69:LYS:HE2	1.98	0.78
1:A:175:VAL:HB	1:D:107:PRO:HB3	1.65	0.78
1:I:93:LYS:HD3	1:U:93:LYS:CD	2.09	0.78
1:J:125:LEU:HA	1:K:136:PRO:HG2	1.64	0.78
1:T:99:LEU:HG	1:T:103:PHE:CE2	2.18	0.78
1:H:48:PRO:HD3	1:H:108:ILE:HG12	1.66	0.78
1:H:145:VAL:CG2	1:I:185:VAL:HG12	2.12	0.78
1:N:58:GLU:HG2	1:N:143:PHE:CZ	2.19	0.78
1:V:85:GLN:HB2	1:V:167:PHE:CZ	2.18	0.78
1:R:86:HIS:HD2	1:R:87:TYR:CE2	2.02	0.77
1:A:177:TRP:CZ2	1:D:104:SER:O	2.37	0.77
1:B:70:LEU:HG	1:E:75:MET:HG2	1.67	0.77
1:D:167:PHE:HD2	1:D:168:TRP:CD1	2.02	0.77
1:H:148:GLY:HA3	1:I:187:GLU:HG3	1.65	0.77
1:C:90:LEU:HB3	1:C:93:LYS:CD	2.07	0.77
1:M:44:ILE:O	1:M:111:MET:HB2	1.85	0.77
1:R:47:LYS:HA	1:R:108:ILE:HD13	1.66	0.77
1:M:184:GLN:O	1:O:49:ASP:HB3	1.85	0.77
1:F:86:HIS:CE1	1:F:168:TRP:HE1	2.02	0.77
1:S:52:GLN:CB	1:T:184:GLN:CG	2.54	0.77
1:B:57:GLY:CA	1:E:60:ILE:HB	2.15	0.77
1:G:185:VAL:HG22	1:I:53:ARG:HD2	1.64	0.76
1:L:179:SER:HB2	1:L:182:VAL:HG23	1.67	0.76
1:W:47:LYS:HE3	1:W:153:HIS:CB	2.15	0.76
1:A:64:GLU:O	1:D:54:CYS:SG	2.43	0.76
1:L:62:ARG:HA	1:L:65:LYS:HE3	1.67	0.76
1:G:126:LEU:HD11	1:G:154:GLY:HA3	1.67	0.76
1:S:148:GLY:CA	1:T:187:GLU:OE1	2.31	0.76
1:H:92:SER:C	1:S:92:SER:O	2.24	0.76
1:Q:55:LEU:HD11	1:Q:143:PHE:HB3	1.67	0.76
1:T:175:VAL:CG1	1:W:107:PRO:HB3	2.16	0.76
1:I:52:GLN:HB3	1:L:180:HIS:HD2	1.50	0.76
1:A:58:GLU:O	1:A:61:GLN:HG2	1.86	0.75
1:K:187:GLU:OE2	1:L:148:GLY:CA	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:46:VAL:O	1:V:108:ILE:HG23	1.85	0.75
1:V:136:PRO:HB2	1:X:138:THR:HG22	1.67	0.75
1:F:46:VAL:CG2	1:F:51:VAL:HG22	2.17	0.75
1:M:149:ARG:NH1	1:N:187:GLU:HG2	2.01	0.75
1:M:66:LYS:NZ	1:O:144:ALA:O	2.19	0.75
1:E:66:LYS:NZ	1:F:141:GLY:O	2.19	0.75
1:F:46:VAL:HG23	1:F:51:VAL:CG2	2.17	0.75
1:O:81:GLU:HA	1:O:81:GLU:OE2	1.87	0.75
1:A:144:ALA:O	1:B:66:LYS:NZ	2.17	0.75
1:A:177:TRP:CD1	1:D:107:PRO:CD	2.70	0.74
1:M:73:LEU:HD11	1:M:109:VAL:CG1	2.17	0.74
1:U:47:LYS:HB3	1:U:48:PRO:CD	2.17	0.74
1:N:180:HIS:HD2	1:Q:52:GLN:HB3	1.50	0.74
1:B:129:THR:O	1:B:147:VAL:HG23	1.86	0.74
1:S:91:ALA:HA	1:S:96:TYR:CE1	2.22	0.74
1:M:67:GLY:HA2	1:O:53:ARG:HH22	1.52	0.74
1:P:66:LYS:NZ	1:Q:144:ALA:H	1.86	0.74
1:U:68:TYR:CE2	1:U:118:VAL:HG23	2.23	0.74
1:A:77:GLN:CD	1:D:177:TRP:HZ2	1.91	0.74
1:A:177:TRP:CZ3	1:D:105:SER:O	2.41	0.74
1:H:99:LEU:HG	1:H:103:PHE:HE2	1.51	0.74
1:H:145:VAL:CG2	1:I:185:VAL:HG13	2.17	0.74
1:M:66:LYS:CE	1:O:144:ALA:O	2.36	0.74
1:O:75:MET:HB3	1:R:73:LEU:HB3	1.70	0.74
1:C:85:GLN:HE22	1:C:88:ILE:HD12	1.53	0.73
1:N:183:LYS:HB3	1:P:180:HIS:NE2	2.03	0.73
1:A:175:VAL:CG1	1:D:107:PRO:CB	2.64	0.73
1:B:51:VAL:HG11	1:B:107:PRO:HG2	1.70	0.73
1:V:136:PRO:CB	1:X:138:THR:HG22	2.16	0.73
1:X:162:LYS:HA	1:X:165:ILE:HD12	1.70	0.73
1:E:58:GLU:O	1:E:62:ARG:HG3	1.89	0.73
1:M:73:LEU:HD12	1:M:110:GLY:O	1.89	0.73
1:D:46:VAL:HG12	1:D:152:CYS:SG	2.28	0.73
1:T:122:GLY:O	1:T:126:LEU:HG	1.88	0.73
1:A:48:PRO:HD3	1:A:108:ILE:HD11	1.71	0.73
1:B:175:VAL:HG12	1:B:177:TRP:HD1	1.52	0.73
1:S:49:ASP:HA	1:T:184:GLN:HB3	1.71	0.73
1:C:131:PRO:HG2	1:C:146:ASP:O	1.89	0.73
1:J:66:LYS:HG3	1:J:68:TYR:CE1	2.23	0.73
1:S:135:LEU:O	1:S:141:GLY:HA3	1.89	0.73
1:D:53:ARG:NH2	1:D:143:PHE:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:PRO:HG3	1:H:108:ILE:HD12	1.70	0.73
1:M:52:GLN:CB	1:N:184:GLN:NE2	2.51	0.73
1:N:93:LYS:O	1:N:96:TYR:HD1	1.72	0.72
1:O:96:TYR:O	1:O:100:VAL:HG23	1.89	0.72
1:T:52:GLN:HB3	1:W:180:HIS:CD2	2.20	0.72
1:K:41:ARG:HH12	1:K:174:LEU:HD13	1.53	0.72
1:U:40:GLU:OE2	1:U:117:GLY:HA2	1.90	0.72
1:I:48:PRO:HD3	1:I:108:ILE:HD11	1.72	0.72
1:M:125:LEU:HA	1:O:136:PRO:HG3	1.70	0.72
1:X:40:GLU:OE2	1:X:119:VAL:HG23	1.89	0.72
1:A:187:GLU:HG3	1:C:149:ARG:CZ	2.18	0.72
1:M:75:MET:HB3	1:P:73:LEU:O	1.89	0.72
1:B:75:MET:SD	1:B:107:PRO:HB2	2.29	0.72
1:T:136:PRO:CG	1:U:125:LEU:HD23	2.19	0.72
1:T:177:TRP:HZ3	1:W:52:GLN:HA	1.53	0.72
1:D:116:LYS:HG2	1:D:186:TYR:HE1	1.53	0.72
1:K:46:VAL:HG22	1:K:109:VAL:HB	1.71	0.72
1:E:42:THR:HB	1:E:118:VAL:HG13	1.72	0.72
1:A:180:HIS:O	1:F:180:HIS:HB3	1.88	0.72
1:H:180:HIS:NE2	1:K:52:GLN:HB3	2.04	0.72
1:U:112:VAL:HG22	1:U:165:ILE:HG12	1.72	0.72
1:O:122:GLY:HA2	1:O:125:LEU:HD12	1.70	0.71
1:A:187:GLU:HG3	1:C:149:ARG:NE	2.05	0.71
1:G:92:SER:OG	1:T:94:PRO:CG	2.38	0.71
1:G:180:HIS:CG	1:L:181:SER:HA	2.24	0.71
1:V:185:VAL:CG1	1:W:145:VAL:HG21	2.12	0.71
1:B:61:GLN:HB2	1:E:57:GLY:CA	2.13	0.71
1:A:46:VAL:HG22	1:A:109:VAL:HB	1.71	0.71
1:B:57:GLY:HA3	1:E:60:ILE:HB	1.71	0.71
1:I:72:ALA:HB2	1:I:173:GLU:O	1.89	0.71
1:V:53:ARG:HD2	1:X:185:VAL:HG22	1.72	0.71
1:M:73:LEU:CB	1:P:75:MET:HB3	2.20	0.71
1:A:177:TRP:CE2	1:D:106:GLY:HA2	2.25	0.71
1:C:93:LYS:HA	1:M:92:SER:HB2	0.73	0.71
1:I:58:GLU:O	1:I:61:GLN:HG2	1.89	0.71
1:S:46:VAL:O	1:S:108:ILE:HG23	1.90	0.71
1:A:177:TRP:CH2	1:D:104:SER:O	2.44	0.71
1:Q:185:VAL:HG13	1:R:145:VAL:HG21	1.72	0.71
1:S:53:ARG:HG2	1:T:181:SER:HB2	1.71	0.71
1:A:72:ALA:HB2	1:A:174:LEU:HD23	1.72	0.71
1:O:130:ASN:HD21	1:O:132:ALA:HB3	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD13	1:B:111:MET:HG2	1.70	0.71
1:G:90:LEU:HB3	1:G:93:LYS:HD2	1.71	0.71
1:P:181:SER:O	1:P:185:VAL:CG2	2.37	0.71
1:T:116:LYS:HB2	1:T:186:TYR:HE1	1.55	0.70
1:M:70:LEU:CD2	1:P:75:MET:HE3	2.20	0.70
1:X:68:TYR:CD2	1:X:118:VAL:HG23	2.26	0.70
1:A:52:GLN:HE22	1:D:179:SER:HA	1.55	0.70
1:K:48:PRO:HB3	1:K:106:GLY:HA3	1.74	0.70
1:O:80:ALA:CB	1:O:100:VAL:HG12	2.20	0.70
1:X:129:THR:HA	1:X:140:ARG:NH1	2.05	0.70
1:C:47:LYS:HB3	1:C:48:PRO:HD3	1.73	0.70
1:G:61:GLN:NE2	1:J:61:GLN:OE1	2.22	0.70
1:I:122:GLY:HA2	1:I:125:LEU:HD12	1.72	0.70
1:N:148:GLY:HA3	1:O:187:GLU:CD	2.12	0.70
1:U:70:LEU:HD23	1:X:75:MET:CE	2.20	0.70
1:G:180:HIS:CD2	1:J:52:GLN:HB3	2.27	0.70
1:J:91:ALA:HA	1:J:96:TYR:CE1	2.27	0.70
1:S:72:ALA:CB	1:S:174:LEU:HD23	2.21	0.70
1:A:92:SER:HB2	1:O:92:SER:O	1.92	0.70
1:P:46:VAL:HG12	1:P:152:CYS:SG	2.32	0.70
1:W:66:LYS:O	1:X:145:VAL:HG13	1.92	0.70
1:M:181:SER:O	1:M:185:VAL:HG23	1.92	0.69
1:P:56:VAL:O	1:P:60:ILE:HG13	1.92	0.69
1:X:68:TYR:CE2	1:X:118:VAL:HG23	2.27	0.69
1:L:50:GLY:HA2	1:L:151:VAL:HG23	1.73	0.69
1:C:52:GLN:NE2	1:F:177:TRP:HE1	1.90	0.69
1:T:64:GLU:OE2	1:W:56:VAL:N	2.25	0.69
1:V:65:LYS:HB2	1:W:143:PHE:CD1	2.27	0.69
1:X:164:GLU:O	1:X:168:TRP:HB2	1.92	0.69
1:A:175:VAL:HG11	1:D:107:PRO:CB	2.22	0.69
1:G:75:MET:HB3	1:J:73:LEU:HB3	1.74	0.69
1:V:49:ASP:HB3	1:X:184:GLN:O	1.91	0.69
1:X:48:PRO:HD3	1:X:108:ILE:HD11	1.74	0.69
1:A:187:GLU:HG3	1:C:149:ARG:HG3	1.71	0.69
1:S:49:ASP:CA	1:T:184:GLN:HE21	2.06	0.69
1:S:75:MET:HE3	1:V:70:LEU:HD23	1.73	0.69
1:K:99:LEU:O	1:K:103:PHE:HD2	1.75	0.69
1:A:77:GLN:CD	1:D:177:TRP:CZ2	2.66	0.69
1:E:58:GLU:HG2	1:E:143:PHE:CZ	2.28	0.69
1:Q:66:LYS:HG3	1:R:145:VAL:HG13	1.75	0.69
1:B:93:LYS:O	1:B:96:TYR:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:TYR:O	1:K:100:VAL:HG23	1.93	0.68
1:N:55:LEU:HD12	1:N:151:VAL:HG21	1.75	0.68
1:H:93:LYS:HE3	1:S:93:LYS:HG2	1.74	0.68
1:H:99:LEU:CG	1:H:103:PHE:HE2	2.06	0.68
1:J:62:ARG:NH1	1:J:137:GLY:O	2.26	0.68
1:S:71:VAL:HG12	1:S:174:LEU:HB3	1.75	0.68
1:W:80:ALA:O	1:W:84:GLN:N	2.25	0.68
1:G:146:ASP:HB2	1:H:116:LYS:NZ	2.09	0.68
1:H:56:VAL:HG12	1:H:60:ILE:HD11	1.76	0.68
1:G:162:LYS:HA	1:G:165:ILE:HD12	1.74	0.68
1:V:143:PHE:HA	1:X:66:LYS:HA	1.74	0.68
1:X:181:SER:O	1:X:185:VAL:HG23	1.93	0.68
1:N:93:LYS:HD3	1:N:95:PHE:CZ	2.28	0.68
1:H:93:LYS:NZ	1:S:94:PRO:HD2	2.08	0.68
1:U:62:ARG:NH1	1:U:137:GLY:O	2.26	0.68
1:A:143:PHE:O	1:B:66:LYS:O	2.11	0.68
1:H:93:LYS:CG	1:S:93:LYS:HA	2.24	0.68
1:P:50:GLY:HA2	1:P:55:LEU:HD12	1.76	0.68
1:H:52:GLN:HB3	1:K:180:HIS:CD2	2.16	0.68
1:A:187:GLU:CG	1:C:149:ARG:HG2	2.24	0.68
1:H:175:VAL:HG11	1:K:107:PRO:HB3	1.76	0.68
1:H:180:HIS:NE2	1:J:184:GLN:CG	2.56	0.68
1:M:73:LEU:HB3	1:P:75:MET:CB	2.24	0.68
1:S:93:LYS:HD3	1:S:95:PHE:HZ	1.58	0.68
1:T:145:VAL:HG12	1:U:66:LYS:HE3	1.73	0.68
1:U:50:GLY:HA3	1:U:151:VAL:CG2	2.24	0.68
1:X:131:PRO:HB2	1:X:145:VAL:O	1.94	0.68
1:A:56:VAL:CB	1:D:64:GLU:OE2	2.37	0.67
1:M:52:GLN:CB	1:N:184:GLN:CD	2.62	0.67
1:M:57:GLY:HA3	1:P:60:ILE:HB	1.76	0.67
1:U:58:GLU:O	1:U:61:GLN:HG2	1.94	0.67
1:N:147:VAL:O	1:N:150:ASN:ND2	2.27	0.67
1:A:180:HIS:CD2	1:D:53:ARG:HG2	2.29	0.67
1:D:73:LEU:HD11	1:D:109:VAL:CG1	2.24	0.67
1:C:64:GLU:HB3	1:F:54:CYS:SG	2.34	0.67
1:E:48:PRO:HD3	1:E:108:ILE:CD1	2.25	0.67
1:I:126:LEU:HD13	1:I:140:ARG:NH2	2.09	0.67
1:B:175:VAL:CG1	1:E:77:GLN:HB2	2.25	0.67
1:H:180:HIS:HD2	1:K:52:GLN:HB3	1.49	0.67
1:T:58:GLU:N	1:W:61:GLN:OE1	2.27	0.67
1:O:58:GLU:O	1:O:61:GLN:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLN:NE2	1:E:177:TRP:CD1	2.62	0.67
1:D:140:ARG:HE	1:D:150:ASN:HD22	1.43	0.67
1:K:58:GLU:HG2	1:K:143:PHE:CZ	2.29	0.67
1:J:169:PHE:HD1	1:J:173:GLU:OE1	1.78	0.67
1:M:73:LEU:CD1	1:M:109:VAL:HG12	2.25	0.67
1:P:43:PHE:CD2	1:P:164:GLU:HB3	2.30	0.67
1:R:37:MET:N	1:R:116:LYS:HZ3	1.91	0.67
1:X:42:THR:HB	1:X:119:VAL:HG22	1.77	0.67
1:A:179:SER:CA	1:D:52:GLN:OE1	2.42	0.67
1:D:140:ARG:HD3	1:D:150:ASN:HB2	1.76	0.67
1:P:73:LEU:HD13	1:P:111:MET:HG2	1.77	0.66
1:A:177:TRP:CD1	1:D:106:GLY:HA2	2.30	0.66
1:B:179:SER:CA	1:E:52:GLN:HE22	1.99	0.66
1:G:73:LEU:H	1:J:75:MET:HB3	1.59	0.66
1:J:91:ALA:HA	1:J:96:TYR:CD1	2.30	0.66
1:T:68:TYR:CE2	1:T:118:VAL:HG23	2.30	0.66
1:B:60:ILE:CD1	1:E:60:ILE:HD12	2.25	0.66
1:M:65:LYS:CA	1:P:54:CYS:SG	2.81	0.66
1:F:47:LYS:O	1:F:51:VAL:HG23	1.94	0.66
1:O:48:PRO:HG2	1:O:102:TYR:O	1.94	0.66
1:C:180:HIS:CD2	1:F:52:GLN:HB3	2.30	0.66
1:H:57:GLY:N	1:K:64:GLU:OE1	2.19	0.66
1:I:161:ALA:O	1:I:165:ILE:HG13	1.96	0.66
1:V:85:GLN:NE2	1:V:88:ILE:HD12	2.11	0.66
1:I:73:LEU:O	1:L:74:LYS:HA	1.95	0.66
1:J:95:PHE:HD1	1:J:95:PHE:C	1.98	0.66
1:R:48:PRO:HD3	1:R:108:ILE:CD1	2.25	0.66
1:R:140:ARG:HD3	1:R:150:ASN:HB2	1.78	0.66
1:G:149:ARG:NH1	1:H:187:GLU:HG2	2.11	0.66
1:H:89:ASP:O	1:S:94:PRO:CG	2.37	0.66
1:H:93:LYS:HG3	1:S:93:LYS:HA	1.78	0.66
1:I:43:PHE:HE2	1:I:45:ALA:HB2	1.58	0.66
1:I:48:PRO:HD3	1:I:108:ILE:CD1	2.25	0.66
1:K:74:LYS:HE2	1:K:76:LEU:HD22	1.75	0.66
1:O:93:LYS:HG3	1:O:94:PRO:CD	2.21	0.66
1:D:116:LYS:HG2	1:D:186:TYR:CE1	2.30	0.66
1:O:47:LYS:HB3	1:O:48:PRO:CD	2.26	0.66
1:O:93:LYS:CG	1:O:94:PRO:HD2	2.22	0.66
1:P:88:ILE:HG22	1:P:163:ARG:NH2	2.11	0.66
1:T:56:VAL:HB	1:W:64:GLU:CD	2.16	0.66
1:A:177:TRP:HD1	1:D:107:PRO:HG3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LYS:HA	1:C:108:ILE:HD12	1.79	0.65
1:A:178:THR:O	1:D:52:GLN:OE1	2.14	0.65
1:E:46:VAL:HG21	1:E:56:VAL:HG22	1.79	0.65
1:A:64:GLU:OE2	1:D:56:VAL:N	2.27	0.65
1:J:88:ILE:HG22	1:J:163:ARG:HH22	1.62	0.65
1:N:175:VAL:HG21	1:Q:76:LEU:HA	1.78	0.65
1:S:49:ASP:HA	1:T:184:GLN:NE2	2.08	0.65
1:A:185:VAL:CA	1:C:53:ARG:HD2	2.26	0.65
1:X:53:ARG:O	1:X:55:LEU:HG	1.96	0.65
