



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:07 PM UTC

PDB ID : 3ZLP / pdb_00003zlp
Title : Crystal structure of Schistosoma mansoni Peroxiredoxin 1 C48P mutant form with four decamers in the asymmetric unit
Authors : Saccoccia, F.; Angelucci, F.; Ardini, M.; Boumis, G.; Brunori, M.; DiLeandro, L.; Ippoliti, R.; Miele, A.E.; Natoli, G.; Scotti, S.; Bellelli, A.
Deposited on : 2013-02-04
Resolution : 3.52 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

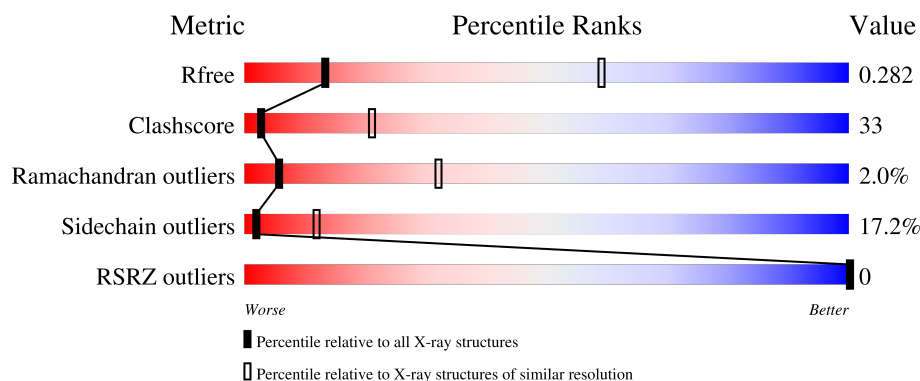
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 Å.

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



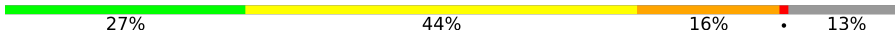
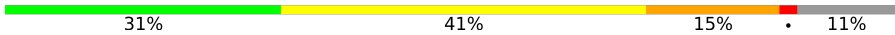
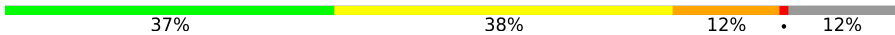
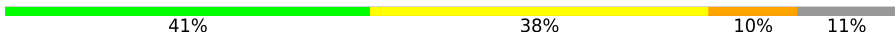
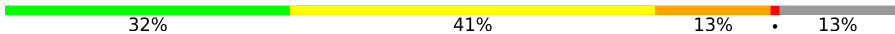
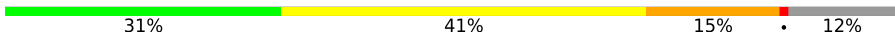
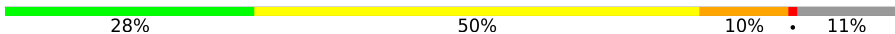
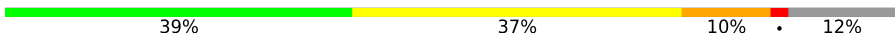
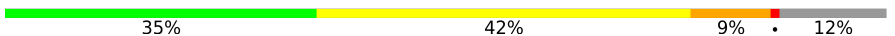
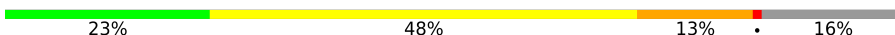
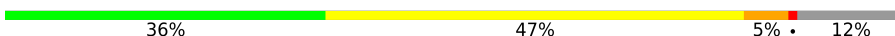
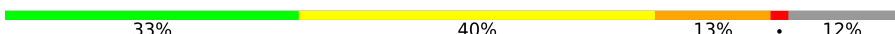
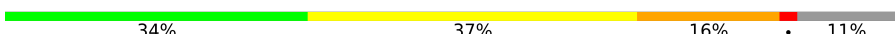
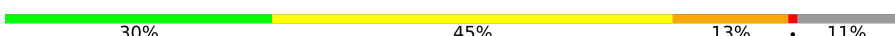
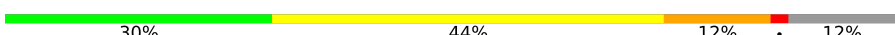
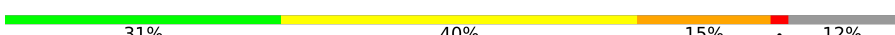
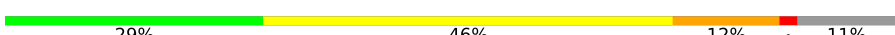
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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

Mol	Chain	Length	Quality of chain
1	A	186	
1	B	186	
1	C	186	
1	D	186	
1	E	186	

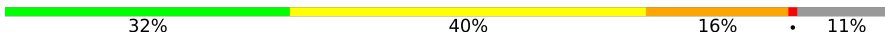
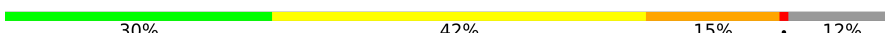
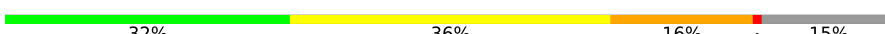
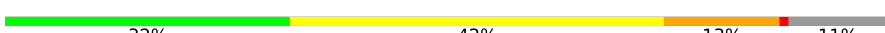
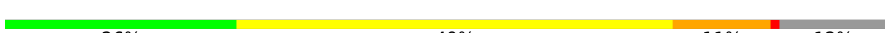
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Mol	Chain	Length	Quality of chain
1	F	186	
1	G	186	
1	H	186	
1	I	186	
1	J	186	
1	K	186	
1	L	186	
1	M	186	
1	N	186	
1	O	186	
1	P	186	
1	Q	186	
1	R	186	
1	S	186	
1	T	186	
1	U	186	
1	V	186	
1	W	186	
1	X	186	
1	Y	186	
1	Z	186	
1	a	186	
1	b	186	
1	c	186	
1	d	186	

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Mol	Chain	Length	Quality of chain
1	e	186	
1	f	186	
1	g	186	
1	h	186	
1	i	186	
1	j	186	
1	k	186	
1	l	186	
1	m	186	
1	n	186	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 52692 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 THIOREDOXIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1310	840	222	244	4			
1	B	165	Total	C	N	O	S	0	2	0
			1337	860	226	246	5			
1	C	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	D	164	Total	C	N	O	S	0	2	0
			1331	854	227	246	4			
1	E	162	Total	C	N	O	S	0	0	0
			1300	834	219	243	4			
1	F	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	G	162	Total	C	N	O	S	0	1	0
			1306	838	219	245	4			
1	H	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	I	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			
1	J	166	Total	C	N	O	S	0	0	0
			1332	854	225	248	5			
1	K	161	Total	C	N	O	S	0	0	0
			1291	828	217	242	4			
1	L	164	Total	C	N	O	S	0	2	0
			1327	854	223	245	5			
1	M	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	N	164	Total	C	N	O	S	0	2	0
			1331	854	227	246	4			
1	O	163	Total	C	N	O	S	0	0	0
			1310	840	222	244	4			
1	P	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	157	Total	C	N	O	S	0	1	0
			1267	810	214	239	4			
1	R	164	Total	C	N	O	S	0	0	0
			1315	844	221	245	5			
1	S	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			
1	T	166	Total	C	N	O	S	0	0	0
			1332	854	225	248	5			
1	U	163	Total	C	N	O	S	0	0	0
			1310	840	222	244	4			
1	V	165	Total	C	N	O	S	0	2	0
			1337	860	226	246	5			
1	W	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	X	164	Total	C	N	O	S	0	2	0
			1331	854	227	246	4			
1	Y	163	Total	C	N	O	S	0	0	0
			1310	840	222	244	4			
1	Z	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	a	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			
1	b	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	c	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			
1	d	166	Total	C	N	O	S	0	0	0
			1332	854	225	248	5			
1	e	162	Total	C	N	O	S	0	0	0
			1300	834	219	243	4			
1	f	165	Total	C	N	O	S	0	2	0
			1337	860	226	246	5			
1	g	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	h	163	Total	C	N	O	S	0	2	0
			1321	848	224	245	4			
1	i	158	Total	C	N	O	S	0	0	0
			1271	812	217	238	4			
1	j	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	k	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	m	157	Total	C	N	O	S	0	1	0
			1267	810	214	239	4			
1	n	166	Total	C	N	O	S	0	0	0
			1332	854	225	248	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	THR	-	expression tag	UNP O97161
A	48	PRO	CYS	engineered mutation	UNP O97161
B	0	THR	-	expression tag	UNP O97161
B	48	PRO	CYS	engineered mutation	UNP O97161
C	0	THR	-	expression tag	UNP O97161
C	48	PRO	CYS	engineered mutation	UNP O97161
D	0	THR	-	expression tag	UNP O97161
D	48	PRO	CYS	engineered mutation	UNP O97161
E	0	THR	-	expression tag	UNP O97161
E	48	PRO	CYS	engineered mutation	UNP O97161
F	0	THR	-	expression tag	UNP O97161
F	48	PRO	CYS	engineered mutation	UNP O97161
G	0	THR	-	expression tag	UNP O97161
G	48	PRO	CYS	engineered mutation	UNP O97161
H	0	THR	-	expression tag	UNP O97161
H	48	PRO	CYS	engineered mutation	UNP O97161
I	0	THR	-	expression tag	UNP O97161
I	48	PRO	CYS	engineered mutation	UNP O97161
J	0	THR	-	expression tag	UNP O97161
J	48	PRO	CYS	engineered mutation	UNP O97161
K	0	THR	-	expression tag	UNP O97161
K	48	PRO	CYS	engineered mutation	UNP O97161
L	0	THR	-	expression tag	UNP O97161
L	48	PRO	CYS	engineered mutation	UNP O97161
M	0	THR	-	expression tag	UNP O97161
M	48	PRO	CYS	engineered mutation	UNP O97161
N	0	THR	-	expression tag	UNP O97161
N	48	PRO	CYS	engineered mutation	UNP O97161
O	0	THR	-	expression tag	UNP O97161
O	48	PRO	CYS	engineered mutation	UNP O97161
P	0	THR	-	expression tag	UNP O97161
P	48	PRO	CYS	engineered mutation	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	THR	-	expression tag	UNP O97161
Q	48	PRO	CYS	engineered mutation	UNP O97161
R	0	THR	-	expression tag	UNP O97161
R	48	PRO	CYS	engineered mutation	UNP O97161
S	0	THR	-	expression tag	UNP O97161
S	48	PRO	CYS	engineered mutation	UNP O97161
T	0	THR	-	expression tag	UNP O97161
T	48	PRO	CYS	engineered mutation	UNP O97161
U	0	THR	-	expression tag	UNP O97161
U	48	PRO	CYS	engineered mutation	UNP O97161
V	0	THR	-	expression tag	UNP O97161
V	48	PRO	CYS	engineered mutation	UNP O97161
W	0	THR	-	expression tag	UNP O97161
W	48	PRO	CYS	engineered mutation	UNP O97161
X	0	THR	-	expression tag	UNP O97161
X	48	PRO	CYS	engineered mutation	UNP O97161
Y	0	THR	-	expression tag	UNP O97161
Y	48	PRO	CYS	engineered mutation	UNP O97161
Z	0	THR	-	expression tag	UNP O97161
Z	48	PRO	CYS	engineered mutation	UNP O97161
a	0	THR	-	expression tag	UNP O97161
a	48	PRO	CYS	engineered mutation	UNP O97161
b	0	THR	-	expression tag	UNP O97161
b	48	PRO	CYS	engineered mutation	UNP O97161
c	0	THR	-	expression tag	UNP O97161
c	48	PRO	CYS	engineered mutation	UNP O97161
d	0	THR	-	expression tag	UNP O97161
d	48	PRO	CYS	engineered mutation	UNP O97161
e	0	THR	-	expression tag	UNP O97161
e	48	PRO	CYS	engineered mutation	UNP O97161
f	0	THR	-	expression tag	UNP O97161
f	48	PRO	CYS	engineered mutation	UNP O97161
g	0	THR	-	expression tag	UNP O97161
g	48	PRO	CYS	engineered mutation	UNP O97161
h	0	THR	-	expression tag	UNP O97161
h	48	PRO	CYS	engineered mutation	UNP O97161
i	0	THR	-	expression tag	UNP O97161
i	48	PRO	CYS	engineered mutation	UNP O97161
j	0	THR	-	expression tag	UNP O97161
j	48	PRO	CYS	engineered mutation	UNP O97161
k	0	THR	-	expression tag	UNP O97161
k	48	PRO	CYS	engineered mutation	UNP O97161

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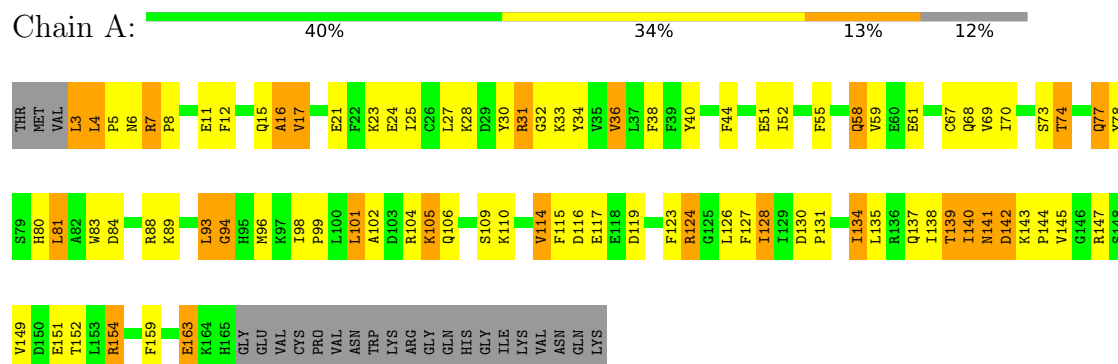
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Chain	Residue	Modelled	Actual	Comment	Reference
l	0	THR	-	expression tag	UNP O97161
l	48	PRO	CYS	engineered mutation	UNP O97161
m	0	THR	-	expression tag	UNP O97161
m	48	PRO	CYS	engineered mutation	UNP O97161
n	0	THR	-	expression tag	UNP O97161
n	48	PRO	CYS	engineered mutation	UNP O97161

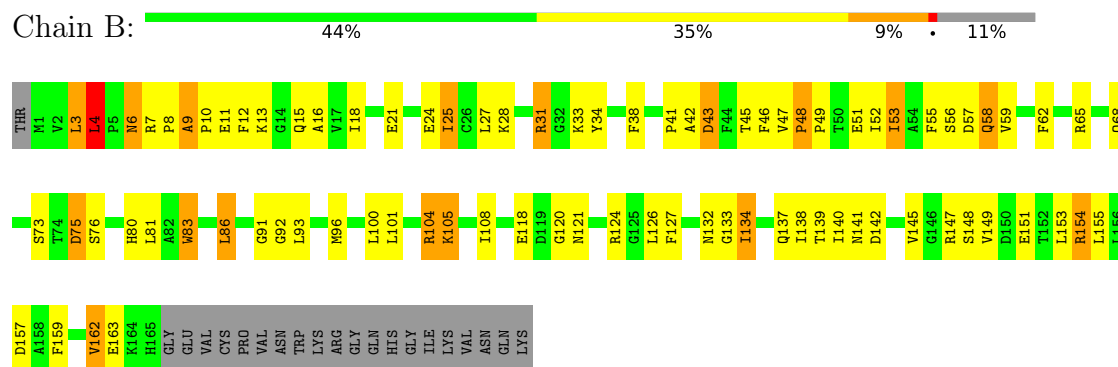
3 Residue-property plots

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

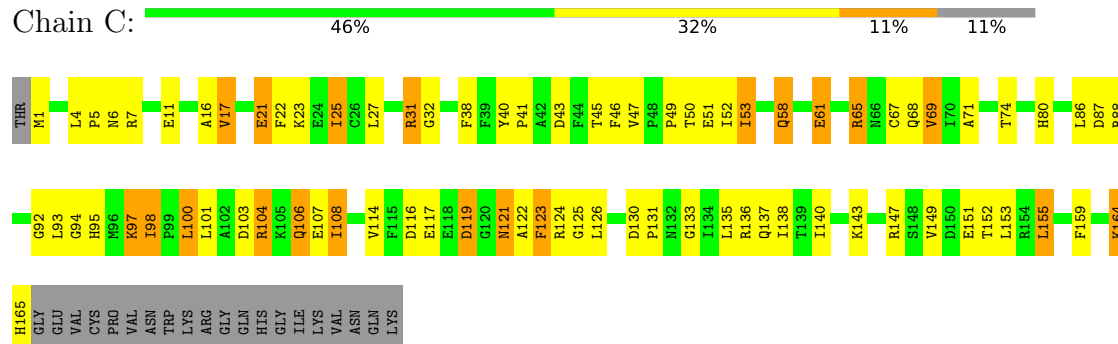
• Molecule 1: THIOREDOXIN PEROXIDASE



• Molecule 1: THIOREDOXIN PEROXIDASE

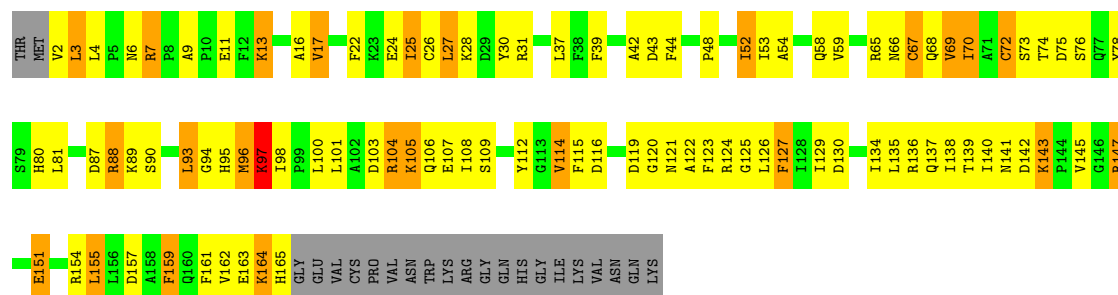


• Molecule 1: THIOREDOXIN PEROXIDASE

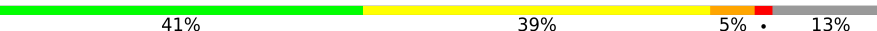


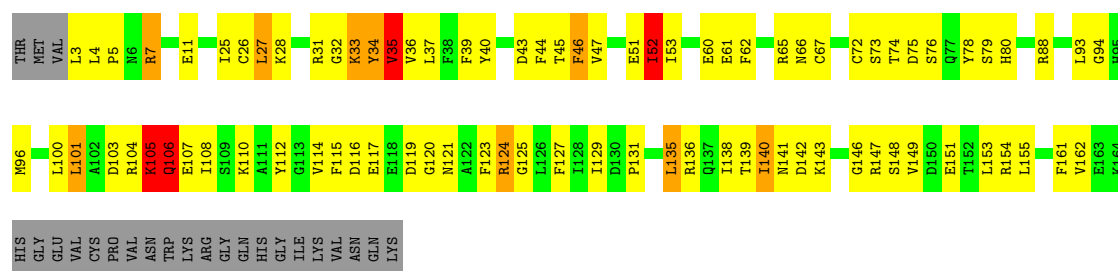
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain D: 



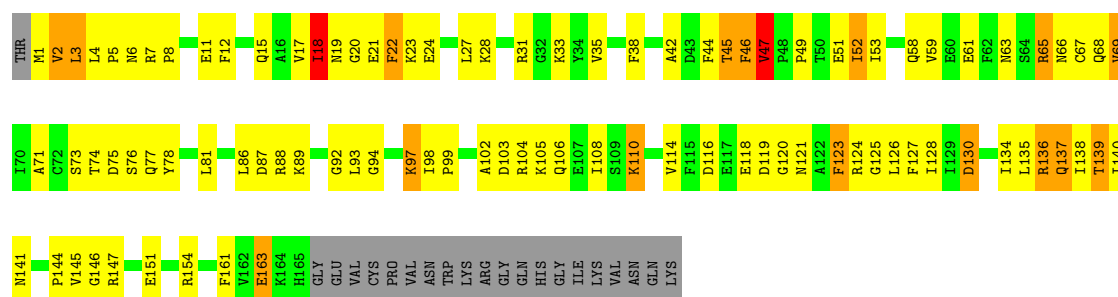
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain E: 

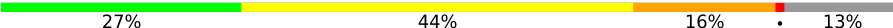


• Molecule 1: THIOREDOXIN PEROXIDASE

Chain F: 



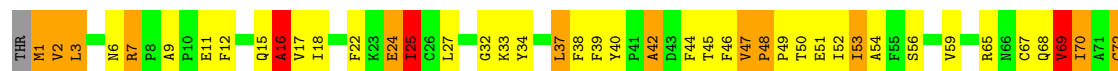
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain G: 

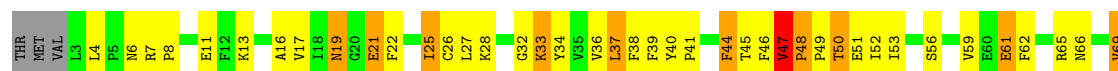




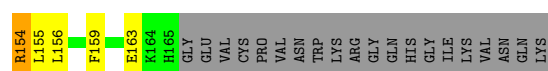
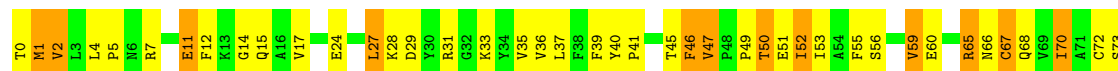
• Molecule 1: THIOREDOXIN PEROXIDASE



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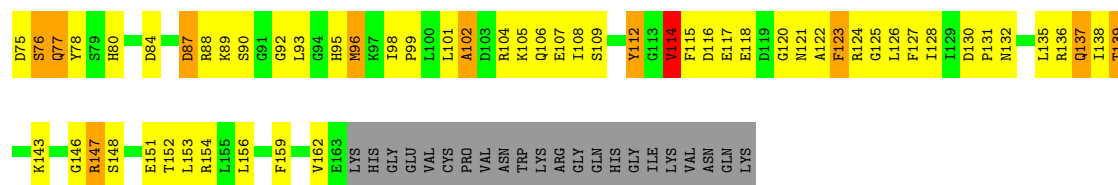


• Molecule 1: THIOREDOXIN PEROXIDASE

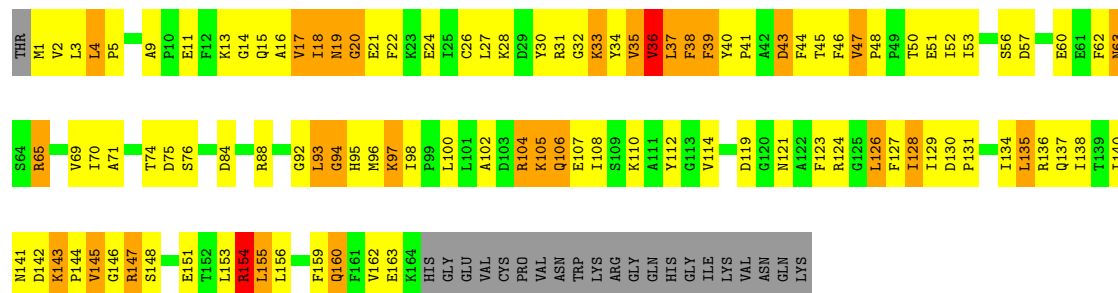


• Molecule 1: THIOREDOXIN PEROXIDASE

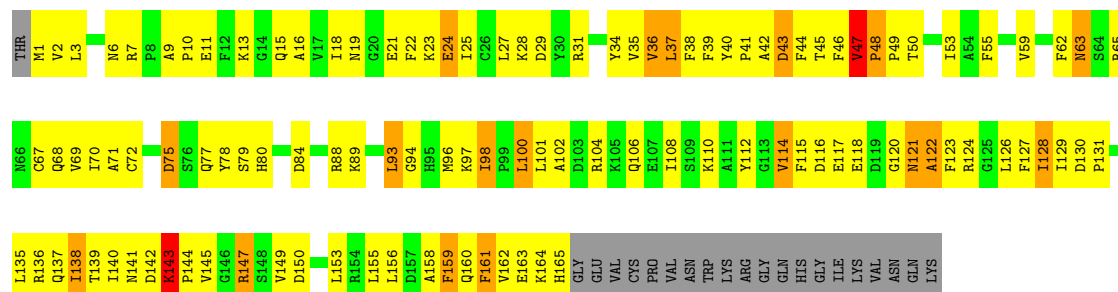




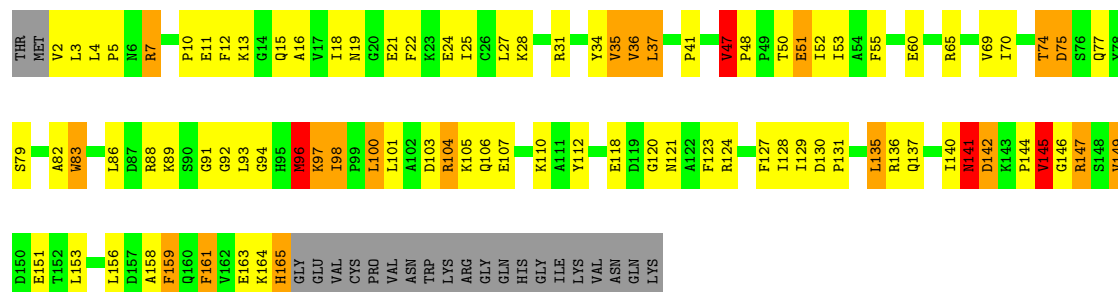
• Molecule 1: THIOREDOXIN PEROXIDASE



• Molecule 1: THIOREDOXIN PEROXIDASE

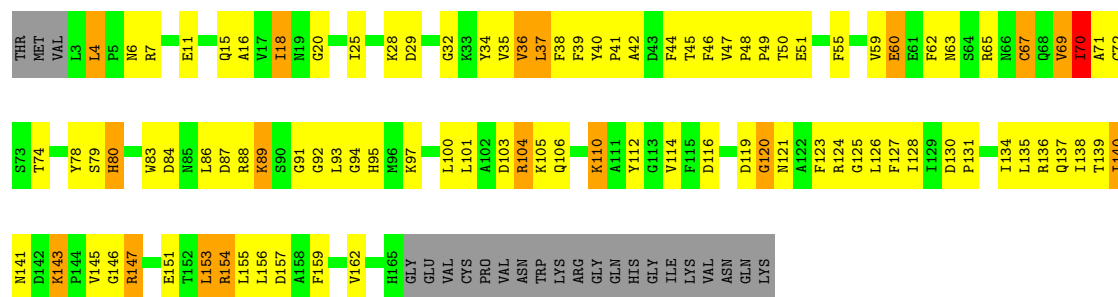


• Molecule 1: THIOREDOXIN PEROXIDASE



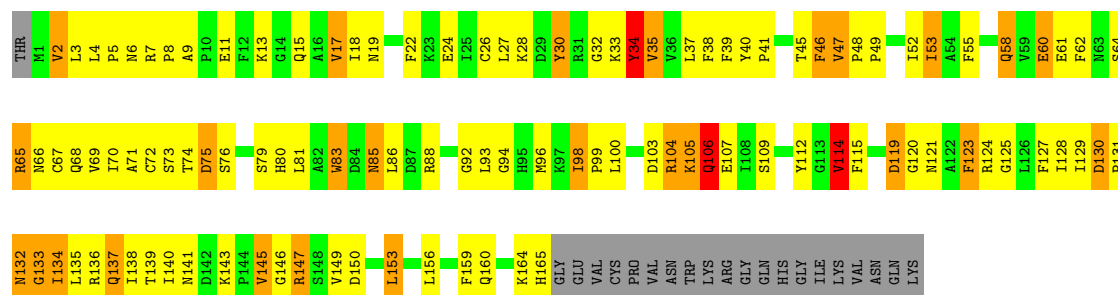
• Molecule 1: THIOREDOXIN PEROXIDASE





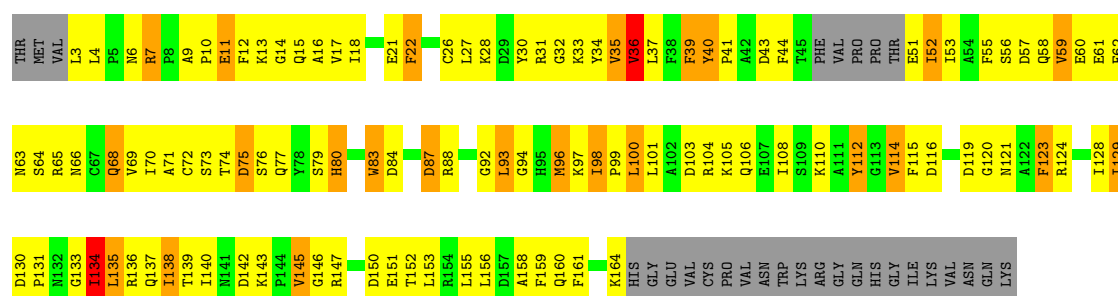
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain P: 30% 44% 14% 11%



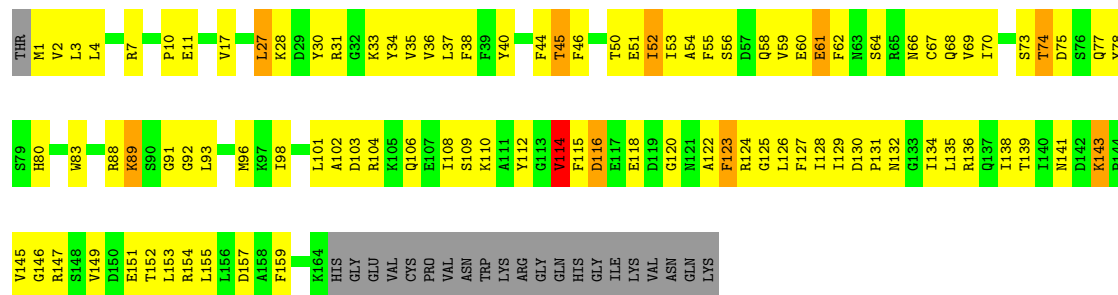
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain Q: 23% 48% 13% 16%