1:B:52:GLN:NE2	1:E:177:TRP:HD1	1.95	0.65
1:C:90:LEU:HD22	1:C:93:LYS:NZ	2.11	0.65
1:R:38:THR:H	1:R:116:LYS:HD3	1.61	0.65
1:A:66:LYS:HD2	1:C:142:ASP:O	1.97	0.65
1:A:177:TRP:CD1	1:D:107:PRO:HD3	2.32	0.65
1:I:107:PRO:HB3	1:L:175:VAL:CG1	2.24	0.65
1:K:46:VAL:CG2	1:K:109:VAL:HB	2.26	0.65
1:M:183:LYS:O	1:O:149:ARG:NE	2.26	0.65
1:S:49:ASP:HB2	1:T:184:GLN:O	1.97	0.65
1:A:177:TRP:CD1	1:D:107:PRO:N	2.65	0.65
1:B:49:ASP:HA	1:C:184:GLN:NE2	2.11	0.65
1:M:57:GLY:CA	1:P:60:ILE:HB	2.27	0.65
1:M:87:TYR:CD1	1:M:99:LEU:HD21	2.32	0.65
1:J:143:PHE:CE1	1:L:65:LYS:HD2	2.31	0.65
1:T:180:HIS:NE2	1:V:184:GLN:CG	2.53	0.65
1:H:93:LYS:HD3	1:H:95:PHE:CZ	2.32	0.64
1:H:130:ASN:ND2	1:H:132:ALA:HB3	2.12	0.64
1:B:145:VAL:HG21	1:C:185:VAL:HG12	1.78	0.64
1:P:144:ALA:O	1:R:66:LYS:NZ	2.29	0.64
1:A:187:GLU:CG	1:C:149:ARG:NH1	2.59	0.64
1:K:89:ASP:O	1:R:92:SER:HB2	1.97	0.64
1:L:52:GLN:OE1	1:L:52:GLN:HA	1.98	0.64
1:M:82:GLN:HA	1:M:167:PHE:HZ	1.61	0.64
1:T:75:MET:N	1:W:73:LEU:HB3	2.13	0.64
1:A:175:VAL:HG11	1:D:107:PRO:HA	1.80	0.64
1:K:184:GLN:HG3	1:L:52:GLN:HB3	1.80	0.64
1:N:52:GLN:HB2	1:O:184:GLN:HE21	1.61	0.64
1:N:180:HIS:O	1:P:180:HIS:CB	2.42	0.64
1:M:90:LEU:O	1:M:92:SER:N	2.30	0.64
1:U:54:CYS:SG	1:X:64:GLU:HB3	2.38	0.64
1:V:145:VAL:HG12	1:X:68:TYR:HE1	1.62	0.64
1:B:90:LEU:HB3	1:B:93:LYS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:VAL:HG22	1:I:185:VAL:HG13	1.79	0.64
1:G:73:LEU:O	1:J:75:MET:N	2.31	0.64
1:V:145:VAL:HG12	1:X:68:TYR:CE1	2.31	0.64
1:W:47:LYS:HA	1:W:108:ILE:HD12	1.78	0.64
1:X:47:LYS:HA	1:X:108:ILE:CD1	2.28	0.64
1:C:181:SER:OG	1:C:184:GLN:HB2	1.98	0.64
1:M:60:ILE:O	1:M:64:GLU:HG3	1.98	0.64
1:T:178:THR:O	1:W:52:GLN:OE1	2.16	0.64
1:J:44:ILE:HD13	1:J:154:GLY:HA2	1.79	0.63
1:W:46:VAL:HG22	1:W:109:VAL:HB	1.81	0.63
1:A:52:GLN:CD	1:D:180:HIS:HD2	2.01	0.63
1:B:65:LYS:HA	1:E:54:CYS:SG	2.38	0.63
1:C:48:PRO:HD2	1:C:102:TYR:CE1	2.32	0.63
1:A:60:ILE:HB	1:D:57:GLY:CA	2.27	0.63
1:B:52:GLN:HE22	1:E:69:LYS:HE2	1.62	0.63
1:S:78:PRO:HG3	1:S:108:ILE:HD12	1.79	0.63
1:C:58:GLU:O	1:C:61:GLN:HG2	1.98	0.63
1:G:92:SER:O	1:T:92:SER:C	2.36	0.63
1:J:40:GLU:OE2	1:J:119:VAL:HG23	1.99	0.63
1:J:95:PHE:C	1:J:95:PHE:CD1	2.71	0.63
1:V:78:PRO:HG3	1:V:108:ILE:HG13	1.80	0.63
1:G:177:TRP:NE1	1:J:77:GLN:OE1	2.31	0.63
1:C:180:HIS:NE2	1:E:184:GLN:CG	2.58	0.63
1:D:90:LEU:O	1:D:92:SER:N	2.31	0.63
1:G:122:GLY:O	1:G:125:LEU:HB3	1.98	0.63
1:B:57:GLY:O	1:E:57:GLY:HA2	1.99	0.63
1:M:73:LEU:HD13	1:M:111:MET:HG3	1.80	0.63
1:S:53:ARG:HG3	1:T:184:GLN:HB2	1.81	0.63
1:G:184:GLN:CG	1:L:180:HIS:CE1	2.82	0.63
1:L:58:GLU:O	1:L:61:GLN:HB3	1.98	0.63
1:M:75:MET:SD	1:M:107:PRO:HB2	2.39	0.63
1:T:50:GLY:HA2	1:T:55:LEU:HD12	1.79	0.63
1:G:73:LEU:N	1:J:75:MET:HB3	2.14	0.63
1:A:65:LYS:O	1:C:143:PHE:CE1	2.52	0.62
1:J:181:SER:O	1:J:185:VAL:HG23	1.99	0.62
1:S:84:GLN:HG2	1:S:96:TYR:OH	1.99	0.62
1:V:144:ALA:O	1:X:66:LYS:NZ	2.32	0.62
1:B:52:GLN:HE21	1:E:177:TRP:HD1	1.47	0.62
1:J:160:SER:HB3	1:J:164:GLU:OE2	1.99	0.62
1:R:58:GLU:O	1:R:62:ARG:HG3	1.99	0.62
1:T:126:LEU:HA	1:T:139:ILE:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:129:THR:HA	1:U:140:ARG:NH1	2.15	0.62
1:C:93:LYS:HE2	1:M:93:LYS:HG2	1.80	0.62
1:D:143:PHE:O	1:F:65:LYS:O	2.16	0.62
1:M:175:VAL:HG12	1:M:177:TRP:HD1	1.64	0.62
1:N:70:LEU:HD11	1:N:73:LEU:HB2	1.82	0.62
1:N:148:GLY:HA3	1:O:187:GLU:OE2	1.99	0.62
1:P:59:ILE:HG12	1:P:139:ILE:HG21	1.80	0.62
1:V:46:VAL:HG11	1:V:59:ILE:HD13	1.81	0.62
1:E:73:LEU:HD13	1:E:111:MET:HG2	1.82	0.62
1:Q:47:LYS:HB3	1:Q:48:PRO:CD	2.30	0.62
1:V:65:LYS:HB2	1:W:143:PHE:HD1	1.64	0.62
1:A:184:GLN:HG3	1:C:52:GLN:C	2.19	0.62
1:B:93:LYS:O	1:B:96:TYR:CD2	2.52	0.62
1:L:120:LYS:O	1:L:124:VAL:HG23	1.99	0.62
1:S:72:ALA:HB2	1:S:174:LEU:HD23	1.82	0.62
1:A:64:GLU:OE1	1:D:57:GLY:N	2.32	0.62
1:C:44:ILE:HD13	1:C:154:GLY:CA	2.27	0.62
1:E:47:LYS:HB3	1:E:49:ASP:OD1	2.00	0.62
1:G:52:GLN:CB	1:H:184:GLN:HG3	2.27	0.62
1:H:52:GLN:OE1	1:K:179:SER:HA	1.99	0.62
1:P:43:PHE:HD2	1:P:164:GLU:HB3	1.63	0.62
1:V:44:ILE:HD13	1:V:154:GLY:HA2	1.81	0.62
1:A:77:GLN:OE1	1:D:177:TRP:NE1	2.32	0.62
1:A:187:GLU:HG3	1:C:149:ARG:CD	2.29	0.62
1:O:78:PRO:HG3	1:O:108:ILE:HG13	1.82	0.62
1:W:47:LYS:CE	1:W:153:HIS:HB2	2.28	0.62
1:N:180:HIS:N	1:Q:52:GLN:OE1	2.32	0.62
1:V:149:ARG:NH2	1:X:187:GLU:HB3	2.14	0.62
1:D:175:VAL:HG12	1:D:177:TRP:HD1	1.64	0.62
1:T:73:LEU:HG	1:W:73:LEU:HD21	1.82	0.62
1:A:186:TYR:CE1	1:C:145:VAL:HG21	2.34	0.61
1:C:93:LYS:CG	1:M:92:SER:HB2	2.30	0.61
1:M:47:LYS:HA	1:M:108:ILE:HG12	1.81	0.61
1:M:185:VAL:O	1:O:149:ARG:HB2	1.99	0.61
1:N:139:ILE:O	1:N:143:PHE:CD2	2.52	0.61
1:P:127:GLY:O	1:P:140:ARG:NH1	2.33	0.61
1:V:143:PHE:N	1:X:66:LYS:HZ2	1.97	0.61
1:X:88:ILE:O	1:X:91:ALA:HB2	1.99	0.61
1:A:57:GLY:HA3	1:D:61:GLN:HB2	1.80	0.61
1:A:73:LEU:O	1:D:74:LYS:HA	2.00	0.61
1:E:56:VAL:HA	1:E:59:ILE:HD12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:ARG:HD3	1:H:150:ASN:HB2	1.82	0.61
1:M:67:GLY:HA3	1:O:53:ARG:HH12	1.64	0.61
1:T:107:PRO:HD3	1:W:177:TRP:CD1	2.36	0.61
1:A:175:VAL:HG12	1:D:107:PRO:HB3	1.75	0.61
1:E:96:TYR:O	1:E:99:LEU:HB3	2.01	0.61
1:J:51:VAL:HG21	1:J:107:PRO:O	2.00	0.61
1:T:75:MET:H	1:W:73:LEU:HB3	1.65	0.61
1:A:57:GLY:HA3	1:D:61:GLN:CB	2.31	0.61
1:O:46:VAL:HG11	1:O:59:ILE:HD12	1.82	0.61
1:N:180:HIS:HD2	1:Q:52:GLN:CB	2.13	0.61
1:P:75:MET:CE	1:P:109:VAL:HG22	2.30	0.61
1:T:42:THR:CG2	1:T:118:VAL:HG22	2.30	0.61
1:A:71:VAL:O	1:D:75:MET:HG2	2.00	0.61
1:A:116:LYS:CB	1:C:145:VAL:HB	2.30	0.61
1:A:116:LYS:HB2	1:C:145:VAL:HG21	1.81	0.61
1:M:68:TYR:CE2	1:M:118:VAL:HG23	2.36	0.61
1:P:47:LYS:HB3	1:P:48:PRO:HD3	1.80	0.61
1:T:143:PHE:HA	1:U:65:LYS:O	2.00	0.61
1:A:74:LYS:HA	1:D:73:LEU:CG	2.30	0.61
1:A:177:TRP:HD1	1:D:107:PRO:CG	2.14	0.61
1:B:75:MET:CE	1:E:70:LEU:HD23	2.31	0.61
1:U:61:GLN:HB2	1:U:65:LYS:NZ	2.15	0.61
1:M:88:ILE:HG22	1:M:163:ARG:HH22	1.64	0.61
1:Q:170:LYS:HB2	1:Q:173:GLU:HG3	1.83	0.61
1:T:70:LEU:HD21	1:T:73:LEU:HD22	1.83	0.61
1:T:93:LYS:HD3	1:T:95:PHE:CZ	2.36	0.61
1:V:55:LEU:HD21	1:V:143:PHE:CG	2.36	0.61
1:J:186:TYR:C	1:K:149:ARG:HG3	2.21	0.61
1:O:102:TYR:CE1	1:O:149:ARG:HD3	2.35	0.60
1:P:68:TYR:HE1	1:Q:145:VAL:CG1	2.14	0.60
1:X:145:VAL:HG23	1:X:146:ASP:N	2.16	0.60
1:A:83:ALA:O	1:A:87:TYR:HD2	1.85	0.60
1:C:93:LYS:HE3	1:M:93:LYS:HA	1.82	0.60
1:P:90:LEU:O	1:P:96:TYR:CD1	2.54	0.60
1:U:70:LEU:HD23	1:X:75:MET:HE1	1.82	0.60
1:B:73:LEU:HD11	1:B:109:VAL:CG1	2.31	0.60
1:E:60:ILE:HG23	1:E:113:TRP:HZ2	1.65	0.60
1:L:86:HIS:HD1	1:L:168:TRP:HE1	1.48	0.60
1:N:130:ASN:ND2	1:N:132:ALA:HB3	2.16	0.60
1:R:38:THR:HG22	1:R:116:LYS:HG2	1.83	0.60
1:U:93:LYS:HG2	1:U:95:PHE:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LYS:HG2	1:M:92:SER:C	2.21	0.60
1:F:112:VAL:HG21	1:F:174:LEU:HD22	1.83	0.60
1:H:72:ALA:HB3	1:H:174:LEU:HD22	1.84	0.60
1:O:77:GLN:HB2	1:R:175:VAL:HG13	1.83	0.60
1:E:75:MET:SD	1:E:109:VAL:HG22	2.42	0.60
1:I:52:GLN:NE2	1:L:177:TRP:CD1	2.70	0.60
1:S:87:TYR:HD1	1:S:90:LEU:HD12	1.65	0.60
1:G:180:HIS:O	1:L:180:HIS:O	2.19	0.60
1:L:38:THR:HG22	1:L:116:LYS:CG	2.26	0.60
1:H:47:LYS:HE2	1:H:103:PHE:CE1	2.37	0.60
1:J:185:VAL:CG1	1:K:145:VAL:HG22	2.26	0.60
1:V:85:GLN:HE22	1:V:88:ILE:HD12	1.66	0.60
1:G:175:VAL:HG12	1:G:177:TRP:CD1	2.36	0.60
1:N:161:ALA:O	1:N:165:ILE:HB	2.02	0.60
1:C:93:LYS:HG2	1:M:92:SER:HB2	1.84	0.60
1:D:73:LEU:HD13	1:D:111:MET:HG2	1.83	0.60
1:G:48:PRO:HD3	1:G:108:ILE:HD11	1.84	0.60
1:G:53:ARG:NH2	1:H:66:LYS:O	2.35	0.60
1:G:175:VAL:HG12	1:G:177:TRP:HD1	1.65	0.60
1:J:71:VAL:HB	1:J:112:VAL:HG12	1.84	0.60
1:P:86:HIS:CE1	1:P:164:GLU:HG2	2.37	0.60
1:V:187:GLU:HG2	1:W:146:ASP:OD2	2.01	0.60
1:A:175:VAL:HG11	1:D:107:PRO:CA	2.31	0.60
1:B:140:ARG:HD3	1:B:150:ASN:HB2	1.84	0.60
1:H:112:VAL:HG13	1:H:165:ILE:HD11	1.84	0.60
1:U:75:MET:HE1	1:U:109:VAL:HG22	1.82	0.60
1:F:51:VAL:HG13	1:F:56:VAL:CG2	2.32	0.59
1:V:141:GLY:C	1:X:66:LYS:HZ3	2.04	0.59
1:N:184:GLN:HG2	1:P:180:HIS:CD2	2.37	0.59
1:U:75:MET:CE	1:U:109:VAL:HG22	2.31	0.59
1:A:80:ALA:O	1:A:84:GLN:HG3	2.01	0.59
1:G:70:LEU:HD23	1:J:75:MET:CE	2.31	0.59
1:L:46:VAL:HG22	1:L:109:VAL:HB	1.83	0.59
1:N:180:HIS:CD2	1:Q:52:GLN:CB	2.85	0.59
1:F:86:HIS:CE1	1:F:164:GLU:HG2	2.38	0.59
1:I:47:LYS:HE3	1:I:153:HIS:HB2	1.84	0.59
1:O:64:GLU:OE2	1:R:54:CYS:HA	2.02	0.59
1:F:42:THR:HB	1:F:118:VAL:HG13	1.83	0.59
1:J:169:PHE:CD1	1:J:173:GLU:OE1	2.55	0.59
1:P:65:LYS:HD2	1:Q:143:PHE:CE1	2.34	0.59
1:B:47:LYS:HE3	1:B:153:HIS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:TRP:CE2	1:E:107:PRO:HG3	2.37	0.59
1:M:93:LYS:HD3	1:M:95:PHE:CZ	2.37	0.59
1:T:72:ALA:HB2	1:T:174:LEU:CD2	2.32	0.59
1:T:72:ALA:HB2	1:T:174:LEU:HD22	1.85	0.59
1:G:70:LEU:HD21	1:G:73:LEU:HB2	1.84	0.59
1:G:146:ASP:HB2	1:H:116:LYS:HZ2	1.66	0.59
1:H:70:LEU:HD11	1:H:73:LEU:HD13	1.84	0.59
1:R:140:ARG:HE	1:R:150:ASN:ND2	2.01	0.59
1:A:50:GLY:HA2	1:A:151:VAL:HG22	1.85	0.59
1:H:62:ARG:HA	1:H:65:LYS:HE3	1.85	0.59
1:P:88:ILE:HG22	1:P:163:ARG:HH22	1.68	0.59
1:S:82:GLN:HA	1:S:167:PHE:HZ	1.67	0.59
1:V:78:PRO:HG2	1:V:103:PHE:O	2.02	0.59
1:O:80:ALA:O	1:O:84:GLN:N	2.35	0.58
1:P:185:VAL:C	1:Q:149:ARG:HG3	2.23	0.58
1:V:53:ARG:CD	1:X:185:VAL:HG22	2.33	0.58
1:A:184:GLN:HG3	1:C:52:GLN:O	2.03	0.58
1:A:184:GLN:HB2	1:C:53:ARG:HG3	1.83	0.58
1:H:93:LYS:HZ1	1:S:94:PRO:HD2	1.65	0.58
1:M:67:GLY:CA	1:O:53:ARG:HH22	2.16	0.58
1:N:183:LYS:CB	1:P:180:HIS:CE1	2.83	0.58
1:T:62:ARG:HA	1:T:65:LYS:HE3	1.85	0.58
1:A:75:MET:N	1:D:73:LEU:HB3	2.18	0.58
1:C:122:GLY:O	1:C:126:LEU:HG	2.02	0.58
1:M:48:PRO:HD3	1:M:108:ILE:HD11	1.84	0.58
1:P:66:LYS:HZ1	1:Q:144:ALA:H	1.49	0.58
1:J:47:LYS:NZ	1:J:150:ASN:OD1	2.24	0.58
1:A:187:GLU:HG2	1:C:149:ARG:NH1	2.18	0.58
1:B:73:LEU:HD11	1:B:109:VAL:HG12	1.85	0.58
1:M:170:LYS:O	1:M:173:GLU:HB2	2.04	0.58
1:S:75:MET:CE	1:V:70:LEU:HD23	2.32	0.58
1:A:64:GLU:HB3	1:D:54:CYS:SG	2.44	0.58
1:A:67:GLY:CA	1:C:53:ARG:HH21	2.17	0.58
1:B:90:LEU:HD22	1:B:93:LYS:CE	2.30	0.58
1:G:91:ALA:HA	1:G:96:TYR:CD1	2.39	0.58
1:L:50:GLY:CA	1:L:151:VAL:HG23	2.33	0.58
1:M:62:ARG:HD2	1:M:139:ILE:HG12	1.85	0.58
1:N:58:GLU:HG2	1:N:143:PHE:HZ	1.68	0.58
1:N:131:PRO:HG3	1:N:140:ARG:HB3	1.85	0.58
1:O:80:ALA:HA	1:O:83:ALA:HB3	1.86	0.58
1:W:81:GLU:HA	1:W:84:GLN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:ALA:HB2	1:F:173:GLU:O	2.03	0.58
1:M:138:THR:HG22	1:O:136:PRO:HG2	1.86	0.58
1:V:185:VAL:HG13	1:W:145:VAL:HG23	1.83	0.58
1:G:53:ARG:HD2	1:H:185:VAL:HG22	1.86	0.58
1:M:53:ARG:HD2	1:N:185:VAL:HG22	1.86	0.58
1:N:52:GLN:NE2	1:Q:177:TRP:HE1	2.02	0.58
1:T:175:VAL:HG11	1:W:107:PRO:CB	2.32	0.58
1:H:73:LEU:HD12	1:H:110:GLY:O	2.03	0.58
1:L:48:PRO:HD2	1:L:102:TYR:CE1	2.39	0.58
1:P:68:TYR:CE1	1:Q:145:VAL:HG12	2.32	0.58
1:P:184:GLN:O	1:Q:49:ASP:HB3	2.04	0.58
1:S:72:ALA:HB3	1:S:174:LEU:HD23	1.85	0.58
1:S:86:HIS:CE1	1:S:168:TRP:NE1	2.70	0.58
1:U:70:LEU:HD23	1:X:75:MET:HE2	1.85	0.58
1:W:137:GLY:O	1:X:136:PRO:HB2	2.03	0.58
1:C:131:PRO:HG2	1:C:146:ASP:C	2.25	0.57
1:G:68:TYR:CE2	1:G:118:VAL:HG23	2.38	0.57
1:G:180:HIS:HD2	1:J:52:GLN:HB3	1.66	0.57
1:I:52:GLN:HG3	1:L:177:TRP:HE1	1.68	0.57
1:P:65:LYS:CD	1:Q:143:PHE:HE1	2.17	0.57
1:S:180:HIS:CE1	1:X:181:SER:HB2	2.39	0.57
1:A:184:GLN:CB	1:C:53:ARG:HG3	2.33	0.57
1:H:93:LYS:HA	1:S:92:SER:O	2.04	0.57
1:L:86:HIS:CE1	1:L:164:GLU:HG2	2.39	0.57
1:M:90:LEU:C	1:M:92:SER:N	2.56	0.57
1:P:51:VAL:HG11	1:P:107:PRO:HG2	1.86	0.57
1:A:43:PHE:CD1	1:A:111:MET:O	2.56	0.57
1:B:58:GLU:O	1:B:62:ARG:HG3	2.04	0.57
1:B:75:MET:HE2	1:E:70:LEU:HD23	1.86	0.57
1:C:56:VAL:O	1:C:60:ILE:HG13	2.04	0.57
1:K:48:PRO:HD3	1:K:108:ILE:HD11	1.86	0.57
1:B:42:THR:OG1	1:B:155:SER:HB2	2.04	0.57
1:C:93:LYS:CG	1:M:92:SER:CB	2.82	0.57
1:P:68:TYR:CE1	1:Q:145:VAL:CG1	2.87	0.57
1:A:60:ILE:HD13	1:D:60:ILE:HD12	1.86	0.57
1:F:147:VAL:O	1:F:150:ASN:ND2	2.37	0.57
1:O:145:VAL:HG23	1:O:146:ASP:N	2.19	0.57
1:P:129:THR:O	1:P:131:PRO:HD3	2.04	0.57
1:Q:71:VAL:HG12	1:Q:174:LEU:HB3	1.86	0.57
1:T:46:VAL:HG22	1:T:109:VAL:HB	1.86	0.57
1:A:77:GLN:CB	1:D:177:TRP:HE1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:GLU:OE2	1:D:119:VAL:HB	2.05	0.57
1:G:46:VAL:O	1:G:108:ILE:HG23	2.04	0.57
1:K:55:LEU:HD12	1:K:151:VAL:CG2	2.35	0.57
1:K:66:LYS:HD3	1:K:125:LEU:HD21	1.85	0.57
1:N:180:HIS:NE2	1:P:184:GLN:CB	2.67	0.57
1:U:55:LEU:HD21	1:U:143:PHE:CG	2.40	0.57
1:X:150:ASN:O	1:X:151:VAL:HG12	2.04	0.57
1:G:75:MET:CB	1:J:73:LEU:HB3	2.35	0.57
1:J:126:LEU:HD11	1:J:154:GLY:HA3	1.87	0.57
1:K:62:ARG:HG2	1:K:65:LYS:HE3	1.85	0.57
1:P:47:LYS:HB3	1:P:48:PRO:HD2	1.86	0.57
1:Q:152:CYS:SG	1:Q:153:HIS:N	2.78	0.57
1:T:41:ARG:HG3	1:T:114:GLU:HB2	1.87	0.57
1:W:66:LYS:HG2	1:W:125:LEU:HD11	1.85	0.57
1:A:177:TRP:CE2	1:D:106:GLY:CA	2.87	0.57
1:J:120:LYS:O	1:J:124:VAL:HG23	2.05	0.57
1:P:86:HIS:HE1	1:P:164:GLU:HG2	1.69	0.57
1:U:93:LYS:HG2	1:U:95:PHE:CD1	2.39	0.57
1:D:66:LYS:HD3	1:D:125:LEU:HD21	1.87	0.56
1:C:52:GLN:NE2	1:F:180:HIS:CD2	2.73	0.56
1:G:177:TRP:CD1	1:J:107:PRO:HD3	2.40	0.56
1:I:62:ARG:NH1	1:I:142:ASP:OD2	2.39	0.56
1:M:119:VAL:O	1:M:123:ARG:HB2	2.05	0.56
1:D:87:TYR:CD1	1:D:99:LEU:HD21	2.40	0.56
1:F:38:THR:H	1:F:116:LYS:HD3	1.71	0.56
1:K:73:LEU:HD13	1:K:111:MET:CG	2.35	0.56
1:L:47:LYS:CE	1:L:153:HIS:HB2	2.26	0.56
1:M:63:PHE:O	1:M:66:LYS:HB3	2.05	0.56
1:R:55:LEU:O	1:R:57:GLY:N	2.39	0.56
1:S:68:TYR:CE2	1:S:118:VAL:HG23	2.40	0.56
1:V:62:ARG:HA	1:V:65:LYS:HE3	1.87	0.56
1:V:144:ALA:H	1:X:66:LYS:HZ1	1.51	0.56
1:V:169:PHE:HD1	1:V:173:GLU:HB3	1.70	0.56
1:O:75:MET:CB	1:R:73:LEU:HB3	2.34	0.56
1:V:147:VAL:O	1:V:150:ASN:ND2	2.38	0.56
1:W:66:LYS:NZ	1:X:144:ALA:O	2.22	0.56
1:A:116:LYS:HE2	1:C:146:ASP:HB2	1.88	0.56
1:B:63:PHE:HD2	1:B:68:TYR:HD2	1.52	0.56
1:H:47:LYS:CD	1:H:103:PHE:HE1	2.17	0.56
1:B:135:LEU:HB3	1:B:136:PRO:CD	2.36	0.56
1:E:60:ILE:HG23	1:E:113:TRP:CZ2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:VAL:HG22	1:F:53:ARG:NH1	2.21	0.56
1:I:74:LYS:HG2	1:I:169:PHE:HE1	1.71	0.56
1:J:124:VAL:HG12	1:K:136:PRO:CD	2.35	0.56
1:S:91:ALA:HA	1:S:96:TYR:CD1	2.40	0.56
1:U:52:GLN:OE1	1:X:180:HIS:HD2	1.89	0.56
1:B:54:CYS:SG	1:E:64:GLU:C	2.84	0.56
1:F:179:SER:HB2	1:F:182:VAL:HG23	1.86	0.56
1:S:149:ARG:HG2	1:T:187:GLU:CG	2.36	0.56
1:T:85:GLN:HB2	1:T:167:PHE:CZ	2.41	0.56
1:E:72:ALA:HB2	1:E:174:LEU:HD23	1.88	0.56
1:I:73:LEU:HD11	1:I:109:VAL:HG12	1.86	0.56
1:M:74:LYS:HA	1:P:74:LYS:HA	1.87	0.56
1:M:88:ILE:CG2	1:M:163:ARG:NH2	2.64	0.56
1:M:171:PRO:HA	1:M:174:LEU:HG	1.87	0.56
1:N:129:THR:HA	1:N:140:ARG:NH1	2.21	0.56
1:Q:46:VAL:HG22	1:Q:109:VAL:HB	1.87	0.56
1:T:178:THR:O	1:W:52:GLN:CD	2.44	0.56
1:H:138:THR:O	1:H:142:ASP:HB2	2.05	0.56
1:I:37:MET:HB2	1:I:116:LYS:HG3	1.87	0.56
1:M:175:VAL:HG12	1:M:177:TRP:CD1	2.40	0.56
1:A:52:GLN:NE2	1:D:180:HIS:CD2	2.74	0.56
1:I:52:GLN:NE2	1:L:177:TRP:NE1	2.53	0.56
1:J:55:LEU:HD11	1:J:143:PHE:HB3	1.88	0.56
1:L:73:LEU:HD13	1:L:111:MET:HG3	1.88	0.56
1:P:80:ALA:O	1:P:84:GLN:HG3	2.06	0.56
1:S:128:ALA:N	1:S:134:SER:OG	2.39	0.56
1:S:180:HIS:HB2	1:X:180:HIS:O	2.06	0.56
1:V:149:ARG:HG3	1:X:185:VAL:O	2.06	0.56
1:B:109:VAL:HG11	1:E:73:LEU:HD23	1.88	0.55
1:F:126:LEU:HA	1:F:139:ILE:HD12	1.87	0.55
1:G:92:SER:OG	1:T:94:PRO:HG3	2.06	0.55
1:F:40:GLU:HB3	1:F:118:VAL:HG12	1.87	0.55
1:G:84:GLN:CA	1:G:96:TYR:OH	2.53	0.55
1:J:52:GLN:CG	1:L:184:GLN:HE21	2.13	0.55
1:Q:87:TYR:O	1:Q:90:LEU:N	2.35	0.55
1:B:73:LEU:HB3	1:E:75:MET:CB	2.37	0.55
1:T:120:LYS:HG2	1:T:123:ARG:HH21	1.70	0.55
1:D:167:PHE:CD2	1:D:168:TRP:CD1	2.92	0.55
1:D:175:VAL:HG12	1:D:177:TRP:CD1	2.40	0.55
1:F:42:THR:HG23	1:F:44:ILE:HD11	1.86	0.55
1:G:60:ILE:O	1:G:64:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:56:VAL:H	1:R:64:GLU:CD	2.09	0.55
1:D:72:ALA:HB2	1:D:174:LEU:HD13	1.89	0.55
1:M:52:GLN:HB3	1:N:184:GLN:CG	2.36	0.55
1:T:180:HIS:O	1:V:180:HIS:CB	2.55	0.55
1:G:172:GLU:N	1:G:172:GLU:OE1	2.40	0.55
1:L:43:PHE:HD2	1:L:164:GLU:OE1	1.89	0.55
1:O:80:ALA:CB	1:O:100:VAL:CG1	2.75	0.55
1:P:181:SER:OG	1:Q:53:ARG:HG2	2.06	0.55
1:T:72:ALA:CB	1:T:174:LEU:HD22	2.37	0.55
1:X:47:LYS:HA	1:X:108:ILE:HD13	1.87	0.55
1:A:178:THR:C	1:D:52:GLN:OE1	2.45	0.55
1:B:53:ARG:O	1:B:55:LEU:HG	2.07	0.55
1:G:87:TYR:CD1	1:G:99:LEU:HD21	2.42	0.55
1:J:66:LYS:NZ	1:K:141:GLY:O	2.37	0.55
1:M:61:GLN:O	1:M:65:LYS:HG3	2.06	0.55
1:O:107:PRO:HG3	1:R:69:LYS:NZ	2.22	0.55
1:V:136:PRO:HG2	1:X:138:THR:CG2	2.30	0.55
1:A:70:LEU:HD13	1:A:113:TRP:CE2	2.42	0.55
1:A:180:HIS:NE2	1:D:53:ARG:CG	2.55	0.55
1:B:122:GLY:HA2	1:B:125:LEU:HD12	1.89	0.55
1:H:88:ILE:HG22	1:H:163:ARG:HH21	1.72	0.55
1:I:53:ARG:NH1	1:I:143:PHE:O	2.39	0.55
1:J:42:THR:OG1	1:J:155:SER:HB2	2.07	0.55
1:J:47:LYS:HB3	1:J:48:PRO:CD	2.36	0.55
1:M:119:VAL:HG12	1:M:155:SER:O	2.07	0.55
1:R:78:PRO:HB3	1:R:168:TRP:CH2	2.42	0.55
1:V:125:LEU:O	1:V:139:ILE:HD12	2.07	0.55
1:A:171:PRO:C	1:A:173:GLU:H	2.09	0.55
1:C:49:ASP:O	1:C:53:ARG:HB2	2.07	0.55
1:K:187:GLU:CD	1:L:148:GLY:HA3	2.27	0.55
1:M:82:GLN:HA	1:M:167:PHE:CZ	2.40	0.55
1:O:46:VAL:HG12	1:O:59:ILE:CD1	2.32	0.55
1:P:66:LYS:NZ	1:Q:140:ARG:O	2.40	0.55
1:Q:55:LEU:HD13	1:Q:151:VAL:HG21	1.88	0.55
1:V:85:GLN:HB2	1:V:167:PHE:CE1	2.42	0.55
1:A:42:THR:HG22	1:A:118:VAL:HG22	1.88	0.55
1:F:41:ARG:HD3	1:F:41:ARG:N	2.22	0.55
1:J:143:PHE:HE1	1:L:65:LYS:HD2	1.71	0.55
1:S:48:PRO:HD3	1:S:108:ILE:CG1	2.37	0.55
1:S:175:VAL:HG11	1:V:77:GLN:HB2	1.89	0.55
1:H:149:ARG:HB2	1:I:185:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:83:ALA:O	1:O:87:TYR:CD2	2.60	0.54
1:U:47:LYS:HB3	1:U:48:PRO:HD2	1.87	0.54
1:X:170:LYS:HB3	1:X:172:GLU:OE1	2.07	0.54
1:A:60:ILE:O	1:A:64:GLU:HG3	2.07	0.54
1:G:47:LYS:HA	1:G:108:ILE:HG12	1.89	0.54
1:H:93:LYS:HE3	1:S:93:LYS:CG	2.37	0.54
1:L:68:TYR:CE2	1:L:118:VAL:HG23	2.42	0.54
1:U:93:LYS:HD2	1:U:94:PRO:HD2	1.89	0.54
1:F:83:ALA:HB3	1:F:100:VAL:HG13	1.88	0.54
1:J:185:VAL:HG12	1:K:145:VAL:HG21	1.85	0.54
1:K:60:ILE:O	1:K:64:GLU:HG3	2.08	0.54
1:B:175:VAL:HG13	1:E:77:GLN:HB2	1.89	0.54
1:M:153:HIS:CG	1:M:154:GLY:N	2.76	0.54
1:O:78:PRO:HG3	1:O:108:ILE:CG1	2.37	0.54
1:T:58:GLU:O	1:T:62:ARG:HG3	2.07	0.54
1:B:72:ALA:HB2	1:B:173:GLU:O	2.08	0.54
1:B:161:ALA:O	1:B:165:ILE:N	2.39	0.54
1:G:74:LYS:HA	1:J:74:LYS:HA	1.89	0.54
1:K:73:LEU:HD12	1:K:74:LYS:H	1.72	0.54
1:N:120:LYS:HG2	1:N:123:ARG:HH21	1.72	0.54
1:C:89:ASP:O	1:M:94:PRO:HD3	2.08	0.54
1:D:116:LYS:CG	1:D:186:TYR:HE1	2.20	0.54
1:J:185:VAL:HG22	1:K:53:ARG:NH2	2.23	0.54
1:M:59:ILE:HG12	1:M:139:ILE:HG21	1.90	0.54
1:O:44:ILE:HD13	1:O:154:GLY:HA2	1.90	0.54
1:O:73:LEU:CD1	1:O:109:VAL:HG12	2.32	0.54
1:O:84:GLN:O	1:O:88:ILE:N	2.41	0.54
1:D:66:LYS:O	1:E:145:VAL:HG13	2.07	0.54
1:M:73:LEU:HD13	1:M:111:MET:CG	2.37	0.54
1:B:73:LEU:CD1	1:B:111:MET:HG2	2.38	0.54
1:E:75:MET:HE3	1:E:107:PRO:HB2	1.89	0.54
1:S:140:ARG:HH21	1:S:150:ASN:ND2	2.06	0.54
1:S:149:ARG:HG2	1:T:187:GLU:HG2	1.90	0.54
1:U:55:LEU:HD11	1:U:143:PHE:HB3	1.89	0.54
1:E:99:LEU:HG	1:E:103:PHE:CE2	2.43	0.54
1:F:69:LYS:HD3	1:F:179:SER:OG	2.07	0.54
1:P:120:LYS:O	1:P:124:VAL:HG23	2.08	0.54
1:S:162:LYS:HD3	1:S:165:ILE:HD12	1.90	0.54
1:U:140:ARG:HD3	1:U:150:ASN:HB2	1.90	0.54
1:V:133:ASP:OD1	1:V:133:ASP:N	2.41	0.54
1:X:48:PRO:HD3	1:X:108:ILE:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:N	1:D:57:GLY:HA3	2.23	0.54
1:G:74:LYS:HE3	1:G:76:LEU:HD22	1.90	0.54
1:G:94:PRO:HD2	1:T:93:LYS:NZ	2.22	0.54
1:K:66:LYS:O	1:L:53:ARG:NH2	2.40	0.54
1:L:46:VAL:HG21	1:L:56:VAL:HG22	1.89	0.54
1:T:42:THR:HG21	1:T:118:VAL:HG22	1.90	0.54
1:A:180:HIS:HB2	1:F:181:SER:HA	1.90	0.53
1:F:46:VAL:O	1:F:108:ILE:HG23	2.08	0.53
1:H:93:LYS:HA	1:S:92:SER:C	2.28	0.53
1:K:78:PRO:HB3	1:K:168:TRP:CH2	2.44	0.53
1:P:161:ALA:O	1:P:165:ILE:HG13	2.08	0.53
1:G:70:LEU:HD23	1:J:75:MET:HE3	1.90	0.53
1:K:73:LEU:HD12	1:K:74:LYS:N	2.22	0.53
1:M:91:ALA:HA	1:M:96:TYR:CE1	2.43	0.53
1:Q:47:LYS:HE3	1:Q:152:CYS:O	2.08	0.53
1:T:68:TYR:CD2	1:T:118:VAL:HG23	2.42	0.53
1:X:171:PRO:HA	1:X:174:LEU:HD12	1.91	0.53
1:B:75:MET:HB3	1:E:73:LEU:H	1.73	0.53
1:B:86:HIS:HD2	1:B:87:TYR:CE2	2.25	0.53
1:C:93:LYS:HA	1:M:92:SER:CA	2.32	0.53
1:E:60:ILE:HG12	1:E:111:MET:SD	2.48	0.53
1:I:91:ALA:HA	1:I:96:TYR:CZ	2.43	0.53
1:E:87:TYR:CD1	1:E:99:LEU:HD21	2.43	0.53
1:G:56:VAL:HB	1:J:64:GLU:CD	2.26	0.53
1:G:70:LEU:HD21	1:G:73:LEU:CB	2.38	0.53
1:N:46:VAL:O	1:N:108:ILE:HG23	2.09	0.53
1:Q:84:GLN:HA	1:Q:96:TYR:OH	2.09	0.53
1:T:175:VAL:CB	1:W:107:PRO:HB3	2.38	0.53
1:U:140:ARG:NH2	1:U:150:ASN:ND2	2.56	0.53
1:A:185:VAL:HB	1:A:186:TYR:CD2	2.43	0.53
1:O:57:GLY:HA2	1:O:60:ILE:HD12	1.90	0.53
1:P:82:GLN:HA	1:P:167:PHE:HZ	1.73	0.53
1:T:53:ARG:HD2	1:U:181:SER:OG	2.08	0.53
1:B:51:VAL:HG21	1:B:107:PRO:O	2.09	0.53
1:G:162:LYS:HA	1:G:165:ILE:CD1	2.38	0.53
1:J:126:LEU:CD1	1:J:154:GLY:HA3	2.38	0.53
1:T:123:ARG:HA	1:T:126:LEU:HD12	1.90	0.53
1:A:49:ASP:HA	1:B:184:GLN:HE21	1.74	0.53
1:A:67:GLY:CA	1:C:53:ARG:NH2	2.56	0.53
1:D:47:LYS:HB3	1:D:48:PRO:CD	2.38	0.53
1:I:85:GLN:HB3	1:I:167:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:83:ALA:HB3	1:N:100:VAL:HG13	1.91	0.53
1:S:75:MET:CE	1:S:109:VAL:HG22	2.38	0.53
1:A:177:TRP:NE1	1:D:77:GLN:OE1	2.40	0.53
1:I:46:VAL:CG1	1:I:152:CYS:SG	2.94	0.53
1:V:149:ARG:HG3	1:X:185:VAL:C	2.29	0.53
1:I:75:MET:CE	1:I:109:VAL:HG22	2.39	0.53
1:J:47:LYS:HB3	1:J:48:PRO:HD2	1.90	0.53
1:J:55:LEU:HD21	1:J:143:PHE:CG	2.43	0.53
1:N:142:ASP:O	1:O:66:LYS:CA	2.52	0.53
1:T:143:PHE:CE1	1:U:65:LYS:HB3	2.43	0.53
1:A:64:GLU:C	1:D:54:CYS:SG	2.87	0.53
1:A:184:GLN:C	1:C:53:ARG:HG3	2.28	0.53
1:F:46:VAL:HG12	1:F:59:ILE:HD13	1.91	0.53
1:M:54:CYS:HA	1:P:64:GLU:CD	2.29	0.53