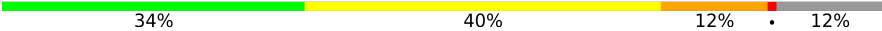


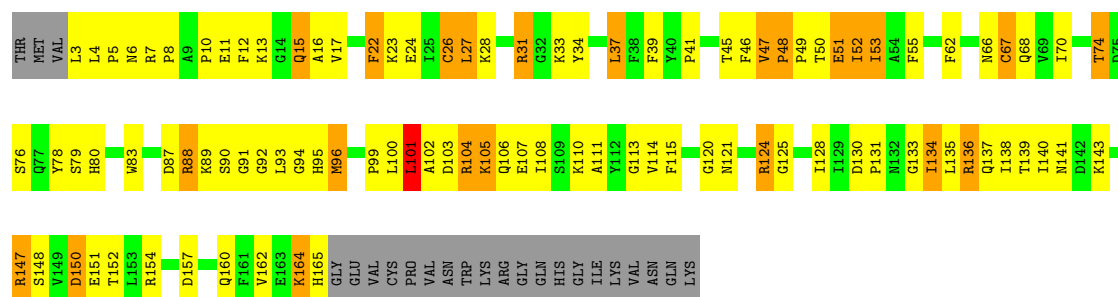
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain R: 36% 47% 5% 12%



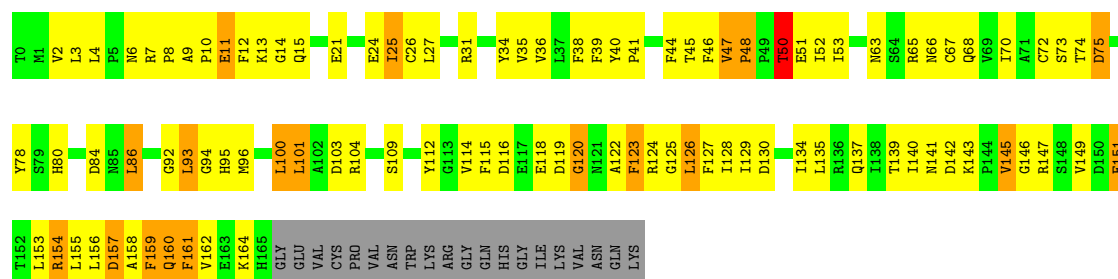
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain S: 

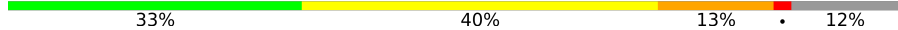


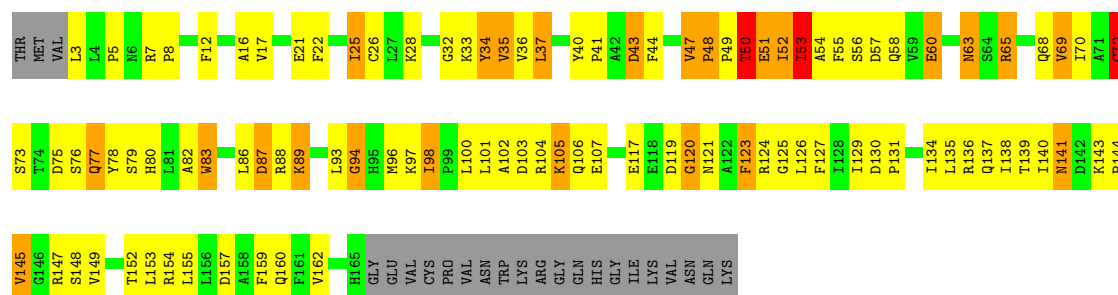
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain T: 

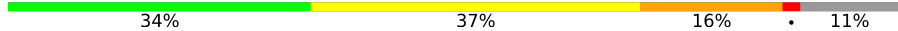


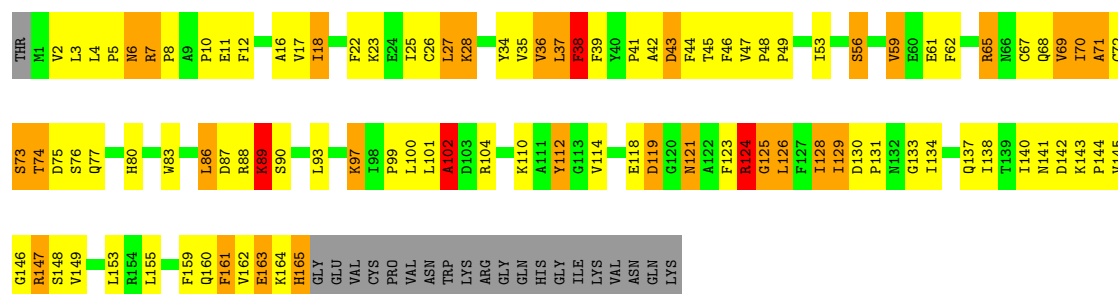
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain U: 

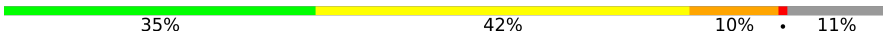


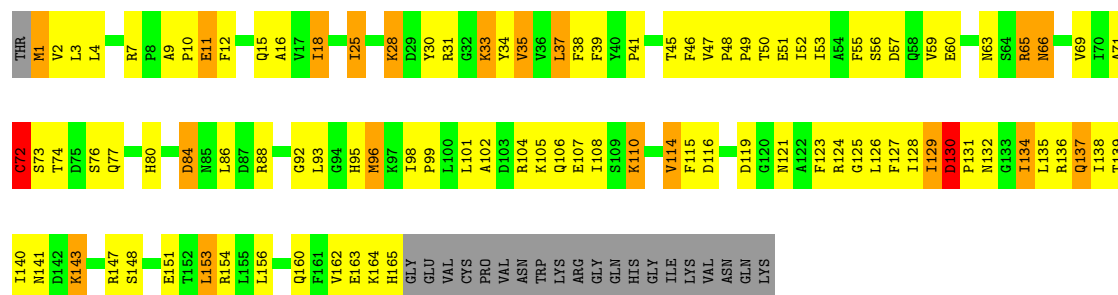
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain V: 



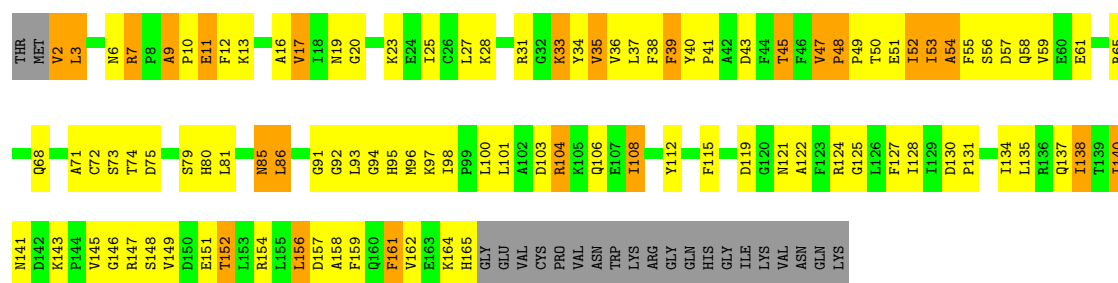
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain W: 

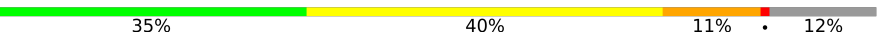


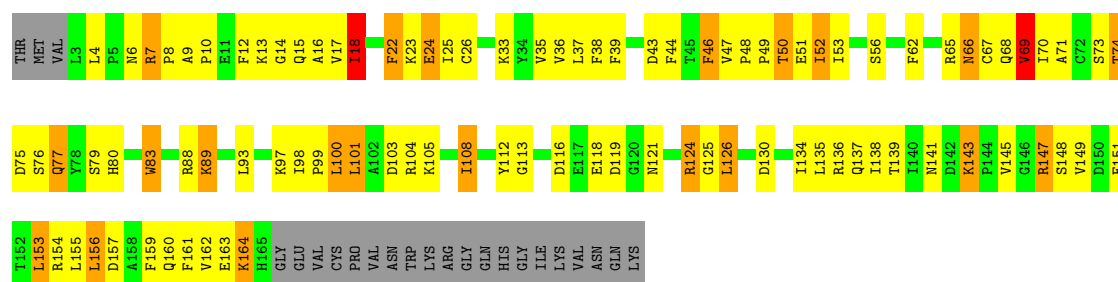
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain X: 

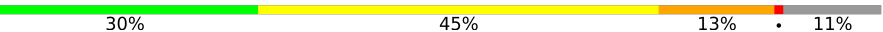


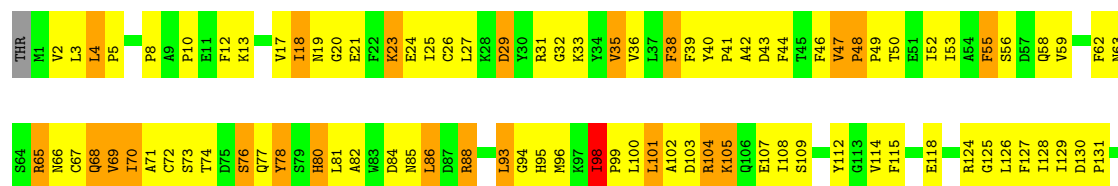
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain Y: 



• Molecule 1: THIOREDOXIN PEROXIDASE

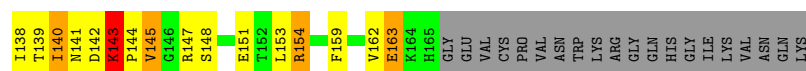
Chain Z: 





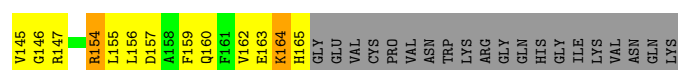
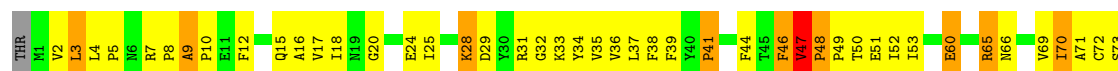
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain a: 30% 44% 12% 12%



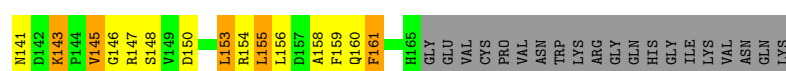
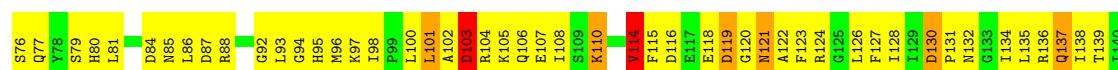
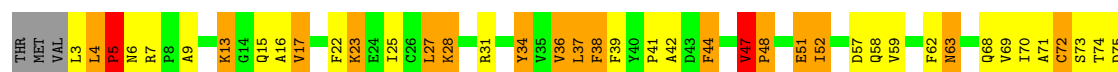
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain b: 32% 45% 10% 11%



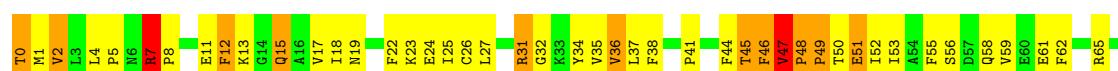
• Molecule 1: THIOREDOXIN PEROXIDASE

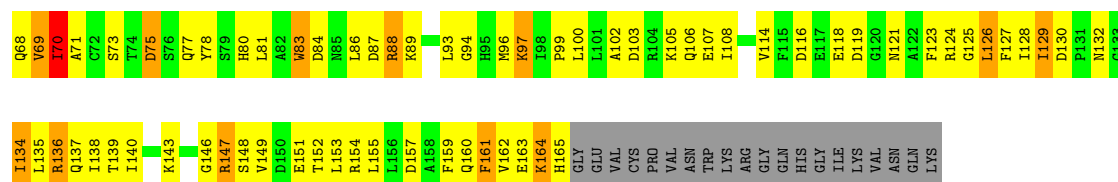
Chain c: 31% 40% 15% 12%



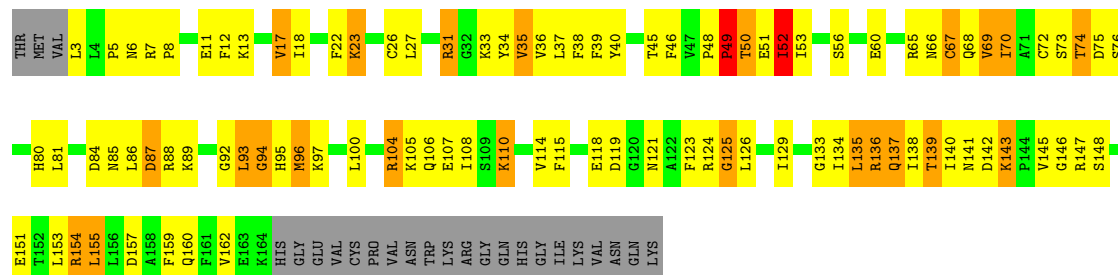
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain d: 29% 46% 12% 11%

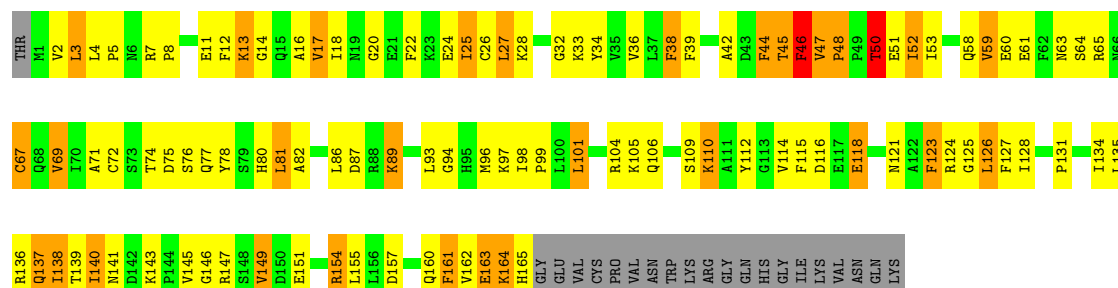




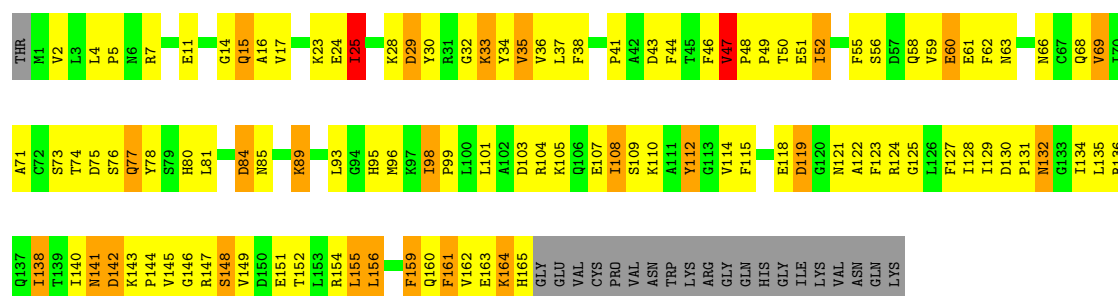
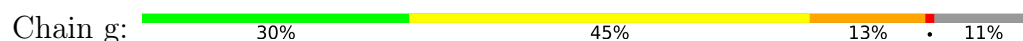
• Molecule 1: THIOREDOXIN PEROXIDASE



• Molecule 1: THIOREDOXIN PEROXIDASE

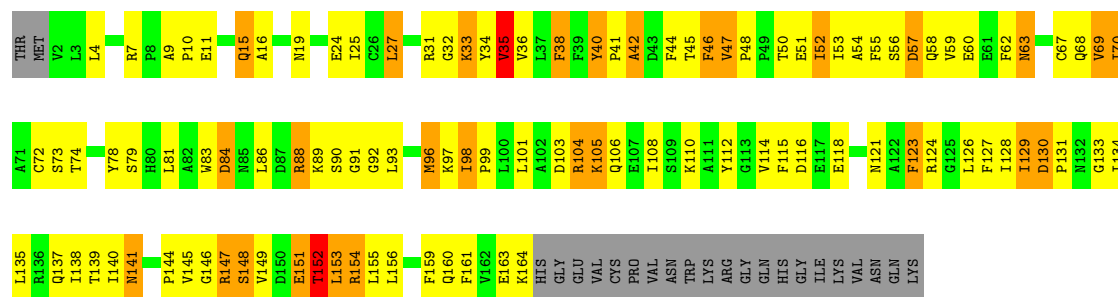


• Molecule 1: THIOREDOXIN PEROXIDASE

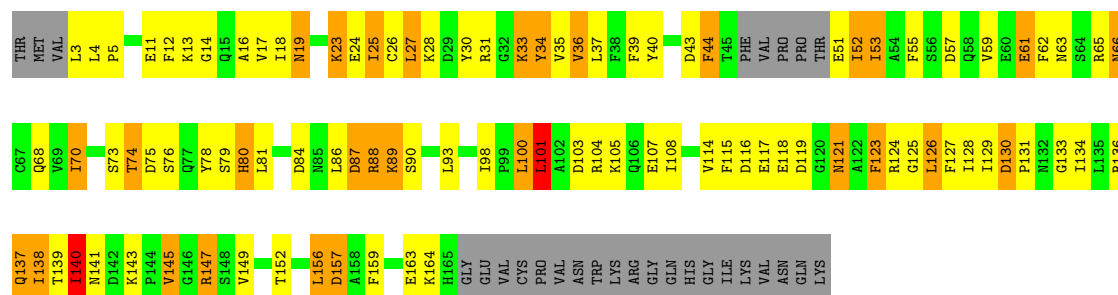


• Molecule 1: THIOREDOXIN PEROXIDASE

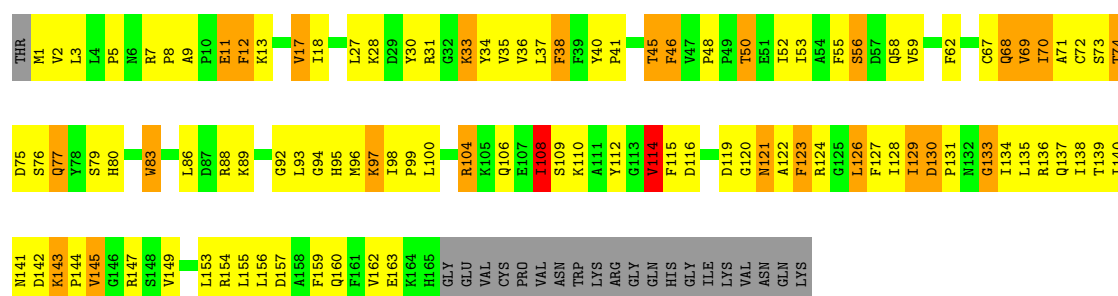




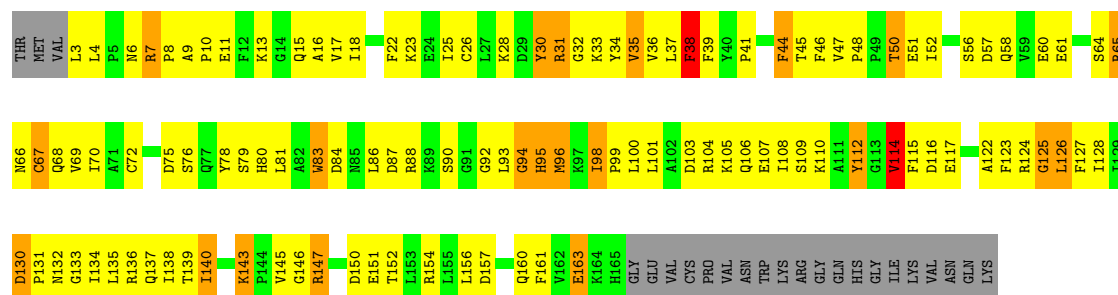
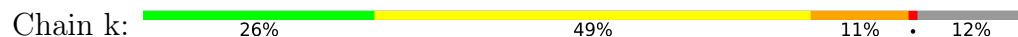
• Molecule 1: THIOREDOXIN PEROXIDASE



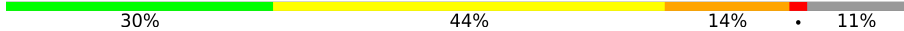
• Molecule 1: THIOREDOXIN PEROXIDASE

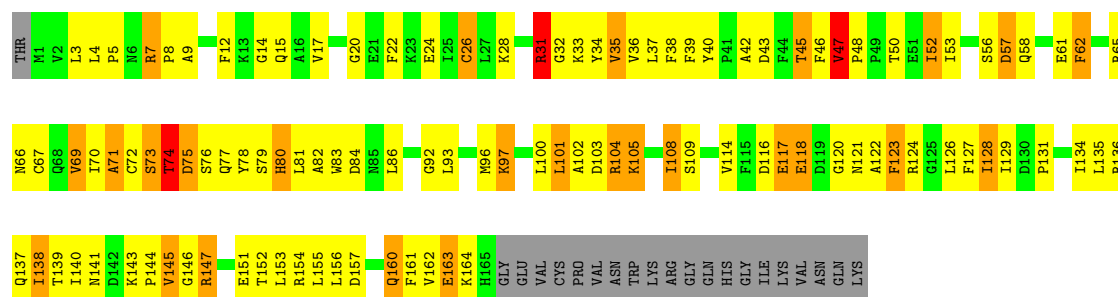


• Molecule 1: THIOREDOXIN PEROXIDASE



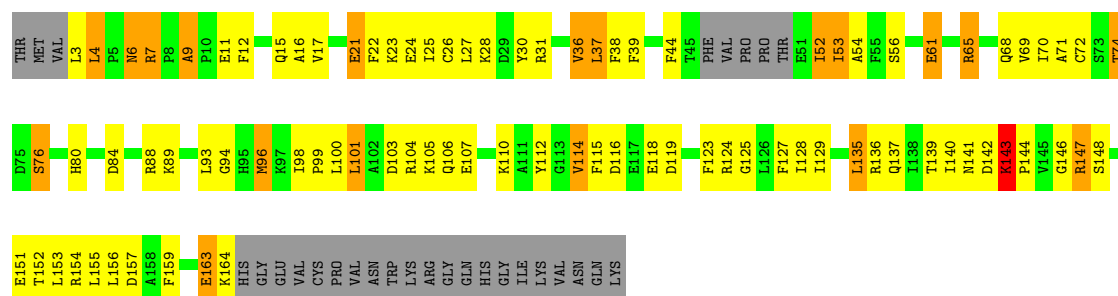
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain l: 



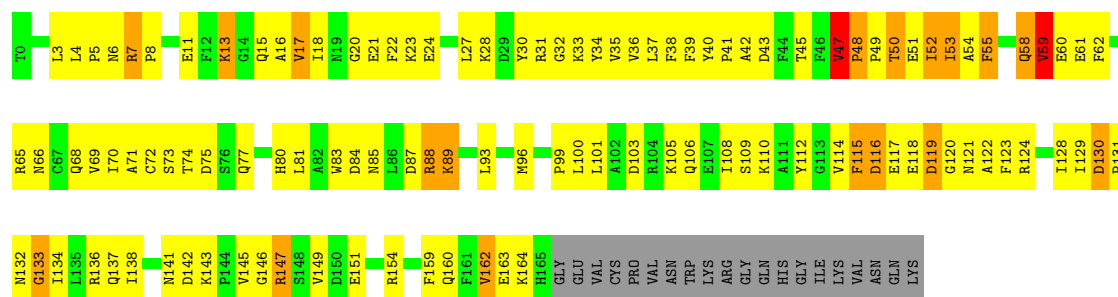
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain m: 



• Molecule 1: THIOREDOXIN PEROXIDASE

Chain n: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.18Å 190.30Å 212.00Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	48.76 – 3.52 48.76 – 3.52	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.76-3.52) 97.7 (48.76-3.52)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.277 , 0.289 0.274 , 0.282	Depositor DCC
R_{free} test set	4589 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.327 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	2 of 91789 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52692	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	1/1341 (0.1%)	1.10	7/1813 (0.4%)
1	B	0.41	0/1374	1.05	7/1855 (0.4%)
1	C	0.39	0/1356	0.94	3/1833 (0.2%)
1	D	0.42	0/1368	1.15	14/1849 (0.8%)
1	E	0.40	0/1330	1.06	5/1798 (0.3%)
1	F	0.38	0/1356	0.95	2/1833 (0.1%)
1	G	0.40	0/1339	1.21	17/1810 (0.9%)
1	H	0.47	0/1356	1.20	13/1833 (0.7%)
1	I	0.45	0/1350	1.15	9/1825 (0.5%)
1	J	0.43	0/1363	1.04	6/1843 (0.3%)
1	K	0.42	0/1321	1.13	15/1787 (0.8%)
1	L	0.43	0/1363	1.13	7/1840 (0.4%)
1	M	0.45	0/1356	1.15	11/1833 (0.6%)
1	N	0.42	0/1368	1.21	15/1849 (0.8%)
1	O	0.41	0/1341	1.07	9/1813 (0.5%)
1	P	0.40	0/1356	1.12	9/1833 (0.5%)
1	Q	0.43	0/1296	1.00	4/1747 (0.2%)
1	R	0.42	0/1345	1.04	7/1818 (0.4%)
1	S	0.43	0/1350	1.20	7/1825 (0.4%)
1	T	0.39	0/1363	1.09	9/1843 (0.5%)
1	U	0.45	0/1341	1.13	11/1813 (0.6%)
1	V	0.44	0/1374	1.13	8/1855 (0.4%)
1	W	0.39	0/1356	1.04	3/1833 (0.2%)
1	X	0.43	0/1368	1.17	12/1849 (0.6%)
1	Y	0.46	1/1341 (0.1%)	1.04	4/1813 (0.2%)
1	Z	0.43	0/1356	1.16	16/1833 (0.9%)
1	a	0.48	0/1350	1.22	14/1825 (0.8%)
1	b	0.47	0/1356	1.21	13/1833 (0.7%)
1	c	0.43	0/1350	1.27	15/1825 (0.8%)
1	d	0.41	0/1363	1.15	14/1843 (0.8%)
1	e	0.41	0/1330	1.05	8/1798 (0.4%)
1	f	0.44	0/1374	1.15	10/1855 (0.5%)
1	g	0.42	0/1356	1.11	10/1833 (0.5%)
1	h	0.44	0/1357	1.27	19/1834 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.38	0/1298	0.86	2/1750 (0.1%)
1	j	0.43	0/1356	1.14	15/1833 (0.8%)
1	k	0.43	0/1350	1.21	8/1825 (0.4%)
1	l	0.43	0/1356	1.12	11/1833 (0.6%)
1	m	0.36	0/1296	0.92	6/1747 (0.3%)
1	n	0.44	0/1363	1.03	8/1843 (0.4%)
All	All	0.42	2/53983 (0.0%)	1.11	383/72953 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	E	0	1
1	G	0	2
1	H	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	2
1	P	0	1
1	Q	0	2
1	R	0	1
1	S	0	2
1	T	0	1
1	U	0	1
1	V	0	4
1	W	0	1
1	X	0	1
1	Y	0	2
1	a	0	3
1	b	0	2
1	c	0	3
1	d	0	3
1	e	0	2
1	f	0	4
1	h	0	4
1	j	0	1
1	k	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	l	0	2
1	m	0	1
1	n	0	1
All	All	0	59

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	69	VAL	CA-CB	5.26	1.61	1.54
1	A	142	ASP	CA-C	5.17	1.55	1.52