1:P:43:PHE:HD1	1:P:111:MET:O	1.92	0.53
1:P:66:LYS:HZ2	1:Q:144:ALA:H	1.57	0.53
1:A:143:PHE:HA	1:B:66:LYS:HA	1.91	0.52
1:B:44:ILE:HG13	1:B:63:PHE:CZ	2.44	0.52
1:C:70:LEU:HD21	1:C:73:LEU:HD22	1.90	0.52
1:E:99:LEU:HG	1:E:103:PHE:HE2	1.73	0.52
1:H:47:LYS:HD3	1:H:103:PHE:HE1	1.73	0.52
1:I:70:LEU:HD21	1:I:73:LEU:HB2	1.91	0.52
1:O:130:ASN:ND2	1:O:132:ALA:HB3	2.24	0.52
1:Q:41:ARG:NH2	1:Q:165:ILE:HG21	2.24	0.52
1:T:66:LYS:HG2	1:T:68:TYR:CE1	2.44	0.52
1:H:56:VAL:O	1:H:60:ILE:HG13	2.09	0.52
1:I:37:MET:HG3	1:I:38:THR:H	1.74	0.52
1:J:95:PHE:HD1	1:J:96:TYR:N	2.06	0.52
1:P:49:ASP:OD1	1:P:49:ASP:N	2.36	0.52
1:Q:55:LEU:CD1	1:Q:151:VAL:HG21	2.39	0.52
1:R:46:VAL:HG21	1:R:56:VAL:HG22	1.92	0.52
1:S:76:LEU:HD21	1:S:168:TRP:CZ3	2.44	0.52
1:U:96:TYR:O	1:U:100:VAL:HG23	2.08	0.52
1:A:175:VAL:CG2	1:D:75:MET:HG3	2.39	0.52
1:B:76:LEU:HD23	1:B:76:LEU:N	2.24	0.52
1:B:148:GLY:HA3	1:C:187:GLU:OE1	2.09	0.52
1:G:60:ILE:HG12	1:G:111:MET:SD	2.49	0.52
1:T:175:VAL:HG13	1:W:77:GLN:HB2	1.91	0.52
1:V:53:ARG:NH2	1:V:143:PHE:O	2.35	0.52
1:V:53:ARG:NH2	1:X:66:LYS:O	2.42	0.52
1:C:89:ASP:O	1:M:94:PRO:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:TYR:CE2	1:F:118:VAL:HG23	2.44	0.52
1:N:52:GLN:CB	1:O:184:GLN:HE21	2.23	0.52
1:V:137:GLY:HA3	1:X:137:GLY:HA3	1.90	0.52
1:A:64:GLU:CD	1:D:57:GLY:H	2.12	0.52
1:A:187:GLU:CD	1:C:149:ARG:HG2	2.29	0.52
1:F:90:LEU:O	1:F:96:TYR:CD1	2.63	0.52
1:H:39:SER:HA	1:H:114:GLU:OE2	2.09	0.52
1:W:93:LYS:HE3	1:W:95:PHE:HE2	1.75	0.52
1:C:112:VAL:HG13	1:C:165:ILE:CD1	2.40	0.52
1:H:42:THR:HB	1:H:118:VAL:HG13	1.92	0.52
1:J:43:PHE:CZ	1:J:168:TRP:CD2	2.97	0.52
1:S:86:HIS:CE1	1:S:164:GLU:HG2	2.45	0.52
1:T:68:TYR:HE2	1:T:118:VAL:HG23	1.75	0.52
1:V:136:PRO:HB2	1:X:138:THR:CG2	2.39	0.52
1:C:130:ASN:HD21	1:C:132:ALA:HB3	1.75	0.52
1:G:111:MET:SD	1:G:113:TRP:NE1	2.81	0.52
1:P:42:THR:HG22	1:P:113:TRP:HB2	1.92	0.52
1:T:53:ARG:O	1:T:54:CYS:HB3	2.09	0.52
1:F:46:VAL:HG22	1:F:109:VAL:HB	1.91	0.52
1:H:56:VAL:HG11	1:H:109:VAL:HG21	1.91	0.52
1:T:56:VAL:HB	1:W:64:GLU:OE1	2.09	0.52
1:V:149:ARG:CZ	1:X:187:GLU:HB3	2.39	0.52
1:W:99:LEU:HG	1:W:103:PHE:HE2	1.74	0.52
1:A:56:VAL:HB	1:D:64:GLU:OE1	2.08	0.52
1:D:145:VAL:HG12	1:F:66:LYS:HE3	1.91	0.52
1:D:181:SER:O	1:D:185:VAL:HG23	2.10	0.52
1:E:70:LEU:HD21	1:E:73:LEU:HB2	1.91	0.52
1:E:130:ASN:HD21	1:E:132:ALA:HB3	1.75	0.52
1:I:107:PRO:HD3	1:L:177:TRP:CD1	2.44	0.52
1:Q:66:LYS:HG3	1:R:145:VAL:CG1	2.40	0.52
1:R:90:LEU:HD13	1:R:95:PHE:HZ	1.74	0.52
1:T:78:PRO:HG3	1:T:108:ILE:HD12	1.90	0.52
1:V:72:ALA:HB1	1:V:169:PHE:CE1	2.45	0.52
1:A:65:LYS:O	1:C:143:PHE:CD1	2.63	0.51
1:C:120:LYS:HA	1:C:123:ARG:HE	1.74	0.51
1:H:47:LYS:CE	1:H:103:PHE:HE1	2.23	0.51
1:J:181:SER:HG	1:K:53:ARG:HG2	1.72	0.51
1:K:55:LEU:HD12	1:K:151:VAL:HG23	1.91	0.51
1:V:49:ASP:CB	1:X:184:GLN:O	2.56	0.51
1:A:175:VAL:HG13	1:D:77:GLN:HB2	1.91	0.51
1:A:177:TRP:CD1	1:D:107:PRO:CG	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:VAL:HG22	1:D:109:VAL:HB	1.91	0.51
1:F:44:ILE:O	1:F:111:MET:HB2	2.10	0.51
1:F:69:LYS:O	1:F:114:GLU:N	2.41	0.51
1:G:68:TYR:CD2	1:G:118:VAL:HG23	2.45	0.51
1:V:149:ARG:HB2	1:X:185:VAL:O	2.11	0.51
1:C:64:GLU:HG3	1:C:113:TRP:HH2	1.75	0.51
1:D:85:GLN:O	1:D:163:ARG:NH2	2.43	0.51
1:G:187:GLU:HG2	1:I:149:ARG:NH1	2.25	0.51
1:I:77:GLN:HB2	1:L:175:VAL:HG13	1.93	0.51
1:T:82:GLN:HA	1:T:167:PHE:CZ	2.46	0.51
1:U:140:ARG:NE	1:U:150:ASN:HB2	2.26	0.51
1:W:46:VAL:HG21	1:W:56:VAL:HG13	1.92	0.51
1:X:126:LEU:CD1	1:X:154:GLY:HA3	2.41	0.51
1:C:52:GLN:CD	1:F:180:HIS:CD2	2.84	0.51
1:F:86:HIS:CE1	1:F:168:TRP:NE1	2.76	0.51
1:G:175:VAL:HG13	1:J:77:GLN:HB2	1.92	0.51
1:I:107:PRO:HD3	1:L:177:TRP:CG	2.45	0.51
1:U:43:PHE:HB2	1:U:165:ILE:HG13	1.93	0.51
1:J:125:LEU:HA	1:K:136:PRO:CG	2.35	0.51
1:P:184:GLN:O	1:Q:49:ASP:CB	2.59	0.51
1:S:59:ILE:HG12	1:S:139:ILE:HD13	1.91	0.51
1:A:38:THR:O	1:A:115:GLY:HA2	2.10	0.51
1:B:165:ILE:CG2	1:B:174:LEU:HD11	2.41	0.51
1:C:112:VAL:HG13	1:C:165:ILE:HD13	1.91	0.51
1:D:78:PRO:HG3	1:D:108:ILE:HG13	1.91	0.51
1:H:93:LYS:HG2	1:S:93:LYS:HA	1.91	0.51
1:H:112:VAL:HG21	1:H:174:LEU:HD21	1.91	0.51
1:J:47:LYS:HE3	1:J:152:CYS:O	2.11	0.51
1:O:57:GLY:HA3	1:R:57:GLY:O	2.10	0.51
1:O:140:ARG:HD3	1:O:150:ASN:HB2	1.93	0.51
1:G:87:TYR:CG	1:G:99:LEU:HD21	2.46	0.51
1:J:124:VAL:HG12	1:K:136:PRO:HD3	1.91	0.51
1:P:73:LEU:HA	1:P:110:GLY:O	2.11	0.51
1:Q:59:ILE:HG12	1:Q:139:ILE:HD13	1.93	0.51
1:W:128:ALA:O	1:W:140:ARG:HD2	2.10	0.51
1:W:170:LYS:O	1:W:173:GLU:HG3	2.11	0.51
1:X:40:GLU:HB3	1:X:115:GLY:O	2.11	0.51
1:E:122:GLY:HA2	1:E:125:LEU:HD12	1.93	0.51
1:H:165:ILE:O	1:H:169:PHE:HB2	2.10	0.51
1:W:90:LEU:O	1:W:96:TYR:CD1	2.63	0.51
1:B:55:LEU:N	1:E:64:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:LEU:HD21	1:E:73:LEU:CB	2.41	0.51
1:G:53:ARG:NH2	1:H:66:LYS:C	2.64	0.51
1:S:87:TYR:CD1	1:S:90:LEU:HD12	2.45	0.51
1:A:77:GLN:HB2	1:D:177:TRP:NE1	2.25	0.51
1:B:177:TRP:CZ2	1:E:107:PRO:HG3	2.46	0.51
1:C:70:LEU:HD12	1:C:71:VAL:N	2.26	0.51
1:E:49:ASP:O	1:E:53:ARG:HG3	2.10	0.51
1:G:48:PRO:HB3	1:G:106:GLY:HA3	1.93	0.51
1:H:93:LYS:N	1:S:92:SER:O	2.43	0.51
1:M:37:MET:N	1:M:116:LYS:HZ2	2.09	0.51
1:M:111:MET:SD	1:M:113:TRP:NE1	2.78	0.51
1:N:69:LYS:HD2	1:N:179:SER:HB2	1.93	0.51
1:Q:68:TYR:O	1:Q:113:TRP:CZ3	2.64	0.51
1:Q:122:GLY:HA2	1:Q:125:LEU:HD12	1.93	0.51
1:U:61:GLN:HB2	1:U:65:LYS:HZ1	1.74	0.51
1:C:112:VAL:HG22	1:C:165:ILE:HG12	1.93	0.50
1:G:75:MET:CE	1:J:70:LEU:HD23	2.41	0.50
1:H:52:GLN:CB	1:K:180:HIS:HD2	2.10	0.50
1:H:128:ALA:O	1:H:140:ARG:HD2	2.11	0.50
1:M:61:GLN:HB3	1:M:65:LYS:NZ	2.26	0.50
1:A:49:ASP:HA	1:B:184:GLN:NE2	2.26	0.50
1:B:180:HIS:H	1:E:52:GLN:NE2	2.09	0.50
1:H:88:ILE:HG22	1:H:163:ARG:NH2	2.25	0.50
1:I:93:LYS:HG2	1:I:95:PHE:CE1	2.46	0.50
1:O:56:VAL:HG12	1:O:60:ILE:HD11	1.94	0.50
1:V:44:ILE:O	1:V:111:MET:HB2	2.12	0.50
1:G:184:GLN:CD	1:L:180:HIS:NE2	2.65	0.50
1:H:92:SER:O	1:S:92:SER:CB	2.50	0.50
1:J:66:LYS:CG	1:J:68:TYR:CE1	2.93	0.50
1:O:145:VAL:HG23	1:O:146:ASP:H	1.74	0.50
1:Q:76:LEU:O	1:Q:108:ILE:N	2.38	0.50
1:S:180:HIS:HD2	1:V:52:GLN:HB3	1.75	0.50
1:T:180:HIS:HD2	1:W:53:ARG:HG3	1.75	0.50
1:W:170:LYS:HB2	1:W:173:GLU:HG3	1.92	0.50
1:A:187:GLU:CG	1:C:149:ARG:CG	2.72	0.50
1:C:64:GLU:HG3	1:C:113:TRP:CH2	2.47	0.50
1:E:43:PHE:CE2	1:E:45:ALA:HB2	2.46	0.50
1:H:112:VAL:HG23	1:H:169:PHE:CE2	2.46	0.50
1:O:57:GLY:CA	1:R:57:GLY:O	2.60	0.50
1:V:143:PHE:N	1:X:66:LYS:HD2	2.26	0.50
1:X:48:PRO:HG2	1:X:102:TYR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:CD1	1:B:109:VAL:HG12	2.42	0.50
1:B:74:LYS:HA	1:E:73:LEU:O	2.12	0.50
1:I:91:ALA:HA	1:I:96:TYR:CE1	2.47	0.50
1:P:90:LEU:HD22	1:P:93:LYS:HG3	1.92	0.50
1:S:86:HIS:HE1	1:S:164:GLU:HG2	1.76	0.50
1:A:74:LYS:C	1:D:73:LEU:HD23	2.32	0.50
1:B:180:HIS:CD2	1:E:52:GLN:HG3	2.45	0.50
1:G:126:LEU:O	1:G:140:ARG:HB2	2.11	0.50
1:T:126:LEU:HD22	1:T:152:CYS:SG	2.52	0.50
1:U:179:SER:O	1:U:182:VAL:HG23	2.11	0.50
1:B:86:HIS:CG	1:B:168:TRP:HE1	2.30	0.50
1:E:48:PRO:HG2	1:E:102:TYR:O	2.10	0.50
1:G:179:SER:HB2	1:G:182:VAL:HG23	1.93	0.50
1:M:61:GLN:CG	1:P:57:GLY:HA3	2.33	0.50
1:U:93:LYS:HG3	1:U:94:PRO:HD2	1.94	0.50
1:V:149:ARG:NH1	1:X:187:GLU:HA	2.27	0.50
1:C:120:LYS:HA	1:C:123:ARG:HH21	1.76	0.50
1:L:138:THR:O	1:L:142:ASP:HB2	2.12	0.50
1:N:82:GLN:HA	1:N:167:PHE:HZ	1.76	0.50
1:O:54:CYS:SG	1:R:64:GLU:HB3	2.51	0.50
1:P:126:LEU:HD13	1:P:140:ARG:NH2	2.25	0.50
1:T:73:LEU:H	1:W:75:MET:HB2	1.77	0.50
1:T:177:TRP:CE3	1:W:52:GLN:HG2	2.47	0.50
1:B:145:VAL:CG2	1:C:185:VAL:HG12	2.41	0.50
1:G:180:HIS:HB2	1:L:180:HIS:O	2.11	0.50
1:J:145:VAL:HG23	1:J:146:ASP:N	2.26	0.50
1:Q:72:ALA:HB2	1:Q:174:LEU:HA	1.94	0.50
1:V:126:LEU:HA	1:V:139:ILE:HB	1.94	0.50
1:V:143:PHE:O	1:X:66:LYS:O	2.29	0.50
1:G:175:VAL:CG1	1:J:107:PRO:HB3	2.23	0.49
1:J:102:TYR:OH	1:J:149:ARG:HD2	2.12	0.49
1:D:86:HIS:HD2	1:D:87:TYR:CZ	2.30	0.49
1:H:58:GLU:N	1:K:61:GLN:OE1	2.45	0.49
1:Q:135:LEU:O	1:Q:141:GLY:HA3	2.13	0.49
1:R:70:LEU:HB2	1:R:113:TRP:CZ3	2.46	0.49
1:T:62:ARG:HD2	1:T:139:ILE:HG12	1.93	0.49
1:T:72:ALA:CB	1:T:174:LEU:CD2	2.90	0.49
1:T:99:LEU:CG	1:T:103:PHE:HE2	2.18	0.49
1:C:47:LYS:HB3	1:C:48:PRO:HD2	1.92	0.49
1:I:69:LYS:HD3	1:I:114:GLU:OE2	2.12	0.49
1:R:59:ILE:HG12	1:R:139:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:43:PHE:HB3	1:T:164:GLU:OE1	2.12	0.49
1:T:47:LYS:HB3	1:T:48:PRO:HD2	1.93	0.49
1:C:66:LYS:HD3	1:C:125:LEU:HD21	1.94	0.49
1:H:82:GLN:HA	1:H:167:PHE:HZ	1.77	0.49
1:N:55:LEU:HD11	1:N:143:PHE:HB3	1.93	0.49
1:O:85:GLN:HA	1:O:88:ILE:HB	1.93	0.49
1:O:98:ASP:OD1	1:O:99:LEU:N	2.46	0.49
1:Q:48:PRO:HG2	1:Q:102:TYR:O	2.11	0.49
1:Q:184:GLN:NE2	1:R:149:ARG:HE	2.09	0.49
1:S:53:ARG:NE	1:T:185:VAL:HG22	2.27	0.49
1:T:177:TRP:CZ2	1:W:51:VAL:HG12	2.47	0.49
1:T:181:SER:O	1:T:185:VAL:HG23	2.12	0.49
1:A:47:LYS:NZ	1:A:153:HIS:HB2	2.27	0.49
1:H:113:TRP:O	1:H:118:VAL:HG21	2.13	0.49
1:H:167:PHE:CD2	1:H:168:TRP:CD1	3.01	0.49
1:J:184:GLN:HE21	1:K:49:ASP:HA	1.76	0.49
1:M:80:ALA:O	1:M:84:GLN:N	2.28	0.49
1:Q:179:SER:CB	1:Q:182:VAL:HG23	2.43	0.49
1:V:142:ASP:C	1:X:66:LYS:HD2	2.33	0.49
1:W:72:ALA:HB2	1:W:174:LEU:HA	1.94	0.49
1:W:140:ARG:NH2	1:W:152:CYS:O	2.45	0.49
1:B:83:ALA:HB3	1:B:100:VAL:HG13	1.95	0.49
1:D:87:TYR:CG	1:D:99:LEU:HD21	2.47	0.49
1:H:72:ALA:HB2	1:H:174:LEU:HA	1.94	0.49
1:M:49:ASP:CA	1:N:184:GLN:HE21	2.13	0.49
1:M:50:GLY:O	1:M:55:LEU:HB2	2.11	0.49
1:N:177:TRP:CD1	1:Q:107:PRO:HG3	2.47	0.49
1:R:68:TYR:CE2	1:R:118:VAL:HG23	2.48	0.49
1:T:56:VAL:HB	1:W:64:GLU:OE2	2.13	0.49
1:T:179:SER:HA	1:W:52:GLN:OE1	2.12	0.49
1:V:145:VAL:HG21	1:X:186:TYR:CZ	2.48	0.49
1:A:177:TRP:CG	1:D:107:PRO:HD3	2.47	0.49
1:C:95:PHE:HA	1:C:98:ASP:OD2	2.12	0.49
1:L:76:LEU:HD11	1:L:168:TRP:HZ3	1.77	0.49
1:M:63:PHE:HD2	1:M:68:TYR:HD2	1.59	0.49
1:O:55:LEU:HD23	1:O:58:GLU:HG3	1.94	0.49
1:S:70:LEU:HD23	1:V:75:MET:HE3	1.93	0.49
1:S:93:LYS:CD	1:S:95:PHE:CZ	2.94	0.49
1:T:175:VAL:HB	1:W:107:PRO:HB3	1.95	0.49
1:U:86:HIS:HD2	1:U:87:TYR:CD1	2.31	0.49
1:D:90:LEU:C	1:D:92:SER:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:LYS:HB3	1:G:48:PRO:CD	2.42	0.49
1:H:112:VAL:CG1	1:H:165:ILE:HD11	2.43	0.49
1:P:46:VAL:HA	1:P:152:CYS:HA	1.95	0.49
1:P:90:LEU:CD2	1:P:93:LYS:HG3	2.43	0.49
1:T:82:GLN:HA	1:T:167:PHE:HZ	1.78	0.49
1:W:99:LEU:HG	1:W:103:PHE:CE2	2.48	0.49
1:B:175:VAL:HG11	1:E:77:GLN:HB2	1.95	0.49
1:F:47:LYS:HD3	1:F:102:TYR:OH	2.13	0.49
1:J:40:GLU:OE2	1:J:119:VAL:CG2	2.61	0.49
1:K:46:VAL:HG12	1:K:152:CYS:SG	2.53	0.49
1:P:74:LYS:NZ	1:P:173:GLU:OE1	2.37	0.49
1:P:156:ASP:OD1	1:P:157:SER:N	2.46	0.49
1:R:38:THR:HA	1:R:116:LYS:HD3	1.95	0.49
1:S:149:ARG:NE	1:T:187:GLU:HA	2.25	0.49
1:T:38:THR:O	1:T:38:THR:HG22	2.13	0.49
1:X:42:THR:HA	1:X:161:ALA:HB1	1.95	0.49
1:A:72:ALA:HA	1:D:75:MET:HB3	1.93	0.49
1:D:44:ILE:HD13	1:D:154:GLY:CA	2.42	0.49
1:I:47:LYS:HB3	1:I:48:PRO:HD2	1.95	0.49
1:N:55:LEU:HD12	1:N:151:VAL:CG2	2.41	0.49
1:S:48:PRO:C	1:T:184:GLN:NE2	2.67	0.49
1:S:140:ARG:HE	1:S:150:ASN:HB2	1.77	0.49
1:B:87:TYR:O	1:B:90:LEU:N	2.31	0.48
1:C:102:TYR:CE1	1:C:149:ARG:HD3	2.47	0.48
1:E:53:ARG:O	1:E:54:CYS:HB3	2.12	0.48
1:M:54:CYS:HA	1:P:64:GLU:OE2	2.13	0.48
1:M:139:ILE:O	1:M:143:PHE:HB2	2.13	0.48
1:N:49:ASP:O	1:N:53:ARG:HG3	2.13	0.48
1:P:74:LYS:HG2	1:P:169:PHE:HE1	1.78	0.48
1:P:139:ILE:O	1:P:143:PHE:N	2.46	0.48
1:S:175:VAL:CG1	1:V:77:GLN:HB2	2.43	0.48
1:W:63:PHE:O	1:W:66:LYS:HB3	2.13	0.48
1:A:124:VAL:HG12	1:C:136:PRO:CG	2.43	0.48
1:M:158:VAL:O	1:M:161:ALA:HB3	2.13	0.48
1:V:112:VAL:HG22	1:V:165:ILE:HG12	1.93	0.48
1:F:48:PRO:HG3	1:F:108:ILE:HD11	1.96	0.48
1:S:140:ARG:NH2	1:S:150:ASN:ND2	2.61	0.48
1:T:64:GLU:CD	1:W:57:GLY:H	2.16	0.48
1:B:58:GLU:HG2	1:B:143:PHE:CZ	2.47	0.48
1:L:45:ALA:HA	1:L:109:VAL:O	2.13	0.48
1:Q:47:LYS:HG3	1:Q:152:CYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:170:LYS:HB3	1:Q:172:GLU:CD	2.33	0.48
1:T:72:ALA:HA	1:W:75:MET:HG2	1.95	0.48
1:U:75:MET:HE2	1:X:73:LEU:HD23	1.94	0.48
1:B:58:GLU:HG2	1:B:143:PHE:HZ	1.77	0.48
1:H:99:LEU:CD1	1:H:103:PHE:HE2	2.27	0.48
1:H:143:PHE:HA	1:I:65:LYS:O	2.13	0.48
1:I:105:SER:O	1:L:177:TRP:CH2	2.67	0.48
1:J:56:VAL:O	1:J:60:ILE:HG13	2.12	0.48
1:J:77:GLN:HE22	1:J:104:SER:HA	1.79	0.48
1:O:60:ILE:HB	1:R:57:GLY:HA2	1.95	0.48
1:R:38:THR:N	1:R:116:LYS:HD3	2.27	0.48
1:G:70:LEU:HD23	1:J:75:MET:HE2	1.95	0.48
1:K:68:TYR:CE2	1:K:118:VAL:HG23	2.49	0.48
1:L:42:THR:HG21	1:L:118:VAL:HG22	1.96	0.48
1:Q:41:ARG:NH1	1:Q:174:LEU:HD13	2.22	0.48
1:T:170:LYS:HB2	1:T:173:GLU:HG3	1.95	0.48
1:W:140:ARG:NE	1:W:150:ASN:HB2	2.28	0.48
1:G:91:ALA:HA	1:G:96:TYR:CE1	2.49	0.48
1:I:121:GLY:O	1:I:124:VAL:HB	2.13	0.48
1:M:180:HIS:CG	1:R:184:GLN:HG3	2.49	0.48
1:O:54:CYS:SG	1:R:65:LYS:HA	2.53	0.48
1:P:186:TYR:N	1:Q:149:ARG:HG3	2.29	0.48
1:Q:66:LYS:HG2	1:Q:68:TYR:CE1	2.48	0.48
1:Q:101:ALA:O	1:Q:105:SER:HB3	2.13	0.48
1:S:149:ARG:HH11	1:T:187:GLU:HG2	1.76	0.48
1:U:46:VAL:CG1	1:U:59:ILE:HD13	2.44	0.48
1:V:47:LYS:HB3	1:V:48:PRO:CD	2.43	0.48
1:X:145:VAL:CG2	1:X:146:ASP:N	2.77	0.48
1:D:66:LYS:HG2	1:D:68:TYR:CE1	2.48	0.48
1:J:149:ARG:NH1	1:L:187:GLU:HA	2.28	0.48
1:M:67:GLY:HA2	1:O:53:ARG:NH2	2.26	0.48
1:N:120:LYS:O	1:N:124:VAL:HG23	2.14	0.48
1:O:46:VAL:CG2	1:O:109:VAL:HG23	2.36	0.48
1:O:47:LYS:HA	1:O:108:ILE:CD1	2.43	0.48
1:O:51:VAL:HG11	1:O:107:PRO:HG2	1.95	0.48
1:P:63:PHE:HE1	1:P:139:ILE:HD11	1.79	0.48
1:U:55:LEU:HD21	1:U:143:PHE:CD1	2.48	0.48
1:W:86:HIS:CE1	1:W:164:GLU:HG2	2.49	0.48
1:B:53:ARG:HD2	1:C:184:GLN:HB3	1.96	0.48
1:D:184:GLN:O	1:E:149:ARG:HG3	2.14	0.48
1:G:137:GLY:HA3	1:I:136:PRO:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:179:SER:HB2	1:I:182:VAL:HG23	1.94	0.48
1:J:46:VAL:HG22	1:J:109:VAL:H	1.78	0.48
1:O:64:GLU:CD	1:R:54:CYS:HA	2.33	0.48
1:S:149:ARG:CZ	1:T:187:GLU:CA	2.76	0.48
1:T:178:THR:O	1:W:52:GLN:NE2	2.47	0.48
1:U:125:LEU:O	1:U:138:THR:HB	2.14	0.48
1:A:48:PRO:HG2	1:A:102:TYR:O	2.14	0.48
1:A:52:GLN:CG	1:D:180:HIS:HD2	2.26	0.48
1:G:126:LEU:HD11	1:G:154:GLY:CA	2.41	0.48
1:H:181:SER:O	1:H:185:VAL:HG23	2.14	0.48
1:I:170:LYS:HB2	1:I:173:GLU:HG3	1.96	0.48
1:J:55:LEU:HD13	1:J:151:VAL:CG2	2.39	0.48
1:J:68:TYR:CE2	1:J:118:VAL:HG23	2.49	0.48
1:L:47:LYS:O	1:L:50:GLY:N	2.47	0.48
1:O:128:ALA:N	1:O:134:SER:OG	2.47	0.48
1:R:49:ASP:HB3	1:R:149:ARG:HD2	1.95	0.48
1:B:122:GLY:O	1:B:126:LEU:HG	2.14	0.47
1:F:112:VAL:HG21	1:F:174:LEU:CD2	2.44	0.47
1:I:56:VAL:HG21	1:L:70:LEU:CD2	2.39	0.47
1:M:52:GLN:HB3	1:N:184:GLN:HG3	1.96	0.47
1:M:149:ARG:CZ	1:N:187:GLU:HG2	2.44	0.47
1:P:44:ILE:HA	1:P:153:HIS:O	2.14	0.47
1:V:47:LYS:HB2	1:V:49:ASP:OD1	2.14	0.47
1:X:66:LYS:HD3	1:X:125:LEU:HD21	1.95	0.47
1:A:84:GLN:HA	1:A:96:TYR:OH	2.15	0.47
1:B:99:LEU:HD11	1:B:103:PHE:HE2	1.78	0.47
1:C:58:GLU:HA	1:C:61:GLN:HG2	1.95	0.47
1:C:61:GLN:O	1:C:65:LYS:HG3	2.15	0.47
1:H:93:LYS:HA	1:S:92:SER:CB	2.44	0.47
1:L:42:THR:CG2	1:L:118:VAL:HG22	2.44	0.47
1:M:171:PRO:C	1:M:173:GLU:H	2.17	0.47
1:M:180:HIS:CB	1:R:184:GLN:HG3	2.43	0.47
1:W:56:VAL:HA	1:W:59:ILE:HD12	1.95	0.47
1:B:62:ARG:HA	1:B:65:LYS:HE3	1.95	0.47
1:J:53:ARG:NH2	1:L:65:LYS:O	2.46	0.47
1:N:47:LYS:O	1:N:50:GLY:N	2.45	0.47
1:Q:61:GLN:O	1:Q:65:LYS:HG2	2.14	0.47
1:R:91:ALA:HA	1:R:96:TYR:CD1	2.49	0.47
1:U:175:VAL:HG11	1:X:107:PRO:HB3	1.96	0.47
1:V:146:ASP:OD2	1:X:116:LYS:HG3	2.14	0.47
1:X:39:SER:O	1:X:41:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:NZ	1:C:132:ALA:HB1	2.29	0.47
1:F:38:THR:HA	1:F:116:LYS:HG2	1.95	0.47
1:G:179:SER:HA	1:J:52:GLN:OE1	2.14	0.47
1:G:184:GLN:HE21	1:I:49:ASP:HA	1.79	0.47
1:H:44:ILE:HB	1:H:111:MET:HB2	1.96	0.47
1:S:61:GLN:O	1:S:65:LYS:HG3	2.14	0.47
1:S:90:LEU:HA	1:S:93:LYS:HG3	1.96	0.47
1:W:111:MET:CE	1:W:113:TRP:HE1	2.27	0.47
1:A:50:GLY:HA2	1:A:151:VAL:CG2	2.45	0.47
1:C:94:PRO:HD2	1:M:92:SER:CB	2.42	0.47
1:C:180:HIS:NE2	1:F:52:GLN:CD	2.68	0.47
1:H:42:THR:OG1	1:H:155:SER:HB2	2.14	0.47
1:H:48:PRO:O	1:H:52:GLN:HB2	2.14	0.47
1:M:49:ASP:OD2	1:M:151:VAL:HA	2.15	0.47
1:M:54:CYS:SG	1:P:64:GLU:CB	2.98	0.47
1:P:45:ALA:O	1:P:153:HIS:N	2.47	0.47
1:Q:62:ARG:HG2	1:Q:65:LYS:HZ1	1.79	0.47
1:Q:73:LEU:HD13	1:Q:111:MET:HG3	1.96	0.47
1:B:72:ALA:CB	1:B:173:GLU:O	2.63	0.47
1:J:126:LEU:HD13	1:J:140:ARG:NH2	2.30	0.47
1:J:175:VAL:HG12	1:J:177:TRP:CD1	2.50	0.47
1:L:102:TYR:C	1:L:104:SER:H	2.18	0.47
1:P:184:GLN:HE21	1:Q:52:GLN:HG3	1.78	0.47
1:V:56:VAL:HG13	1:V:109:VAL:HG21	1.96	0.47
1:A:143:PHE:CE1	1:B:65:LYS:HD2	2.50	0.47
1:B:175:VAL:HG12	1:B:177:TRP:CD1	2.41	0.47
1:C:180:HIS:HD2	1:F:52:GLN:HB3	1.76	0.47
1:E:51:VAL:HG11	1:E:107:PRO:HG2	1.96	0.47
1:E:145:VAL:HG23	1:E:146:ASP:N	2.30	0.47
1:G:140:ARG:O	1:G:144:ALA:HB3	2.15	0.47
1:K:187:GLU:OE2	1:L:148:GLY:N	2.47	0.47
1:L:62:ARG:HD2	1:L:139:ILE:HG12	1.97	0.47
1:L:76:LEU:HD11	1:L:168:TRP:CZ3	2.50	0.47
1:N:55:LEU:HD21	1:N:143:PHE:CD1	2.49	0.47
1:P:145:VAL:HG12	1:R:66:LYS:HE3	1.96	0.47
1:S:76:LEU:HD21	1:S:168:TRP:HZ3	1.79	0.47
1:V:55:LEU:O	1:V:58:GLU:HB2	2.15	0.47
1:X:46:VAL:HG22	1:X:109:VAL:HB	1.95	0.47
1:A:74:LYS:HB2	1:D:73:LEU:O	2.15	0.47
1:F:56:VAL:HG12	1:F:60:ILE:HD12	1.96	0.47
1:J:38:THR:HG23	1:J:114:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:66:LYS:O	1:K:143:PHE:O	2.33	0.47
1:K:73:LEU:HD13	1:K:111:MET:HG3	1.95	0.47
1:M:53:ARG:HG2	1:N:181:SER:HB2	1.97	0.47
1:N:49:ASP:HA	1:O:184:GLN:NE2	2.30	0.47
1:V:149:ARG:HD2	1:X:184:GLN:O	2.15	0.47
1:A:83:ALA:O	1:A:87:TYR:CD2	2.65	0.47
1:A:138:THR:OG1	1:A:141:GLY:HA3	2.14	0.47
1:C:140:ARG:HH21	1:C:150:ASN:ND2	2.13	0.47
1:D:145:VAL:CG2	1:F:185:VAL:HG13	2.44	0.47
1:G:93:LYS:CG	1:T:93:LYS:HG2	2.38	0.47
1:G:158:VAL:O	1:G:162:LYS:HG2	2.15	0.47
1:P:145:VAL:HA	1:R:66:LYS:HE3	1.96	0.47
1:V:62:ARG:HD2	1:V:139:ILE:HG13	1.95	0.47
1:X:74:LYS:HE3	1:X:169:PHE:CE1	2.50	0.47
1:X:170:LYS:HB3	1:X:172:GLU:CD	2.35	0.47
1:B:135:LEU:HB3	1:B:136:PRO:HD2	1.97	0.47
1:K:43:PHE:HB3	1:K:155:SER:OG	2.15	0.47
1:M:48:PRO:HG2	1:M:102:TYR:O	2.15	0.47
1:N:180:HIS:HB3	1:P:181:SER:HA	1.97	0.47
1:T:131:PRO:HG3	1:T:140:ARG:HB3	1.97	0.47
1:U:50:GLY:CA	1:U:151:VAL:CG2	2.79	0.47
1:A:177:TRP:CZ2	1:D:77:GLN:OE1	2.69	0.46
1:D:43:PHE:CD2	1:D:164:GLU:HB3	2.50	0.46
1:E:66:LYS:HD3	1:E:125:LEU:HD21	1.96	0.46
1:F:86:HIS:HE1	1:F:164:GLU:HG2	1.79	0.46
1:M:49:ASP:HB3	1:M:149:ARG:HD2	1.96	0.46
1:M:61:GLN:HG3	1:P:57:GLY:CA	2.33	0.46
1:M:105:SER:O	1:P:177:TRP:CZ2	2.69	0.46
1:S:115:GLY:O	1:S:118:VAL:HB	2.15	0.46
1:U:179:SER:HA	1:X:52:GLN:HE22	1.80	0.46
1:C:45:ALA:HA	1:C:109:VAL:O	2.15	0.46
1:I:74:LYS:NZ	1:I:173:GLU:OE1	2.47	0.46
1:J:66:LYS:HG3	1:J:68:TYR:CD1	2.49	0.46
1:V:44:ILE:HD12	1:V:126:LEU:HD11	1.97	0.46
1:V:116:LYS:O	1:V:118:VAL:N	2.48	0.46
1:A:57:GLY:HA3	1:D:61:GLN:CD	2.36	0.46
1:A:184:GLN:NE2	1:C:49:ASP:HA	2.30	0.46
1:A:184:GLN:HE21	1:C:49:ASP:HA	1.80	0.46
1:H:128:ALA:N	1:H:134:SER:OG	2.48	0.46
1:I:110:GLY:O	1:I:169:PHE:HZ	1.98	0.46
1:K:58:GLU:HG2	1:K:143:PHE:HZ	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:LYS:HD3	1:L:179:SER:OG	2.16	0.46
1:N:180:HIS:CD2	1:P:184:GLN:HB2	2.50	0.46
1:T:57:GLY:C	1:W:61:GLN:OE1	2.53	0.46
1:T:177:TRP:CH2	1:W:51:VAL:O	2.68	0.46
1:U:64:GLU:OE2	1:X:56:VAL:HG23	2.15	0.46
1:U:93:LYS:HG3	1:U:94:PRO:CD	2.45	0.46
1:V:65:LYS:HB2	1:W:143:PHE:CE1	2.51	0.46
1:X:69:LYS:HD3	1:X:179:SER:OG	2.15	0.46
1:B:123:ARG:HD3	1:B:156:ASP:HA	1.95	0.46
1:J:60:ILE:O	1:J:64:GLU:HG3	2.16	0.46
1:Q:109:VAL:HG12	1:Q:111:MET:HE2	1.97	0.46
1:W:61:GLN:O	1:W:65:LYS:HG2	2.16	0.46
1:A:169:PHE:CD1	1:A:173:GLU:OE1	2.69	0.46
1:I:107:PRO:HD3	1:L:177:TRP:CB	2.46	0.46
1:I:107:PRO:CD	1:L:177:TRP:CD1	2.99	0.46
1:K:112:VAL:HG21	1:K:174:LEU:HD22	1.97	0.46
1:O:75:MET:CE	1:O:109:VAL:HG22	2.45	0.46
1:Q:126:LEU:O	1:Q:140:ARG:HG3	2.16	0.46
1:T:167:PHE:HD2	1:T:168:TRP:CD1	2.33	0.46
1:A:184:GLN:O	1:C:49:ASP:HB2	2.16	0.46
1:B:78:PRO:HG3	1:B:108:ILE:HD12	1.97	0.46
1:D:145:VAL:HG23	1:D:146:ASP:N	2.30	0.46
1:E:82:GLN:O	1:E:167:PHE:HZ	1.97	0.46
1:G:86:HIS:HD2	1:G:87:TYR:CE2	2.33	0.46
1:L:130:ASN:C	1:L:132:ALA:H	2.18	0.46
1:O:150:ASN:O	1:O:151:VAL:HG12	2.16	0.46
1:P:49:ASP:O	1:P:53:ARG:N	2.48	0.46
1:P:114:GLU:HG2	1:P:115:GLY:N	2.31	0.46
1:P:175:VAL:HG12	1:P:177:TRP:CD1	2.51	0.46
1:R:42:THR:HG22	1:R:113:TRP:HB2	1.98	0.46
1:R:86:HIS:CD2	1:R:87:TYR:CE2	2.93	0.46
1:T:75:MET:CB	1:W:73:LEU:HB3	2.46	0.46
1:T:118:VAL:O	1:T:122:GLY:N	2.46	0.46
1:U:140:ARG:CD	1:U:150:ASN:HB2	2.46	0.46
1:U:150:ASN:O	1:U:152:CYS:N	2.48	0.46
1:B:61:GLN:CA	1:E:57:GLY:HA3	2.45	0.46
1:D:73:LEU:CD1	1:D:109:VAL:CG1	2.93	0.46
1:G:93:LYS:HE3	1:T:95:PHE:CE2	2.51	0.46
1:P:187:GLU:HA	1:Q:149:ARG:HH22	1.76	0.46
1:U:49:ASP:OD1	1:U:49:ASP:N	2.44	0.46
1:V:46:VAL:HG12	1:V:152:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:58:GLU:O	1:V:62:ARG:HG3	2.16	0.46
1:J:126:LEU:HD11	1:J:154:GLY:CA	2.46	0.46
1:L:102:TYR:C	1:L:102:TYR:CD1	2.90	0.46
1:M:76:LEU:O	1:M:78:PRO:HD3	2.15	0.46
1:M:122:GLY:O	1:M:125:LEU:HB3	2.16	0.46
1:S:54:CYS:SG	1:V:64:GLU:HB3	2.56	0.46
1:S:73:LEU:HD13	1:S:111:MET:HG2	1.97	0.46
1:U:175:VAL:HG12	1:U:177:TRP:HD1	1.80	0.46
1:A:38:THR:HG23	1:A:186:TYR:CZ	2.50	0.46
1:A:52:GLN:CD	1:D:180:HIS:CD2	2.87	0.46
1:A:77:GLN:HG3	1:D:177:TRP:CZ2	2.51	0.46
1:H:85:GLN:HB2	1:H:167:PHE:CZ	2.51	0.46
1:I:74:LYS:HG2	1:I:169:PHE:CE1	2.50	0.46
1:M:73:LEU:HA	1:M:110:GLY:O	2.16	0.46
1:U:110:GLY:O	1:U:111:MET:HG3	2.16	0.46
1:V:74:LYS:NZ	1:V:76:LEU:HD13	2.31	0.46
1:A:60:ILE:CB	1:D:57:GLY:HA2	2.36	0.46
1:E:130:ASN:ND2	1:E:132:ALA:HB3	2.30	0.46
1:H:148:GLY:HA3	1:I:187:GLU:CG	2.40	0.46