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	4	LEU	CA-C-N	13.26	136.41	119.84
1	c	4	LEU	C-N-CA	13.26	136.41	119.84
1	N	48	PRO	CA-C-N	-13.06	103.52	119.84
1	N	48	PRO	C-N-CA	-13.06	103.52	119.84
1	e	45	THR	N-CA-C	-12.45	97.45	112.89
1	G	125	GLY	N-CA-C	11.34	127.32	112.13
1	W	130	ASP	CA-C-N	-11.27	105.76	119.84
1	W	130	ASP	C-N-CA	-11.27	105.76	119.84
1	f	47	VAL	CA-C-N	10.99	131.70	120.38
1	f	47	VAL	C-N-CA	10.99	131.70	120.38
1	l	47	VAL	CA-C-N	-10.80	109.26	120.38
1	l	47	VAL	C-N-CA	-10.80	109.26	120.38
1	f	46	PHE	N-CA-C	-10.61	93.70	110.14
1	V	125	GLY	N-CA-C	10.56	126.40	112.25
1	a	49	PRO	CA-C-O	-10.07	113.62	121.38
1	B	48	PRO	N-CA-C	10.06	122.97	110.70
1	b	47	VAL	CA-C-N	-10.04	112.43	119.66
1	b	47	VAL	C-N-CA	-10.04	112.43	119.66
1	a	143	LYS	CA-C-N	-9.86	110.15	119.82
1	a	143	LYS	C-N-CA	-9.86	110.15	119.82
1	d	47	VAL	N-CA-C	9.77	124.88	112.67
1	N	120	GLY	N-CA-C	-9.62	101.14	115.00
1	d	48	PRO	N-CA-C	9.62	122.44	110.70
1	I	47	VAL	CA-C-N	-9.55	110.54	120.38
1	I	47	VAL	C-N-CA	-9.55	110.54	120.38
1	X	9	ALA	CA-C-N	9.36	131.54	119.84
1	X	9	ALA	C-N-CA	9.36	131.54	119.84
1	L	20	GLY	N-CA-C	9.35	125.81	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	47	VAL	CA-C-N	-9.33	110.77	120.38
1	H	47	VAL	C-N-CA	-9.33	110.77	120.38
1	K	48	PRO	N-CA-C	9.33	122.08	110.70
1	S	48	PRO	CA-C-N	9.18	131.31	119.84
1	S	48	PRO	C-N-CA	9.18	131.31	119.84
1	f	45	THR	N-CA-C	9.14	125.31	109.96
1	d	45	THR	N-CA-C	9.03	121.12	111.28
1	h	27	LEU	N-CA-C	8.73	121.59	111.11
1	G	32	GLY	N-CA-C	-8.73	102.43	115.00
1	j	40	TYR	CA-C-N	8.65	127.97	118.97
1	j	40	TYR	C-N-CA	8.65	127.97	118.97
1	S	48	PRO	N-CA-C	8.53	121.10	110.70
1	K	120	GLY	N-CA-C	-8.52	102.74	115.00
1	h	130	ASP	CA-C-N	8.36	128.09	119.56
1	h	130	ASP	C-N-CA	8.36	128.09	119.56
1	A	17	VAL	N-CA-C	8.33	119.70	107.37
1	Z	52	ILE	N-CA-C	8.15	118.93	110.62
1	c	72	CYS	N-CA-C	8.11	118.65	108.19
1	j	130	ASP	CA-C-N	-8.10	109.72	119.84
1	j	130	ASP	C-N-CA	-8.10	109.72	119.84
1	B	91	GLY	N-CA-C	8.09	126.49	115.32
1	H	117	GLU	N-CA-C	8.05	120.06	111.28
1	d	47	VAL	CB-CA-C	-8.02	106.08	113.70
1	L	4	LEU	CA-C-N	7.99	127.88	120.21
1	L	4	LEU	C-N-CA	7.99	127.88	120.21
1	a	46	PHE	CB-CA-C	-7.97	106.30	115.79
1	G	126	LEU	N-CA-C	7.96	120.22	110.91
1	e	92	GLY	N-CA-C	7.95	121.62	111.37
1	T	9	ALA	N-CA-C	-7.88	100.16	109.93
1	m	143	LYS	CA-C-N	-7.87	113.70	121.65
1	m	143	LYS	C-N-CA	-7.87	113.70	121.65
1	X	91	GLY	N-CA-C	-7.83	104.39	115.43
1	U	72	CYS	N-CA-C	7.82	127.46	110.80
1	h	149	VAL	N-CA-C	7.76	118.56	110.72
1	P	120	GLY	N-CA-C	-7.71	104.39	115.27
1	K	76	SER	CB-CA-C	-7.70	106.63	115.79
1	a	48	PRO	CA-C-N	7.70	129.43	121.65
1	a	48	PRO	C-N-CA	7.70	129.43	121.65
1	b	46	PHE	CA-C-N	7.66	135.50	121.70
1	b	46	PHE	C-N-CA	7.66	135.50	121.70
1	R	52	ILE	N-CA-C	7.65	119.34	110.62
1	d	7	ARG	CA-C-N	7.64	129.40	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	7	ARG	C-N-CA	7.64	129.40	119.84
1	D	48	PRO	CA-C-N	-7.64	111.88	119.90
1	D	48	PRO	C-N-CA	-7.64	111.88	119.90
1	R	92	GLY	N-CA-C	7.60	123.31	112.82
1	Q	53	ILE	N-CA-C	-7.59	105.32	112.83
1	f	48	PRO	N-CA-C	7.58	119.95	110.70
1	X	39	PHE	N-CA-C	7.50	122.01	113.02
1	D	67	CYS	CB-CA-C	-7.49	106.88	115.79
1	h	151	GLU	N-CA-C	7.40	119.43	111.36
1	P	47	VAL	CA-C-N	-7.37	112.79	120.38
1	P	47	VAL	C-N-CA	-7.37	112.79	120.38
1	S	26	CYS	N-CA-C	7.37	121.98	112.92
1	l	105	LYS	N-CA-C	-7.33	103.93	113.17
1	h	47	VAL	CA-C-N	7.29	127.89	120.38
1	h	47	VAL	C-N-CA	7.29	127.89	120.38
1	H	9	ALA	CA-C-N	7.28	128.94	119.84
1	H	9	ALA	C-N-CA	7.28	128.94	119.84
1	B	162	VAL	N-CA-C	7.27	118.92	111.00
1	T	47	VAL	CA-C-N	-7.26	112.90	120.38
1	T	47	VAL	C-N-CA	-7.26	112.90	120.38
1	Z	48	PRO	CA-C-N	7.25	128.90	119.84
1	Z	48	PRO	C-N-CA	7.25	128.90	119.84
1	T	50	THR	CB-CA-C	-7.22	108.23	116.54
1	J	2	VAL	N-CA-C	7.22	118.26	107.80
1	D	67	CYS	N-CA-C	7.17	122.51	109.32
1	l	48	PRO	CA-C-N	7.15	128.78	119.84
1	l	48	PRO	C-N-CA	7.15	128.78	119.84
1	M	47	VAL	CA-C-N	-7.13	113.03	120.38
1	M	47	VAL	C-N-CA	-7.13	113.03	120.38
1	H	48	PRO	CA-C-N	-7.13	110.92	119.84
1	H	48	PRO	C-N-CA	-7.13	110.92	119.84
1	g	69	VAL	N-CA-C	7.02	117.97	107.51
1	c	47	VAL	CA-C-N	-7.01	113.16	120.38
1	c	47	VAL	C-N-CA	-7.01	113.16	120.38
1	G	117	GLU	N-CA-C	6.99	119.79	111.33
1	Z	143	LYS	CA-C-N	-6.98	112.49	121.91
1	Z	143	LYS	C-N-CA	-6.98	112.49	121.91
1	P	132	ASN	N-CA-C	-6.97	103.77	112.90
1	Z	47	VAL	N-CA-C	6.89	115.49	107.84
1	O	48	PRO	CA-C-N	-6.89	112.55	119.99
1	O	48	PRO	C-N-CA	-6.89	112.55	119.99
1	G	76	SER	N-CA-C	6.88	118.18	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	61	GLU	N-CA-C	6.84	118.82	111.36
1	E	101	LEU	N-CA-C	6.81	118.78	111.36
1	k	125	GLY	N-CA-C	6.79	121.23	112.13
1	D	143	LYS	CA-C-N	-6.77	112.77	121.91
1	D	143	LYS	C-N-CA	-6.77	112.77	121.91
1	k	95	HIS	N-CA-C	-6.77	105.02	113.28
1	X	7	ARG	CA-C-N	6.75	128.27	119.84
1	X	7	ARG	C-N-CA	6.75	128.27	119.84
1	M	43	ASP	N-CA-C	-6.74	104.81	113.16
1	U	48	PRO	CA-C-N	6.74	126.19	118.85
1	U	48	PRO	C-N-CA	6.74	126.19	118.85
1	M	48	PRO	CA-C-N	-6.72	112.78	119.56
1	M	48	PRO	C-N-CA	-6.72	112.78	119.56
1	D	162	VAL	N-CA-C	6.69	120.41	111.44
1	Y	52	ILE	N-CA-C	6.69	117.44	110.62
1	Z	50	THR	N-CA-C	6.67	119.14	108.41
1	A	142	ASP	N-CA-C	6.66	118.71	108.12
1	N	98	ILE	CA-C-N	-6.63	112.29	119.98
1	N	98	ILE	C-N-CA	-6.63	112.29	119.98
1	S	101	LEU	N-CA-C	6.62	119.96	110.24
1	j	68	GLN	CB-CA-C	-6.61	107.17	115.89
1	L	94	GLY	N-CA-C	-6.58	100.31	112.62
1	l	117	GLU	N-CA-C	6.58	118.45	111.28
1	k	38	PHE	N-CA-C	6.58	119.91	110.24
1	K	162	VAL	N-CA-C	6.57	116.72	110.74
1	P	2	VAL	N-CA-C	6.57	118.06	108.53
1	D	163	GLU	N-CA-C	6.57	118.52	111.36
1	l	145	VAL	N-CA-C	6.55	122.96	109.34
1	I	25	ILE	N-CA-C	6.53	119.51	108.86
1	g	48	PRO	N-CA-C	6.53	118.67	110.70
1	B	9	ALA	CA-C-N	6.52	126.87	119.83
1	B	9	ALA	C-N-CA	6.52	126.87	119.83
1	V	56	SER	N-CA-C	6.51	118.46	111.36
1	R	69	VAL	N-CA-C	6.50	116.08	106.85
1	c	103	ASP	N-CA-C	6.49	124.63	110.80
1	X	48	PRO	N-CA-C	6.47	118.60	110.70
1	j	46	PHE	N-CA-C	6.46	120.13	108.69
1	b	44	PHE	N-CA-C	6.45	120.61	112.87
1	k	130	ASP	CA-C-N	-6.45	111.78	119.84
1	k	130	ASP	C-N-CA	-6.45	111.78	119.84
1	e	52	ILE	N-CA-C	6.45	117.19	110.62
1	U	25	ILE	N-CA-C	6.43	117.74	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	94	GLY	N-CA-C	6.43	120.03	111.03
1	n	47	VAL	CA-C-N	6.41	126.98	120.38
1	n	47	VAL	C-N-CA	6.41	126.98	120.38
1	P	133	GLY	N-CA-C	6.39	128.32	113.18
1	Q	76	SER	N-CA-C	6.36	118.07	110.19
1	n	20	GLY	N-CA-C	6.36	122.25	114.69
1	U	117	GLU	N-CA-C	6.35	118.21	111.28
1	Z	98	ILE	CA-C-N	6.35	127.78	119.84
1	Z	98	ILE	C-N-CA	6.35	127.78	119.84
1	G	7	ARG	CA-C-N	-6.34	113.25	119.78
1	G	7	ARG	C-N-CA	-6.34	113.25	119.78
1	M	122	ALA	N-CA-C	6.32	117.83	108.60
1	h	48	PRO	CA-C-N	-6.30	111.96	119.84
1	h	48	PRO	C-N-CA	-6.30	111.96	119.84
1	K	9	ALA	CA-C-N	6.30	126.63	119.83
1	K	9	ALA	C-N-CA	6.30	126.63	119.83
1	T	52	ILE	N-CA-C	6.30	117.80	110.62
1	n	21	GLU	N-CA-C	6.29	120.96	113.16
1	N	145	VAL	N-CA-C	6.26	118.41	108.89
1	k	31	ARG	N-CA-C	-6.25	102.28	110.53
1	f	48	PRO	CA-C-N	6.24	141.97	127.00
1	f	48	PRO	C-N-CA	6.24	141.97	127.00
1	G	115	PHE	N-CA-C	6.21	118.17	110.91
1	G	98	ILE	CA-C-N	6.19	126.40	119.90
1	G	98	ILE	C-N-CA	6.19	126.40	119.90
1	Z	88	ARG	N-CA-C	6.19	117.69	111.07
1	N	48	PRO	N-CA-C	6.19	118.25	110.70
1	K	118	GLU	N-CA-C	-6.18	105.69	113.72
1	F	47	VAL	CA-C-N	6.16	126.72	120.38
1	F	47	VAL	C-N-CA	6.16	126.72	120.38
1	G	112	TYR	N-CA-C	6.13	120.37	113.01
1	X	108	ILE	N-CA-C	6.13	116.87	110.62
1	S	67	CYS	N-CA-C	6.12	117.53	108.60
1	T	50	THR	N-CA-C	6.10	117.58	108.31
1	e	69	VAL	N-CA-C	6.09	116.25	110.53
1	M	158	ALA	N-CA-C	6.08	117.90	111.28
1	Y	143	LYS	CA-C-N	-6.08	113.71	121.91
1	Y	143	LYS	C-N-CA	-6.08	113.71	121.91
1	J	56	SER	N-CA-C	6.08	119.16	111.69
1	L	154	ARG	N-CA-C	6.07	117.98	111.36
1	G	76	SER	CB-CA-C	-6.07	107.85	116.34
1	f	48	PRO	C-N-CD	-6.05	107.29	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	20	GLY	N-CA-C	6.04	122.11	114.25
1	K	16	ALA	N-CA-C	6.02	117.39	108.60
1	b	139	THR	N-CA-C	6.01	120.74	113.17
1	g	155	LEU	N-CA-C	6.01	117.83	111.28
1	c	13	LYS	N-CA-C	6.00	116.20	108.34
1	h	98	ILE	CA-C-N	5.98	127.32	119.84
1	h	98	ILE	C-N-CA	5.98	127.32	119.84
1	S	15	GLN	N-CA-C	-5.98	100.55	109.94
1	U	79	SER	N-CA-C	5.98	117.88	111.36
1	J	59	VAL	N-CA-C	5.98	118.52	111.05
1	O	4	LEU	CA-C-N	5.97	125.36	118.85
1	O	4	LEU	C-N-CA	5.97	125.36	118.85
1	L	135	LEU	N-CA-C	5.96	119.23	110.59
1	Q	39	PHE	CB-CA-C	-5.96	108.70	115.79
1	G	67	CYS	N-CA-C	5.93	116.42	108.23
1	I	50	THR	N-CA-C	-5.93	105.70	113.17
1	H	121	ASN	N-CA-C	5.92	117.91	107.61
1	m	76	SER	N-CA-C	5.90	116.73	108.00
1	j	108	ILE	N-CA-C	5.89	116.63	110.62
1	V	89	LYS	N-CA-C	5.89	117.39	110.97
1	D	72	CYS	N-CA-C	5.88	117.89	110.24
1	Y	66	ASN	N-CA-C	5.88	117.79	110.91
1	g	98	ILE	N-CA-C	5.88	114.30	107.89
1	G	40	TYR	CA-C-N	5.83	127.13	119.84
1	G	40	TYR	C-N-CA	5.83	127.13	119.84
1	R	157	ASP	N-CA-C	5.83	118.51	111.40
1	e	125	GLY	N-CA-C	5.82	120.04	112.25
1	O	143	LYS	CA-C-N	-5.81	114.06	121.91
1	O	143	LYS	C-N-CA	-5.81	114.06	121.91
1	E	124	ARG	CA-C-N	-5.81	116.42	122.69
1	E	124	ARG	C-N-CA	-5.81	116.42	122.69
1	V	126	LEU	N-CA-C	5.80	118.19	108.96
1	O	37	LEU	N-CA-C	5.79	117.73	108.41
1	h	123	PHE	CA-C-N	-5.78	114.81	122.85
1	h	123	PHE	C-N-CA	-5.78	114.81	122.85
1	c	42	ALA	N-CA-C	5.77	117.56	108.96
1	N	130	ASP	CA-C-N	-5.75	112.95	119.28
1	N	130	ASP	C-N-CA	-5.75	112.95	119.28
1	d	15	GLN	N-CA-C	-5.75	100.81	109.95
1	V	69	VAL	N-CA-C	5.72	117.65	111.58
1	H	144	PRO	N-CA-C	5.72	121.06	113.40
1	J	47	VAL	CA-C-N	-5.72	114.49	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	47	VAL	C-N-CA	-5.72	114.49	120.38
1	L	163	GLU	N-CA-C	5.72	116.63	108.74
1	f	38	PHE	N-CA-C	5.72	118.22	108.90
1	I	48	PRO	N-CA-C	5.70	117.66	110.70
1	P	134	ILE	N-CA-C	-5.68	100.05	107.88
1	k	50	THR	N-CA-C	5.64	115.73	108.34
1	X	94	GLY	N-CA-C	-5.64	106.29	112.04
1	n	162	VAL	N-CA-C	5.64	119.00	111.44
1	C	21	GLU	N-CA-C	5.64	120.18	112.68
1	A	16	ALA	N-CA-C	5.63	116.33	108.00
1	j	68	GLN	N-CA-C	5.63	118.48	109.02
1	X	37	LEU	N-CA-C	5.63	117.82	108.99
1	f	42	ALA	N-CA-C	5.62	116.50	108.74
1	j	129	ILE	N-CA-C	5.62	121.04	109.34
1	c	48	PRO	N-CA-C	5.62	117.55	110.70
1	Z	62	PHE	N-CA-C	5.61	117.26	111.03
1	V	38	PHE	N-CA-C	5.61	120.23	113.17
1	m	9	ALA	CA-C-N	5.60	125.60	119.89
1	m	9	ALA	C-N-CA	5.60	125.60	119.89
1	N	69	VAL	N-CA-C	5.59	115.65	107.37
1	i	101	LEU	CB-CA-C	-5.58	108.52	115.89
1	H	48	PRO	N-CA-C	5.58	117.51	110.70
1	l	69	VAL	N-CA-C	5.58	116.34	108.36
1	N	7	ARG	CA-C-N	5.57	126.80	119.84
1	N	7	ARG	C-N-CA	5.57	126.80	119.84
1	a	49	PRO	N-CA-C	5.56	122.30	113.12
1	A	141	ASN	CA-C-N	-5.55	114.48	121.98
1	A	141	ASN	C-N-CA	-5.55	114.48	121.98
1	b	25	ILE	N-CA-C	5.55	116.90	108.80
1	H	150	ASP	N-CA-C	5.55	117.13	111.14
1	b	98	ILE	CA-C-N	5.54	126.77	119.84
1	b	98	ILE	C-N-CA	5.54	126.77	119.84
1	Z	4	LEU	CA-C-N	5.54	126.76	119.84
1	Z	4	LEU	C-N-CA	5.54	126.76	119.84
1	X	47	VAL	CA-C-N	-5.54	114.68	120.38
1	X	47	VAL	C-N-CA	-5.54	114.68	120.38
1	a	16	ALA	N-CA-C	5.53	117.25	108.79
1	n	48	PRO	N-CA-C	5.53	117.44	110.70
1	N	96	MET	N-CA-C	5.53	118.47	108.69
1	c	76	SER	CB-CA-C	-5.53	110.19	116.54
1	a	154	ARG	N-CA-C	5.51	118.47	111.69
1	Z	76	SER	N-CA-C	5.50	118.58	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	133	GLY	CA-C-N	5.49	129.32	121.96
1	P	133	GLY	C-N-CA	5.49	129.32	121.96
1	h	161	PHE	CA-C-N	-5.49	115.64	123.10
1	h	161	PHE	C-N-CA	-5.49	115.64	123.10
1	I	21	GLU	N-CA-C	5.47	122.45	110.80
1	G	4	LEU	CA-C-N	-5.45	114.56	121.91
1	G	4	LEU	C-N-CA	-5.45	114.56	121.91
1	c	121	ASN	N-CA-C	5.44	117.11	108.79
1	c	101	LEU	N-CA-C	5.44	118.59	109.95
1	h	48	PRO	N-CA-C	5.43	117.33	110.70
1	d	47	VAL	CA-C-N	-5.43	114.79	120.38
1	d	47	VAL	C-N-CA	-5.43	114.79	120.38
1	d	87	ASP	CB-CA-C	-5.43	109.33	115.79
1	E	105	LYS	N-CA-C	5.43	117.54	107.99
1	V	102	ALA	CA-C-N	-5.43	114.94	123.13
1	V	102	ALA	C-N-CA	-5.43	114.94	123.13
1	A	89	LYS	N-CA-C	5.42	116.88	110.97
1	n	50	THR	N-CA-C	-5.42	106.64	113.20
1	W	12	PHE	N-CA-C	5.40	116.47	108.86
1	c	44	PHE	N-CA-C	5.40	118.84	111.39
1	c	4	LEU	N-CA-C	5.39	118.37	109.58
1	M	37	LEU	N-CA-C	5.39	117.12	107.80
1	Z	163	GLU	N-CA-C	5.39	117.23	111.36
1	C	106	GLN	CB-CA-C	-5.39	110.34	116.54
1	N	141	ASN	CA-C-N	-5.38	111.27	121.54
1	N	141	ASN	C-N-CA	-5.38	111.27	121.54
1	K	76	SER	N-CA-C	5.37	119.20	109.32
1	l	20	GLY	N-CA-C	5.37	121.23	114.25
1	d	83	TRP	N-CA-C	5.37	118.99	112.23
1	j	17	VAL	N-CA-C	5.37	115.04	106.88
1	e	72	CYS	N-CA-C	5.37	117.41	108.99
1	h	81	LEU	N-CA-C	5.36	117.20	111.36
1	H	42	ALA	N-CA-C	5.36	116.41	108.86
1	a	133	GLY	N-CA-C	5.36	125.87	113.18
1	d	49	PRO	CA-C-O	-5.34	114.90	121.31
1	j	133	GLY	N-CA-C	-5.33	105.70	114.76
1	U	130	ASP	CA-C-N	5.32	124.99	119.56
1	U	130	ASP	C-N-CA	5.32	124.99	119.56
1	j	38	PHE	N-CA-C	5.32	117.63	109.07
1	C	108	ILE	N-CA-C	-5.30	105.22	111.00
1	M	63	ASN	N-CA-C	5.30	118.91	112.23
1	J	72	CYS	N-CA-C	5.30	122.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	56	SER	N-CA-C	5.29	117.13	111.36
1	n	85	ASN	N-CA-C	5.29	116.85	111.14
1	U	120	GLY	N-CA-C	-5.29	107.75	115.63
1	R	143	LYS	CA-C-N	-5.28	114.78	121.91
1	R	143	LYS	C-N-CA	-5.28	114.78	121.91
1	T	120	GLY	N-CA-C	-5.28	107.40	115.00
1	T	145	VAL	N-CA-C	5.27	116.17	110.21
1	k	133	GLY	N-CA-C	-5.27	106.97	115.08
1	h	152	THR	N-CA-C	5.24	116.99	111.28
1	b	140	ILE	N-CA-C	5.24	117.00	109.51
1	U	34	TYR	N-CA-C	5.23	121.93	110.80
1	B	4	LEU	CA-C-N	-5.22	115.20	120.21
1	B	4	LEU	C-N-CA	-5.22	115.20	120.21
1	m	76	SER	CB-CA-C	-5.21	109.05	116.34
1	e	67	CYS	N-CA-C	5.18	117.50	111.02
1	e	74	THR	N-CA-C	5.18	118.70	112.38
1	g	98	ILE	CA-C-N	5.17	125.98	119.98
1	g	98	ILE	C-N-CA	5.17	125.98	119.98
1	R	116	ASP	N-CA-C	-5.17	102.25	109.96
1	c	51	GLU	N-CA-C	5.17	116.60	110.97
1	K	102	ALA	N-CA-C	5.16	117.77	108.48
1	d	70	ILE	N-CA-C	5.16	115.39	108.17
1	D	112	TYR	N-CA-C	5.16	119.20	113.01
1	g	48	PRO	CA-C-N	-5.15	114.49	119.90
1	g	48	PRO	C-N-CA	-5.15	114.49	119.90
1	d	118	GLU	N-CA-C	5.15	116.70	111.14
1	j	143	LYS	N-CA-C	5.14	119.24	112.35
1	T	154	ARG	N-CA-C	-5.14	105.75	111.36
1	A	16	ALA	CB-CA-C	-5.14	109.15	116.34
1	j	95	HIS	N-CA-C	5.14	117.10	108.73
1	g	47	VAL	CA-C-N	5.13	125.67	120.38
1	g	47	VAL	C-N-CA	5.13	125.67	120.38
1	b	20	GLY	N-CA-C	5.12	120.91	114.25
1	a	88	ARG	N-CA-C	5.12	117.25	111.11
1	I	40	TYR	CA-C-N	5.12	126.23	119.84
1	I	40	TYR	C-N-CA	5.12	126.23	119.84
1	l	45	THR	N-CA-C	-5.11	102.48	110.10
1	Z	136	ARG	N-CA-C	5.11	117.97	111.69
1	H	25	ILE	N-CA-C	5.10	119.95	109.34
1	h	42	ALA	N-CA-C	5.10	115.78	108.74
1	b	143	LYS	CA-C-N	-5.10	115.03	121.91
1	b	143	LYS	C-N-CA	-5.10	115.03	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	44	PHE	N-CA-C	5.09	118.26	111.24
1	i	126	LEU	N-CA-C	5.08	118.35	110.17
1	K	40	TYR	CA-C-N	5.08	124.25	118.97
1	K	40	TYR	C-N-CA	5.08	124.25	118.97
1	a	113	GLY	N-CA-C	5.08	123.06	115.64
1	O	120	GLY	N-CA-C	-5.08	107.69	115.00
1	a	17	VAL	N-CA-C	5.07	115.06	107.51
1	M	48	PRO	N-CA-C	5.06	116.87	110.70
1	I	44	PHE	CB-CA-C	-5.06	104.70	111.89
1	Q	36	VAL	N-CA-C	5.05	119.85	109.34
1	M	24	GLU	N-CA-C	5.05	117.01	109.59
1	l	144	PRO	N-CA-C	5.04	120.16	113.40
1	D	9	ALA	CA-C-N	5.04	126.14	119.84
1	D	9	ALA	C-N-CA	5.04	126.14	119.84
1	D	97	LYS	N-CA-C	-5.03	106.99	113.02
1	K	7	ARG	CA-C-N	5.02	126.12	119.84
1	K	7	ARG	C-N-CA	5.02	126.12	119.84
1	D	3	LEU	N-CA-C	5.02	116.49	108.41
1	E	27	LEU	N-CA-C	-5.01	105.29	111.40

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	GLU	Peptide
1	A	94	GLY	Peptide
1	B	105	LYS	Peptide
1	B	31	ARG	Peptide
1	B	43	ASP	Peptide
1	E	45	THR	Peptide
1	G	10	PRO	Peptide
1	G	5	PRO	Peptide
1	H	16	ALA	Peptide
1	K	117	GLU	Peptide
1	L	18	ILE	Peptide
1	M	143	LYS	Peptide
1	N	47	VAL	Peptide
1	N	96	MET	Peptide
1	P	34	TYR	Peptide
1	Q	60	GLU	Peptide
1	Q	87	ASP	Peptide
1	R	132	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	S	47	VAL	Peptide
1	S	91	GLY	Peptide
1	T	48	PRO	Peptide
1	U	47	VAL	Peptide
1	V	102	ALA	Peptide
1	V	124	ARG	Peptide
1	V	49	PRO	Peptide
1	V	73	SER	Peptide
1	W	132	ASN	Peptide
1	X	33	LYS	Peptide
1	Y	46	PHE	Peptide
1	Y	50	THR	Peptide
1	a	46	PHE	Peptide
1	a	65	ARG	Peptide
1	a	67	CYS	Peptide
1	b	121	ASN	Peptide
1	b	48	PRO	Peptide
1	c	103	ASP	Peptide
1	c	119	ASP	Peptide
1	c	5	PRO	Peptide
1	d	46	PHE	Peptide
1	d	47	VAL	Peptide
1	d	48	PRO	Peptide
1	e	49	PRO	Peptide
1	e	94	GLY	Peptide
1	f	44	PHE	Peptide
1	f	45	THR	Peptide
1	f	46	PHE	Peptide
1	f	50	THR	Peptide
1	h	105	LYS	Peptide
1	h	148	SER	Peptide
1	h	33	LYS	Peptide
1	h	35	VAL	Peptide
1	j	45	THR	Peptide
1	k	44	PHE	Peptide
1	k	48	PRO	Peptide
1	k	94	GLY	Peptide
1	l	46	PHE	Peptide
1	l	71	ALA	Peptide
1	m	146	GLY	Peptide
1	n	47	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1310	0	1282	94	0
1	B	1337	0	1329	82	0
1	C	1325	0	1303	85	0
1	D	1331	0	1312	106	0
1	E	1300	0	1275	78	0
1	F	1325	0	1303	92	0
1	G	1306	0	1281	114	0
1	H	1325	0	1303	101	0
1	I	1316	0	1288	86	0
1	J	1332	0	1310	85	0
1	K	1291	0	1262	78	0
1	L	1327	0	1322	105	0
1	M	1325	0	1303	103	0
1	N	1331	0	1312	80	1
1	O	1310	0	1282	88	0
1	P	1325	0	1303	108	0
1	Q	1267	0	1241	102	0
1	R	1315	0	1296	86	1
1	S	1316	0	1288	108	0
1	T	1332	0	1310	89	0
1	U	1310	0	1282	114	0
1	V	1337	0	1329	113	0
1	W	1325	0	1303	91	0
1	X	1331	0	1312	102	0
1	Y	1310	0	1282	89	1
1	Z	1325	0	1303	110	0
1	a	1316	0	1288	113	0
1	b	1325	0	1303	109	1
1	c	1316	0	1288	90	0
1	d	1332	0	1310	113	0
1	e	1300	0	1275	82	0
1	f	1337	0	1329	87	0
1	g	1325	0	1303	97	0
1	h	1321	0	1305	103	0
1	i	1271	0	1242	89	0
1	j	1325	0	1303	99	0
1	k	1316	0	1288	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	l	1325	0	1303	94	0
1	m	1267	0	1241	83	0
1	n	1332	0	1310	107	0
All	All	52692	0	51804	3465	2

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 33.