1:I:125:LEU:O	1:I:138:THR:HB	2.16	0.46
1:I:126:LEU:O	1:I:140:ARG:HG3	2.16	0.46
1:J:62:ARG:NH2	1:J:142:ASP:OD2	2.49	0.46
1:K:62:ARG:HD2	1:K:139:ILE:HD11	1.98	0.46
1:M:53:ARG:CG	1:N:184:GLN:CB	2.73	0.46
1:N:53:ARG:HH12	1:N:144:ALA:HA	1.79	0.46
1:P:56:VAL:CG1	1:P:109:VAL:HG21	2.46	0.46
1:T:80:ALA:O	1:T:84:GLN:N	2.36	0.46
1:W:40:GLU:OE2	1:W:119:VAL:HG23	2.16	0.46
1:C:48:PRO:HG2	1:C:102:TYR:O	2.16	0.45
1:E:55:LEU:HD11	1:E:143:PHE:HB3	1.97	0.45
1:H:72:ALA:HB3	1:H:174:LEU:CD2	2.46	0.45
1:K:65:LYS:HD2	1:L:143:PHE:HE1	1.80	0.45
1:M:68:TYR:CE1	1:O:145:VAL:HG12	2.51	0.45
1:N:76:LEU:HD21	1:N:168:TRP:HZ3	1.80	0.45
1:P:66:LYS:NZ	1:Q:144:ALA:O	2.41	0.45
1:S:150:ASN:O	1:S:152:CYS:N	2.40	0.45
1:T:39:SER:O	1:T:114:GLU:HG3	2.16	0.45
1:T:140:ARG:NH2	1:T:152:CYS:O	2.46	0.45
1:W:73:LEU:HD11	1:W:109:VAL:HG13	1.97	0.45
1:A:116:LYS:HB2	1:C:145:VAL:CG2	2.46	0.45
1:B:73:LEU:HB3	1:E:75:MET:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:VAL:HG13	1:E:77:GLN:CB	2.45	0.45
1:H:60:ILE:HG23	1:H:113:TRP:HZ2	1.82	0.45
1:H:145:VAL:HG22	1:I:185:VAL:CG1	2.38	0.45
1:I:40:GLU:HG2	1:I:118:VAL:HG12	1.97	0.45
1:P:72:ALA:CB	1:P:174:LEU:HD13	2.46	0.45
1:Q:41:ARG:NH2	1:Q:165:ILE:HD13	2.31	0.45
1:R:68:TYR:CD2	1:R:118:VAL:HG23	2.51	0.45
1:R:91:ALA:HA	1:R:96:TYR:CE1	2.52	0.45
1:R:140:ARG:HE	1:R:150:ASN:HD22	1.65	0.45
1:X:42:THR:OG1	1:X:155:SER:HB2	2.17	0.45
1:B:89:ASP:O	1:B:93:LYS:NZ	2.46	0.45
1:E:76:LEU:HD21	1:E:168:TRP:HZ3	1.82	0.45
1:G:75:MET:HE3	1:J:70:LEU:HD23	1.99	0.45
1:H:179:SER:O	1:H:182:VAL:HB	2.17	0.45
1:M:64:GLU:HG2	1:M:113:TRP:HH2	1.81	0.45
1:M:180:HIS:CD2	1:R:184:GLN:HG3	2.51	0.45
1:R:97:LYS:HD2	1:R:97:LYS:HA	1.76	0.45
1:A:73:LEU:HG	1:D:73:LEU:HD21	1.96	0.45
1:C:49:ASP:HB3	1:C:149:ARG:HD2	1.97	0.45
1:C:63:PHE:O	1:C:66:LYS:HB3	2.17	0.45
1:D:44:ILE:HD13	1:D:154:GLY:HA3	1.98	0.45
1:D:131:PRO:HB2	1:D:145:VAL:O	2.16	0.45
1:F:62:ARG:HA	1:F:65:LYS:HG2	1.97	0.45
1:I:93:LYS:HG2	1:I:95:PHE:CZ	2.51	0.45
1:J:184:GLN:O	1:K:53:ARG:HD2	2.17	0.45
1:K:48:PRO:HB3	1:K:106:GLY:CA	2.43	0.45
1:M:67:GLY:O	1:O:145:VAL:HG11	2.16	0.45
1:O:49:ASP:OD2	1:O:151:VAL:N	2.47	0.45
1:S:71:VAL:CG1	1:S:174:LEU:HB3	2.44	0.45
1:S:180:HIS:CD2	1:V:52:GLN:HB3	2.49	0.45
1:T:167:PHE:CD2	1:T:168:TRP:CD1	3.05	0.45
1:U:95:PHE:CD1	1:U:95:PHE:C	2.90	0.45
1:V:85:GLN:CB	1:V:167:PHE:CE1	3.00	0.45
1:B:57:GLY:O	1:E:57:GLY:CA	2.65	0.45
1:T:116:LYS:HB2	1:T:186:TYR:CE1	2.44	0.45
1:V:103:PHE:HE2	1:V:168:TRP:CH2	2.34	0.45
1:G:43:PHE:HE1	1:G:169:PHE:CE2	2.34	0.45
1:G:65:LYS:HB3	1:I:143:PHE:HE1	1.82	0.45
1:J:41:ARG:HD3	1:J:165:ILE:HD13	1.99	0.45
1:M:93:LYS:HB3	1:M:95:PHE:CE2	2.52	0.45
1:N:180:HIS:NE2	1:P:184:GLN:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:53:ARG:O	1:P:55:LEU:HG	2.17	0.45
1:R:55:LEU:HD21	1:R:143:PHE:CD2	2.52	0.45
1:R:63:PHE:HB2	1:R:113:TRP:CZ2	2.52	0.45
1:C:170:LYS:HB2	1:C:173:GLU:HG3	1.98	0.45
1:J:51:VAL:HG22	1:J:75:MET:HE1	1.99	0.45
1:J:95:PHE:CD1	1:J:96:TYR:N	2.85	0.45
1:L:49:ASP:OD1	1:L:49:ASP:N	2.39	0.45
1:L:112:VAL:HG23	1:L:169:PHE:CE2	2.52	0.45
1:R:78:PRO:HB3	1:R:168:TRP:HH2	1.79	0.45
1:G:175:VAL:CG2	1:J:76:LEU:HA	2.46	0.45
1:H:93:LYS:CA	1:S:92:SER:O	2.65	0.45
1:H:99:LEU:CG	1:H:103:PHE:CE2	2.88	0.45
1:I:103:PHE:HE2	1:I:168:TRP:HH2	1.65	0.45
1:L:83:ALA:CB	1:L:100:VAL:HG13	2.47	0.45
1:O:47:LYS:HB3	1:O:48:PRO:HD2	1.97	0.45
1:P:184:GLN:O	1:Q:149:ARG:HD2	2.16	0.45
1:Q:109:VAL:HG11	1:Q:111:MET:HE1	1.98	0.45
1:R:140:ARG:NE	1:R:150:ASN:HD22	2.14	0.45
1:S:49:ASP:CA	1:T:184:GLN:NE2	2.74	0.45
1:T:150:ASN:O	1:T:152:CYS:N	2.43	0.45
1:U:77:GLN:NE2	1:U:104:SER:O	2.50	0.45
1:U:95:PHE:C	1:U:95:PHE:HD1	2.20	0.45
1:A:57:GLY:CA	1:D:61:GLN:HB2	2.47	0.45
1:B:42:THR:HG22	1:B:118:VAL:HG22	1.99	0.45
1:G:115:GLY:HA2	1:G:186:TYR:OH	2.17	0.45
1:J:74:LYS:HG2	1:J:169:PHE:CZ	2.52	0.45
1:J:135:LEU:HD13	1:L:135:LEU:HD13	1.97	0.45
1:M:161:ALA:O	1:M:165:ILE:N	2.47	0.45
1:N:57:GLY:N	1:Q:64:GLU:OE1	2.50	0.45
1:O:82:GLN:HA	1:O:167:PHE:HZ	1.81	0.45
1:T:162:LYS:O	1:T:165:ILE:HB	2.17	0.45
1:V:56:VAL:CG1	1:V:109:VAL:HG21	2.47	0.45
1:A:70:LEU:HD21	1:A:73:LEU:HB2	1.99	0.45
1:A:95:PHE:HE1	1:A:99:LEU:HD22	1.82	0.45
1:A:181:SER:O	1:A:185:VAL:HG23	2.17	0.45
1:E:167:PHE:HD2	1:E:168:TRP:CD1	2.34	0.45
1:H:58:GLU:HG2	1:H:143:PHE:CE2	2.47	0.45
1:U:75:MET:HE2	1:X:70:LEU:HD21	1.99	0.45
1:V:128:ALA:O	1:V:140:ARG:HD2	2.17	0.45
1:A:60:ILE:HG22	1:D:57:GLY:N	2.32	0.44
1:A:91:ALA:HA	1:A:96:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HD23	1:C:139:ILE:HD12	1.99	0.44
1:D:103:PHE:CE2	1:D:168:TRP:HH2	2.34	0.44
1:E:37:MET:HG3	1:E:39:SER:H	1.82	0.44
1:H:64:GLU:CD	1:K:57:GLY:H	2.20	0.44
1:I:55:LEU:O	1:I:59:ILE:HD12	2.18	0.44
1:I:73:LEU:CD1	1:I:109:VAL:HG12	2.46	0.44
1:L:164:GLU:O	1:L:168:TRP:N	2.43	0.44
1:M:130:ASN:HA	1:M:131:PRO:HD3	1.81	0.44
1:N:75:MET:SD	1:N:107:PRO:HB2	2.58	0.44
1:O:41:ARG:O	1:O:118:VAL:HG13	2.17	0.44
1:P:86:HIS:HB2	1:P:168:TRP:HE1	1.82	0.44
1:T:62:ARG:HH21	1:T:143:PHE:HE2	1.64	0.44
1:C:90:LEU:HD13	1:C:93:LYS:HZ2	1.83	0.44
1:F:71:VAL:HB	1:F:112:VAL:HB	1.98	0.44
1:G:41:ARG:HG3	1:G:114:GLU:HG3	1.98	0.44
1:N:177:TRP:CG	1:Q:107:PRO:HG3	2.51	0.44
1:N:184:GLN:HG2	1:P:180:HIS:HD2	1.80	0.44
1:T:64:GLU:OE2	1:W:55:LEU:C	2.56	0.44
1:T:82:GLN:O	1:T:167:PHE:HE2	2.00	0.44
1:A:66:LYS:HE2	1:A:68:TYR:CZ	2.52	0.44
1:A:122:GLY:O	1:A:126:LEU:HG	2.17	0.44
1:B:64:GLU:C	1:E:54:CYS:HG	2.20	0.44
1:C:62:ARG:O	1:C:66:LYS:HB2	2.17	0.44
1:C:90:LEU:CB	1:C:93:LYS:HD2	2.08	0.44
1:D:63:PHE:O	1:D:68:TYR:HB2	2.17	0.44
1:E:86:HIS:HD2	1:E:87:TYR:CE2	2.35	0.44
1:I:90:LEU:O	1:I:96:TYR:CD1	2.71	0.44
1:V:103:PHE:HE2	1:V:168:TRP:HH2	1.64	0.44
1:A:77:GLN:HB2	1:D:177:TRP:HE1	1.83	0.44
1:C:90:LEU:HD22	1:C:93:LYS:HZ2	1.80	0.44
1:D:68:TYR:CE2	1:D:118:VAL:HG23	2.52	0.44
1:G:94:PRO:HD2	1:T:93:LYS:HZ3	1.81	0.44
1:M:86:HIS:HD2	1:M:87:TYR:CE2	2.36	0.44
1:O:70:LEU:HD13	1:O:113:TRP:CE2	2.53	0.44
1:V:55:LEU:HD11	1:V:143:PHE:HB3	2.00	0.44
1:W:128:ALA:N	1:W:134:SER:OG	2.51	0.44
1:A:116:LYS:CB	1:C:145:VAL:CB	2.96	0.44
1:B:42:THR:CG2	1:B:118:VAL:HG22	2.48	0.44
1:B:179:SER:HB3	1:B:182:VAL:HG23	1.99	0.44
1:F:63:PHE:HD2	1:F:68:TYR:HD2	1.64	0.44
1:F:177:TRP:CG	1:F:178:THR:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:PRO:HG2	1:I:102:TYR:O	2.18	0.44
1:K:51:VAL:HG21	1:K:107:PRO:O	2.18	0.44
1:M:184:GLN:O	1:O:49:ASP:CB	2.60	0.44
1:S:82:GLN:HA	1:S:167:PHE:CZ	2.49	0.44
1:S:90:LEU:HB3	1:S:93:LYS:HD2	1.97	0.44
1:X:158:VAL:O	1:X:162:LYS:HG2	2.18	0.44
1:L:55:LEU:HD12	1:L:151:VAL:HG21	1.99	0.44
1:M:184:GLN:OE1	1:R:180:HIS:NE2	2.51	0.44
1:N:73:LEU:HA	1:N:110:GLY:O	2.17	0.44
1:O:120:LYS:O	1:O:124:VAL:HG23	2.17	0.44
1:P:72:ALA:HB2	1:P:174:LEU:HA	2.00	0.44
1:S:84:GLN:CG	1:S:96:TYR:OH	2.66	0.44
1:S:180:HIS:NE2	1:V:52:GLN:O	2.51	0.44
1:D:66:LYS:HG3	1:E:145:VAL:HG12	2.00	0.44
1:G:180:HIS:ND1	1:L:181:SER:HA	2.33	0.44
1:J:77:GLN:NE2	1:J:104:SER:HA	2.32	0.44
1:J:185:VAL:HG22	1:K:53:ARG:CZ	2.48	0.44
1:O:47:LYS:HA	1:O:108:ILE:HD12	1.99	0.44
1:U:69:LYS:HE3	1:U:177:TRP:O	2.17	0.44
1:U:86:HIS:CD2	1:U:87:TYR:CE1	3.06	0.44
1:A:66:LYS:CA	1:C:142:ASP:O	2.61	0.44
1:C:93:LYS:HE3	1:M:93:LYS:HG2	1.96	0.44
1:D:130:ASN:HA	1:D:131:PRO:HD3	1.78	0.44
1:F:76:LEU:HD23	1:F:76:LEU:H	1.83	0.44
1:G:179:SER:HA	1:J:52:GLN:HE22	1.82	0.44
1:J:73:LEU:HD11	1:J:109:VAL:CG1	2.48	0.44
1:N:102:TYR:CD1	1:N:102:TYR:C	2.90	0.44
1:O:56:VAL:HG23	1:R:64:GLU:OE2	2.18	0.44
1:T:52:GLN:OE1	1:T:52:GLN:HA	2.17	0.44
1:T:52:GLN:NE2	1:W:177:TRP:NE1	2.65	0.44
1:B:64:GLU:OE1	1:E:56:VAL:HB	2.17	0.44
1:F:100:VAL:O	1:F:104:SER:N	2.50	0.44
1:J:52:GLN:HG3	1:L:184:GLN:CD	2.36	0.44
1:M:142:ASP:O	1:N:66:LYS:CA	2.42	0.44
1:O:77:GLN:HB2	1:R:175:VAL:CG1	2.46	0.44
1:P:59:ILE:HG12	1:P:139:ILE:CG2	2.48	0.44
1:T:126:LEU:HD11	1:T:154:GLY:HA3	2.00	0.44
1:U:75:MET:CE	1:X:73:LEU:HD23	2.47	0.44
1:V:40:GLU:HB3	1:V:118:VAL:HG12	1.99	0.44
1:M:180:HIS:NE2	1:P:52:GLN:O	2.51	0.43
1:R:46:VAL:HG23	1:R:46:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:123:ARG:HH22	1:R:156:ASP:HB3	1.83	0.43
1:A:56:VAL:O	1:A:60:ILE:HG13	2.17	0.43
1:A:149:ARG:NH2	1:B:187:GLU:HA	2.34	0.43
1:I:179:SER:CB	1:I:182:VAL:HG23	2.49	0.43
1:J:112:VAL:HG11	1:J:174:LEU:CD1	2.48	0.43
1:K:185:VAL:HG13	1:L:53:ARG:CZ	2.48	0.43
1:M:68:TYR:CD2	1:M:118:VAL:HG23	2.52	0.43
1:N:145:VAL:HG21	1:O:186:TYR:CZ	2.53	0.43
1:R:47:LYS:HB3	1:R:48:PRO:HD2	2.00	0.43
1:D:46:VAL:CG2	1:D:109:VAL:HG23	2.48	0.43
1:E:131:PRO:HG3	1:E:140:ARG:HD3	2.00	0.43
1:G:184:GLN:HG2	1:L:180:HIS:CE1	2.53	0.43
1:P:44:ILE:HG13	1:P:113:TRP:CD1	2.54	0.43
1:P:46:VAL:HG21	1:P:56:VAL:HG22	2.01	0.43
1:S:49:ASP:N	1:T:184:GLN:NE2	2.66	0.43
1:T:143:PHE:CD1	1:U:65:LYS:HB3	2.53	0.43
1:W:46:VAL:HG12	1:W:152:CYS:SG	2.58	0.43
1:G:92:SER:O	1:T:93:LYS:HA	2.19	0.43
1:I:39:SER:HA	1:I:114:GLU:HG3	2.00	0.43
1:J:144:ALA:O	1:L:66:LYS:NZ	2.39	0.43
1:K:45:ALA:HB3	1:K:153:HIS:HD2	1.84	0.43
1:T:64:GLU:HB3	1:W:54:CYS:SG	2.58	0.43
1:T:99:LEU:O	1:T:103:PHE:CD2	2.72	0.43
1:U:177:TRP:NE1	1:X:107:PRO:HG3	2.33	0.43
1:V:103:PHE:CE2	1:V:168:TRP:HH2	2.36	0.43
1:A:77:GLN:CG	1:D:177:TRP:CZ2	3.01	0.43
1:B:180:HIS:HD2	1:E:52:GLN:HG3	1.83	0.43
1:F:78:PRO:HD3	1:F:108:ILE:HG12	2.00	0.43
1:H:85:GLN:HA	1:H:88:ILE:HB	2.00	0.43
1:L:86:HIS:CE1	1:L:168:TRP:HE1	2.36	0.43
1:M:62:ARG:O	1:M:66:LYS:HB2	2.18	0.43
1:S:149:ARG:HG2	1:T:187:GLU:HG3	2.01	0.43
1:U:93:LYS:CG	1:U:94:PRO:HD2	2.48	0.43
1:V:47:LYS:HB3	1:V:48:PRO:HD2	2.00	0.43
1:A:149:ARG:HG3	1:B:185:VAL:O	2.18	0.43
1:D:56:VAL:O	1:D:60:ILE:HG13	2.18	0.43
1:J:88:ILE:HG22	1:J:163:ARG:NH2	2.31	0.43
1:K:95:PHE:CD1	1:K:99:LEU:HD13	2.53	0.43
1:B:93:LYS:NZ	1:N:93:LYS:HG2	2.34	0.43
1:E:58:GLU:HG2	1:E:143:PHE:HZ	1.79	0.43
1:H:48:PRO:HD3	1:H:108:ILE:CG1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:LEU:O	1:H:92:SER:N	2.52	0.43
1:H:90:LEU:HD22	1:H:93:LYS:NZ	2.32	0.43
1:L:48:PRO:HG3	1:L:108:ILE:HD11	2.01	0.43
1:W:81:GLU:O	1:W:84:GLN:HB2	2.18	0.43
1:W:84:GLN:HA	1:W:96:TYR:OH	2.18	0.43
1:A:177:TRP:NE1	1:D:106:GLY:C	2.72	0.43
1:A:184:GLN:OE1	1:F:180:HIS:CD2	2.72	0.43
1:D:40:GLU:HG2	1:D:119:VAL:HG23	2.00	0.43
1:D:77:GLN:NE2	1:D:104:SER:OG	2.52	0.43
1:F:70:LEU:HD11	1:F:73:LEU:HB2	2.00	0.43
1:N:123:ARG:HD3	1:N:156:ASP:HA	2.01	0.43
1:S:93:LYS:HB3	1:S:95:PHE:CE2	2.53	0.43
1:V:51:VAL:HG11	1:V:107:PRO:HG2	2.01	0.43
1:X:73:LEU:HA	1:X:110:GLY:O	2.19	0.43
1:D:70:LEU:HD21	1:D:73:LEU:HD22	2.00	0.43
1:G:177:TRP:CZ2	1:J:104:SER:O	2.72	0.43
1:M:53:ARG:HG3	1:N:184:GLN:HB3	1.88	0.43
1:T:143:PHE:CZ	1:U:65:LYS:HD2	2.53	0.43
1:W:185:VAL:HG13	1:X:145:VAL:HG22	2.01	0.43
1:A:175:VAL:HG21	1:D:75:MET:HG3	2.01	0.43
1:A:187:GLU:HG2	1:C:149:ARG:NH2	2.34	0.43
1:G:75:MET:HA	1:G:108:ILE:O	2.19	0.43