All (3465) 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:i:65:ARG:NH1	1:i:157:ASP:OD2	1.84	1.09
1:H:76:SER:HB2	1:H:104:ARG:HH11	1.17	1.06
1:U:33:LYS:HZ3	1:U:68:GLN:HG3	1.15	1.06
1:D:119:ASP:OD2	1:D:143:LYS:NZ	1.89	1.06
1:g:11:GLU:OE1	1:g:28:LYS:NZ	1.89	1.04
1:e:18:ILE:HG12	1:e:23:LYS:HZ2	1.17	1.03
1:a:124:ARG:NH1	1:a:143:LYS:O	1.94	1.00
1:Y:7:ARG:NH1	1:Z:118:GLU:OE1	1.93	0.99
1:L:151:GLU:HB2	1:L:154:ARG:HH11	1.26	0.99
1:Y:36:VAL:HB	1:Y:69:VAL:HG23	1.45	0.98
1:K:125:GLY:O	1:K:147:ARG:NH1	1.97	0.97
1:G:124:ARG:NH1	1:G:145:VAL:O	1.97	0.97
1:Y:119:ASP:OD2	1:Y:143:LYS:NZ	1.96	0.97
1:D:65:ARG:NH1	1:D:157:ASP:OD1	1.97	0.97
1:j:88:ARG:NH1	1:j:93:LEU:O	1.97	0.97
1:T:103:ASP:OD2	1:T:109:SER:OG	1.83	0.96
1:Y:69:VAL:HG22	1:Y:70:ILE:H	1.32	0.95
1:e:39:PHE:O	1:e:147:ARG:NH1	2.00	0.94
1:U:51:GLU:OE2	1:U:124:ARG:NH1	2.01	0.93
1:Z:76:SER:HB2	1:Z:104:ARG:HG2	1.50	0.92
1:M:1:MET:HG3	1:N:3:LEU:H	1.34	0.92
1:O:151:GLU:OE2	1:O:154:ARG:NH1	2.03	0.92
1:T:122:ALA:O	1:T:143:LYS:NZ	2.02	0.92
1:l:124:ARG:NH1	1:l:143:LYS:O	2.03	0.91
1:S:5:PRO:O	1:S:7:ARG:NH1	2.02	0.91
1:k:38:PHE:HA	1:k:125:GLY:HA3	1.53	0.91
1:m:88:ARG:HH11	1:m:94:GLY:H	0.99	0.91
1:R:31:ARG:NH1	1:R:131:PRO:O	2.03	0.90
1:K:39:PHE:O	1:K:147:ARG:NH2	2.04	0.90
1:a:62:PHE:O	1:a:65:ARG:NH1	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:115:PHE:HA	1:k:122:ALA:HA	1.54	0.88
1:O:38:PHE:HB3	1:O:126:LEU:HD23	1.54	0.88
1:K:84:ASP:HA	1:K:93:LEU:HB2	1.53	0.88
1:D:109:SER:HB2	1:D:115:PHE:HB2	1.56	0.88
1:Y:124:ARG:NH1	1:Y:143:LYS:O	2.06	0.87
1:j:33:LYS:NZ	1:j:68:GLN:OE1	2.07	0.87
1:Y:24:GLU:OE1	1:Y:25:ILE:N	2.08	0.87
1:J:39:PHE:O	1:J:147:ARG:NH2	2.08	0.86
1:C:65:ARG:HH12	1:C:153:LEU:HG	1.41	0.86
1:I:154:ARG:HH11	1:J:148:SER:HB3	1.39	0.86
1:U:72:CYS:SG	1:U:73:SER:N	2.49	0.85
1:k:109:SER:HB3	1:k:115:PHE:HB2	1.58	0.85
1:G:89:LYS:HB2	1:X:13:LYS:HZ2	1.38	0.85
1:P:74:THR:O	1:Q:104:ARG:NH1	2.08	0.85
1:X:122:ALA:O	1:X:143:LYS:NZ	2.10	0.85
1:c:72:CYS:SG	1:c:73:SER:N	2.46	0.85
1:m:84:ASP:HA	1:m:93:LEU:HB2	1.58	0.85
1:C:122:ALA:O	1:C:143:LYS:NZ	2.10	0.85
1:j:9:ALA:N	1:j:133:GLY:O	2.10	0.85
1:F:75:ASP:OD1	1:G:104:ARG:NH1	2.10	0.84
1:Q:74:THR:HA	1:Q:103:ASP:HB3	1.58	0.84
1:h:88:ARG:H	1:h:88:ARG:HE	1.25	0.84
1:k:8:PRO:HA	1:k:134:ILE:HA	1.56	0.84
1:U:126:LEU:HD22	1:U:152:THR:HG21	1.59	0.84
1:g:16:ALA:HB3	1:g:24:GLU:HA	1.60	0.84
1:X:115:PHE:HA	1:X:122:ALA:HA	1.58	0.84
1:W:65:ARG:HD3	1:W:156:LEU:HD11	1.57	0.84
1:V:53:ILE:HD11	1:V:88:ARG:HH11	1.41	0.84
1:k:56:SER:OG	1:k:88:ARG:NH2	2.10	0.84
1:D:74:THR:HA	1:D:103:ASP:HB3	1.59	0.84
1:c:71:ALA:HB3	1:c:100:LEU:HA	1.60	0.84
1:A:104:ARG:NH1	1:J:74:THR:OG1	2.11	0.83
1:n:116:ASP:H	1:n:122:ALA:HA	1.41	0.83
1:D:72:CYS:HB2	1:D:101:LEU:HB3	1.60	0.83
1:N:128:ILE:HG23	1:N:136:ARG:HB2	1.60	0.83
1:m:88:ARG:NH1	1:m:94:GLY:H	1.76	0.83
1:E:51:GLU:HG3	1:E:124:ARG:HH12	1.43	0.83
1:N:103:ASP:OD1	1:N:106:GLN:N	2.11	0.83
1:R:130:ASP:OD1	1:R:136:ARG:NH1	2.12	0.82
1:H:7:ARG:HH11	1:H:7:ARG:H	1.23	0.82
1:G:38:PHE:HA	1:G:126:LEU:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:ASP:OD2	1:H:136:ARG:NH1	2.12	0.82
1:O:39:PHE:O	1:O:147:ARG:NH2	2.11	0.82
1:g:119:ASP:N	1:g:119:ASP:OD1	2.12	0.82
1:g:151:GLU:OE2	1:g:154:ARG:NH1	2.12	0.81
1:i:125:GLY:HA3	1:i:140:ILE:HA	1.61	0.81
1:H:118:GLU:O	1:I:105:LYS:NZ	2.13	0.81
1:P:52:ILE:HD13	1:P:124:ARG:HH12	1.43	0.81
1:S:151:GLU:HB2	1:T:151:GLU:HG3	1.62	0.81
1:P:75:ASP:HA	1:Q:104:ARG:HH12	1.45	0.81
1:a:128:ILE:HG23	1:a:136:ARG:HB3	1.63	0.81
1:n:32:GLY:HA2	1:n:131:PRO:HB3	1.61	0.81
1:A:151:GLU:HB2	1:B:151:GLU:HG3	1.62	0.81
1:I:118:GLU:OE2	1:J:7:ARG:NH2	2.14	0.81
1:Q:160:GLN:OE1	1:Q:164:LYS:NZ	2.14	0.80
1:C:1:MET:HE2	1:D:3:LEU:HB2	1.63	0.80
1:B:137:GLN:HB3	1:B:159:PHE:HZ	1.46	0.80
1:N:11:GLU:OE2	1:N:27:LEU:HB3	1.82	0.80
1:a:114:VAL:HG11	1:a:140:ILE:HG21	1.64	0.80
1:e:138:ILE:HB	1:f:140:ILE:HG23	1.63	0.80
1:A:38:PHE:HA	1:A:126:LEU:H	1.47	0.80
1:U:78:TYR:HB3	1:d:44:PHE:HB3	1.61	0.80
1:Y:16:ALA:HB2	1:Y:25:ILE:HB	1.63	0.80
1:I:36:VAL:HB	1:I:69:VAL:HA	1.64	0.80
1:X:74:THR:HA	1:X:103:ASP:HB3	1.63	0.80
1:d:75:ASP:OD2	1:d:80:HIS:NE2	2.15	0.80
1:Z:65:ARG:HG2	1:Z:156:LEU:HD11	1.62	0.80
1:f:13[A]:LYS:NZ	1:f:25:ILE:O	2.14	0.79
1:I:136:ARG:HH22	1:J:144:PRO:HG2	1.48	0.79
1:U:154:ARG:HH11	1:U:155:LEU:HA	1.47	0.79
1:D:121:ASN:OD1	1:E:104:ARG:NH1	2.15	0.79
1:V:25:ILE:HD11	1:V:101:LEU:HD21	1.63	0.79
1:m:38:PHE:HB2	1:m:147:ARG:HH12	1.48	0.79
1:F:15:GLN:HB2	1:F:77:GLN:HE22	1.48	0.79
1:b:124:ARG:HG3	1:b:124:ARG:HH11	1.48	0.79
1:h:16:ALA:HB2	1:h:101:LEU:HD23	1.65	0.79
1:Z:104:ARG:NH1	1:a:121:ASN:OD1	2.16	0.78
1:C:124:ARG:HB3	1:C:147:ARG:HH12	1.46	0.78
1:Z:39:PHE:O	1:Z:147:ARG:NH1	2.16	0.78
1:B:105:LYS:NZ	1:C:117:GLU:O	2.14	0.78
1:H:48:PRO:HG2	1:H:49:PRO:HD3	1.65	0.78
1:G:11:GLU:OE1	1:G:27:LEU:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:5:PRO:HB3	1:S:136:ARG:HA	1.66	0.78
1:e:119:ASP:OD2	1:e:143:LYS:NZ	2.17	0.78
1:E:51:GLU:HG3	1:E:124:ARG:NH1	1.98	0.78
1:n:47:VAL:HA	1:n:49:PRO:HD2	1.66	0.78
1:l:56:SER:HB3	1:l:96:MET:HE2	1.65	0.78
1:D:114:VAL:HG22	1:D:115:PHE:H	1.48	0.78
1:W:140:ILE:HB	1:X:138:ILE:HG13	1.66	0.78
1:e:33:LYS:HG3	1:e:66:ASN:HB3	1.65	0.78
1:D:115:PHE:HA	1:D:122:ALA:HA	1.66	0.78
1:f:124:ARG:HE	1:f:146:GLY:HA2	1.47	0.78
1:i:80:HIS:HD2	1:i:100:LEU:HD23	1.47	0.78
1:G:67:CYS:SG	1:G:68:GLN:N	2.51	0.77
1:l:124:ARG:HB2	1:l:141:ASN:HB3	1.65	0.77
1:S:105:LYS:H	1:S:105:LYS:NZ	1.82	0.77
1:C:6:ASN:OD1	1:C:136:ARG:NH1	2.17	0.77
1:b:65:ARG:NH1	1:b:157:ASP:OD1	2.16	0.77
1:T:67:CYS:SG	1:T:68:GLN:N	2.53	0.77
1:C:137:GLN:HB2	1:C:159:PHE:HE2	1.48	0.77
1:G:76:SER:HB2	1:G:104:ARG:HD2	1.67	0.77
1:H:76:SER:HB2	1:H:104:ARG:NH1	1.96	0.77
1:e:154:ARG:NH2	1:f:146:GLY:O	2.18	0.77
1:n:39:PHE:HB2	1:n:124:ARG:HA	1.67	0.77
1:Y:162:VAL:HG11	1:Z:144:PRO:HB2	1.68	0.76
1:l:28:LYS:HD2	1:l:31:ARG:NH1	2.01	0.76
1:T:41:PRO:HB3	1:T:143:LYS:HZ2	1.50	0.76
1:a:50:THR:HG23	1:a:54:ALA:HB2	1.68	0.76
1:b:104:ARG:HG3	1:c:120:GLY:HA3	1.67	0.76
1:i:65:ARG:HB3	1:i:156:LEU:HD11	1.65	0.76
1:n:73:SER:OG	1:n:80:HIS:NE2	2.16	0.76
1:J:50:THR:HB	1:J:53:ILE:HB	1.68	0.76
1:O:87:ASP:HB3	1:O:89:LYS:NZ	2.01	0.76
1:S:39:PHE:O	1:S:147:ARG:NH2	2.18	0.76
1:P:124:ARG:HB3	1:P:141:ASN:HB2	1.66	0.76
1:U:41:PRO:HD3	1:U:147:ARG:HH22	1.48	0.76
1:Z:125:GLY:HA2	1:Z:140:ILE:HG13	1.68	0.76
1:m:38:PHE:HB2	1:m:147:ARG:NH1	2.01	0.76
1:g:51:GLU:HG2	1:g:52:ILE:HG13	1.66	0.76
1:j:11:GLU:OE1	1:j:12:PHE:N	2.19	0.76
1:i:40:TYR:HB2	1:i:124:ARG:NH1	2.00	0.75
1:b:34:TYR:OH	1:b:163:GLU:OE1	2.03	0.75
1:B:38:PHE:HB2	1:B:147:ARG:HH12	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:33:LYS:NZ	1:S:67:CYS:O	2.19	0.75
1:n:61:GLU:O	1:n:65:ARG:NH1	2.19	0.75
1:U:162:VAL:HG21	1:V:144:PRO:HB2	1.68	0.75
1:m:74:THR:O	1:m:80:HIS:NE2	2.19	0.75
1:b:46:PHE:HB3	1:b:47:VAL:HG22	1.67	0.75
1:b:74:THR:OG1	1:b:121:ASN:ND2	2.19	0.75
1:Z:78:TYR:HA	1:Z:81:LEU:HB3	1.67	0.75
1:C:41:PRO:HB3	1:C:143:LYS:HZ1	1.51	0.75
1:V:16:ALA:HB2	1:V:101:LEU:HD13	1.69	0.75
1:c:137:GLN:NE2	1:d:140:ILE:O	2.20	0.75
1:g:35:VAL:HG12	1:g:68:GLN:HB3	1.68	0.75
1:S:124:ARG:NH2	1:S:143:LYS:O	2.20	0.75
1:g:160:GLN:O	1:g:164:LYS:NZ	2.20	0.75
1:O:65:ARG:NH1	1:O:157:ASP:OD1	2.20	0.74
1:S:50:THR:HG22	1:S:51:GLU:H	1.52	0.74
1:V:124:ARG:NH1	1:V:145:VAL:O	2.19	0.74
1:X:74:THR:O	1:Y:104:ARG:NH1	2.20	0.74
1:F:49:PRO:HG2	1:F:52:ILE:HD13	1.69	0.74
1:V:70:ILE:HG22	1:V:99:PRO:HG2	1.70	0.74
1:e:31:ARG:HH12	1:e:133:GLY:HA3	1.51	0.74
1:N:88:ARG:HG2	1:N:94:GLY:HA3	1.69	0.74
1:b:104:ARG:NH1	1:c:104:ARG:NH1	2.36	0.74
1:n:34:TYR:OH	1:n:163:GLU:OE2	2.04	0.74
1:O:140:ILE:HG23	1:P:138:ILE:HB	1.70	0.74
1:P:75:ASP:HA	1:Q:104:ARG:NH1	2.01	0.74
1:Z:18:ILE:O	1:Z:20:GLY:N	2.21	0.73
1:I:49:PRO:HA	1:I:53:ILE:HD13	1.68	0.73
1:i:141:ASN:HA	1:j:137:GLN:HG3	1.69	0.73
1:O:69:VAL:HG12	1:O:70:ILE:H	1.53	0.73
1:T:45:THR:OG1	1:T:48:PRO:O	2.06	0.73
1:d:35:VAL:H	1:d:129:ILE:HG22	1.51	0.73
1:m:21:GLU:HG3	1:m:23:LYS:NZ	2.03	0.73
1:c:141:ASN:HA	1:d:137:GLN:HG2	1.68	0.73
1:g:59:VAL:HG13	1:g:60:GLU:H	1.52	0.73
1:A:15:GLN:HA	1:A:24:GLU:HA	1.71	0.73
1:V:160:GLN:HB3	1:V:164:LYS:HZ2	1.53	0.73
1:n:88:ARG:NH1	1:n:88:ARG:H	1.86	0.73
1:A:114:VAL:HG23	1:A:123:PHE:HB2	1.71	0.73
1:E:36:VAL:HG23	1:E:67:CYS:SG	2.29	0.73
1:d:51:GLU:HG2	1:d:146:GLY:HA3	1.71	0.73
1:m:88:ARG:HH11	1:m:94:GLY:N	1.83	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:SER:HB3	1:E:104:ARG:NH1	2.03	0.73
1:I:34:TYR:OH	1:I:163:GLU:OE2	2.05	0.73
1:X:12:PHE:HB2	1:X:108:ILE:HG22	1.69	0.73
1:a:68:GLN:HE22	1:a:99:PRO:HG2	1.52	0.73
1:F:28:LYS:HG2	1:F:31:ARG:HH21	1.54	0.72
1:Q:35:VAL:HB	1:Q:129:ILE:HG23	1.69	0.72
1:X:151:GLU:OE1	1:X:154:ARG:NH1	2.19	0.72
1:e:151:GLU:HG3	1:f:151:GLU:HB2	1.70	0.72
1:M:28:LYS:HG2	1:M:31:ARG:HH21	1.53	0.72
1:Q:151:GLU:HG3	1:R:151:GLU:HB2	1.71	0.72
1:i:156:LEU:HA	1:i:159:PHE:HB2	1.71	0.72
1:P:85:ASN:OD1	1:P:85:ASN:N	2.23	0.72
1:K:151:GLU:HG2	1:L:151:GLU:HG2	1.71	0.72
1:c:75:ASP:HB3	1:c:79:SER:HB3	1.71	0.72
1:h:35:VAL:HA	1:h:68:GLN:HB3	1.71	0.72
1:W:51:GLU:C	1:W:53:ILE:H	1.98	0.72
1:n:6:ASN:OD1	1:n:136:ARG:NH1	2.22	0.72
1:D:16:ALA:HB2	1:D:101:LEU:HD23	1.70	0.72
1:P:96:MET:HG3	1:P:98:ILE:H	1.54	0.72
1:i:74:THR:HA	1:i:103:ASP:HB3	1.72	0.72
1:V:160:GLN:HB3	1:V:164:LYS:NZ	2.05	0.72
1:h:104:ARG:NH1	1:i:121:ASN:OD1	2.22	0.72
1:k:124:ARG:NH1	1:k:147:ARG:NH1	2.38	0.72
1:F:103:ASP:OD2	1:F:108:ILE:N	2.23	0.72
1:L:50:THR:HB	1:L:53:ILE:H	1.55	0.72
1:Y:50:THR:H	1:Y:53:ILE:HG22	1.53	0.72
1:S:76:SER:HB2	1:S:104:ARG:NH1	2.04	0.71
1:b:104:ARG:NH1	1:c:104:ARG:HH12	1.87	0.71
1:h:124:ARG:HB3	1:h:147:ARG:HE	1.52	0.71
1:J:127:PHE:HB3	1:J:135:LEU:HD21	1.72	0.71
1:L:147:ARG:HB2	1:L:147:ARG:HH11	1.55	0.71
1:I:137:GLN:NE2	1:I:139:THR:OG1	2.22	0.71
1:m:9:ALA:HB2	1:m:135:LEU:HB2	1.70	0.71
1:B:33[A]:LYS:HZ1	1:B:68:GLN:HB3	1.54	0.71
1:G:89:LYS:HB2	1:X:13:LYS:NZ	2.04	0.71
1:J:27:LEU:HD22	1:J:31:ARG:HH12	1.56	0.71
1:O:4:LEU:HB3	1:O:7:ARG:HD3	1.72	0.71
1:Q:3:LEU:HD21	1:R:2:VAL:HG22	1.71	0.71
1:Q:30:TYR:HD1	1:Q:33:LYS:HZ2	1.37	0.71
1:f:50:THR:HA	1:f:51:GLU:HB2	1.72	0.71
1:P:52:ILE:HD13	1:P:124:ARG:NH1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:51:GLU:OE2	1:n:147:ARG:HD2	1.91	0.71
1:H:104:ARG:NH2	1:I:74:THR:O	2.23	0.71
1:U:86:LEU:HD21	1:d:86:LEU:HD21	1.72	0.71
1:Y:53:ILE:HD11	1:Y:88:ARG:HH21	1.55	0.71
1:m:129:ILE:HG12	1:m:135:LEU:HD22	1.72	0.71
1:E:53:ILE:HG12	1:E:96:MET:HE1	1.71	0.71
1:D:27:LEU:HD22	1:D:31[B]:ARG:NH1	2.06	0.71
1:M:18:ILE:HG13	1:M:19:ASN:H	1.56	0.71
1:a:147:ARG:O	1:b:154:ARG:NH2	2.23	0.71
1:l:71:ALA:HB3	1:l:100:LEU:HA	1.71	0.71
1:A:124:ARG:NH1	1:A:143:LYS:O	2.23	0.71
1:B:31:ARG:NH1	1:B:133:GLY:HA3	2.06	0.71
1:D:88:ARG:HD2	1:D:94:GLY:HA3	1.71	0.71
1:R:36:VAL:HG22	1:R:128:ILE:HG12	1.73	0.71
1:Y:65:ARG:HD2	1:Y:156:LEU:HD21	1.73	0.71
1:n:110:LYS:HA	1:n:115:PHE:HB2	1.72	0.71
1:G:96:MET:HG2	1:G:98:ILE:H	1.53	0.70
1:L:76:SER:HB2	1:L:104:ARG:HG2	1.73	0.70
1:W:28:LYS:HA	1:W:31:ARG:NH1	2.06	0.70
1:a:3:LEU:HD11	1:a:113:GLY:HA3	1.72	0.70
1:g:105:LYS:HD2	1:g:107:GLU:OE1	1.91	0.70
1:i:12:PHE:HB3	1:i:108:ILE:HG21	1.72	0.70
1:N:105:LYS:HA	1:O:106:GLN:HE22	1.55	0.70
1:c:84:ASP:OD1	1:c:95:HIS:HA	1.91	0.70
1:K:154:ARG:NH1	1:L:148:SER:HB3	2.04	0.70
1:S:124:ARG:HB3	1:S:141:ASN:HB2	1.72	0.70
1:a:41:PRO:HG3	1:a:143:LYS:HB2	1.74	0.70
1:j:157:ASP:HA	1:j:160:GLN:HE21	1.55	0.70
1:F:53:ILE:HD12	1:F:94:GLY:H	1.55	0.70
1:Z:142:ASP:OD2	1:Z:144:PRO:HD2	1.92	0.70
1:e:13:LYS:HD3	1:e:26:CYS:HB3	1.71	0.70
1:k:30:TYR:HD2	1:k:70:ILE:HD11	1.57	0.70
1:A:116:ASP:OD1	1:B:7:ARG:NH2	2.24	0.70
1:Y:148:SER:OG	1:Z:151:GLU:OE2	2.09	0.70
1:d:164:LYS:O	1:d:165:HIS:ND1	2.24	0.70
1:l:145:VAL:HG13	1:l:146:GLY:H	1.55	0.70
1:A:51:GLU:OE2	1:A:147:ARG:N	2.24	0.70
1:H:6:ASN:HB3	1:H:7:ARG:HH12	1.56	0.70
1:H:141:ASN:N	1:H:141:ASN:OD1	2.25	0.70
1:i:23:LYS:HD3	1:i:24:GLU:H	1.55	0.70
1:k:39:PHE:O	1:k:147:ARG:NH2	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:36:VAL:HG13	1:M:128:ILE:HG23	1.73	0.70
1:N:16:ALA:HB3	1:N:25:ILE:HD12	1.72	0.70
1:g:35:VAL:HA	1:g:68:GLN:H	1.56	0.70
1:k:7:ARG:NH2	1:l:116:ASP:OD1	2.23	0.70
1:m:39:PHE:O	1:m:147:ARG:NH2	2.23	0.70
1:H:40:TYR:CZ	1:H:73:SER:HB2	2.27	0.70
1:S:80:HIS:CE1	1:S:102:ALA:HB2	2.26	0.70
1:V:130:ASP:OD1	1:V:134:ILE:N	2.25	0.70
1:l:104:ARG:HA	1:l:104:ARG:HH11	1.56	0.70
1:Y:50:THR:HB	1:Y:51:GLU:HA	1.74	0.69
1:d:124:ARG:NH1	1:d:143:LYS:O	2.22	0.69
1:k:143:LYS:HB3	1:k:143:LYS:HZ3	1.57	0.69
1:m:53:ILE:HG12	1:m:54:ALA:H	1.57	0.69
1:B:12:PHE:HB2	1:B:108:ILE:HD12	1.73	0.69
1:H:6:ASN:HB3	1:H:7:ARG:NH1	2.06	0.69
1:N:5:PRO:HA	1:N:135:LEU:HB3	1.72	0.69
1:O:125:GLY:HA2	1:O:140:ILE:HA	1.75	0.69
1:Y:46:PHE:HA	1:Y:48:PRO:HD3	1.75	0.69
1:c:5:PRO:O	1:c:7:ARG:N	2.25	0.69
1:E:7:ARG:HE	1:E:7:ARG:H	1.40	0.69
1:I:32:GLY:H	1:I:131:PRO:HB3	1.58	0.69
1:h:151:GLU:HG2	1:h:155:LEU:HD23	1.74	0.69
1:l:120:GLY:HA3	1:m:104:ARG:HB3	1.73	0.69
1:E:140:ILE:HG22	1:F:138:ILE:HB	1.73	0.69
1:F:42:ALA:HB2	1:F:121:ASN:ND2	2.08	0.69
1:O:47:VAL:HG12	1:O:91:GLY:HA2	1.72	0.69
1:U:72:CYS:HB2	1:U:80:HIS:NE2	2.06	0.69
1:d:49:PRO:HA	1:d:50:THR:HB	1.74	0.69
1:W:1:MET:N	1:W:1:MET:SD	2.66	0.69
1:h:141:ASN:HB2	1:h:145:VAL:HG21	1.75	0.69
1:e:6:ASN:HA	1:e:136:ARG:NH1	2.07	0.69
1:g:38:PHE:HB2	1:g:147:ARG:HH12	1.57	0.69
1:C:119:ASP:OD2	1:C:121:ASN:ND2	2.25	0.69
1:G:80:HIS:HD2	1:G:100:LEU:HB3	1.58	0.69
1:L:45:THR:HA	1:M:78:TYR:HB3	1.74	0.69
1:Q:36:VAL:HB	1:Q:128:ILE:HG13	1.74	0.69
1:Q:59:VAL:HG22	1:Q:97:LYS:HG2	1.74	0.69
1:X:35:VAL:HG22	1:X:68:GLN:HB2	1.73	0.69
1:Z:18:ILE:HG22	1:Z:99:PRO:HG3	1.74	0.69
1:f:60:GLU:O	1:f:64:SER:N	2.20	0.69
1:k:84:ASP:OD1	1:k:96:MET:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:116:ASP:OD1	1:l:7:ARG:NH2	2.25	0.69
1:n:130:ASP:N	1:n:134:ILE:O	2.22	0.69
1:V:164:LYS:HG3	1:V:165:HIS:H	1.57	0.69
1:W:51:GLU:O	1:W:53:ILE:N	2.24	0.69
1:i:117:GLU:H	1:j:7:ARG:HH22	1.41	0.69
1:P:60:GLU:O	1:P:64:SER:OG	2.11	0.69
1:b:8:PRO:HA	1:b:134:ILE:HA	1.75	0.69
1:N:52:ILE:HG21	1:N:147:ARG:HE	1.58	0.68
1:U:44:PHE:HB2	1:d:78:TYR:HB3	1.75	0.68
1:Y:33:LYS:NZ	1:Y:66:ASN:OD1	2.23	0.68
1:Z:124:ARG:NH2	1:Z:143:LYS:O	2.26	0.68
1:a:137:GLN:HG2	1:b:141:ASN:HA	1.73	0.68
1:E:11:GLU:HG2	1:E:27:LEU:HB3	1.74	0.68
1:I:17:VAL:HA	1:I:22:PHE:HA	1.75	0.68
1:M:65:ARG:NH1	1:M:153:LEU:HD12	2.08	0.68
1:R:104:ARG:HG3	1:S:120:GLY:H	1.58	0.68
1:e:104:ARG:HH12	1:n:121:ASN:CA	2.07	0.68
1:j:83:TRP:HB3	1:j:93:LEU:HG	1.75	0.68
1:Q:87:ASP:HA	1:Q:94:GLY:HA2	1.75	0.68
1:R:83:TRP:NE1	1:R:91:GLY:O	2.26	0.68
1:S:33:LYS:HZ3	1:S:67:CYS:H	1.41	0.68
1:C:137:GLN:HG3	1:C:155:LEU:HG	1.76	0.68
1:D:17:VAL:HG13	1:D:100:LEU:HB2	1.76	0.68
1:M:160:GLN:O	1:M:164:LYS:NZ	2.25	0.68
1:X:53:ILE:O	1:X:55:PHE:N	2.24	0.68
1:n:88:ARG:H	1:n:88:ARG:HH11	1.40	0.68
1:i:51:GLU:N	1:i:51:GLU:OE1	2.26	0.68
1:J:27:LEU:HD22	1:J:31:ARG:NH1	2.09	0.68
1:V:34:TYR:CE1	1:V:131:PRO:HD3	2.29	0.68
1:a:53:ILE:HG23	1:a:96:MET:HE1	1.76	0.68
1:d:130:ASP:HB3	1:d:134:ILE:HG23	1.76	0.68
1:C:45:THR:HG23	1:C:46:PHE:H	1.58	0.68
1:X:11:GLU:HB3	1:X:27:LEU:HD22	1.74	0.68
1:k:30:TYR:CZ	1:k:68:GLN:HG2	2.29	0.68
1:P:41:PRO:HD2	1:P:124:ARG:NH1	2.09	0.68
1:Q:123:PHE:HE1	1:Q:142:ASP:HA	1.59	0.68
1:R:74:THR:HA	1:R:103:ASP:HB3	1.76	0.68
1:U:52:ILE:O	1:U:54:ALA:N	2.26	0.68
1:C:38:PHE:HE1	1:C:69:VAL:HG23	1.56	0.68
1:c:36:VAL:HB	1:c:128:ILE:HD13	1.74	0.68
1:U:33:LYS:NZ	1:U:68:GLN:HG3	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:125:GLY:HA2	1:a:140:ILE:HA	1.74	0.68