1:G:94:PRO:CG	1:T:89:ASP:O	2.48	0.43
1:G:103:PHE:CE2	1:G:168:TRP:HH2	2.37	0.43
1:L:119:VAL:HG11	1:L:157:SER:HA	2.00	0.43
1:M:44:ILE:HG21	1:M:63:PHE:CE1	2.54	0.43
1:T:57:GLY:HA3	1:W:61:GLN:HA	2.01	0.43
1:A:66:LYS:CD	1:C:142:ASP:O	2.66	0.42
1:B:75:MET:HE3	1:E:70:LEU:HD23	1.99	0.42
1:G:146:ASP:HB2	1:H:116:LYS:HZ1	1.81	0.42
1:H:93:LYS:HE3	1:S:93:LYS:HE3	2.00	0.42
1:H:126:LEU:HD11	1:H:154:GLY:HA3	2.00	0.42
1:O:128:ALA:O	1:O:140:ARG:HD2	2.18	0.42
1:R:58:GLU:OE2	1:R:62:ARG:NE	2.31	0.42
1:T:180:HIS:NE2	1:W:52:GLN:HB3	2.34	0.42
1:W:48:PRO:HD3	1:W:108:ILE:CD1	2.49	0.42
1:A:47:LYS:HB3	1:A:48:PRO:HD2	2.01	0.42
1:A:185:VAL:HG22	1:C:53:ARG:CZ	2.49	0.42
1:D:102:TYR:CZ	1:D:149:ARG:HD3	2.54	0.42
1:E:46:VAL:HG22	1:E:109:VAL:H	1.84	0.42
1:E:76:LEU:HD21	1:E:168:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:185:VAL:HG22	1:L:53:ARG:NE	2.34	0.42
1:L:146:ASP:OD1	1:L:147:VAL:N	2.52	0.42
1:N:42:THR:HG21	1:N:118:VAL:HG22	2.01	0.42
1:N:172:GLU:H	1:N:172:GLU:CD	2.22	0.42
1:Q:55:LEU:CD1	1:Q:143:PHE:HB3	2.44	0.42
1:R:73:LEU:HD13	1:R:111:MET:HG2	2.01	0.42
1:W:62:ARG:NH1	1:W:137:GLY:O	2.52	0.42
1:X:139:ILE:HG22	1:X:151:VAL:HG11	2.00	0.42
1:A:138:THR:OG1	1:A:141:GLY:N	2.52	0.42
1:A:144:ALA:O	1:B:66:LYS:CE	2.67	0.42
1:B:43:PHE:HE1	1:B:169:PHE:HE2	1.67	0.42
1:B:54:CYS:C	1:E:64:GLU:CD	2.78	0.42
1:B:126:LEU:HA	1:B:139:ILE:HB	2.01	0.42
1:H:170:LYS:HE2	1:H:173:GLU:OE2	2.18	0.42
1:I:99:LEU:O	1:I:102:TYR:HB3	2.18	0.42
1:M:70:LEU:CD2	1:P:75:MET:CE	2.94	0.42
1:N:53:ARG:NH2	1:N:143:PHE:O	2.52	0.42
1:S:176:ASN:O	1:S:177:TRP:CD1	2.72	0.42
1:V:126:LEU:HD23	1:V:139:ILE:HD13	2.00	0.42
1:X:147:VAL:O	1:X:150:ASN:ND2	2.52	0.42
1:A:66:LYS:O	1:C:53:ARG:NH2	2.51	0.42
1:B:150:ASN:O	1:B:152:CYS:N	2.44	0.42
1:E:68:TYR:N	1:E:68:TYR:CD1	2.87	0.42
1:G:93:LYS:HB3	1:G:94:PRO:HD2	2.02	0.42
1:J:186:TYR:HD1	1:K:146:ASP:OD2	2.03	0.42
1:V:44:ILE:HD13	1:V:154:GLY:CA	2.47	0.42
1:V:136:PRO:HG3	1:X:124:VAL:C	2.35	0.42
1:A:177:TRP:CD1	1:D:106:GLY:CA	3.00	0.42
1:D:68:TYR:CD2	1:D:118:VAL:HG23	2.54	0.42
1:D:84:GLN:HG2	1:D:96:TYR:OH	2.19	0.42
1:E:64:GLU:HG3	1:E:113:TRP:HH2	1.85	0.42
1:F:140:ARG:HE	1:F:150:ASN:HB2	1.84	0.42
1:G:136:PRO:HG2	1:H:138:THR:HG22	2.01	0.42
1:H:126:LEU:HD11	1:H:154:GLY:N	2.33	0.42
1:K:66:LYS:HG2	1:K:125:LEU:HD11	2.01	0.42
1:O:56:VAL:O	1:O:60:ILE:HG13	2.18	0.42
1:P:150:ASN:O	1:P:152:CYS:N	2.45	0.42
1:Q:179:SER:HB2	1:Q:182:VAL:HG23	2.01	0.42
1:T:42:THR:HG22	1:T:113:TRP:HB2	2.01	0.42
1:T:46:VAL:HG21	1:T:56:VAL:HG22	2.00	0.42
1:T:72:ALA:HB3	1:T:112:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:140:ARG:HH21	1:U:150:ASN:ND2	2.18	0.42
1:F:83:ALA:CB	1:F:100:VAL:HG13	2.49	0.42
1:G:180:HIS:NE2	1:J:53:ARG:HG2	2.34	0.42
1:H:99:LEU:CD1	1:H:103:PHE:CE2	3.03	0.42
1:H:130:ASN:HD21	1:H:132:ALA:HB3	1.83	0.42
1:I:95:PHE:CD1	1:I:95:PHE:C	2.93	0.42
1:N:116:LYS:HB2	1:N:186:TYR:HE1	1.84	0.42
1:R:59:ILE:O	1:R:62:ARG:HB2	2.19	0.42
1:S:47:LYS:O	1:S:50:GLY:N	2.47	0.42
1:T:40:GLU:HG2	1:T:41:ARG:N	2.35	0.42
1:U:47:LYS:HB3	1:U:48:PRO:HD3	1.96	0.42
1:G:73:LEU:HA	1:G:110:GLY:O	2.19	0.42
1:H:58:GLU:CA	1:K:61:GLN:OE1	2.67	0.42
1:Q:51:VAL:HG11	1:Q:107:PRO:HG2	2.01	0.42
1:S:38:THR:HA	1:S:116:LYS:HG3	2.02	0.42
1:U:93:LYS:CD	1:U:94:PRO:HD2	2.49	0.42
1:W:69:LYS:HD3	1:W:179:SER:OG	2.20	0.42
1:X:44:ILE:HA	1:X:153:HIS:O	2.19	0.42
1:A:95:PHE:CE1	1:A:99:LEU:HD22	2.54	0.42
1:D:103:PHE:HE2	1:D:168:TRP:HH2	1.67	0.42
1:L:167:PHE:HD2	1:L:168:TRP:CD1	2.38	0.42
1:O:73:LEU:HD13	1:O:111:MET:HG2	2.02	0.42
1:Q:102:TYR:CE1	1:Q:149:ARG:HD3	2.55	0.42
1:R:68:TYR:CD1	1:R:68:TYR:N	2.87	0.42
1:G:83:ALA:HB3	1:G:100:VAL:HG13	2.01	0.42
1:G:131:PRO:HG3	1:G:140:ARG:HD3	2.02	0.42
1:H:180:HIS:NE2	1:K:52:GLN:CB	2.79	0.42
1:K:93:LYS:CE	1:R:89:ASP:O	2.67	0.42
1:M:43:PHE:CD2	1:M:164:GLU:HB3	2.55	0.42
1:O:93:LYS:HG2	1:O:95:PHE:CE1	2.54	0.42
1:U:72:ALA:HB3	1:U:112:VAL:HB	2.01	0.42
1:V:51:VAL:HG22	1:V:75:MET:HE1	2.02	0.42
1:V:83:ALA:HA	1:V:86:HIS:HB3	2.00	0.42
1:E:62:ARG:HA	1:E:65:LYS:HE3	2.01	0.42
1:G:93:LYS:HE3	1:T:95:PHE:HE2	1.85	0.42
1:I:60:ILE:O	1:I:64:GLU:HG3	2.20	0.42
1:N:180:HIS:CE1	1:P:184:GLN:CG	2.96	0.42
1:U:73:LEU:HB3	1:X:75:MET:CB	2.50	0.42
1:D:126:LEU:HD23	1:D:139:ILE:HD12	2.02	0.41
1:H:86:HIS:HB2	1:H:168:TRP:HE1	1.85	0.41
1:J:119:VAL:HG13	1:J:155:SER:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:127:GLY:O	1:L:140:ARG:NH1	2.53	0.41
1:N:53:ARG:HD2	1:O:184:GLN:O	2.20	0.41
1:N:99:LEU:HG	1:N:103:PHE:CE2	2.55	0.41
1:P:46:VAL:HG22	1:P:109:VAL:HB	2.02	0.41
1:P:75:MET:SD	1:P:107:PRO:HB2	2.59	0.41
1:Q:112:VAL:HG11	1:Q:174:LEU:HD22	2.01	0.41
1:S:102:TYR:OH	1:S:149:ARG:HA	2.20	0.41
1:B:97:LYS:HA	1:B:97:LYS:HD2	1.91	0.41
1:D:170:LYS:HB2	1:D:173:GLU:HG3	2.02	0.41
1:I:92:SER:O	1:U:93:LYS:HD2	2.20	0.41
1:K:62:ARG:HA	1:K:65:LYS:HG2	2.01	0.41
1:L:83:ALA:HB3	1:L:100:VAL:HG13	2.00	0.41
1:M:171:PRO:C	1:M:173:GLU:N	2.73	0.41
1:R:102:TYR:CE1	1:R:149:ARG:HD3	2.54	0.41
1:S:149:ARG:NH2	1:T:187:GLU:CA	2.73	0.41
1:T:183:LYS:HB3	1:V:180:HIS:CE1	2.55	0.41
1:U:84:GLN:HG2	1:U:96:TYR:OH	2.20	0.41
1:F:63:PHE:CD2	1:F:68:TYR:HD2	2.38	0.41
1:K:41:ARG:HH21	1:K:162:LYS:NZ	2.17	0.41
1:K:72:ALA:HB3	1:K:112:VAL:CG2	2.51	0.41
1:K:78:PRO:HB3	1:K:168:TRP:CZ3	2.55	0.41
1:L:73:LEU:HD11	1:L:109:VAL:CG1	2.49	0.41
1:L:179:SER:O	1:L:182:VAL:HB	2.20	0.41
1:N:49:ASP:OD2	1:N:149:ARG:HB3	2.20	0.41
1:R:71:VAL:HG13	1:R:175:VAL:O	2.20	0.41
1:R:116:LYS:HD2	1:R:116:LYS:HA	1.83	0.41
1:V:46:VAL:HG22	1:V:109:VAL:HB	2.01	0.41
1:X:126:LEU:HD11	1:X:154:GLY:HA3	2.03	0.41
1:A:42:THR:OG1	1:A:155:SER:HB2	2.21	0.41
1:C:89:ASP:O	1:M:94:PRO:CD	2.69	0.41
1:G:73:LEU:O	1:J:74:LYS:HA	2.20	0.41
1:I:177:TRP:CZ3	1:I:179:SER:HA	2.55	0.41
1:L:161:ALA:O	1:L:165:ILE:HG13	2.20	0.41
1:M:106:GLY:HA2	1:P:177:TRP:NE1	2.35	0.41
1:P:145:VAL:HG13	1:R:66:LYS:O	2.19	0.41
1:S:126:LEU:O	1:S:140:ARG:HB2	2.21	0.41
1:V:53:ARG:NE	1:X:185:VAL:HG22	2.35	0.41
1:W:48:PRO:HD3	1:W:108:ILE:HD11	2.01	0.41
1:W:62:ARG:HA	1:W:65:LYS:HE3	2.02	0.41
1:G:153:HIS:CE1	1:G:154:GLY:O	2.73	0.41
1:J:146:ASP:OD1	1:J:147:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:LEU:HD13	1:K:111:MET:HG2	2.02	0.41
1:N:71:VAL:HB	1:N:112:VAL:HG12	2.01	0.41
1:N:119:VAL:HG11	1:N:157:SER:O	2.21	0.41
1:O:84:GLN:HG2	1:O:96:TYR:OH	2.20	0.41
1:P:184:GLN:HB3	1:Q:49:ASP:HA	2.01	0.41
1:Q:62:ARG:HD2	1:Q:139:ILE:HG12	2.02	0.41
1:V:149:ARG:CB	1:X:185:VAL:O	2.69	0.41
1:V:150:ASN:O	1:V:151:VAL:HG12	2.20	0.41
1:W:58:GLU:HA	1:W:58:GLU:OE2	2.21	0.41
1:A:179:SER:N	1:D:52:GLN:OE1	2.53	0.41
1:B:70:LEU:HB3	1:E:75:MET:HE1	2.01	0.41
1:C:47:LYS:CB	1:C:48:PRO:CD	2.87	0.41
1:C:85:GLN:NE2	1:C:88:ILE:HD12	2.29	0.41
1:C:126:LEU:HA	1:C:139:ILE:HB	2.01	0.41
1:E:68:TYR:N	1:E:68:TYR:HD1	2.19	0.41
1:G:124:VAL:HG12	1:I:136:PRO:CD	2.50	0.41
1:G:185:VAL:HG22	1:I:53:ARG:CD	2.44	0.41
1:O:145:VAL:CG2	1:O:146:ASP:N	2.84	0.41
1:R:146:ASP:OD1	1:R:147:VAL:N	2.53	0.41
1:A:74:LYS:NZ	1:A:76:LEU:HD13	2.35	0.41
1:A:92:SER:HB2	1:O:92:SER:C	2.41	0.41
1:A:116:LYS:HB2	1:C:145:VAL:CB	2.51	0.41
1:A:169:PHE:HD1	1:A:173:GLU:OE1	2.03	0.41
1:C:48:PRO:HB3	1:C:106:GLY:HA3	2.02	0.41
1:H:56:VAL:HB	1:K:64:GLU:OE2	2.20	0.41
1:H:155:SER:OG	1:H:161:ALA:HA	2.21	0.41
1:N:83:ALA:O	1:N:86:HIS:HB3	2.21	0.41
1:P:41:ARG:HD3	1:P:165:ILE:HD13	2.02	0.41
1:T:47:LYS:HE2	1:T:103:PHE:HE1	1.83	0.41
1:T:180:HIS:CD2	1:W:52:GLN:HB3	2.56	0.41
1:W:111:MET:HE3	1:W:113:TRP:HE1	1.85	0.41
1:A:175:VAL:HG12	1:A:177:TRP:CD1	2.55	0.41
1:A:178:THR:N	1:D:52:GLN:HE22	2.18	0.41
1:F:62:ARG:HA	1:F:65:LYS:HE3	2.03	0.41
1:I:126:LEU:HB3	1:I:140:ARG:CZ	2.51	0.41
1:P:66:LYS:HE3	1:Q:144:ALA:O	2.20	0.41
1:T:73:LEU:HA	1:T:110:GLY:O	2.20	0.41
1:U:50:GLY:N	1:U:151:VAL:HG23	2.35	0.41
1:V:63:PHE:HD2	1:V:68:TYR:HD2	1.68	0.41
1:W:137:GLY:C	1:X:136:PRO:HB2	2.41	0.41
1:X:130:ASN:HA	1:X:131:PRO:HD2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:HG2	1:B:138:THR:HG22	2.02	0.41
1:A:171:PRO:C	1:A:173:GLU:N	2.74	0.41
1:B:76:LEU:HD23	1:B:76:LEU:H	1.84	0.41
1:C:93:LYS:HG3	1:M:92:SER:O	2.21	0.41
1:E:122:GLY:O	1:E:125:LEU:HB2	2.20	0.41
1:E:126:LEU:HD21	1:E:152:CYS:HB3	2.03	0.41
1:E:140:ARG:HD3	1:E:150:ASN:HB2	2.02	0.41
1:G:62:ARG:CG	1:G:139:ILE:HD11	2.50	0.41
1:H:58:GLU:HB2	1:K:61:GLN:OE1	2.20	0.41
1:H:61:GLN:NE2	1:K:58:GLU:OE2	2.54	0.41
1:K:64:GLU:HG3	1:K:113:TRP:HH2	1.86	0.41
1:M:61:GLN:OE1	1:P:58:GLU:HG2	2.20	0.41
1:M:73:LEU:HD23	1:P:75:MET:CB	2.36	0.41
1:M:186:TYR:CD1	1:O:146:ASP:HB2	2.56	0.41
1:P:66:LYS:HZ2	1:Q:143:PHE:N	2.18	0.41
1:R:46:VAL:CG2	1:R:109:VAL:HB	2.50	0.41
1:S:115:GLY:HA2	1:S:186:TYR:OH	2.21	0.41
1:S:128:ALA:O	1:S:140:ARG:HD2	2.21	0.41
1:T:96:TYR:O	1:T:100:VAL:HG23	2.20	0.41
1:U:49:ASP:O	1:U:53:ARG:N	2.54	0.41
1:W:47:LYS:HB3	1:W:48:PRO:CD	2.50	0.41
1:X:93:LYS:HA	1:X:94:PRO:HD2	1.74	0.41
1:A:59:ILE:HG12	1:A:139:ILE:HD13	2.02	0.41
1:G:37:MET:O	1:G:40:GLU:HB2	2.21	0.41
1:G:130:ASN:HA	1:G:131:PRO:HD3	1.90	0.41
1:J:153:HIS:NE2	1:J:164:GLU:OE1	2.54	0.41
1:K:42:THR:HG22	1:K:118:VAL:HG22	2.02	0.41
1:K:55:LEU:HD12	1:K:151:VAL:HG21	2.01	0.41
1:M:102:TYR:CE1	1:M:149:ARG:HD3	2.56	0.41
1:Q:62:ARG:HA	1:Q:65:LYS:HZ2	1.86	0.41
1:Q:109:VAL:CG1	1:Q:111:MET:HE1	2.51	0.41
1:R:55:LEU:O	1:R:56:VAL:C	2.59	0.41
1:R:86:HIS:HD2	1:R:87:TYR:CZ	2.35	0.41
1:S:140:ARG:NH2	1:S:152:CYS:O	2.54	0.41
1:A:177:TRP:HZ2	1:D:77:GLN:CD	2.25	0.40
1:D:53:ARG:O	1:D:54:CYS:HB3	2.21	0.40
1:K:39:SER:O	1:K:41:ARG:HD3	2.21	0.40
1:K:63:PHE:HB3	1:K:113:TRP:CZ3	2.55	0.40
1:M:151:VAL:HG13	1:M:152:CYS:HB2	2.03	0.40
1:Q:109:VAL:HG12	1:Q:111:MET:CE	2.51	0.40
1:S:70:LEU:CD2	1:V:75:MET:HE3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:47:LYS:HE2	1:T:103:PHE:CE1	2.56	0.40
1:X:45:ALA:O	1:X:153:HIS:N	2.43	0.40
1:X:63:PHE:O	1:X:66:LYS:HB3	2.21	0.40
1:A:52:GLN:NE2	1:D:179:SER:HA	2.28	0.40
1:A:85:GLN:O	1:A:163:ARG:NH2	2.54	0.40
1:B:50:GLY:HA2	1:B:151:VAL:HG23	2.02	0.40
1:D:72:ALA:HB3	1:D:112:VAL:HB	2.02	0.40
1:G:58:GLU:HG2	1:J:61:GLN:NE2	2.36	0.40
1:H:86:HIS:CD2	1:H:87:TYR:CE2	3.10	0.40
1:H:123:ARG:HD3	1:H:156:ASP:HA	2.03	0.40
1:H:136:PRO:HG2	1:I:125:LEU:HD23	2.03	0.40
1:N:63:PHE:HD2	1:N:68:TYR:HD2	1.69	0.40
1:O:41:ARG:O	1:O:119:VAL:HG23	2.22	0.40
1:Q:62:ARG:HA	1:Q:65:LYS:NZ	2.36	0.40
1:R:43:PHE:HB2	1:R:165:ILE:HG13	2.03	0.40
1:T:120:LYS:CG	1:T:123:ARG:HH21	2.34	0.40
1:A:177:TRP:CZ3	1:D:105:SER:C	2.94	0.40
1:B:52:GLN:HB3	1:E:180:HIS:HD2	1.87	0.40
1:B:54:CYS:SG	1:E:65:LYS:N	2.94	0.40
1:E:102:TYR:C	1:E:104:SER:H	2.24	0.40
1:G:109:VAL:O	1:G:109:VAL:HG12	2.21	0.40
1:I:73:LEU:HD11	1:I:109:VAL:CG1	2.50	0.40
1:L:121:GLY:O	1:L:125:LEU:HG	2.20	0.40
1:O:87:TYR:HB3	1:O:90:LEU:HD12	2.02	0.40