1:h:38:PHE:HD2	1:h:147:ARG:HH12	1.40	0.68
1:S:88:ARG:HE	1:S:88:ARG:H	1.42	0.67
1:f:38:PHE:HE2	1:f:52:ILE:HG12	1.57	0.67
1:C:16:ALA:HB1	1:C:101:LEU:HA	1.76	0.67
1:H:34:TYR:OH	1:H:163:GLU:OE2	2.10	0.67
1:K:4:LEU:HD23	1:K:7:ARG:HH21	1.58	0.67
1:O:84:ASP:HA	1:O:93:LEU:HB2	1.76	0.67
1:g:141:ASN:OD1	1:g:141:ASN:N	2.25	0.67
1:l:9:ALA:HA	1:l:135:LEU:HG	1.76	0.67
1:B:73:SER:OG	1:B:80:HIS:NE2	2.27	0.67
1:S:55:PHE:HB3	1:S:62:PHE:HE2	1.60	0.67
1:X:54:ALA:O	1:X:58[A]:GLN:NE2	2.28	0.67
1:e:17:VAL:HG13	1:e:100:LEU:HB2	1.75	0.67
1:e:51:GLU:HG2	1:e:146:GLY:HA3	1.76	0.67
1:H:38:PHE:HB3	1:H:126:LEU:HD23	1.75	0.67
1:K:137:GLN:NE2	1:L:140:ILE:O	2.26	0.67
1:b:130:ASP:OD2	1:b:132:ASN:ND2	2.27	0.67
1:f:76:SER:HB3	1:f:104:ARG:HH21	1.58	0.67
1:K:75:ASP:HA	1:K:104:ARG:HE	1.58	0.67
1:V:53:ILE:HD11	1:V:88:ARG:NH1	2.10	0.67
1:D:42:ALA:HA	1:D:75:ASP:OD1	1.94	0.67
1:D:107:GLU:HG3	1:D:108:ILE:HG13	1.77	0.67
1:R:73:SER:HB3	1:R:80:HIS:CE1	2.29	0.67
1:V:36:VAL:HG13	1:V:69:VAL:HG13	1.75	0.67
1:I:65:ARG:HH12	1:I:153:LEU:HD21	1.59	0.67
1:g:124:ARG:NH1	1:g:124:ARG:HB2	2.09	0.67
1:g:161:PHE:O	1:g:165:HIS:ND1	2.28	0.67
1:k:22:PHE:HE2	1:k:78:TYR:HA	1.59	0.67
1:k:123:PHE:HE2	1:l:4:LEU:HB3	1.60	0.67
1:A:11:GLU:HG3	1:A:27:LEU:HB3	1.77	0.67
1:X:130:ASP:OD1	1:X:131:PRO:HD2	1.94	0.67
1:Z:12:PHE:HB2	1:Z:108:ILE:HD12	1.75	0.67
1:g:41:PRO:HD3	1:g:124:ARG:NH1	2.09	0.67
1:G:18:ILE:HG12	1:G:99:PRO:HB3	1.76	0.67
1:I:11:GLU:OE2	1:I:28:LYS:HE2	1.95	0.67
1:P:119:ASP:OD2	1:P:143:LYS:NZ	2.28	0.67
1:Q:15:GLN:NE2	1:Q:77:GLN:OE1	2.27	0.67
1:S:47:VAL:HG22	1:S:49:PRO:HD3	1.77	0.67
1:k:39:PHE:H	1:k:125:GLY:HA3	1.60	0.67
1:m:124:ARG:NH2	1:m:143:LYS:O	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:41:PRO:HB3	1:N:121:ASN:HB3	1.75	0.66
1:h:84:ASP:HA	1:h:93:LEU:HB2	1.76	0.66
1:j:52:ILE:HG13	1:j:53:ILE:HD12	1.77	0.66
1:k:130:ASP:OD2	1:k:132:ASN:ND2	2.25	0.66
1:F:18:ILE:HG22	1:F:99:PRO:HG3	1.77	0.66
1:G:43:ASP:OD1	1:G:43:ASP:N	2.26	0.66
1:R:120:GLY:HA3	1:S:105:LYS:HB3	1.76	0.66
1:j:120:GLY:HA2	1:k:105:LYS:HG2	1.77	0.66
1:Y:12:PHE:HB2	1:Y:108:ILE:HD12	1.77	0.66
1:Y:13:LYS:HD2	1:Y:26:CYS:HB3	1.77	0.66
1:k:45:THR:HA	1:k:46:PHE:HB3	1.75	0.66
1:I:154:ARG:NH1	1:J:148:SER:HB3	2.11	0.66
1:M:124:ARG:HH21	1:M:141:ASN:HD22	1.42	0.66
1:g:162:VAL:HG21	1:h:144:PRO:HB2	1.76	0.66
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.61	0.66
1:L:151:GLU:OE1	1:L:154:ARG:NH1	2.28	0.66
1:a:118[B]:GLU:CD	1:b:7:ARG:HH12	2.02	0.66
1:L:36:VAL:HG23	1:L:128:ILE:HG23	1.78	0.66
1:l:122:ALA:O	1:l:143:LYS:NZ	2.27	0.66
1:m:4:LEU:HD22	1:m:7:ARG:HH21	1.60	0.66
1:A:140:ILE:HG12	1:B:138:ILE:HB	1.78	0.66
1:E:123:PHE:HB2	1:E:140:ILE:HD11	1.77	0.66
1:F:44:PHE:O	1:F:45:THR:OG1	2.10	0.66
1:T:149:VAL:HG12	1:T:153:LEU:HD23	1.76	0.66
1:a:140:ILE:HD12	1:a:141:ASN:H	1.61	0.66
1:O:41:PRO:HG2	1:O:124:ARG:NH1	2.10	0.66
1:a:15:GLN:HA	1:a:24:GLU:HA	1.78	0.66
1:e:114:VAL:HG12	1:e:123:PHE:H	1.60	0.66
1:D:28:LYS:HA	1:D:31[B]:ARG:HD3	1.77	0.66
1:G:41:PRO:HG2	1:G:124:ARG:HH21	1.59	0.66
1:L:151:GLU:HB2	1:L:154:ARG:NH1	2.07	0.66
1:M:143:LYS:O	1:M:145:VAL:N	2.29	0.66
1:Q:129:ILE:HD11	1:Q:133:GLY:C	2.20	0.66
1:S:34:TYR:CE1	1:S:131:PRO:HD3	2.31	0.66
1:U:144:PRO:HB3	1:V:162:VAL:HB	1.77	0.66
1:W:76:SER:HB3	1:W:104:ARG:HD2	1.77	0.66
1:W:119:ASP:OD2	1:W:121:ASN:HB2	1.94	0.66
1:k:6:ASN:ND2	1:l:118:GLU:OE2	2.29	0.66
1:M:7:ARG:NH2	1:N:118:GLU:OE2	2.29	0.66
1:Q:33:LYS:HB2	1:Q:66:ASN:HB3	1.77	0.66
1:b:2:VAL:HG13	1:b:3:LEU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:104:ARG:HH12	1:n:121:ASN:HA	1.59	0.66
1:f:74:THR:OG1	1:g:104:ARG:NH2	2.28	0.66
1:n:70:ILE:HG22	1:n:101:LEU:HB2	1.78	0.66
1:G:15:GLN:HA	1:G:24:GLU:HA	1.78	0.65
1:P:39:PHE:O	1:P:147:ARG:NH2	2.23	0.65
1:S:128:ILE:HB	1:S:137:GLN:HB3	1.77	0.65
1:d:11:GLU:OE2	1:d:27:LEU:HD23	1.95	0.65
1:j:48:PRO:HB2	1:j:50:THR:HG23	1.78	0.65
1:k:96:MET:HG2	1:k:100:LEU:HD21	1.78	0.65
1:m:12:PHE:HB2	1:m:26:CYS:HA	1.78	0.65
1:L:123:PHE:HD2	1:L:142:ASP:HA	1.61	0.65
1:O:87:ASP:HB3	1:O:89:LYS:HZ3	1.59	0.65
1:R:114:VAL:HG12	1:R:123:PHE:H	1.62	0.65
1:k:28:LYS:HG3	1:k:31:ARG:HH12	1.62	0.65
1:A:74:THR:HG23	1:J:104:ARG:NH1	2.11	0.65
1:D:136:ARG:HB3	1:D:159:PHE:CZ	2.31	0.65
1:M:1:MET:HE3	1:M:2:VAL:HG12	1.78	0.65
1:P:134:ILE:HD11	1:P:136:ARG:HH12	1.61	0.65
1:c:88:ARG:NH2	1:c:96:MET:SD	2.70	0.65
1:c:127:PHE:HB3	1:c:135:LEU:HD11	1.78	0.65
1:e:38:PHE:HD2	1:e:147:ARG:NH1	1.93	0.65
1:G:53:ILE:HG22	1:G:93:LEU:HG	1.77	0.65
1:G:73:SER:HB3	1:G:80:HIS:CE1	2.32	0.65
1:M:98:ILE:HG22	1:M:100:LEU:HD13	1.77	0.65
1:e:124:ARG:HB2	1:e:141:ASN:HB2	1.78	0.65
1:g:162:VAL:HG11	1:h:144:PRO:HG2	1.78	0.65
1:l:73:SER:O	1:l:75:ASP:N	2.30	0.65
1:B:141:ASN:ND2	1:B:142:ASP:O	2.29	0.65
1:D:39:PHE:O	1:D:147:ARG:NH2	2.30	0.65
1:L:143:LYS:HB2	1:L:143:LYS:HZ2	1.61	0.65
1:Z:26:CYS:HB3	1:Z:29:ASP:OD2	1.96	0.65
1:m:140:ILE:HB	1:n:138:ILE:HG13	1.79	0.65
1:K:109:SER:HB3	1:K:115:PHE:HB2	1.79	0.65
1:L:32:GLY:N	1:L:131:PRO:O	2.27	0.65
1:L:43:ASP:O	1:M:79:SER:OG	2.11	0.65
1:T:157:ASP:OD1	1:T:157:ASP:N	2.29	0.65
1:X:164:LYS:NZ	1:X:164:LYS:HB3	2.12	0.65
1:l:45:THR:HG22	1:l:47:VAL:HG21	1.78	0.65
1:M:16:ALA:HB2	1:M:101:LEU:HD23	1.79	0.65
1:U:154:ARG:NH1	1:U:155:LEU:HA	2.12	0.65
1:V:6:ASN:HB3	1:V:7:ARG:HH21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:112:TYR:HB3	1:X:127:PHE:HE2	1.62	0.65
1:d:105:LYS:HB3	1:d:107:GLU:OE1	1.97	0.65
1:k:86:LEU:HB2	1:k:92:GLY:HA3	1.78	0.65
1:P:9:ALA:HB2	1:P:135:LEU:HB2	1.79	0.65
1:e:129:ILE:HG13	1:e:135:LEU:HB2	1.79	0.65
1:k:103:ASP:OD2	1:k:107:GLU:N	2.30	0.65
1:D:6:ASN:N	1:D:135:LEU:O	2.26	0.64
1:Y:125:GLY:O	1:Y:147:ARG:NH2	2.30	0.64
1:a:128:ILE:HG22	1:a:137:GLN:HB3	1.78	0.64
1:h:115:PHE:HZ	1:i:105:LYS:HD3	1.62	0.64
1:j:74:THR:HB	1:j:121:ASN:HB2	1.77	0.64
1:F:130:ASP:HB3	1:F:136:ARG:HD3	1.79	0.64
1:J:130:ASP:OD1	1:J:134:ILE:N	2.24	0.64
1:G:159:PHE:HA	1:G:162:VAL:HG22	1.80	0.64
1:S:16:ALA:HB3	1:S:23:LYS:H	1.62	0.64
1:a:62:PHE:HB3	1:a:153:LEU:HD23	1.80	0.64
1:e:84:ASP:HA	1:e:93:LEU:HD22	1.80	0.64
1:j:126:LEU:HB3	1:j:139:THR:HB	1.80	0.64
1:k:28:LYS:HG3	1:k:31:ARG:NH1	2.11	0.64
1:k:124:ARG:HH12	1:k:147:ARG:NH1	1.94	0.64
1:G:52:ILE:HG12	1:G:93:LEU:HD11	1.78	0.64
1:K:124:ARG:HD3	1:K:147:ARG:HH21	1.61	0.64
1:A:105:LYS:HD3	1:A:105:LYS:H	1.63	0.64
1:F:59:VAL:HG12	1:F:69:VAL:HG23	1.80	0.64
1:I:141:ASN:OD1	1:J:137:GLN:NE2	2.30	0.64
1:P:124:ARG:NH2	1:P:143:LYS:O	2.23	0.64
1:V:124:ARG:HB3	1:V:141:ASN:HB2	1.80	0.64
1:b:4:LEU:HB2	1:b:7:ARG:HD3	1.78	0.64
1:m:118:GLU:OE2	1:n:7:ARG:NH1	2.31	0.64
1:m:164:LYS:H	1:m:164:LYS:HE2	1.62	0.64
1:B:75:ASP:HA	1:C:104:ARG:HH21	1.62	0.64
1:L:105:LYS:HZ3	1:L:107:GLU:HB2	1.63	0.64
1:O:41:PRO:HB3	1:O:143:LYS:HZ1	1.62	0.64
1:V:26:CYS:HB3	1:V:28:LYS:HE2	1.78	0.64
1:c:143:LYS:NZ	1:c:143:LYS:HB2	2.13	0.64
1:i:119:ASP:OD2	1:i:121:ASN:ND2	2.31	0.64
1:m:68:GLN:HG2	1:m:99:PRO:HG2	1.80	0.64
1:n:134:ILE:HG21	1:n:136:ARG:NH1	2.13	0.64
1:n:134:ILE:HG21	1:n:136:ARG:HH11	1.63	0.64
1:B:47:VAL:HB	1:B:48:PRO:HD2	1.80	0.64
1:K:69:VAL:HG21	1:K:98:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:56:SER:HB2	1:U:97:LYS:H	1.61	0.64
1:U:76:SER:HB2	1:U:104:ARG:NH1	2.13	0.64
1:W:2:VAL:HB	1:X:3:LEU:HB3	1.80	0.64
1:W:119:ASP:O	1:W:121:ASN:ND2	2.31	0.64
1:S:11:GLU:HG3	1:S:27:LEU:HB3	1.79	0.64
1:T:161:PHE:HA	1:T:164:LYS:HG2	1.80	0.64
1:U:43:ASP:OD2	1:U:83:TRP:HB2	1.98	0.64
1:f:105:LYS:NZ	1:g:118:GLU:O	2.18	0.64
1:D:59:VAL:HG21	1:D:97:LYS:HG3	1.79	0.64
1:F:51:GLU:OE2	1:F:124:ARG:NH2	2.31	0.64
1:T:48:PRO:HB2	1:T:50:THR:H	1.62	0.64
1:A:93:LEU:HG	1:A:96:MET:SD	2.38	0.63
1:Q:57:ASP:OD1	1:Q:58:GLN:N	2.31	0.63
1:n:45:THR:O	1:n:48:PRO:HD2	1.98	0.63
1:n:72:CYS:HB2	1:n:101:LEU:HB3	1.78	0.63
1:J:125:GLY:H	1:J:147:ARG:HH12	1.44	0.63
1:J:128:ILE:HG12	1:J:137:GLN:HB2	1.79	0.63
1:M:137:GLN:NE2	1:M:138:ILE:O	2.31	0.63
1:S:5:PRO:HA	1:S:135:LEU:HB3	1.80	0.63
1:X:47:VAL:HG22	1:X:49:PRO:HA	1.80	0.63
1:j:31:ARG:HA	1:j:131:PRO:HB2	1.79	0.63
1:T:39:PHE:O	1:T:147:ARG:NH1	2.28	0.63
1:O:46:PHE:C	1:O:49:PRO:HD2	2.24	0.63
1:S:105:LYS:H	1:S:105:LYS:HZ3	1.47	0.63
1:d:107:GLU:HG2	1:d:108:ILE:N	2.13	0.63
1:A:139:THR:HB	1:B:139:THR:HG23	1.81	0.63
1:I:103:ASP:OD2	1:I:108:ILE:N	2.30	0.63
1:S:80:HIS:ND1	1:S:100:LEU:O	2.31	0.63
1:V:125:GLY:HA3	1:V:140:ILE:HA	1.80	0.63
1:X:130:ASP:N	1:X:134:ILE:O	2.32	0.63
1:e:31:ARG:HH12	1:e:133:GLY:CA	2.12	0.63
1:D:151:GLU:OE1	1:D:154:ARG:NH1	2.29	0.63
1:L:65:ARG:HH21	1:L:153:LEU:HB3	1.62	0.63
1:P:17:VAL:HB	1:P:81:LEU:HD12	1.81	0.63
1:R:30:TYR:HE2	1:R:70:ILE:HD11	1.62	0.63
1:b:32:GLY:C	1:b:131:PRO:HB3	2.23	0.63
1:d:45:THR:H	1:d:47:VAL:HA	1.63	0.63
1:f:135:LEU:HD21	1:f:138:ILE:HD11	1.80	0.63
1:h:96:MET:HG2	1:h:98:ILE:HG13	1.81	0.63
1:B:58:GLN:NE2	1:B:58:GLN:O	2.30	0.63
1:F:52:ILE:HG13	1:F:53:ILE:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:135:LEU:HD23	1:W:138:ILE:HD11	1.81	0.63
1:e:18:ILE:HG12	1:e:23:LYS:NZ	2.04	0.63
1:n:80:HIS:CG	1:n:100:LEU:HD21	2.33	0.63
1:A:44:PHE:HD2	1:J:79:SER:HA	1.63	0.63
1:A:80:HIS:NE2	1:A:101:LEU:O	2.31	0.63
1:Q:136:ARG:HB3	1:Q:159:PHE:HE2	1.62	0.63
1:Z:94:GLY:O	1:Z:95:HIS:ND1	2.31	0.63
1:f:60:GLU:O	1:f:63:ASN:N	2.31	0.63
1:n:15:GLN:HG2	1:n:24:GLU:HG2	1.81	0.63
1:G:122:ALA:O	1:G:143:LYS:NZ	2.32	0.63
1:J:125:GLY:CA	1:J:147:ARG:HH12	2.12	0.63
1:N:105:LYS:HB2	1:N:107:GLU:HG3	1.80	0.63
1:N:121:ASN:HA	1:O:104:ARG:NH1	2.14	0.63
1:V:119:ASP:N	1:V:119:ASP:OD1	2.32	0.63
1:Y:69:VAL:CG2	1:Y:70:ILE:H	2.10	0.63
1:h:34:TYR:CG	1:h:131:PRO:HD3	2.34	0.63
1:D:11:GLU:O	1:M:89:LYS:NZ	2.20	0.62
1:G:37:LEU:HD23	1:G:70:ILE:HB	1.81	0.62
1:O:45:THR:HG22	1:O:46:PHE:H	1.63	0.62
1:S:94:GLY:O	1:S:95:HIS:ND1	2.32	0.62
1:e:50:THR:HA	1:e:53:ILE:HG12	1.81	0.62
1:J:17:VAL:HB	1:J:100:LEU:HB2	1.81	0.62
1:J:60:GLU:HG3	1:J:97:LYS:NZ	2.13	0.62
1:S:138:ILE:HB	1:T:140:ILE:HG22	1.81	0.62
1:X:140:ILE:HG12	1:X:141:ASN:H	1.64	0.62
1:m:143:LYS:HB2	1:m:143:LYS:NZ	2.14	0.62
1:D:87:ASP:HB2	1:D:89:LYS:HE3	1.79	0.62
1:O:137:GLN:HB2	1:O:159:PHE:HE2	1.64	0.62
1:P:11:GLU:OE2	1:P:28:LYS:HE2	2.00	0.62
1:Q:9:ALA:HB2	1:Q:135:LEU:HD22	1.81	0.62
1:h:72:CYS:HB2	1:h:101:LEU:HD12	1.81	0.62
1:E:116:ASP:OD1	1:E:117:GLU:N	2.32	0.62
1:Y:163:GLU:HG3	1:Y:164:LYS:H	1.64	0.62
1:g:132:ASN:OD1	1:g:132:ASN:N	2.33	0.62
1:j:11:GLU:HG2	1:j:27:LEU:HD23	1.81	0.62
1:j:106:GLN:HG3	1:j:115:PHE:CE2	2.35	0.62
1:I:103:ASP:OD2	1:I:107:GLU:N	2.31	0.62
1:O:130:ASP:OD2	1:O:134:ILE:HB	1.99	0.62
1:W:39:PHE:H	1:W:147:ARG:HH12	1.47	0.62
1:i:103:ASP:OD1	1:i:107:GLU:N	2.30	0.62
1:m:76:SER:HB3	1:m:104:ARG:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:HA	1:A:27:LEU:HD13	1.81	0.62
1:T:41:PRO:HB3	1:T:143:LYS:NZ	2.15	0.62
1:U:7:ARG:NH2	1:V:118:GLU:OE1	2.29	0.62
1:U:8:PRO:HA	1:U:134:ILE:HG22	1.82	0.62
1:Y:36:VAL:HG13	1:Y:126:LEU:HG	1.81	0.62
1:b:129:ILE:HG13	1:b:135:LEU:HA	1.80	0.62
1:e:38:PHE:HB3	1:e:126:LEU:HD13	1.81	0.62
1:A:151:GLU:OE2	1:A:154:ARG:NH1	2.33	0.62
1:H:104:ARG:HH21	1:I:74:THR:HG23	1.65	0.62
1:I:156:LEU:O	1:I:160:GLN:HG2	2.00	0.62
1:L:9:ALA:HA	1:L:135:LEU:HD23	1.82	0.62
1:S:33:LYS:NZ	1:S:67:CYS:H	1.96	0.62
1:T:8:PRO:HA	1:T:134:ILE:HA	1.82	0.62
1:T:35:VAL:H	1:T:129:ILE:HG22	1.65	0.62
1:U:75:ASP:HB2	1:U:80:HIS:HE1	1.65	0.62
1:A:8:PRO:HA	1:A:134:ILE:HA	1.82	0.62
1:K:15:GLN:O	1:K:102:ALA:N	2.32	0.62
1:L:105:LYS:NZ	1:L:107:GLU:HB2	2.13	0.62
1:N:34:TYR:CE1	1:N:131:PRO:HD3	2.35	0.62
1:P:46:PHE:HD1	1:P:46:PHE:H	1.46	0.62
1:S:134:ILE:HG22	1:S:135:LEU:H	1.63	0.62
1:V:97:LYS:HZ2	1:V:97:LYS:HB3	1.64	0.62
1:j:36:VAL:HG13	1:j:156:LEU:HD13	1.82	0.62
1:G:38:PHE:O	1:G:71:ALA:HA	2.00	0.62
1:Q:16:ALA:HB2	1:Q:101:LEU:HD12	1.80	0.62
1:Q:139:THR:HG23	1:R:139:THR:HG22	1.82	0.62
1:c:75:ASP:HB2	1:c:80:HIS:CE1	2.35	0.62
1:l:57:ASP:N	1:l:57:ASP:OD1	2.33	0.62
1:L:44:PHE:HB2	1:M:79:SER:HA	1.82	0.61
1:M:106:GLN:NE2	1:M:120:GLY:O	2.33	0.61
1:N:142:ASP:OD1	1:N:142:ASP:N	2.31	0.61
1:R:53:ILE:HD13	1:R:88:ARG:NH1	2.15	0.61
1:R:141:ASN:HB2	1:R:147:ARG:HH22	1.65	0.61
1:U:123:PHE:HD2	1:V:4:LEU:HD12	1.63	0.61
1:b:124:ARG:HG3	1:b:124:ARG:NH1	2.15	0.61
1:c:86:LEU:HG	1:c:92:GLY:HA3	1.80	0.61
1:m:144:PRO:HB2	1:n:162:VAL:HG11	1.81	0.61
1:D:69:VAL:HG22	1:D:98:ILE:HB	1.82	0.61
1:F:61:GLU:O	1:F:65:ARG:NH1	2.31	0.61
1:H:77:GLN:HG2	1:H:102:ALA:HB3	1.81	0.61
1:W:137:GLN:NE2	1:X:141:ASN:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:18:ILE:C	1:Z:20:GLY:H	2.07	0.61
1:B:33[A]:LYS:NZ	1:B:68:GLN:HB3	2.15	0.61
1:k:60:GLU:O	1:k:64:SER:OG	2.18	0.61
1:a:124:ARG:HD3	1:a:147:ARG:NH1	2.14	0.61
1:k:13:LYS:NZ	1:k:26:CYS:HB3	2.14	0.61
1:F:86:LEU:HB2	1:F:92:GLY:HA3	1.82	0.61
1:H:137:GLN:HB2	1:H:159:PHE:HE2	1.66	0.61
1:X:28:LYS:HA	1:X:31[B]:ARG:HG2	1.82	0.61
1:Z:104:ARG:NH2	1:a:75:ASP:OD2	2.33	0.61
1:b:126:LEU:HG	1:b:147:ARG:HH12	1.65	0.61
1:d:49:PRO:HB3	1:d:51:GLU:OE1	1.99	0.61
1:k:4:LEU:HD22	1:l:123:PHE:HZ	1.63	0.61
1:A:16:ALA:N	1:A:102:ALA:HB2	2.15	0.61
1:B:15:GLN:HA	1:B:24:GLU:HA	1.82	0.61
1:B:137:GLN:HB3	1:B:159:PHE:CZ	2.33	0.61
1:G:67:CYS:HG	1:G:68:GLN:H	1.45	0.61
1:H:7:ARG:H	1:H:7:ARG:NH1	1.94	0.61
1:a:52:ILE:HG23	1:a:53:ILE:H	1.65	0.61
1:d:70:ILE:HG22	1:d:99:PRO:HB2	1.83	0.61
1:e:8:PRO:HA	1:e:134:ILE:HA	1.82	0.61
1:e:110:LYS:HB2	1:e:110:LYS:NZ	2.15	0.61
1:B:8:PRO:HA	1:B:134:ILE:HA	1.83	0.61
1:C:151:GLU:HB2	1:D:151:GLU:HG3	1.82	0.61
1:S:3:LEU:HD21	1:S:10:PRO:HD3	1.83	0.61
1:X:96:MET:HE3	1:X:98:ILE:HD11	1.82	0.61
1:c:38:PHE:HZ	1:c:52:ILE:HG13	1.64	0.61
1:d:31:ARG:HG2	1:d:31:ARG:HH11	1.66	0.61
1:k:11:GLU:OE1	1:k:28:LYS:HE3	2.00	0.61
1:A:16:ALA:HA	1:A:77:GLN:HB3	1.82	0.61
1:H:73:SER:HB3	1:H:80:HIS:CE1	2.36	0.61
1:H:75:ASP:O	1:H:102:ALA:HB1	2.01	0.61
1:H:106:GLN:NE2	1:I:104:ARG:O	2.34	0.61
1:J:116:ASP:HB3	1:J:121:ASN:O	2.01	0.61
1:R:67:CYS:SG	1:R:68:GLN:N	2.74	0.61
1:R:74:THR:HG21	1:R:122:ALA:H	1.65	0.61
1:f:46:PHE:O	1:f:47:VAL:HG12	2.01	0.61
1:j:141:ASN:OD1	1:j:147:ARG:NH2	2.29	0.61
1:M:47:VAL:HG13	1:M:49:PRO:HD2	1.83	0.61
1:O:88:ARG:HG2	1:O:94:GLY:HA3	1.82	0.61
1:R:109:SER:HB2	1:R:115:PHE:HB2	1.81	0.61
1:U:141:ASN:HB3	1:U:145:VAL:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:23:LYS:NZ	1:Z:23:LYS:HB3	2.16	0.61
1:a:17:VAL:HG11	1:a:81:LEU:HB2	1.81	0.61
1:n:30:TYR:HA	1:n:33:LYS:HE3	1.83	0.61
1:A:70:ILE:HD11	1:A:101:LEU:HD23	1.83	0.61
1:D:93:LEU:HD22	1:D:96:MET:HE1	1.83	0.61
1:N:121:ASN:OD1	1:O:104:ARG:NH1	2.34	0.61
1:X:119:ASP:OD2	1:X:121:ASN:HB2	2.00	0.61
1:Z:23:LYS:HB3	1:Z:23:LYS:HZ2	1.64	0.61
1:f:3:LEU:HD23	1:f:4:LEU:H	1.65	0.61
1:i:61:GLU:O	1:i:65:ARG:NH2	2.33	0.61
1:I:50:THR:HB	1:I:52:ILE:HG13	1.82	0.60
1:K:127:PHE:HB3	1:K:135:LEU:HD11	1.82	0.60
1:M:128:ILE:HG13	1:M:137:GLN:HB3	1.81	0.60
1:Z:88:ARG:HA	1:Z:93:LEU:HA	1.83	0.60
1:Z:130:ASP:HB2	1:Z:136:ARG:HD3	1.82	0.60
1:k:143:LYS:HB3	1:k:143:LYS:NZ	2.16	0.60
1:C:43:ASP:OD2	1:C:80:HIS:HA	2.00	0.60
1:C:88:ARG:NH1	1:C:94:GLY:HA3	2.16	0.60
1:F:15:GLN:HG3	1:F:24:GLU:HA	1.82	0.60
1:P:75:ASP:CA	1:Q:104:ARG:HH12	2.13	0.60
1:X:43:ASP:OD2	1:X:80:HIS:HD2	1.84	0.60
1:Z:76:SER:HA	1:Z:102:ALA:HB1	1.82	0.60
1:i:114:VAL:HG11	1:i:140:ILE:HD13	1.82	0.60
1:n:116:ASP:OD2	1:n:119:ASP:HB2	2.01	0.60
1:B:65:ARG:HH12	1:B:157:ASP:CG	2.09	0.60
1:C:69:VAL:HG13	1:C:98:ILE:HG21	1.82	0.60
1:D:52:ILE:HD11	1:D:147:ARG:HH22	1.66	0.60
1:F:18:ILE:HD12	1:F:23:LYS:HE2	1.82	0.60
1:J:125:GLY:N	1:J:147:ARG:HH12	1.98	0.60
1:Q:116:ASP:HB2	1:Q:123:PHE:HD2	1.67	0.60
1:T:80:HIS:NE2	1:T:101:LEU:O	2.35	0.60
1:U:32:GLY:HA2	1:U:131:PRO:HB3	1.82	0.60
1:c:148:SER:HB2	1:d:154:ARG:NH1	2.17	0.60
1:e:139:THR:HA	1:f:139:THR:HA	1.83	0.60
1:A:44:PHE:O	1:J:78:TYR:HB3	2.01	0.60
1:D:96:MET:HB3	1:D:98:ILE:HG12	1.84	0.60
1:G:64:SER:HB2	1:G:65:ARG:NH1	2.16	0.60
1:J:46:PHE:HA	1:J:47:VAL:C	2.25	0.60
1:a:59:VAL:HA	1:a:62:PHE:CZ	2.36	0.60
1:j:114:VAL:HG12	1:j:123:PHE:H	1.66	0.60
1:A:124:ARG:NH1	1:A:145:VAL:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:PRO:HB2	1:C:50:THR:C	2.26	0.60
1:R:38:PHE:HB3	1:R:126:LEU:HD23	1.83	0.60
1:T:125:GLY:O	1:T:147:ARG:NH2	2.33	0.60
1:U:82:ALA:HB2	1:d:83:TRP:CD1	2.36	0.60
1:g:56:SER:HB2	1:g:96:MET:HE3	1.83	0.60
1:n:36:VAL:O	1:n:69:VAL:HA	2.02	0.60
1:L:104:ARG:NE	1:M:121:ASN:OD1	2.34	0.60
1:d:38:PHE:HB3	1:d:126:LEU:HB3	1.84	0.60
1:l:103:ASP:O	1:l:105:LYS:N	2.32	0.60
1:H:103:ASP:HB3	1:H:108:ILE:HD13	1.83	0.60
1:J:11:GLU:OE2	1:J:28:LYS:HG2	2.01	0.60
1:W:53:ILE:HG12	1:W:96:MET:HE1	1.82	0.60
1:W:108:ILE:HD12	1:W:108:ILE:H	1.66	0.60
1:X:41:PRO:HB3	1:X:143:LYS:NZ	2.17	0.60
1:X:130:ASP:CG	1:X:131:PRO:HD2	2.27	0.60
1:h:110:LYS:NZ	1:h:115:PHE:CE2	2.69	0.60
1:j:8:PRO:HA	1:j:134:ILE:HD13	1.83	0.60
1:H:15:GLN:O	1:H:25:ILE:HG12	2.00	0.60
1:L:57:ASP:HA	1:L:97:LYS:NZ	2.17	0.60
1:U:82:ALA:HB2	1:d:83:TRP:HD1	1.67	0.60
1:W:88:ARG:HA	1:W:92:GLY:O	2.02	0.60
1:b:105:LYS:HG2	1:b:107:GLU:HB2	1.83	0.60
1:e:37:LEU:HA	1:e:70:ILE:O	2.01	0.60
1:L:60:GLU:O	1:L:63:ASN:ND2	2.35	0.60
1:L:130:ASP:HB2	1:L:134:ILE:O	2.02	0.60
1:b:49:PRO:HA	1:b:51:GLU:HB2	1.84	0.60
1:g:23:LYS:O	1:g:24:GLU:HG3	2.01	0.60
1:n:42:ALA:N	1:n:121:ASN:OD1	2.35	0.60
1:K:16:ALA:HB2	1:K:101:LEU:HA	1.83	0.59
1:M:25:ILE:HG12	1:M:101:LEU:HD21	1.83	0.59
1:S:15:GLN:H	1:S:101:LEU:HD13	1.67	0.59
1:c:154:ARG:HH21	1:c:155:LEU:HD22	1.66	0.59
1:d:47:VAL:HB	1:d:83:TRP:HH2	1.66	0.59
1:J:12:PHE:HB2	1:J:108:ILE:HG22	1.84	0.59
1:L:15:GLN:H	1:L:102:ALA:HB2	1.66	0.59
1:R:155:LEU:O	1:R:159:PHE:HB3	2.01	0.59
1:b:50:THR:N	1:b:51:GLU:HB2	2.17	0.59
1:G:4:LEU:HB2	1:G:7:ARG:NH2	2.17	0.59
1:M:80:HIS:CE1	1:M:100:LEU:HB2	2.38	0.59
1:N:104:ARG:NH1	1:O:121:ASN:OD1	2.36	0.59
1:T:93:LEU:HD21	1:T:96:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:114:VAL:HG13	1:W:115:PHE:H	1.67	0.59
1:d:44:PHE:HD2	1:d:83:TRP:HE1	1.50	0.59
1:k:132:ASN:HB2	1:k:134:ILE:HG12	1.83	0.59
1:V:71:ALA:O	1:V:101:LEU:N	2.31	0.59
1:L:36:VAL:HA	1:L:128:ILE:HA	1.85	0.59
1:Q:114:VAL:HG12	1:Q:115:PHE:H	1.68	0.59
1:S:136:ARG:HG3	1:T:142:ASP:HB2	1.85	0.59
1:W:28:LYS:HA	1:W:31:ARG:HH12	1.67	0.59
1:X:45:THR:HB	1:X:47:VAL:HG12	1.84	0.59
1:Z:159:PHE:HA	1:Z:162:VAL:HG22	1.84	0.59
1:c:28:LYS:HE2	1:c:31:ARG:HD2	1.84	0.59
1:L:105:LYS:HZ1	1:L:108:ILE:HD12	1.67	0.59
1:V:47:VAL:HB	1:V:48:PRO:HD2	1.84	0.59
1:X:53:ILE:C	1:X:55:PHE:H	2.10	0.59
1:X:157:ASP:O	1:X:161:PHE:HB3	2.01	0.59
1:H:73:SER:HB3	1:H:80:HIS:HE1	1.67	0.59
1:T:137:GLN:NE2	1:T:139:THR:OG1	2.26	0.59
1:U:124:ARG:HG2	1:U:147:ARG:NH1	2.18	0.59
1:Z:2:VAL:HG22	1:Z:3:LEU:H	1.68	0.59
1:a:159:PHE:HE1	1:b:145:VAL:HG21	1.68	0.59
1:F:38:PHE:HA	1:F:126:LEU:HA	1.84	0.59
1:T:36:VAL:HG12	1:T:128:ILE:HG13	1.85	0.59
1:U:41:PRO:HG3	1:U:124:ARG:HG3	1.85	0.59
1:Z:68:GLN:HE22	1:Z:70:ILE:HG23	1.68	0.59
1:d:34:TYR:OH	1:d:163:GLU:OE2	2.16	0.59
1:n:87:ASP:CG	1:n:89:LYS:HZ2	2.11	0.59
1:G:89:LYS:HD3	1:X:13:LYS:HZ1	1.68	0.59
1:f:75:ASP:HB2	1:f:80:HIS:CE1	2.37	0.59
1:G:85:ASN:OD1	1:G:86:LEU:N	2.35	0.59
1:G:89:LYS:HD3	1:X:13:LYS:NZ	2.17	0.59
1:R:115:PHE:HE1	1:R:120:GLY:HA2	1.67	0.59
1:U:87:ASP:HB2	1:U:89:LYS:HE2	1.85	0.59
1:i:87:ASP:OD2	1:i:89:LYS:NZ	2.36	0.59
1:F:42:ALA:HB2	1:F:121:ASN:HD21	1.68	0.58
1:G:22:PHE:CZ	1:G:77:GLN:HB3	2.38	0.58
1:H:96:MET:HG2	1:H:98:ILE:H	1.67	0.58
1:N:53:ILE:HG21	1:N:93:LEU:HB2	1.85	0.58
1:N:104:ARG:NH1	1:O:121:ASN:HA	2.18	0.58
1:Q:123:PHE:HA	1:Q:143:LYS:HE3	1.83	0.58
1:R:93:LEU:HG	1:R:96:MET:HE2	1.85	0.58
1:Z:105:LYS:NZ	1:Z:107:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LYS:O	1:D:106:GLN:HG2	2.02	0.58
1:n:103:ASP:OD2	1:n:109:SER:N	2.27	0.58
1:G:76:SER:OG	1:G:77:GLN:N	2.37	0.58
1:Q:134:ILE:HD12	1:Q:136:ARG:NH1	2.18	0.58
1:Y:47:VAL:HG23	1:Y:49:PRO:HD2	1.85	0.58
1:b:41:PRO:HA	1:b:122:ALA:HB3	1.86	0.58
1:d:119:ASP:OD2	1:d:121:ASN:HB2	2.03	0.58
1:g:58:GLN:HG3	1:g:149:VAL:HG11	1.84	0.58
1:n:40:TYR:CZ	1:n:73:SER:HB3	2.38	0.58
1:D:120:GLY:HA3	1:E:105:LYS:HG2	1.83	0.58
1:I:151:GLU:HG3	1:J:151:GLU:HB2	1.86	0.58
1:R:2:VAL:HG23	1:R:3:LEU:H	1.69	0.58
1:Y:69:VAL:HG22	1:Y:70:ILE:N	2.13	0.58
1:j:58:GLN:HE22	1:j:62:PHE:HE2	1.52	0.58
1:m:147:ARG:O	1:n:154:ARG:NH2	2.37	0.58
1:I:141:ASN:HD21	1:I:147:ARG:HG3	1.68	0.58
1:M:36:VAL:O	1:M:70:ILE:HG12	2.04	0.58
1:R:89:LYS:HA	1:R:89:LYS:NZ	2.19	0.58
1:U:119:ASP:OD1	1:U:120:GLY:N	2.36	0.58
1:X:74:THR:HG21	1:X:121:ASN:HA	1.86	0.58
1:e:36:VAL:HB	1:e:126:LEU:HD11	1.86	0.58
1:g:125:GLY:HA3	1:g:140:ILE:HG22	1.85	0.58
1:U:36:VAL:HB	1:U:69:VAL:HG13	1.86	0.58
1:V:124:ARG:NH1	1:V:146:GLY:HA2	2.19	0.58
1:W:38:PHE:HB2	1:W:147:ARG:NH1	2.19	0.58
1:a:40:TYR:HA	1:a:124:ARG:HG2	1.84	0.58
1:g:52:ILE:HG21	1:g:93:LEU:HD22	1.85	0.58
1:n:5:PRO:HB3	1:n:136:ARG:C	2.29	0.58
1:I:141:ASN:ND2	1:I:147:ARG:HG3	2.19	0.58
1:S:105:LYS:HG2	1:S:106:GLN:HG2	1.85	0.58
1:X:41:PRO:HB3	1:X:143:LYS:HZ1	1.68	0.58
1:a:34:TYR:H	1:a:131:PRO:HA	1.68	0.58
1:f:93:LEU:HD13	1:f:96:MET:HG3	1.85	0.58
1:h:52:ILE:CG2	1:h:124:ARG:HH12	2.15	0.58
1:k:83:TRP:O	1:k:93:LEU:N	2.23	0.58
1:D:107:GLU:HG3	1:D:108:ILE:H	1.69	0.58
1:Q:30:TYR:HD1	1:Q:33:LYS:NZ	2.01	0.58
1:C:31:ARG:HH12	1:C:133:GLY:HA3	1.69	0.58
1:G:65:ARG:HD3	1:G:156:LEU:HD11	1.86	0.58
1:K:47:VAL:HG23	1:K:48:PRO:HD3	1.85	0.58
1:L:38:PHE:O	1:L:71:ALA:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:6:ASN:OD1	1:O:136:ARG:NH1	2.37	0.58
1:Q:39:PHE:HA	1:Q:72:CYS:H	1.69	0.58
1:V:130:ASP:CG	1:V:134:ILE:H	2.10	0.58
1:d:135:LEU:HD21	1:d:138:ILE:HD11	1.86	0.58
1:i:126:LEU:HD13	1:i:128:ILE:HD11	1.85	0.58
1:m:152:THR:HA	1:m:155:LEU:HD12	1.86	0.58
1:C:38:PHE:HE2	1:C:52:ILE:HG23	1.68	0.58
1:I:47:VAL:HB	1:I:49:PRO:O	2.04	0.58
1:U:41:PRO:HD3	1:U:147:ARG:NH2	2.18	0.58
1:c:4:LEU:HG	1:d:1:MET:HE2	1.86	0.58
1:d:22:PHE:HE2	1:d:77:GLN:HB2	1.69	0.58
1:j:59:VAL:HG11	1:j:97:LYS:HG3	1.86	0.58
1:C:137:GLN:HG2	1:D:141:ASN:HA	1.86	0.57
1:G:36:VAL:HG13	1:G:69:VAL:HG22	1.86	0.57
1:H:1:MET:SD	1:H:1:MET:N	2.67	0.57
1:K:62:PHE:HB2	1:K:67:CYS:HB3	1.85	0.57
1:O:124:ARG:O	1:O:147:ARG:NE	2.37	0.57
1:U:44:PHE:HE1	1:U:86:LEU:HD12	1.69	0.57
1:X:125:GLY:CA	1:X:140:ILE:HA	2.33	0.57
1:Z:3:LEU:HD22	1:Z:4:LEU:H	1.69	0.57
1:e:106:GLN:HG2	1:e:115:PHE:CE1	2.39	0.57
1:Q:65:ARG:HE	1:Q:156:LEU:HD21	1.68	0.57
1:Q:145:VAL:HG23	1:R:154:ARG:NH1	2.18	0.57
1:Z:88:ARG:NH1	1:Z:93:LEU:HB2	2.19	0.57
1:g:17:VAL:HG11	1:g:81:LEU:HD13	1.86	0.57
1:k:22:PHE:CE2	1:k:78:TYR:HA	2.38	0.57
1:E:3:LEU:N	1:F:1:MET:O	2.37	0.57
1:M:159:PHE:HA	1:M:162:VAL:HG12	1.85	0.57
1:P:105:LYS:HD3	1:P:107:GLU:OE2	2.05	0.57
1:P:114:VAL:HG12	1:P:123:PHE:H	1.69	0.57
1:a:48:PRO:C	1:a:50:THR:HA	2.29	0.57
1:F:18:ILE:O	1:F:20:GLY:N	2.37	0.57
1:H:129:ILE:HG13	1:H:130:ASP:N	2.18	0.57
1:H:130:ASP:OD2	1:H:134:ILE:HB	2.04	0.57
1:O:86:LEU:HB2	1:O:92:GLY:HA3	1.87	0.57
1:S:106:GLN:HB2	1:S:110:LYS:HE2	1.84	0.57
1:c:143:LYS:HB2	1:c:143:LYS:HZ2	1.67	0.57
1:f:110:LYS:HD2	1:f:115:PHE:CD2	2.39	0.57
1:h:88:ARG:HG2	1:h:89:LYS:H	1.69	0.57
1:F:18:ILE:C	1:F:20:GLY:H	2.11	0.57
1:J:11:GLU:HA	1:J:27:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:44:PHE:O	1:T:78:TYR:HB3	2.05	0.57
1:N:83:TRP:NE1	1:N:92:GLY:HA3	2.19	0.57
1:S:7:ARG:NH2	1:T:118:GLU:OE2	2.37	0.57
1:W:72:CYS:SG	1:W:73:SER:N	2.76	0.57
1:a:97:LYS:NZ	1:a:97:LYS:HB3	2.19	0.57
1:b:96:MET:HG3	1:b:100:LEU:HD21	1.86	0.57
1:c:105:LYS:HD2	1:c:107:GLU:OE2	2.04	0.57
1:c:126:LEU:H	1:c:139:THR:HG23	1.68	0.57
1:h:156:LEU:O	1:h:160:GLN:HG2	2.04	0.57
1:I:44:PHE:HE2	1:I:86:LEU:HD22	1.70	0.57
1:Y:136:ARG:HB3	1:Y:159:PHE:CE1	2.40	0.57
1:c:115:PHE:H	1:c:122:ALA:HA	1.69	0.57
1:E:154:ARG:NH2	1:F:146:GLY:O	2.35	0.57
1:L:2:VAL:HG22	1:L:3:LEU:H	1.70	0.57
1:O:32:GLY:N	1:O:131:PRO:HB3	2.19	0.57
1:X:51:GLU:HG3	1:X:146:GLY:HA3	1.86	0.57
1:g:24:GLU:OE1	1:g:25:ILE:N	2.36	0.57
1:n:38:PHE:CE2	1:n:69:VAL:HG11	2.40	0.57
1:D:130:ASP:OD1	1:D:134:ILE:N	2.29	0.57
1:F:104:ARG:NE	1:G:74:THR:HB	2.20	0.57
1:J:125:GLY:H	1:J:147:ARG:NH1	2.02	0.57
1:N:55:PHE:HE1	1:N:149:VAL:HG22	1.70	0.57
1:Q:40:TYR:CD1	1:Q:71:ALA:HB1	2.40	0.57
1:i:53:ILE:HD11	1:i:88:ARG:HD2	1.87	0.57
1:C:1:MET:HG3	1:D:2:VAL:HA	1.87	0.57
1:F:104:ARG:NH2	1:G:121:ASN:OD1	2.22	0.57
1:T:2:VAL:HG22	1:T:4:LEU:H	1.70	0.57
1:T:65:ARG:NE	1:T:157:ASP:OD1	2.38	0.57
1:U:136:ARG:NE	1:V:142:ASP:OD2	2.26	0.57
1:V:124:ARG:CB	1:V:141:ASN:HB2	2.35	0.57
1:X:152:THR:O	1:X:156:LEU:HB2	2.05	0.57
1:a:16:ALA:HB2	1:a:101:LEU:HD23	1.87	0.57
1:a:72:CYS:SG	1:a:73:SER:N	2.78	0.57
1:a:124:ARG:HB3	1:a:147:ARG:CZ	2.35	0.57
1:d:77:GLN:HG3	1:d:78:TYR:H	1.70	0.57
1:g:50:THR:N	1:g:51:GLU:OE1	2.37	0.57
1:n:17:VAL:HG21	1:n:81:LEU:HD23	1.85	0.57
1:n:110:LYS:HG2	1:n:115:PHE:CG	2.40	0.57
1:E:155:LEU:HD13	1:F:145:VAL:HG21	1.86	0.57
1:G:32:GLY:N	1:G:131:PRO:O	2.36	0.57
1:N:135:LEU:HD23	1:N:136:ARG:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:96:MET:HG3	1:U:98:ILE:HG13	1.87	0.57
1:V:130:ASP:OD1	1:V:133:GLY:N	2.38	0.57
1:Y:89:LYS:NZ	1:Y:89:LYS:HB3	2.19	0.57
1:j:159:PHE:HA	1:j:162:VAL:HG12	1.86	0.57
1:k:34:TYR:CD1	1:k:131:PRO:HD3	2.40	0.57
1:n:116:ASP:HB2	1:n:122:ALA:O	2.05	0.57
1:R:62:PHE:HA	1:R:67:CYS:HB3	1.87	0.56
1:T:34:TYR:N	1:T:67:CYS:HA	2.20	0.56
1:X:17:VAL:HG22	1:X:100:LEU:HB2	1.86	0.56
1:Z:26:CYS:SG	1:Z:27:LEU:N	2.77	0.56
1:f:13[A]:LYS:NZ	1:f:24:GLU:HG2	2.20	0.56
1:i:87:ASP:OD1	1:i:87:ASP:N	2.30	0.56
1:A:144:PRO:HB2	1:B:162:VAL:HB	1.87	0.56
1:C:7:ARG:HH12	1:D:116:ASP:CG	2.14	0.56
1:G:11:GLU:HG3	1:G:12:PHE:H	1.69	0.56
1:H:80:HIS:CD2	1:H:102:ALA:HB2	2.40	0.56
1:J:15:GLN:HA	1:J:24:GLU:HA	1.87	0.56
1:R:106:GLN:HB3	1:R:115:PHE:HE2	1.70	0.56
1:h:36:VAL:HG13	1:h:69:VAL:HB	1.87	0.56
1:l:40:TYR:CE2	1:l:73:SER:HB2	2.41	0.56
1:B:16:ALA:HB3	1:B:25:ILE:HD11	1.87	0.56
1:I:114:VAL:HG23	1:I:123:PHE:HB2	1.86	0.56
1:Q:41:PRO:HG3	1:Q:143:LYS:HD2	1.86	0.56
1:S:134:ILE:HG22	1:S:135:LEU:N	2.21	0.56
1:X:36:VAL:HB	1:X:127:PHE:O	2.06	0.56
1:X:38:PHE:HA	1:X:125:GLY:O	2.05	0.56
1:X:41:PRO:HD3	1:X:124:ARG:HB3	1.86	0.56
1:Z:44:PHE:HZ	1:Z:82:ALA:HB3	1.69	0.56
1:a:127:PHE:HD2	1:a:138:ILE:HG13	1.70	0.56
1:c:148:SER:HB2	1:d:154:ARG:CZ	2.34	0.56
1:d:130:ASP:HB2	1:d:136:ARG:HD2	1.87	0.56
1:g:130:ASP:OD1	1:g:134:ILE:N	2.23	0.56
1:g:156:LEU:HD13	1:g:156:LEU:H	1.70	0.56
1:E:28:LYS:HD3	1:E:31:ARG:NH1	2.20	0.56
1:I:136:ARG:NH1	1:J:142:ASP:OD2	2.39	0.56
1:U:75:ASP:HB2	1:U:80:HIS:CE1	2.40	0.56
1:Z:126:LEU:HB2	1:Z:139:THR:HB	1.87	0.56
1:a:81:LEU:O	1:a:85:ASN:ND2	2.36	0.56
1:e:159:PHE:HA	1:e:162:VAL:HG22	1.87	0.56
1:N:74:THR:HG23	1:O:104:ARG:NH1	2.21	0.56
1:P:75:ASP:O	1:P:104:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:125:GLY:O	1:P:147:ARG:NH1	2.38	0.56
1:Y:6:ASN:OD1	1:Y:7:ARG:N	2.34	0.56
1:Y:136:ARG:NH1	1:Z:142:ASP:OD2	2.38	0.56
1:f:8:PRO:HA	1:f:134:ILE:HA	1.87	0.56
1:j:128:ILE:HG22	1:j:136:ARG:HB3	1.85	0.56
1:n:130:ASP:OD1	1:n:132:ASN:N	2.39	0.56
1:I:147:ARG:O	1:J:154:ARG:NH2	2.29	0.56
1:T:109:SER:HB3	1:T:115:PHE:HB2	1.87	0.56
1:X:49:PRO:HG2	1:X:53:ILE:HD11	1.88	0.56
1:j:147:ARG:NH1	1:j:147:ARG:HB2	2.20	0.56
1:l:103:ASP:C	1:l:105:LYS:H	2.13	0.56
1:A:154:ARG:HH11	1:B:148:SER:HB2	1.70	0.56
1:B:6:ASN:O	1:B:6:ASN:ND2	2.39	0.56
1:P:52:ILE:HG21	1:P:124:ARG:HH11	1.71	0.56
1:R:30:TYR:CE2	1:R:70:ILE:HD11	2.40	0.56
1:S:135:LEU:O	1:S:136:ARG:HB2	2.06	0.56
1:T:125:GLY:HA3	1:T:140:ILE:HA	1.86	0.56
1:V:83:TRP:CE3	1:V:93:LEU:HG	2.40	0.56
1:X:104:ARG:NH2	1:Y:75:ASP:OD1	2.33	0.56
1:Y:18:ILE:HD12	1:Y:98:ILE:H	1.70	0.56
1:b:37:LEU:HD11	1:b:127:PHE:CD2	2.40	0.56
1:b:75:ASP:HB2	1:b:80:HIS:HE2	1.71	0.56
1:b:127:PHE:CE1	1:b:138:ILE:HG23	2.40	0.56
1:d:114:VAL:HG23	1:d:123:PHE:HB2	1.88	0.56
1:k:80:HIS:HD2	1:k:100:LEU:HB3	1.71	0.56
1:l:73:SER:HB3	1:l:80:HIS:NE2	2.21	0.56
1:m:142:ASP:HB2	1:n:136:ARG:O	2.06	0.56
1:D:44:PHE:O	1:E:78:TYR:HB3	2.06	0.56
1:I:7:ARG:NE	1:J:118:GLU:OE2	2.38	0.56
1:I:130:ASP:HB3	1:I:134:ILE:O	2.05	0.56
1:L:105:LYS:NZ	1:L:105:LYS:HB2	2.21	0.56
1:M:53:ILE:HG22	1:M:88:ARG:NH1	2.20	0.56
1:S:28:LYS:O	1:S:31:ARG:HG2	2.06	0.56
1:W:56:SER:HA	1:W:98:ILE:HG23	1.87	0.56
1:a:38:PHE:O	1:a:71:ALA:HA	2.06	0.56
1:A:7:ARG:NH2	1:B:118:GLU:OE2	2.39	0.56
1:K:11:GLU:HA	1:K:27:LEU:HD12	1.87	0.56
1:X:6:ASN:N	1:X:135:LEU:O	2.39	0.56
1:X:48:PRO:HB2	1:X:50:THR:H	1.70	0.56
1:b:160:GLN:O	1:b:164:LYS:HG2	2.05	0.56
1:e:106:GLN:O	1:e:110:LYS:NZ	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:114:VAL:HG13	1:f:140:ILE:HD12	1.88	0.56
1:g:76:SER:OG	1:g:104:ARG:NH1	2.39	0.56
1:h:130:ASP:CG	1:h:131:PRO:HD2	2.30	0.56
1:l:35:VAL:HG12	1:l:37:LEU:H	1.71	0.56
1:l:78:TYR:HB3	1:m:44:PHE:HB2	1.88	0.56
1:C:97:LYS:HZ2	1:C:97:LYS:HB3	1.70	0.56
1:Q:75:ASP:OD2	1:Q:79:SER:OG	2.16	0.56
1:g:14:GLY:HA3	1:g:101:LEU:HD11	1.88	0.56
1:i:147:ARG:H	1:i:147:ARG:NE	2.03	0.56
1:j:108:ILE:HD13	1:j:108:ILE:H	1.70	0.56
1:n:84:ASP:OD2	1:n:96:MET:HG3	2.05	0.56
1:n:114:VAL:HG13	1:n:115:PHE:H	1.70	0.56
1:A:110:LYS:NZ	1:A:115:PHE:CE2	2.73	0.55
1:D:13:LYS:HB2	1:D:13:LYS:NZ	2.21	0.55
1:N:135:LEU:O	1:N:136:ARG:HD3	2.05	0.55
1:U:88:ARG:HG2	1:U:94:GLY:H	1.72	0.55
1:W:135:LEU:H	1:W:135:LEU:HD12	1.70	0.55
1:Y:51:GLU:HB2	1:Y:147:ARG:HB2	1.88	0.55
1:Z:13:LYS:HB2	1:Z:24:GLU:OE2	2.07	0.55
1:b:33:LYS:HG3	1:b:66:ASN:HB3	1.88	0.55
1:e:35:VAL:HG22	1:e:129:ILE:HD13	1.88	0.55
1:g:47:VAL:O	1:g:49:PRO:HD3	2.06	0.55
1:k:87:ASP:OD1	1:k:90:SER:HB2	2.05	0.55
1:E:73:SER:HB3	1:E:80:HIS:NE2	2.21	0.55
1:M:37:LEU:HD13	1:M:70:ILE:HG13	1.87	0.55
1:T:84:ASP:OD1	1:T:95:HIS:HA	2.06	0.55
1:V:75:ASP:HB2	1:V:80:HIS:CE1	2.41	0.55
1:d:73:SER:HB3	1:d:75:ASP:OD2	2.05	0.55
1:h:46:PHE:HD1	1:h:47:VAL:H	1.54	0.55
1:h:112:TYR:HE2	1:h:127:PHE:HB2	1.72	0.55
1:l:17:VAL:HG22	1:l:22:PHE:HD1	1.71	0.55
1:A:142:ASP:CG	1:A:143:LYS:H	2.14	0.55
1:E:112:TYR:HB3	1:E:127:PHE:HE2	1.72	0.55
1:G:10:PRO:HB2	1:G:111:ALA:HB1	1.89	0.55
1:L:45:THR:C	1:L:47:VAL:H	2.13	0.55
1:Q:28:LYS:HD3	1:Q:31:ARG:HE	1.70	0.55
1:R:50:THR:HG23	1:R:53:ILE:CG1	2.36	0.55
1:T:86:LEU:HD11	1:T:92:GLY:HA3	1.88	0.55
1:U:52:ILE:C	1:U:54:ALA:H	2.15	0.55
1:U:138:ILE:HB	1:V:140:ILE:HB	1.88	0.55
1:X:124:ARG:HH11	1:X:146:GLY:HA2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:22:PHE:HZ	1:Y:77:GLN:HB3	1.71	0.55
1:b:39:PHE:O	1:b:124:ARG:NH2	2.40	0.55
1:i:141:ASN:HB3	1:j:159:PHE:HZ	1.71	0.55
1:G:142:ASP:OD1	1:G:143:LYS:N	2.32	0.55
1:K:104:ARG:HH11	1:T:74:THR:HB	1.71	0.55
1:Q:11:GLU:HG2	1:Q:27:LEU:HB3	1.88	0.55
1:a:141:ASN:HA	1:b:137:GLN:HG3	1.87	0.55
1:d:13:LYS:HD3	1:d:26:CYS:HB2	1.88	0.55
1:h:38:PHE:HB2	1:h:147:ARG:NH1	2.22	0.55
1:H:142:ASP:CG	1:H:143:LYS:H	2.14	0.55
1:K:93:LEU:HB3	1:K:96:MET:HE3	1.88	0.55
1:L:142:ASP:OD2	1:L:144:PRO:HD2	2.05	0.55
1:O:137:GLN:HB2	1:O:159:PHE:CE2	2.41	0.55
1:P:52:ILE:HG21	1:P:124:ARG:NH1	2.22	0.55
1:U:89:LYS:H	1:U:89:LYS:HD3	1.71	0.55
1:X:125:GLY:HA3	1:X:140:ILE:HA	1.88	0.55
1:d:88:ARG:NH1	1:d:94:GLY:HA3	2.22	0.55
1:F:17:VAL:O	1:F:99:PRO:HA	2.05	0.55
1:K:12:PHE:HE2	1:K:37:LEU:HG	1.72	0.55
1:M:15:GLN:NE2	1:M:24:GLU:HB2	2.22	0.55
1:M:126:LEU:HG	1:M:139:THR:HB	1.88	0.55
1:S:37:LEU:HD22	1:S:70:ILE:HB	1.88	0.55
1:U:105:LYS:HB3	1:U:105:LYS:HZ3	1.71	0.55