1:P:47:LYS:CB	1:P:48:PRO:HD3	2.49	0.40
1:P:88:ILE:CG2	1:P:163:ARG:NH2	2.83	0.40
1:Q:130:ASN:HA	1:Q:131:PRO:HD3	1.86	0.40
1:U:69:LYS:HD3	1:U:114:GLU:OE2	2.22	0.40
1:A:73:LEU:HD21	1:D:60:ILE:HD11	2.04	0.40
1:A:77:GLN:CG	1:D:177:TRP:HZ2	2.34	0.40
1:A:180:HIS:CD2	1:D:53:ARG:CG	3.00	0.40
1:H:46:VAL:HA	1:H:152:CYS:HA	2.03	0.40
1:H:145:VAL:HG23	1:H:146:ASP:HB2	2.03	0.40
1:I:78:PRO:HG3	1:I:108:ILE:HG13	2.03	0.40
1:K:42:THR:HB	1:K:119:VAL:HG22	2.02	0.40
1:Q:47:LYS:HB3	1:Q:48:PRO:HD3	2.03	0.40
1:R:73:LEU:HA	1:R:110:GLY:O	2.21	0.40
1:R:135:LEU:HA	1:R:136:PRO:HD3	1.96	0.40
1:S:38:THR:HG23	1:S:186:TYR:CE1	2.56	0.40
1:T:51:VAL:HG11	1:T:107:PRO:HG2	2.03	0.40
1:T:64:GLU:O	1:W:54:CYS:SG	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:126:LEU:HA	1:U:139:ILE:HB	2.04	0.40
1:V:137:GLY:CA	1:X:137:GLY:HA3	2.51	0.40
1:A:177:TRP:CD1	1:D:107:PRO:HG3	2.49	0.40
1:A:178:THR:O	1:D:52:GLN:CD	2.59	0.40
1:E:86:HIS:HB2	1:E:167:PHE:CE2	2.57	0.40
1:G:42:THR:HG23	1:G:44:ILE:HG12	2.03	0.40
1:G:143:PHE:HA	1:H:66:LYS:HA	2.03	0.40
1:H:93:LYS:HZ2	1:S:94:PRO:HD2	1.81	0.40
1:M:65:LYS:N	1:P:54:CYS:SG	2.95	0.40
1:M:138:THR:HG22	1:O:136:PRO:HB2	2.03	0.40
1:M:180:HIS:HD2	1:P:52:GLN:HB3	1.87	0.40
1:N:47:LYS:HE3	1:N:153:HIS:HB2	2.03	0.40
1:Q:157:SER:O	1:Q:160:SER:HB2	2.21	0.40
1:T:72:ALA:HB2	1:T:174:LEU:HD23	2.02	0.40
1:T:177:TRP:CD1	1:W:107:PRO:HG3	2.56	0.40
1:U:57:GLY:HA2	1:X:57:GLY:HA2	2.04	0.40
1:X:74:LYS:HE3	1:X:169:PHE:CD1	2.56	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:M:172:GLU:OE1	1:O:78:PRO:O[3_555]	2.07	0.13

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	12	48
1	B	149/151 (99%)	141 (95%)	7 (5%)	1 (1%)	22	61
1	C	149/151 (99%)	145 (97%)	3 (2%)	1 (1%)	22	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	12	48
1	E	149/151 (99%)	141 (95%)	6 (4%)	2 (1%)	12	48
1	F	149/151 (99%)	145 (97%)	3 (2%)	1 (1%)	22	61
1	G	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
1	H	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	12	48
1	I	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	12	48
1	J	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
1	K	149/151 (99%)	141 (95%)	7 (5%)	1 (1%)	22	61
1	L	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	12	48
1	M	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	22	61
1	N	149/151 (99%)	132 (89%)	13 (9%)	4 (3%)	5	33
1	O	149/151 (99%)	135 (91%)	12 (8%)	2 (1%)	12	48
1	P	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	12	48
1	Q	149/151 (99%)	138 (93%)	9 (6%)	2 (1%)	12	48
1	R	149/151 (99%)	136 (91%)	10 (7%)	3 (2%)	7	39
1	S	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	12	48
1	T	149/151 (99%)	137 (92%)	8 (5%)	4 (3%)	5	33
1	U	149/151 (99%)	138 (93%)	8 (5%)	3 (2%)	7	39
1	V	149/151 (99%)	132 (89%)	15 (10%)	2 (1%)	12	48
1	W	149/151 (99%)	143 (96%)	4 (3%)	2 (1%)	12	48
1	X	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	22	61
All	All	3576/3624 (99%)	3343 (94%)	189 (5%)	44 (1%)	13	50

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	VAL
1	F	151	VAL
1	L	151	VAL
1	R	56	VAL
1	R	151	VAL
1	U	91	ALA
1	U	151	VAL
1	V	117	GLY
1	W	151	VAL

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Mol	Chain	Res	Type
1	B	151	VAL
1	D	91	ALA
1	H	91	ALA
1	M	91	ALA
1	N	151	VAL
1	R	182	VAL
1	T	54	CYS
1	X	151	VAL
1	A	172	GLU
1	Q	151	VAL
1	U	38	THR
1	E	54	CYS
1	E	91	ALA
1	H	151	VAL
1	L	103	PHE
1	O	95	PHE
1	S	86	HIS
1	S	151	VAL
1	I	151	VAL
1	I	182	VAL
1	N	96	TYR
1	N	103	PHE
1	N	182	VAL
1	O	151	VAL
1	T	91	ALA
1	D	151	VAL
1	K	151	VAL
1	Q	118	VAL
1	T	67	GLY
1	T	151	VAL
1	C	151	VAL
1	P	56	VAL
1	V	151	VAL
1	W	145	VAL
1	P	151	VAL

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	A	126/126 (100%)	119 (94%)	7 (6%)	21 54
1	B	126/126 (100%)	121 (96%)	5 (4%)	31 64
1	C	126/126 (100%)	112 (89%)	14 (11%)	6 28
1	D	126/126 (100%)	117 (93%)	9 (7%)	14 46
1	E	126/126 (100%)	119 (94%)	7 (6%)	21 54
1	F	126/126 (100%)	118 (94%)	8 (6%)	18 51
1	G	126/126 (100%)	122 (97%)	4 (3%)	39 69
1	H	126/126 (100%)	114 (90%)	12 (10%)	8 34
1	I	126/126 (100%)	121 (96%)	5 (4%)	31 64
1	J	126/126 (100%)	121 (96%)	5 (4%)	31 64
1	K	126/126 (100%)	114 (90%)	12 (10%)	8 34
1	L	126/126 (100%)	118 (94%)	8 (6%)	18 51
1	M	126/126 (100%)	116 (92%)	10 (8%)	12 41
1	N	126/126 (100%)	116 (92%)	10 (8%)	12 41
1	O	126/126 (100%)	113 (90%)	13 (10%)	7 32
1	P	126/126 (100%)	118 (94%)	8 (6%)	18 51
1	Q	126/126 (100%)	121 (96%)	5 (4%)	31 64
1	R	126/126 (100%)	115 (91%)	11 (9%)	10 38
1	S	126/126 (100%)	120 (95%)	6 (5%)	25 60
1	T	126/126 (100%)	124 (98%)	2 (2%)	62 83
1	U	126/126 (100%)	121 (96%)	5 (4%)	31 64
1	V	126/126 (100%)	120 (95%)	6 (5%)	25 60
1	W	126/126 (100%)	119 (94%)	7 (6%)	21 54
1	X	126/126 (100%)	119 (94%)	7 (6%)	21 54
All	All	3024/3024 (100%)	2838 (94%)	186 (6%)	18 51

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	76	LEU
1	A	85	GLN
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	151	VAL
1	A	179	SER
1	A	182	VAL
1	B	41	ARG
1	B	76	LEU
1	B	102	TYR
1	B	139	ILE
1	B	160	SER
1	C	41	ARG
1	C	70	LEU
1	C	76	LEU
1	C	81	GLU
1	C	88	ILE
1	C	89	ASP
1	C	92	SER
1	C	102	TYR
1	C	114	GLU
1	C	120	LYS
1	C	124	VAL
1	C	126	LEU
1	C	147	VAL
1	C	179	SER
1	D	54	CYS
1	D	62	ARG
1	D	79	SER
1	D	114	GLU
1	D	124	VAL
1	D	126	LEU
1	D	151	VAL
1	D	153	HIS
1	D	155	SER
1	E	38	THR
1	E	41	ARG
1	E	68	TYR
1	E	99	LEU
1	E	120	LYS
1	E	151	VAL
1	E	179	SER
1	F	41	ARG
1	F	70	LEU
1	F	102	TYR
1	F	112	VAL

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Mol	Chain	Res	Type
1	F	133	ASP
1	F	134	SER
1	F	145	VAL
1	F	151	VAL
1	G	41	ARG
1	G	46	VAL
1	G	90	LEU
1	G	143	PHE
1	H	38	THR
1	H	41	ARG
1	H	44	ILE
1	H	54	CYS
1	H	102	TYR
1	H	129	THR
1	H	134	SER
1	H	160	SER
1	H	165	ILE
1	H	170	LYS
1	H	174	LEU
1	H	182	VAL
1	I	85	GLN
1	I	95	PHE
1	I	135	LEU
1	I	151	VAL
1	I	179	SER
1	J	42	THR
1	J	90	LEU
1	J	95	PHE
1	J	114	GLU
1	J	129	THR
1	K	41	ARG
1	K	70	LEU
1	K	73	LEU
1	K	76	LEU
1	K	92	SER
1	K	102	TYR
1	K	114	GLU
1	K	120	LYS
1	K	160	SER
1	K	165	ILE
1	K	174	LEU
1	K	179	SER

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Mol	Chain	Res	Type
1	L	41	ARG
1	L	49	ASP
1	L	62	ARG
1	L	76	LEU
1	L	81	GLU
1	L	102	TYR
1	L	133	ASP
1	L	182	VAL
1	M	41	ARG
1	M	52	GLN
1	M	62	ARG
1	M	119	VAL
1	M	151	VAL
1	M	156	ASP
1	M	158	VAL
1	M	172	GLU
1	M	179	SER
1	M	182	VAL
1	N	41	ARG
1	N	88	ILE
1	N	90	LEU
1	N	96	TYR
1	N	102	TYR
1	N	125	LEU
1	N	147	VAL
1	N	149	ARG
1	N	151	VAL
1	N	165	ILE
1	O	41	ARG
1	O	64	GLU
1	O	71	VAL
1	O	79	SER
1	O	81	GLU
1	O	85	GLN
1	O	90	LEU
1	O	95	PHE
1	O	98	ASP
1	O	109	VAL
1	O	114	GLU
1	O	129	THR
1	O	160	SER
1	P	49	ASP

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Mol	Chain	Res	Type
1	P	68	TYR
1	P	76	LEU
1	P	112	VAL
1	P	147	VAL
1	P	156	ASP
1	P	174	LEU
1	P	179	SER
1	Q	41	ARG
1	Q	76	LEU
1	Q	160	SER
1	Q	174	LEU
1	Q	179	SER
1	R	37	MET
1	R	41	ARG
1	R	76	LEU
1	R	81	GLU
1	R	126	LEU
1	R	133	ASP
1	R	140	ARG
1	R	145	VAL
1	R	151	VAL
1	R	153	HIS
1	R	185	VAL
1	S	41	ARG
1	S	77	GLN
1	S	99	LEU
1	S	109	VAL
1	S	175	VAL
1	S	179	SER
1	T	41	ARG
1	T	116	LYS
1	U	41	ARG
1	U	74	LYS
1	U	81	GLU
1	U	95	PHE
1	U	179	SER
1	V	41	ARG
1	V	55	LEU
1	V	133	ASP
1	V	160	SER
1	V	173	GLU
1	V	179	SER

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Mol	Chain	Res	Type
1	W	41	ARG
1	W	62	ARG
1	W	120	LYS
1	W	145	VAL
1	W	151	VAL
1	W	153	HIS
1	W	179	SER
1	X	41	ARG
1	X	81	GLU
1	X	88	ILE
1	X	99	LEU
1	X	133	ASP
1	X	151	VAL
1	X	158	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	86	HIS
1	B	180	HIS
1	C	52	GLN
1	C	61	GLN
1	C	77	GLN
1	C	85	GLN
1	C	184	GLN
1	D	85	GLN
1	D	86	HIS
1	D	153	HIS
1	D	180	HIS
1	E	52	GLN
1	E	82	GLN
1	E	84	GLN
1	E	86	HIS
1	E	130	ASN
1	F	180	HIS
1	G	86	HIS
1	G	184	GLN
1	H	86	HIS
1	H	184	GLN
1	I	85	GLN
1	I	180	HIS
1	J	184	GLN

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Mol	Chain	Res	Type
1	K	153	HIS
1	K	180	HIS
1	L	184	GLN
1	M	85	GLN
1	N	52	GLN
1	N	85	GLN
1	N	184	GLN
1	O	77	GLN
1	O	130	ASN
1	O	184	GLN
1	P	85	GLN
1	P	86	HIS
1	P	184	GLN
1	Q	180	HIS
1	R	86	HIS
1	R	150	ASN
1	R	153	HIS
1	S	86	HIS
1	T	184	GLN
1	U	86	HIS
1	U	184	GLN
1	V	85	GLN
1	V	180	HIS
1	W	77	GLN
1	W	86	HIS
1	W	153	HIS
1	W	180	HIS
1	X	180	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	151/151 (100%)	-0.09	2 (1%)	77	71	4, 7, 57, 141	0
1	B	151/151 (100%)	-0.00	4 (2%)	56	49	4, 7, 48, 105	0
1	C	151/151 (100%)	0.01	7 (4%)	32	28	4, 7, 51, 107	0
1	D	151/151 (100%)	-0.04	1 (0%)	87	83	2, 7, 46, 95	0
1	E	151/151 (100%)	0.02	2 (1%)	77	71	4, 7, 41, 74	0
1	F	151/151 (100%)	-0.19	1 (0%)	87	83	4, 7, 48, 78	0
1	G	151/151 (100%)	-0.03	3 (1%)	65	60	4, 7, 53, 95	0
1	H	151/151 (100%)	0.05	3 (1%)	65	60	4, 7, 54, 97	0
1	I	151/151 (100%)	-0.09	1 (0%)	87	83	4, 7, 54, 105	0
1	J	151/151 (100%)	-0.14	1 (0%)	87	83	4, 7, 54, 91	0
1	K	151/151 (100%)	-0.10	1 (0%)	87	83	4, 7, 46, 84	0
1	L	151/151 (100%)	-0.06	3 (1%)	65	60	4, 7, 43, 79	0
1	M	151/151 (100%)	0.04	2 (1%)	77	71	4, 7, 60, 93	0
1	N	151/151 (100%)	0.01	0	100	100	4, 7, 47, 105	0
1	O	151/151 (100%)	-0.08	1 (0%)	87	83	4, 7, 52, 96	0
1	P	151/151 (100%)	-0.10	1 (0%)	87	83	4, 7, 51, 89	0
1	Q	151/151 (100%)	-0.00	3 (1%)	65	60	4, 7, 42, 73	0
1	R	151/151 (100%)	-0.09	2 (1%)	77	71	4, 7, 45, 90	0
1	S	151/151 (100%)	0.05	5 (3%)	46	41	4, 7, 49, 88	0
1	T	151/151 (100%)	0.02	2 (1%)	77	71	4, 7, 52, 118	0
1	U	151/151 (100%)	-0.01	2 (1%)	77	71	4, 7, 53, 98	0
1	V	151/151 (100%)	0.10	3 (1%)	65	60	4, 7, 47, 98	0
1	W	151/151 (100%)	-0.14	0	100	100	4, 7, 42, 68	0
1	X	151/151 (100%)	-0.14	2 (1%)	77	71	4, 7, 44, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3624/3624 (100%)	-0.04	52 (1%)	75	69	2, 7, 51, 141	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	180	HIS	3.9
1	Q	105	SER	3.5
1	I	180	HIS	3.2
1	J	91	ALA	3.1
1	C	122	GLY	2.9
1	G	104	SER	2.9
1	T	121	GLY	2.9
1	D	122	GLY	2.9
1	C	121	GLY	2.8
1	X	157	SER	2.7
1	R	101	ALA	2.7
1	X	122	GLY	2.6
1	Q	159	ASP	2.6
1	S	101	ALA	2.6
1	S	52	GLN	2.6
1	B	86	HIS	2.6
1	O	79	SER	2.5
1	H	86	HIS	2.5
1	B	124	VAL	2.5
1	U	124	VAL	2.4
1	L	105	SER	2.4
1	L	129	THR	2.3
1	A	104	SER	2.3
1	E	105	SER	2.3
1	E	80	ALA	2.3
1	C	181	SER	2.3
1	M	180	HIS	2.2
1	C	180	HIS	2.2
1	A	179	SER	2.2
1	R	157	SER	2.2
1	L	124	VAL	2.2
1	V	79	SER	2.2
1	C	92	SER	2.2
1	Q	134	SER	2.2
1	G	179	SER	2.1
1	H	78	PRO	2.1
1	B	52	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	91	ALA	2.1
1	G	180	HIS	2.1
1	C	96	TYR	2.1
1	K	80	ALA	2.1
1	V	83	ALA	2.1
1	B	129	THR	2.1
1	S	109	VAL	2.1
1	S	105	SER	2.1
1	M	183	LYS	2.1
1	U	121	GLY	2.1
1	H	150	ASN	2.0
1	S	106	GLY	2.0
1	V	142	ASP	2.0
1	F	124	VAL	2.0
1	P	134	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.