1:W:164:LYS:HE2	1:W:165:HIS:CE1	2.41	0.55
1:Y:139:THR:HG23	1:Z:139:THR:HG23	1.89	0.55
1:f:104:ARG:NH1	1:g:121:ASN:HA	2.22	0.55
1:h:62:PHE:HB3	1:h:67:CYS:HB3	1.88	0.55
1:C:41:PRO:HB3	1:C:143:LYS:NZ	2.22	0.55
1:K:104:ARG:NH2	1:T:75:ASP:OD2	2.39	0.55
1:Q:43:ASP:HB2	1:Q:83:TRP:CD2	2.41	0.55
1:T:125:GLY:C	1:T:147:ARG:HH21	2.14	0.55
1:Y:135:LEU:HD21	1:Y:138:ILE:HG13	1.89	0.55
1:e:80:HIS:O	1:e:84:ASP:HB2	2.07	0.55
1:h:38:PHE:H	1:h:38:PHE:HD1	1.53	0.55
1:k:36:VAL:O	1:k:70:ILE:N	2.30	0.55
1:F:12:PHE:HB2	1:F:108:ILE:HG12	1.89	0.55
1:G:39:PHE:H	1:G:125:GLY:HA3	1.72	0.55
1:M:38:PHE:H	1:M:71:ALA:HA	1.72	0.55
1:Q:51:GLU:OE1	1:Q:146:GLY:HA2	2.06	0.55
1:W:18:ILE:HG22	1:W:99:PRO:HA	1.87	0.55
1:a:63:ASN:ND2	1:a:67:CYS:HB3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:70:ILE:HG22	1:b:99:PRO:HB2	1.88	0.55
1:c:136:ARG:HG3	1:c:159:PHE:CZ	2.42	0.55
1:d:88:ARG:NH1	1:d:93:LEU:O	2.40	0.55
1:g:140:ILE:HG12	1:h:138:ILE:HB	1.89	0.55
1:R:44:PHE:O	1:S:78:TYR:HB3	2.06	0.55
1:S:67:CYS:SG	1:S:68:GLN:N	2.79	0.55
1:b:15:GLN:HA	1:b:24:GLU:HA	1.88	0.55
1:h:51:GLU:HG3	1:h:52:ILE:H	1.70	0.55
1:A:34:TYR:CD1	1:A:131:PRO:HD3	2.42	0.55
1:D:161:PHE:HA	1:D:164:LYS:NZ	2.22	0.55
1:G:56:SER:HB3	1:G:96:MET:HG3	1.87	0.55
1:G:124:ARG:HB2	1:G:141:ASN:HB2	1.89	0.55
1:L:137:GLN:HG3	1:L:155:LEU:HD22	1.88	0.55
1:V:76:SER:HB3	1:V:104:ARG:CZ	2.37	0.55
1:Z:74:THR:HA	1:Z:103:ASP:O	2.06	0.55
1:c:39:PHE:CE2	1:c:114:VAL:HG21	2.42	0.55
1:h:74:THR:HA	1:h:103:ASP:HB3	1.89	0.55
1:j:115:PHE:HA	1:j:122:ALA:HA	1.88	0.55
1:l:72:CYS:HA	1:l:101:LEU:HB3	1.88	0.55
1:D:11:GLU:HB2	1:M:89:LYS:HZ3	1.72	0.54
1:D:25:ILE:HG12	1:D:26:CYS:N	2.21	0.54
1:E:142:ASP:OD1	1:E:143:LYS:N	2.38	0.54
1:L:57:ASP:HA	1:L:97:LYS:HZ2	1.71	0.54
1:M:37:LEU:HD21	1:M:108:ILE:HD11	1.89	0.54
1:M:55:PHE:HD1	1:M:149:VAL:HG22	1.71	0.54
1:i:73:SER:HB3	1:i:80:HIS:CE1	2.42	0.54
1:i:127:PHE:HD2	1:i:138:ILE:HD11	1.72	0.54
1:j:17:VAL:HG21	1:j:80:HIS:HB2	1.88	0.54
1:k:135:LEU:HD13	1:k:138:ILE:HD11	1.89	0.54
1:n:11:GLU:OE2	1:n:27:LEU:HB3	2.07	0.54
1:n:34:TYR:HA	1:n:129:ILE:O	2.06	0.54
1:n:35:VAL:HA	1:n:68:GLN:H	1.70	0.54
1:n:70:ILE:CG2	1:n:101:LEU:HB2	2.36	0.54
1:A:106:GLN:O	1:A:110:LYS:HG3	2.07	0.54
1:L:45:THR:O	1:L:47:VAL:N	2.40	0.54
1:S:11:GLU:HA	1:S:27:LEU:HD13	1.87	0.54
1:S:107:GLU:O	1:S:111:ALA:N	2.40	0.54
1:W:4:LEU:CD2	1:W:7:ARG:HH12	2.20	0.54
1:a:41:PRO:HG3	1:a:143:LYS:CB	2.37	0.54
1:k:112:TYR:HB3	1:k:114:VAL:HG23	1.88	0.54
1:k:139:THR:HB	1:l:139:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:GLY:HA3	1:G:104:ARG:HG3	1.90	0.54
1:H:160:GLN:O	1:H:164:LYS:HB2	2.07	0.54
1:S:13:LYS:HB3	1:S:13:LYS:NZ	2.22	0.54
1:i:159:PHE:CE1	1:j:145:VAL:HG12	2.43	0.54
1:C:88:ARG:HH11	1:C:94:GLY:HA3	1.72	0.54
1:P:74:THR:C	1:Q:104:ARG:HH12	2.14	0.54
1:R:146:GLY:C	1:R:147:ARG:HH11	2.16	0.54
1:S:16:ALA:HB3	1:S:23:LYS:N	2.22	0.54
1:a:140:ILE:O	1:a:141:ASN:HB2	2.06	0.54
1:h:124:ARG:HB3	1:h:147:ARG:NE	2.21	0.54
1:A:159:PHE:HB3	1:A:163:GLU:OE2	2.07	0.54
1:E:141:ASN:HA	1:F:137:GLN:HG2	1.89	0.54
1:G:34:TYR:HB2	1:G:66:ASN:HB2	1.88	0.54
1:L:17:VAL:HB	1:L:22:PHE:HE1	1.73	0.54
1:P:34:TYR:CD2	1:P:67:CYS:HB2	2.43	0.54
1:Q:61:GLU:HB3	1:Q:65:ARG:HH22	1.72	0.54
1:S:154:ARG:HA	1:S:157:ASP:OD2	2.07	0.54
1:a:59:VAL:HA	1:a:62:PHE:CE2	2.43	0.54
1:k:34:TYR:OH	1:k:163:GLU:OE2	2.25	0.54
1:k:61:GLU:O	1:k:65:ARG:NH1	2.41	0.54
1:l:52:ILE:HG23	1:l:96:MET:HE1	1.89	0.54
1:D:119:ASP:CG	1:D:143:LYS:HZ2	2.16	0.54
1:I:11:GLU:OE2	1:I:27:LEU:HD11	2.06	0.54
1:N:52:ILE:HG12	1:N:146:GLY:HA3	1.88	0.54
1:O:34:TYR:O	1:O:67:CYS:HA	2.06	0.54
1:S:12:PHE:HB3	1:S:108:ILE:HG21	1.90	0.54
1:W:37:LEU:HB2	1:W:71:ALA:H	1.73	0.54
1:b:124:ARG:NH1	1:b:147:ARG:CZ	2.71	0.54
1:d:103:ASP:OD2	1:d:106:GLN:HA	2.07	0.54
1:f:76:SER:HB3	1:f:104:ARG:NH2	2.22	0.54
1:i:18:ILE:HG12	1:i:19:ASN:H	1.72	0.54
1:i:125:GLY:HA2	1:i:147:ARG:HG3	1.89	0.54
1:A:154:ARG:NH1	1:B:148:SER:HB2	2.23	0.54
1:B:96:MET:HB2	1:B:100:LEU:HD11	1.89	0.54
1:C:41:PRO:HD3	1:C:124:ARG:HD3	1.88	0.54
1:F:104:ARG:HH12	1:G:75:ASP:CG	2.16	0.54
1:G:35:VAL:HB	1:G:129:ILE:HB	1.90	0.54
1:O:36:VAL:HG22	1:O:126:LEU:HD21	1.88	0.54
1:P:58:GLN:HE21	1:P:149:VAL:HG21	1.73	0.54
1:P:105:LYS:HA	1:Q:120:GLY:HA3	1.88	0.54
1:Q:39:PHE:HA	1:Q:72:CYS:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:38:PHE:HD2	1:Z:147:ARG:HD2	1.72	0.54
1:Z:151:GLU:OE1	1:Z:151:GLU:HA	2.08	0.54
1:f:34:TYR:O	1:f:67:CYS:HA	2.07	0.54
1:f:104:ARG:NH1	1:g:74:THR:OG1	2.41	0.54
1:i:117:GLU:N	1:j:7:ARG:HH22	2.06	0.54
1:j:38:PHE:HA	1:j:126:LEU:HD22	1.89	0.54
1:l:43:ASP:OD1	1:l:73:SER:OG	2.25	0.54
1:l:83:TRP:NE1	1:l:92:GLY:HA2	2.23	0.54
1:A:127:PHE:O	1:A:128:ILE:HB	2.08	0.54
1:A:137:GLN:HG2	1:B:141:ASN:HA	1.88	0.54
1:B:41:PRO:HD3	1:B:124:ARG:HG2	1.89	0.54
1:B:132:ASN:HD21	1:g:164:LYS:HB2	1.72	0.54
1:E:33:LYS:HB2	1:E:66:ASN:O	2.08	0.54
1:H:15:GLN:HA	1:H:24:GLU:HA	1.90	0.54
1:L:14:GLY:O	1:L:24:GLU:HG3	2.08	0.54
1:L:88:ARG:HA	1:L:92:GLY:O	2.08	0.54
1:P:13:LYS:HE2	1:P:26:CYS:HB2	1.90	0.54
1:S:125:GLY:HA2	1:S:140:ILE:HA	1.89	0.54
1:T:112:TYR:HB3	1:T:127:PHE:HE2	1.73	0.54
1:Z:124:ARG:HH11	1:Z:147:ARG:NH2	2.04	0.54
1:j:79:SER:HA	1:k:44:PHE:CE2	2.42	0.54
1:k:151:GLU:HG2	1:l:151:GLU:HG2	1.90	0.54
1:D:11:GLU:C	1:M:89:LYS:HZ1	2.10	0.54
1:D:53:ILE:HD11	1:D:93:LEU:HA	1.90	0.54
1:L:126:LEU:HD12	1:L:147:ARG:HD3	1.90	0.54
1:P:73:SER:HB3	1:P:75:ASP:OD2	2.08	0.54
1:W:28:LYS:HB3	1:W:28:LYS:HZ3	1.72	0.54
1:W:47:VAL:O	1:W:49:PRO:HD3	2.08	0.54
1:a:83:TRP:CD1	1:a:92:GLY:HA2	2.43	0.54
1:e:18:ILE:H	1:e:23:LYS:NZ	2.06	0.54
1:f:89:LYS:NZ	1:f:89:LYS:HB3	2.22	0.54
1:g:29:ASP:OD1	1:g:29:ASP:N	2.41	0.54
1:k:57:ASP:OD1	1:k:58:GLN:HG2	2.08	0.54
1:m:147:ARG:HG2	1:m:148:SER:H	1.73	0.54
1:n:51:GLU:OE2	1:n:146:GLY:HA2	2.08	0.54
1:A:34:TYR:HD1	1:A:131:PRO:HD3	1.72	0.54
1:E:105:LYS:O	1:E:107:GLU:N	2.41	0.54
1:H:72:CYS:SG	1:H:74:THR:N	2.81	0.54
1:I:145:VAL:HG11	1:J:159:PHE:CZ	2.43	0.54
1:R:115:PHE:CE1	1:R:120:GLY:HA2	2.43	0.54
1:V:104:ARG:NH2	1:W:121:ASN:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:4:LEU:HD22	1:W:7:ARG:HH12	1.71	0.54
1:j:8:PRO:HA	1:j:134:ILE:HA	1.89	0.54
1:A:114:VAL:HG13	1:A:115:PHE:H	1.72	0.53
1:I:56:SER:HA	1:I:59:VAL:HG13	1.91	0.53
1:I:105:LYS:HB2	1:I:107:GLU:HG3	1.90	0.53
1:N:35:VAL:O	1:N:128:ILE:HD12	2.08	0.53
1:S:41:PRO:HB3	1:S:121:ASN:HB3	1.90	0.53
1:U:137:GLN:HG3	1:U:159:PHE:CZ	2.42	0.53
1:b:48:PRO:HA	1:b:49:PRO:O	2.08	0.53
1:g:142:ASP:OD2	1:g:144:PRO:HD2	2.08	0.53
1:B:159:PHE:HA	1:B:162:VAL:HG22	1.90	0.53
1:E:51:GLU:OE2	1:E:146:GLY:HA3	2.08	0.53
1:W:162:VAL:HG23	1:W:163:GLU:H	1.73	0.53
1:f:53:ILE:HD12	1:f:96:MET:HE2	1.90	0.53
1:n:38:PHE:HB2	1:n:147:ARG:HE	1.73	0.53
1:C:137:GLN:HB2	1:C:159:PHE:CE2	2.37	0.53
1:F:89:LYS:HD2	1:Z:8:PRO:HD2	1.89	0.53
1:F:121:ASN:OD1	1:G:104:ARG:HD3	2.09	0.53
1:G:76:SER:OG	1:G:77:GLN:HG2	2.08	0.53
1:G:156:LEU:O	1:G:160:GLN:HG2	2.08	0.53
1:M:164:LYS:HG3	1:M:165:HIS:ND1	2.22	0.53
1:R:73:SER:HB3	1:R:80:HIS:NE2	2.23	0.53
1:S:151:GLU:HA	1:S:154:ARG:HG2	1.89	0.53
1:V:86:LEU:HD23	1:V:87:ASP:H	1.73	0.53
1:W:84:ASP:HA	1:W:93:LEU:HB2	1.89	0.53
1:Y:154:ARG:HA	1:Y:157:ASP:OD2	2.09	0.53
1:b:72:CYS:SG	1:b:103:ASP:HB2	2.48	0.53
1:c:38:PHE:O	1:c:72:CYS:HB2	2.09	0.53
1:h:116:ASP:HB2	1:h:118:GLU:HG2	1.90	0.53
1:B:45:THR:HG22	1:B:83:TRP:HZ2	1.73	0.53
1:C:21:GLU:HG3	1:C:23:LYS:HE3	1.91	0.53
1:C:86:LEU:HB3	1:C:92:GLY:HA3	1.89	0.53
1:I:139:THR:HA	1:J:139:THR:HA	1.91	0.53
1:L:123:PHE:HB2	1:L:140:ILE:HD11	1.90	0.53
1:N:16:ALA:HB1	1:N:100:LEU:O	2.09	0.53
1:O:65:ARG:HD2	1:O:156:LEU:HD13	1.90	0.53
1:S:130:ASP:CG	1:S:131:PRO:HD2	2.33	0.53
1:V:12:PHE:H	1:V:27:LEU:HB2	1.72	0.53
1:a:97:LYS:HB3	1:a:97:LYS:HZ3	1.70	0.53
1:k:136:ARG:HA	1:k:136:ARG:HE	1.74	0.53
1:C:164:LYS:NZ	1:C:165:HIS:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LYS:HA	1:D:31[A]:ARG:HG2	1.91	0.53
1:D:129:ILE:HG12	1:D:135:LEU:HD23	1.89	0.53
1:H:45:THR:HG23	1:H:49:PRO:HG2	1.90	0.53
1:Q:6:ASN:HB2	1:R:123:PHE:CZ	2.43	0.53
1:e:151:GLU:O	1:e:155:LEU:HG	2.08	0.53
1:j:67:CYS:HB2	1:j:156:LEU:HD21	1.89	0.53
1:n:54:ALA:O	1:n:58:GLN:HG3	2.08	0.53
1:B:38:PHE:CE1	1:B:52:ILE:HD12	2.43	0.53
1:G:151:GLU:HB2	1:H:151:GLU:HG3	1.91	0.53
1:J:40:TYR:CZ	1:J:73:SER:HB2	2.44	0.53
1:J:116:ASP:HB2	1:J:123:PHE:CE2	2.43	0.53
1:L:51:GLU:OE1	1:L:52:ILE:HG13	2.09	0.53
1:N:75:ASP:OD1	1:O:104:ARG:NH2	2.26	0.53
1:U:137:GLN:HG3	1:U:159:PHE:HZ	1.74	0.53
1:W:38:PHE:H	1:W:71:ALA:HA	1.73	0.53
1:Z:39:PHE:CD2	1:Z:114:VAL:HB	2.43	0.53
1:Z:86:LEU:O	1:Z:94:GLY:HA2	2.09	0.53
1:b:17:VAL:N	1:b:100:LEU:O	2.34	0.53
1:c:3:LEU:HB3	1:c:138:ILE:HG12	1.90	0.53
1:m:137:GLN:HB2	1:m:159:PHE:HE2	1.74	0.53
1:D:94:GLY:O	1:D:95:HIS:ND1	2.42	0.53
1:E:116:ASP:HB2	1:E:121:ASN:O	2.09	0.53
1:F:74:THR:O	1:G:104:ARG:NH2	2.40	0.53
1:M:161:PHE:HA	1:M:164:LYS:HZ3	1.72	0.53
1:O:46:PHE:HD1	1:O:49:PRO:HG2	1.74	0.53
1:O:121:ASN:HB3	1:O:143:LYS:HZ1	1.73	0.53
1:S:106:GLN:HG3	1:S:107:GLU:H	1.74	0.53
1:W:2:VAL:HG13	1:W:3:LEU:H	1.74	0.53
1:j:38:PHE:HD2	1:j:71:ALA:HA	1.74	0.53
1:C:16:ALA:CB	1:C:101:LEU:HA	2.38	0.53
1:G:45:THR:O	1:G:48:PRO:HD2	2.09	0.53
1:L:130:ASP:OD1	1:L:136:ARG:NH1	2.42	0.53
1:O:36:VAL:O	1:O:69:VAL:HA	2.08	0.53
1:O:153:LEU:HA	1:O:156:LEU:HD12	1.89	0.53
1:g:71:ALA:O	1:g:101:LEU:N	2.36	0.53
1:h:137:GLN:HB2	1:h:159:PHE:CZ	2.43	0.53
1:h:153:LEU:HA	1:h:156:LEU:HD12	1.89	0.53
1:C:5:PRO:C	1:C:7:ARG:H	2.17	0.53
1:C:71:ALA:O	1:C:101:LEU:N	2.26	0.53
1:D:39:PHE:HD2	1:D:125:GLY:HA3	1.74	0.53
1:F:59:VAL:O	1:F:63:ASN:ND2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:GLN:OE1	1:I:104:ARG:NH1	2.32	0.53
1:J:60:GLU:HG3	1:J:97:LYS:HZ1	1.73	0.53
1:N:4:LEU:HB2	1:N:7:ARG:HG2	1.89	0.53
1:O:32:GLY:H	1:O:131:PRO:HB3	1.74	0.53
1:O:139:THR:HG22	1:P:139:THR:HG23	1.89	0.53
1:Q:103:ASP:HA	1:Q:108:ILE:HD12	1.91	0.53
1:R:37:LEU:HD13	1:R:112:TYR:HE2	1.74	0.53
1:U:141:ASN:N	1:U:141:ASN:OD1	2.42	0.53
1:V:89:LYS:NZ	1:V:89:LYS:HB3	2.24	0.53
1:W:9:ALA:HA	1:W:135:LEU:HD11	1.90	0.53
1:Y:50:THR:N	1:Y:53:ILE:HG22	2.24	0.53
1:Z:142:ASP:CG	1:Z:144:PRO:HD2	2.33	0.53
1:d:19:ASN:O	1:d:19:ASN:ND2	2.42	0.53
1:d:26:CYS:SG	1:d:27:LEU:N	2.81	0.53
1:g:16:ALA:H	1:g:24:GLU:HB3	1.73	0.53
1:g:69:VAL:HB	1:g:98:ILE:HD12	1.91	0.53
1:H:109:SER:HB2	1:H:115:PHE:HB2	1.91	0.53
1:K:9:ALA:HB2	1:K:135:LEU:HD22	1.90	0.53
1:L:35:VAL:HG23	1:L:70:ILE:HD12	1.91	0.53
1:L:114:VAL:HG12	1:L:123:PHE:H	1.74	0.53
1:P:105:LYS:HB2	1:P:107:GLU:OE1	2.09	0.53
1:V:104:ARG:HE	1:W:121:ASN:HD21	1.56	0.53
1:W:127:PHE:CD2	1:W:138:ILE:HD12	2.44	0.53
1:Z:59:VAL:HG12	1:Z:63:ASN:OD1	2.09	0.53
1:h:36:VAL:CG1	1:h:69:VAL:HB	2.38	0.53
1:k:75:ASP:O	1:k:104:ARG:NH1	2.42	0.53
1:m:163:GLU:HG2	1:m:164:LYS:HE2	1.90	0.53
1:I:38:PHE:O	1:I:72:CYS:N	2.42	0.52
1:L:43:ASP:HB2	1:L:75:ASP:CG	2.34	0.52
1:Q:68:GLN:O	1:Q:68:GLN:NE2	2.43	0.52
1:R:44:PHE:HD2	1:S:79:SER:HA	1.73	0.52
1:e:104:ARG:HH22	1:n:121:ASN:HA	1.74	0.52
1:g:124:ARG:HB2	1:g:124:ARG:HH11	1.74	0.52
1:n:36:VAL:HB	1:n:69:VAL:HG22	1.91	0.52
1:A:145:VAL:HG11	1:B:159:PHE:HE1	1.74	0.52
1:D:164:LYS:HZ3	1:D:165:HIS:CE1	2.27	0.52
1:G:17:VAL:O	1:G:99:PRO:HA	2.09	0.52
1:H:25:ILE:HD11	1:H:101:LEU:HD23	1.90	0.52
1:M:164:LYS:HE2	1:M:165:HIS:CE1	2.44	0.52
1:N:106:GLN:HE22	1:O:105:LYS:HA	1.72	0.52
1:Z:88:ARG:HA	1:Z:94:GLY:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:124:ARG:HB3	1:b:143:LYS:HA	1.91	0.52
1:h:42:ALA:HB2	1:i:104:ARG:HH22	1.73	0.52
1:E:112:TYR:HB3	1:E:127:PHE:CE2	2.45	0.52
1:F:18:ILE:HD11	1:F:21:GLU:HB3	1.90	0.52
1:F:104:ARG:CZ	1:G:74:THR:HB	2.39	0.52
1:J:35:VAL:HG12	1:J:129:ILE:HB	1.91	0.52
1:K:72:CYS:HB2	1:K:101:LEU:HB3	1.91	0.52
1:K:104:ARG:NH1	1:T:74:THR:HB	2.24	0.52
1:L:93:LEU:H	1:L:93:LEU:HD12	1.73	0.52
1:P:88:ARG:HA	1:P:92:GLY:O	2.10	0.52
1:U:101:LEU:HD23	1:U:102:ALA:N	2.25	0.52
1:Z:38:PHE:HB3	1:Z:126:LEU:HD23	1.90	0.52
1:a:141:ASN:O	1:a:145:VAL:HG12	2.10	0.52
1:b:126:LEU:HD23	1:b:147:ARG:NH2	2.24	0.52
1:i:59:VAL:HA	1:i:62:PHE:CE2	2.45	0.52
1:k:88:ARG:HG2	1:k:94:GLY:H	1.74	0.52
1:m:56:SER:HB3	1:m:96:MET:HE2	1.91	0.52
1:G:115:PHE:HA	1:G:122:ALA:HA	1.90	0.52
1:L:11:GLU:HA	1:L:27:LEU:HD12	1.92	0.52
1:O:112:TYR:HB3	1:O:127:PHE:HE2	1.74	0.52
1:U:106:GLN:OE1	1:d:106:GLN:NE2	2.43	0.52
1:V:161:PHE:HB2	1:V:165:HIS:HE1	1.75	0.52
1:Y:116:ASP:OD2	1:Y:119:ASP:OD1	2.28	0.52
1:d:17:VAL:HG11	1:d:81:LEU:HD23	1.92	0.52
1:k:114:VAL:HG12	1:k:115:PHE:H	1.74	0.52
1:A:130:ASP:OD2	1:A:134:ILE:HG12	2.10	0.52
1:C:164:LYS:HG2	1:C:165:HIS:N	2.23	0.52
1:L:65:ARG:NH2	1:L:153:LEU:HB3	2.25	0.52
1:L:156:LEU:O	1:L:160:GLN:NE2	2.43	0.52
1:N:164:LYS:HD3	1:N:165:HIS:CE1	2.45	0.52
1:P:3:LEU:HD21	1:P:112:TYR:HA	1.92	0.52
1:Q:28:LYS:HA	1:Q:31:ARG:HG3	1.92	0.52
1:V:37:LEU:HD13	1:V:70:ILE:HG13	1.91	0.52
1:W:1:MET:HG2	1:X:2:VAL:HB	1.90	0.52
1:Y:154:ARG:NH1	1:Y:155:LEU:HD23	2.25	0.52
1:e:46:PHE:O	1:e:49:PRO:HD2	2.10	0.52
1:h:52:ILE:HG22	1:h:124:ARG:HH12	1.73	0.52
1:i:139:THR:HA	1:j:138:ILE:O	2.09	0.52
1:l:97:LYS:HZ2	1:l:97:LYS:H	1.58	0.52
1:G:73:SER:HB3	1:G:80:HIS:HE1	1.74	0.52
1:X:36:VAL:HG12	1:X:128:ILE:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:15:GLN:O	1:Y:101:LEU:HA	2.09	0.52
1:d:41:PRO:HB3	1:d:143:LYS:NZ	2.25	0.52
1:i:35:VAL:HB	1:i:129:ILE:HG12	1.92	0.52
1:B:154:ARG:HG3	1:B:155:LEU:N	2.24	0.52
1:F:103:ASP:C	1:F:105:LYS:H	2.18	0.52
1:F:151:GLU:OE2	1:F:154:ARG:NH2	2.32	0.52
1:H:18:ILE:HD11	1:H:25:ILE:HG21	1.91	0.52
1:I:118:GLU:OE1	1:I:118:GLU:N	2.38	0.52
1:P:96:MET:HG3	1:P:98:ILE:HB	1.91	0.52
1:Q:3:LEU:HD23	1:R:1:MET:HB3	1.90	0.52
1:V:62:PHE:CZ	1:V:149:VAL:HG13	2.44	0.52
1:X:151:GLU:HA	1:X:154:ARG:HG2	1.92	0.52
1:i:36:VAL:HG21	1:i:152:THR:HG23	1.92	0.52
1:m:136:ARG:NH2	1:n:142:ASP:OD2	2.43	0.52
1:A:124:ARG:HG2	1:A:141:ASN:HB2	1.90	0.52
1:E:5:PRO:HD3	1:F:140:ILE:HD12	1.91	0.52
1:F:147:ARG:NH1	1:F:147:ARG:HB2	2.25	0.52
1:G:105:LYS:H	1:G:105:LYS:HD2	1.74	0.52
1:I:61:GLU:O	1:I:65:ARG:HD3	2.10	0.52
1:I:65:ARG:HH12	1:I:153:LEU:CD2	2.22	0.52
1:L:50:THR:HA	1:L:51:GLU:HB3	1.92	0.52
1:L:106:GLN:HB2	1:L:110:LYS:HG3	1.91	0.52
1:N:141:ASN:OD1	1:N:141:ASN:N	2.31	0.52
1:P:73:SER:O	1:P:74:THR:OG1	2.22	0.52
1:V:41:PRO:HB3	1:V:143:LYS:HZ1	1.75	0.52
1:W:11:GLU:CD	1:W:28:LYS:HB2	2.34	0.52
1:W:51:GLU:C	1:W:53:ILE:N	2.66	0.52
1:a:17:VAL:HA	1:a:21:GLU:O	2.10	0.52
1:a:130:ASP:HB2	1:a:134:ILE:HG22	1.92	0.52
1:d:4:LEU:HD12	1:d:7:ARG:HH22	1.74	0.52
1:f:87:ASP:HA	1:f:94:GLY:HA2	1.91	0.52
1:h:127:PHE:HD1	1:h:139:THR:H	1.57	0.52
1:h:163:GLU:HG3	1:h:164:LYS:H	1.74	0.52
1:m:53:ILE:HD13	1:m:53:ILE:H	1.74	0.52
1:n:72:CYS:SG	1:n:103:ASP:N	2.79	0.52
1:G:13:LYS:HD2	1:G:26:CYS:HB2	1.92	0.52
1:R:50:THR:HG23	1:R:53:ILE:HG12	1.91	0.52
1:U:37:LEU:H	1:U:37:LEU:HD12	1.75	0.52
1:a:65:ARG:NH1	1:a:65:ARG:HB2	2.25	0.52
1:b:83:TRP:NE1	1:b:92:GLY:HA2	2.24	0.52
1:j:116:ASP:HB3	1:j:119:ASP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:37:LEU:O	1:m:127:PHE:N	2.41	0.52
1:A:138:ILE:O	1:B:140:ILE:HG13	2.09	0.52
1:G:39:PHE:H	1:G:125:GLY:CA	2.23	0.52
1:I:52:ILE:HG22	1:I:96:MET:HE3	1.91	0.52
1:O:39:PHE:CD1	1:O:72:CYS:HB3	2.45	0.52
1:V:42:ALA:HB2	1:V:121:ASN:HB3	1.91	0.52
1:d:80:HIS:ND1	1:d:100:LEU:O	2.36	0.52
1:e:18:ILE:N	1:e:23:LYS:HZ1	2.08	0.52
1:A:83:TRP:HB3	1:A:93:LEU:HD22	1.92	0.51
1:A:128:ILE:HG22	1:A:137:GLN:H	1.76	0.51
1:C:16:ALA:HB2	1:C:101:LEU:HG	1.91	0.51
1:M:72:CYS:HB2	1:M:101:LEU:O	2.09	0.51
1:M:75:ASP:O	1:M:102:ALA:HB1	2.10	0.51
1:O:70:ILE:HG12	1:O:101:LEU:HD23	1.91	0.51
1:Q:4:LEU:HG	1:R:123:PHE:HE2	1.75	0.51
1:Q:70:ILE:HG22	1:Q:99:PRO:HB2	1.91	0.51
1:R:4:LEU:HB3	1:R:7:ARG:HG2	1.92	0.51
1:a:141:ASN:O	1:a:142:ASP:OD1	2.28	0.51
1:a:142:ASP:HB3	1:b:5:PRO:HB2	1.92	0.51
1:g:46:PHE:CD2	1:g:47:VAL:HG23	2.44	0.51
1:l:34:TYR:HE1	1:l:131:PRO:HG3	1.74	0.51
1:A:114:VAL:CG2	1:A:123:PHE:HB2	2.37	0.51
1:F:33:LYS:HG2	1:F:66:ASN:HB3	1.92	0.51
1:L:53:ILE:HD13	1:L:93:LEU:HG	1.92	0.51
1:M:59:VAL:HG12	1:M:63:ASN:ND2	2.25	0.51
1:Q:112:TYR:O	1:Q:114:VAL:HG23	2.10	0.51
1:V:72:CYS:HB2	1:V:102:ALA:H	1.74	0.51
1:b:104:ARG:NH2	1:c:74:THR:OG1	2.42	0.51
1:i:26:CYS:SG	1:i:28:LYS:HB2	2.49	0.51
1:i:119:ASP:OD2	1:i:143:LYS:NZ	2.43	0.51
1:i:130:ASP:OD1	1:i:134:ILE:HG12	2.11	0.51
1:j:53:ILE:HG23	1:j:96:MET:HE1	1.91	0.51
1:l:34:TYR:HB2	1:l:67:CYS:HB3	1.91	0.51
1:l:123:PHE:HA	1:l:143:LYS:HZ3	1.74	0.51
1:E:74:THR:HA	1:E:103:ASP:HB3	1.91	0.51
1:E:123:PHE:CD1	1:E:143:LYS:HE2	2.46	0.51
1:H:88:ARG:HD2	1:H:94:GLY:HA3	1.91	0.51
1:J:51:GLU:C	1:J:53:ILE:H	2.18	0.51
1:M:114:VAL:HG12	1:M:140:ILE:HG23	1.92	0.51
1:P:72:CYS:HA	1:P:80:HIS:HE1	1.76	0.51
1:T:127:PHE:HB3	1:T:135:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:70:ILE:CG2	1:U:101:LEU:HB2	2.40	0.51
1:U:145:VAL:HG21	1:V:155:LEU:HD23	1.91	0.51
1:b:126:LEU:HD23	1:b:147:ARG:HH22	1.75	0.51
1:f:44:PHE:HZ	1:f:82:ALA:HB3	1.75	0.51
1:g:61:GLU:OE1	1:g:61:GLU:N	2.42	0.51
1:j:55:PHE:HA	1:j:58:GLN:HE21	1.74	0.51
1:l:104:ARG:HA	1:l:104:ARG:NH1	2.24	0.51
1:n:130:ASP:HB3	1:n:134:ILE:HB	1.93	0.51
1:I:4:LEU:HB2	1:I:7:ARG:HG2	1.91	0.51
1:I:53:ILE:HG13	1:I:88:ARG:HH12	1.76	0.51
1:N:28:LYS:O	1:N:31[A]:ARG:HG2	2.10	0.51
1:P:76:SER:HA	1:P:104:ARG:HG2	1.91	0.51
1:W:74:THR:OG1	1:W:121:ASN:OD1	2.26	0.51
1:W:148:SER:HB3	1:X:151:GLU:OE2	2.10	0.51
1:Z:88:ARG:HH12	1:Z:93:LEU:HD23	1.75	0.51
1:b:38:PHE:CE1	1:b:52:ILE:HG22	2.45	0.51
1:g:148:SER:O	1:g:152:THR:OG1	2.13	0.51
1:i:130:ASP:OD1	1:i:133:GLY:N	2.44	0.51
1:n:160:GLN:HA	1:n:164:LYS:HZ3	1.76	0.51
1:B:86:LEU:HB3	1:B:92:GLY:HA3	1.92	0.51
1:H:105:LYS:HG3	1:H:107:GLU:HG3	1.92	0.51
1:Q:7:ARG:O	1:Q:135:LEU:HB2	2.11	0.51
1:R:89:LYS:HA	1:R:89:LYS:HZ3	1.75	0.51
1:V:56:SER:HA	1:V:59:VAL:HG23	1.93	0.51
1:a:127:PHE:CE2	1:a:138:ILE:HG23	2.45	0.51
1:e:3:LEU:HD13	1:f:2:VAL:HG13	1.93	0.51
1:l:122:ALA:C	1:l:143:LYS:HZ1	2.17	0.51
1:m:151:GLU:HB3	1:n:151:GLU:OE2	2.11	0.51
1:G:8:PRO:HA	1:G:133:GLY:O	2.10	0.51
1:I:128:ILE:HG22	1:I:137:GLN:HB3	1.93	0.51
1:Q:52:ILE:HD13	1:Q:147:ARG:HH22	1.75	0.51
1:R:50:THR:N	1:R:51:GLU:HB3	2.25	0.51
1:U:154:ARG:NH1	1:U:155:LEU:HD12	2.25	0.51
1:V:37:LEU:HG	1:V:39:PHE:CE1	2.45	0.51
1:V:89:LYS:HB3	1:V:89:LYS:HZ2	1.75	0.51
1:Y:71:ALA:N	1:Y:99:PRO:O	2.39	0.51
1:a:37:LEU:HD22	1:a:127:PHE:H	1.76	0.51
1:g:7:ARG:HH12	1:h:123:PHE:HZ	1.58	0.51
1:h:134:ILE:HG22	1:h:135:LEU:H	1.76	0.51
1:A:25:ILE:HD12	1:A:30:TYR:OH	2.11	0.51
1:N:121:ASN:HA	1:O:104:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:41:PRO:HB3	1:d:143:LYS:HZ3	1.75	0.51
1:d:116:ASP:HB3	1:d:123:PHE:CZ	2.45	0.51
1:g:145:VAL:HG21	1:h:159:PHE:HE1	1.75	0.51
1:A:139:THR:HA	1:B:139:THR:HA	1.93	0.51
1:G:76:SER:HB2	1:G:104:ARG:HB2	1.91	0.51
1:R:130:ASP:HB2	1:R:134:ILE:HB	1.92	0.51
1:T:13:LYS:HG3	1:T:26:CYS:HB3	1.91	0.51
1:Y:43:ASP:OD2	1:Y:83:TRP:HB2	2.11	0.51
1:d:4:LEU:HD12	1:d:7:ARG:HH12	1.76	0.51
1:g:156:LEU:HA	1:g:159:PHE:CE1	2.46	0.51
1:i:137:GLN:HG3	1:j:140:ILE:O	2.11	0.51
1:A:16:ALA:H	1:A:102:ALA:HB2	1.76	0.51
1:A:88:ARG:HA	1:A:94:GLY:H	1.76	0.51
1:C:95:HIS:O	1:C:97:LYS:NZ	2.44	0.51
1:G:75:ASP:HB3	1:G:79:SER:HB2	1.93	0.51
1:G:101:LEU:HD13	1:G:102:ALA:H	1.75	0.51
1:H:56:SER:HB2	1:H:96:MET:HG3	1.93	0.51
1:M:38:PHE:CE2	1:M:147:ARG:HD2	2.45	0.51
1:N:127:PHE:CZ	1:N:140:ILE:HD11	2.46	0.51
1:W:60:GLU:OE1	1:W:60:GLU:HA	2.11	0.51
1:a:36:VAL:HG23	1:a:128:ILE:HB	1.93	0.51
1:b:9:ALA:HB2	1:b:129:ILE:HD11	1.93	0.51
1:g:16:ALA:N	1:g:24:GLU:HB3	2.25	0.51
1:E:43:ASP:OD2	1:E:80:HIS:HD2	1.94	0.51
1:G:7:ARG:O	1:G:135:LEU:N	2.39	0.51
1:K:116:ASP:HB2	1:K:123:PHE:CD2	2.46	0.51
1:M:38:PHE:CZ	1:M:126:LEU:HB3	2.46	0.51
1:M:130:ASP:HB3	1:M:136:ARG:HD3	1.93	0.51
1:N:35:VAL:HG13	1:N:129:ILE:HD11	1.93	0.51
1:P:8:PRO:HA	1:P:134:ILE:HA	1.92	0.51
1:W:11:GLU:OE2	1:W:28:LYS:HB2	2.10	0.51
1:W:59:VAL:HG12	1:W:63:ASN:OD1	2.11	0.51
1:Z:32:GLY:C	1:Z:131:PRO:HB3	2.35	0.51
1:a:25:ILE:HG12	1:a:26:CYS:H	1.75	0.51
1:d:58:GLN:HG2	1:d:149:VAL:HG11	1.94	0.51
1:h:70:ILE:HG13	1:h:99:PRO:O	2.11	0.51
1:E:72:CYS:SG	1:E:101:LEU:HD12	2.51	0.50
1:L:119:ASP:OD1	1:L:121:ASN:HB2	2.11	0.50
1:Q:32:GLY:C	1:Q:131:PRO:HB3	2.36	0.50
1:Q:106:GLN:O	1:Q:110:LYS:HB2	2.11	0.50
1:T:73:SER:HB3	1:T:80:HIS:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:96:MET:HG3	1:T:100:LEU:HD11	1.92	0.50
1:U:36:VAL:HG12	1:U:36:VAL:O	2.11	0.50
1:U:105:LYS:HZ3	1:U:107:GLU:HG3	1.75	0.50
1:V:35:VAL:O	1:V:128:ILE:HA	2.11	0.50
1:a:76:SER:HB2	1:a:78:TYR:CE1	2.47	0.50
1:g:89:LYS:NZ	1:g:89:LYS:HB3	2.25	0.50
1:k:41:PRO:HB3	1:k:143:LYS:NZ	2.26	0.50
1:k:106:GLN:O	1:k:110:LYS:HG2	2.11	0.50
1:l:37:LEU:HD23	1:l:70:ILE:HB	1.92	0.50
1:n:4:LEU:HB3	1:n:7:ARG:HE	1.74	0.50
1:B:28:LYS:HD2	1:B:31:ARG:HE	1.76	0.50
1:B:42:ALA:HB2	1:B:121:ASN:HD21	1.75	0.50
1:F:87:ASP:OD1	1:F:88:ARG:N	2.44	0.50
1:J:154:ARG:HH11	1:J:154:ARG:HB2	1.76	0.50
1:Q:40:TYR:HD1	1:Q:71:ALA:HB1	1.77	0.50
1:U:52:ILE:HA	1:U:55:PHE:HE1	1.77	0.50
1:U:70:ILE:HG21	1:U:101:LEU:HD12	1.93	0.50
1:V:89:LYS:H	1:V:89:LYS:HZ3	1.58	0.50
1:Z:88:ARG:NH1	1:Z:93:LEU:HD23	2.26	0.50
1:b:156:LEU:O	1:b:160:GLN:HG2	2.12	0.50
1:i:4:LEU:HD21	1:j:116:ASP:CG	2.35	0.50
1:i:33:LYS:HE2	1:i:66:ASN:HD22	1.75	0.50
1:i:52:ILE:HG21	1:i:124:ARG:NH1	2.26	0.50
1:l:147:ARG:HG3	1:l:147:ARG:NH1	2.26	0.50
1:n:37:LEU:HD23	1:n:70:ILE:HB	1.93	0.50
1:A:6:ASN:N	1:A:135:LEU:O	2.44	0.50
1:H:17:VAL:N	1:H:100:LEU:O	2.44	0.50
1:N:79:SER:HA	1:O:44:PHE:HB2	1.93	0.50
1:W:9:ALA:HB2	1:W:129:ILE:HD11	1.92	0.50
1:f:116:ASP:HB3	1:f:123:PHE:HE1	1.77	0.50
1:j:35:VAL:O	1:j:129:ILE:HG22	2.12	0.50
1:n:8:PRO:HA	1:n:133:GLY:O	2.11	0.50
1:B:34:TYR:OH	1:B:163:GLU:OE2	2.27	0.50
1:F:21:GLU:HG3	1:F:22:PHE:H	1.75	0.50
1:G:114:VAL:HG12	1:G:123:PHE:H	1.75	0.50
1:I:11:GLU:HA	1:I:27:LEU:HD21	1.94	0.50
1:J:5:PRO:C	1:J:7:ARG:H	2.18	0.50
1:J:14:GLY:O	1:J:24:GLU:HG3	2.11	0.50
1:L:137:GLN:HB2	1:L:159:PHE:CZ	2.46	0.50
1:O:87:ASP:HB3	1:O:89:LYS:HZ1	1.76	0.50
1:Q:75:ASP:OD1	1:Q:80:HIS:ND1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:105:LYS:O	1:S:107:GLU:HG2	2.11	0.50
1:U:123:PHE:CD2	1:V:4:LEU:HD12	2.45	0.50
1:X:61:GLU:O	1:X:65:ARG:HG2	2.10	0.50
1:Z:53:ILE:HD11	1:Z:88:ARG:HD3	1.92	0.50
1:a:159:PHE:CE1	1:b:145:VAL:HG21	2.47	0.50
1:i:74:THR:O	1:i:74:THR:OG1	2.28	0.50
1:m:116:ASP:HB3	1:m:119:ASP:O	2.11	0.50
1:n:49:PRO:HG3	1:n:83:TRP:HZ2	1.76	0.50
1:C:38:PHE:CE2	1:C:52:ILE:HG23	2.46	0.50
1:D:122:ALA:O	1:D:143:LYS:HE2	2.11	0.50
1:E:138:ILE:HB	1:F:140:ILE:HG12	1.92	0.50
1:J:142:ASP:OD1	1:J:143:LYS:N	2.44	0.50
1:J:151:GLU:O	1:J:155:LEU:HB2	2.12	0.50
1:M:77:GLN:HG3	1:M:102:ALA:HB3	1.94	0.50
1:S:6:ASN:H	1:S:136:ARG:HD2	1.76	0.50
1:S:76:SER:HB2	1:S:104:ARG:HH12	1.75	0.50
1:U:137:GLN:NE2	1:V:141:ASN:OD1	2.44	0.50
1:c:103:ASP:HB2	1:c:105:LYS:HB2	1.94	0.50
1:d:51:GLU:HB3	1:d:147:ARG:HH12	1.76	0.50
1:f:47:VAL:N	1:f:48:PRO:HD3	2.25	0.50
1:h:151:GLU:HA	1:h:154:ARG:HD3	1.94	0.50
1:l:160:GLN:O	1:l:164:LYS:HG3	2.11	0.50
1:D:87:ASP:HA	1:D:94:GLY:HA2	1.92	0.50
1:F:18:ILE:HD13	1:F:23:LYS:HB2	1.93	0.50
1:H:88:ARG:HA	1:H:92:GLY:O	2.12	0.50
1:J:36:VAL:HG22	1:J:128:ILE:HG22	1.94	0.50
1:K:37:LEU:HD11	1:K:39:PHE:CE2	2.47	0.50
1:O:36:VAL:HG13	1:O:69:VAL:HG22	1.93	0.50
1:T:4:LEU:HB3	1:T:7:ARG:HD3	1.93	0.50
1:U:56:SER:HA	1:U:98:ILE:HG23	1.94	0.50
1:U:126:LEU:HD21	1:U:147:ARG:HB3	1.93	0.50
1:X:35:VAL:HA	1:X:68:GLN:O	2.12	0.50
1:X:127:PHE:HB3	1:X:135:LEU:HD11	1.94	0.50
1:Y:39:PHE:HB2	1:Y:125:GLY:H	1.77	0.50
1:Z:124:ARG:HG3	1:Z:141:ASN:HB3	1.94	0.50
1:b:28:LYS:HA	1:b:31:ARG:HG2	1.93	0.50
1:c:158:ALA:O	1:c:161:PHE:HD1	1.95	0.50
1:n:105:LYS:O	1:n:106:GLN:HG2	2.11	0.50
1:A:116:ASP:OD2	1:A:119:ASP:OD2	2.30	0.50
1:A:124:ARG:O	1:A:147:ARG:HD3	2.12	0.50
1:F:76:SER:HB3	1:F:104:ARG:CZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:PHE:CE2	1:G:138:ILE:HG23	2.47	0.50
1:I:39:PHE:O	1:I:124:ARG:HG3	2.12	0.50
1:L:97:LYS:H	1:L:97:LYS:HD2	1.77	0.50
1:M:96:MET:HA	1:M:96:MET:HE2	1.92	0.50
1:U:124:ARG:HG2	1:U:147:ARG:HH12	1.75	0.50
1:Z:105:LYS:CB	1:Z:105:LYS:HZ3	2.24	0.50
1:b:53:ILE:HD12	1:b:96:MET:HE1	1.94	0.50
1:b:117:GLU:O	1:c:105:LYS:HD3	2.11	0.50
1:d:38:PHE:CZ	1:d:71:ALA:HB2	2.47	0.50
1:g:85:ASN:HA	1:g:95:HIS:CE1	2.47	0.50
1:h:128:ILE:HG22	1:h:137:GLN:HB3	1.93	0.50
1:k:7:ARG:NH2	1:l:118:GLU:OE2	2.44	0.50
1:D:6:ASN:O	1:D:7:ARG:NH1	2.39	0.50
1:D:67:CYS:O	1:D:68:GLN:HG2	2.11	0.50
1:I:19:ASN:HB3	1:I:97:LYS:HA	1.94	0.50
1:N:141:ASN:ND2	1:N:145:VAL:O	2.45	0.50
1:O:16:ALA:HB2	1:O:101:LEU:HD22	1.93	0.50
1:P:119:ASP:OD2	1:P:121:ASN:HB2	2.12	0.50
1:S:22:PHE:HD1	1:S:22:PHE:H	1.60	0.50
1:S:33:LYS:C	1:S:131:PRO:HA	2.37	0.50
1:S:105:LYS:H	1:S:105:LYS:HZ2	1.55	0.50
1:V:10:PRO:HD2	1:V:112:TYR:HE1	1.77	0.50
1:Z:10:PRO:HD2	1:Z:112:TYR:CE1	2.46	0.50
1:Z:40:TYR:HE1	1:Z:43:ASP:OD1	1.93	0.50
1:a:12:PHE:HB2	1:a:108:ILE:HB	1.93	0.50
1:e:6:ASN:HA	1:e:136:ARG:HH12	1.75	0.50
1:g:49:PRO:O	1:g:124:ARG:NH2	2.42	0.50
1:g:55:PHE:HA	1:g:62:PHE:HE2	1.76	0.50
1:k:137:GLN:HG2	1:l:147:ARG:HH22	1.76	0.50
1:l:40:TYR:CZ	1:l:73:SER:HB2	2.47	0.50
1:l:76:SER:HB3	1:l:104:ARG:HB2	1.92	0.50
1:B:104:ARG:HG3	1:B:104:ARG:NH1	2.26	0.50
1:I:62:PHE:HZ	1:I:149:VAL:HG23	1.77	0.50
1:K:76:SER:OG	1:K:104:ARG:HB2	2.12	0.50
1:R:127:PHE:CE2	1:R:138:ILE:HG23	2.47	0.50
1:S:33:LYS:HZ2	1:S:67:CYS:C	2.20	0.50
1:T:40:TYR:CZ	1:T:73:SER:HB2	2.47	0.50
1:V:17:VAL:O	1:V:99:PRO:HA	2.12	0.50
1:a:16:ALA:HB1	1:a:100:LEU:O	2.11	0.50
1:d:88:ARG:HH12	1:d:94:GLY:HA3	1.77	0.50
1:g:33:LYS:NZ	1:g:33:LYS:HB3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:37:LEU:HA	1:j:70:ILE:HB	1.93	0.50
1:j:136:ARG:NH1	1:j:163:GLU:OE1	2.42	0.50
1:k:139:THR:HA	1:l:139:THR:HA	1.93	0.50
1:l:8:PRO:HA	1:l:134:ILE:HA	1.94	0.50
1:l:126:LEU:HD11	1:l:152:THR:HG22	1.94	0.50
1:n:124:ARG:HD3	1:n:147:ARG:NH1	2.26	0.50
1:A:11:GLU:OE1	1:A:28:LYS:HB2	2.11	0.49
1:A:44:PHE:CD2	1:J:79:SER:HA	2.47	0.49
1:A:67:CYS:SG	1:A:68:GLN:N	2.85	0.49
1:B:3:LEU:O	1:B:4:LEU:HB2	2.12	0.49
1:B:57:ASP:OD1	1:B:58:GLN:HG3	2.12	0.49
1:G:70:ILE:HG22	1:G:71:ALA:H	1.77	0.49
1:R:104:ARG:HG3	1:S:120:GLY:N	2.26	0.49
1:S:164:LYS:H	1:S:164:LYS:HD3	1.76	0.49
1:V:129:ILE:O	1:V:130:ASP:HB3	2.11	0.49
1:W:33:LYS:C	1:W:131:PRO:HG3	2.36	0.49
1:a:126:LEU:HB3	1:a:139:THR:HG23	1.94	0.49
1:e:154:ARG:HG3	1:e:155:LEU:N	2.27	0.49
1:g:74:THR:HG23	1:g:122:ALA:HB2	1.93	0.49
1:i:16:ALA:HB2	1:i:25:ILE:HG12	1.93	0.49
1:j:38:PHE:HZ	1:j:52:ILE:HG22	1.77	0.49
1:D:104:ARG:C	1:D:106:GLN:H	2.20	0.49
1:K:77:GLN:HG2	1:K:78:TYR:H	1.76	0.49
1:L:105:LYS:HD3	1:L:105:LYS:H	1.77	0.49
1:N:106:GLN:O	1:N:110:LYS:HG2	2.12	0.49
1:P:5:PRO:C	1:P:7:ARG:H	2.20	0.49
1:Q:33:LYS:CB	1:Q:66:ASN:HB3	2.42	0.49
1:T:15:GLN:NE2	1:T:24:GLU:HB2	2.27	0.49
1:T:73:SER:HB3	1:T:80:HIS:CE1	2.47	0.49
1:T:123:PHE:HB3	1:T:140:ILE:HD11	1.95	0.49
1:a:36:VAL:HA	1:a:127:PHE:O	2.12	0.49
1:a:72:CYS:HA	1:a:101:LEU:O	2.12	0.49
1:g:127:PHE:CE1	1:g:138:ILE:HB	2.46	0.49
1:g:128:ILE:HD12	1:g:136:ARG:HB2	1.93	0.49
1:n:38:PHE:O	1:n:71:ALA:HA	2.12	0.49
1:n:132:ASN:O	1:n:134:ILE:HG12	2.12	0.49
1:I:53:ILE:HG13	1:I:88:ARG:NH1	2.27	0.49
1:Y:137:GLN:HG3	1:Z:141:ASN:HA	1.95	0.49
1:b:164:LYS:HG3	1:b:165:HIS:H	1.78	0.49
1:d:17:VAL:HB	1:d:100:LEU:HB2	1.94	0.49
1:d:105:LYS:O	1:d:106:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:22:PHE:CZ	1:f:81:LEU:HD23	2.47	0.49
1:h:110:LYS:NZ	1:h:115:PHE:HE2	2.09	0.49
1:G:128:ILE:HB	1:G:137:GLN:HB3	1.93	0.49
1:I:154:ARG:HH21	1:I:158:ALA:HB2	1.76	0.49
1:M:116:ASP:OD2	1:M:118:GLU:OE2	2.30	0.49
1:Q:73:SER:O	1:Q:75:ASP:N	2.46	0.49
1:U:123:PHE:CD2	1:V:5:PRO:HD2	2.47	0.49
1:X:147:ARG:HB2	1:X:147:ARG:NH1	2.28	0.49
1:Z:55:PHE:HA	1:Z:149:VAL:HG13	1.94	0.49
1:a:114:VAL:CG1	1:a:140:ILE:HG21	2.40	0.49
1:b:136:ARG:HD3	1:b:159:PHE:CD1	2.47	0.49
1:c:15:GLN:O	1:c:102:ALA:HB2	2.12	0.49
1:f:3:LEU:HD11	1:f:112:TYR:HD1	1.76	0.49
1:f:69:VAL:O	1:f:99:PRO:HD2	2.13	0.49
1:l:5:PRO:HA	1:l:135:LEU:HD13	1.94	0.49
1:l:39:PHE:CE2	1:l:109:SER:HA	2.48	0.49
1:m:105:LYS:HD2	1:m:107:GLU:OE2	2.12	0.49
1:A:69:VAL:HG13	1:A:98:ILE:HG13	1.93	0.49
1:D:124:ARG:HG3	1:D:147:ARG:CZ	2.43	0.49
1:J:80:HIS:O	1:J:84:ASP:HB3	2.12	0.49
1:J:96:MET:HB2	1:J:100:LEU:HD21	1.95	0.49
1:Q:116:ASP:HB2	1:Q:123:PHE:CD2	2.45	0.49
1:V:8:PRO:HA	1:V:134:ILE:HA	1.95	0.49
1:V:41:PRO:HB3	1:V:143:LYS:NZ	2.27	0.49
1:X:53:ILE:HG23	1:X:96:MET:SD	2.52	0.49
1:f:128:ILE:O	1:f:135:LEU:HD12	2.13	0.49
1:i:17:VAL:H	1:i:101:LEU:HA	1.76	0.49
1:n:88:ARG:HH11	1:n:88:ARG:N	2.09	0.49
1:E:123:PHE:HD1	1:E:143:LYS:HE2	1.78	0.49
1:F:2:VAL:HG22	1:F:3:LEU:H	1.78	0.49
1:F:68:GLN:NE2	1:F:98:ILE:HG22	2.27	0.49
1:H:39:PHE:HB2	1:H:125:GLY:H	1.78	0.49
1:O:41:PRO:HG2	1:O:124:ARG:HH11	1.76	0.49
1:R:74:THR:HG23	1:S:104:ARG:HH21	1.77	0.49
1:V:18:ILE:HG12	1:V:99:PRO:HB3	1.94	0.49
1:b:16:ALA:HA	1:b:101:LEU:HA	1.94	0.49
1:f:126:LEU:HB3	1:f:139:THR:OG1	2.12	0.49
1:h:11:GLU:HG2	1:h:27:LEU:HD11	1.94	0.49
1:j:36:VAL:CG1	1:j:156:LEU:HD13	2.43	0.49
1:l:77:GLN:C	1:l:79:SER:H	2.21	0.49
1:m:21:GLU:HG3	1:m:23:LYS:HZ2	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PHE:CE1	1:B:153:LEU:HD23	2.48	0.49
1:D:161:PHE:HA	1:D:164:LYS:HZ2	1.77	0.49
1:G:12:PHE:HB3	1:G:108:ILE:HG23	1.95	0.49
1:N:15:GLN:HG2	1:N:24:GLU:HG2	1.95	0.49
1:T:10:PRO:O	1:T:11:GLU:HB2	2.13	0.49
1:W:129:ILE:HD13	1:W:135:LEU:HA	1.94	0.49
1:m:110:LYS:HG2	1:m:115:PHE:CG	2.48	0.49
1:G:44:PHE:HZ	1:G:82:ALA:HB3	1.77	0.49
1:K:6:ASN:HD21	1:L:142:ASP:HB2	1.77	0.49
1:K:137:GLN:HB2	1:L:141:ASN:HA	1.94	0.49
1:P:45:THR:HB	1:P:48:PRO:HD2	1.94	0.49
1:S:105:LYS:HG2	1:S:105:LYS:O	2.13	0.49
1:W:124:ARG:O	1:W:140:ILE:HA	2.12	0.49
1:Y:76:SER:HB3	1:Y:104:ARG:HH21	1.78	0.49
1:Y:141:ASN:ND2	1:Y:145:VAL:HG13	2.28	0.49
1:d:25:ILE:HG12	1:d:26:CYS:H	1.77	0.49
1:g:33:LYS:NZ	1:g:66:ASN:OD1	2.45	0.49
1:g:96:MET:HE2	1:g:98:ILE:HB	1.94	0.49
1:D:114:VAL:HG22	1:D:115:PHE:N	2.24	0.49
1:Q:6:ASN:HB2	1:R:123:PHE:HZ	1.76	0.49
1:V:164:LYS:HG3	1:V:165:HIS:N	2.26	0.49
1:W:39:PHE:HD2	1:W:125:GLY:HA3	1.78	0.49
1:b:46:PHE:HB3	1:b:47:VAL:CG2	2.37	0.49
1:c:22:PHE:HE2	1:c:77:GLN:HB3	1.76	0.49
1:f:75:ASP:HB2	1:f:80:HIS:HE1	1.77	0.49
1:m:137:GLN:NE2	1:m:139:THR:OG1	2.35	0.49
1:A:17:VAL:HG22	1:A:81:LEU:HD22	1.95	0.49
1:G:36:VAL:HG22	1:G:69:VAL:HG13	1.94	0.49
1:M:39:PHE:HB2	1:M:122:ALA:HB1	1.94	0.49
1:N:96:MET:HE2	1:N:98:ILE:HD11	1.95	0.49
1:N:124:ARG:O	1:N:141:ASN:N	2.46	0.49
1:O:128:ILE:HG22	1:O:137:GLN:HB3	1.95	0.49
1:P:5:PRO:HA	1:P:135:LEU:O	2.12	0.49
1:U:55:PHE:HZ	1:U:147:ARG:HB2	1.78	0.49
1:U:119:ASP:OD1	1:U:121:ASN:N	2.34	0.49
1:X:56:SER:OG	1:X:96:MET:HA	2.13	0.49
1:Z:68:GLN:NE2	1:Z:70:ILE:HG23	2.28	0.49
1:Z:77:GLN:O	1:Z:81:LEU:N	2.40	0.49
1:a:162:VAL:HG23	1:a:163:GLU:H	1.78	0.49
1:i:75:ASP:OD1	1:i:79:SER:OG	2.28	0.49
1:F:73:SER:O	1:F:102:ALA:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:ILE:CG1	1:M:137:GLN:HB3	2.43	0.48
1:O:138:ILE:HB	1:P:140:ILE:HB	1.94	0.48
1:V:34:TYR:OH	1:V:159:PHE:O	2.31	0.48
1:W:55:PHE:HB3	1:W:69:VAL:HG11	1.94	0.48
1:W:129:ILE:HG23	1:W:130:ASP:O	2.13	0.48
1:a:128:ILE:HG21	1:a:159:PHE:HE2	1.77	0.48
1:a:142:ASP:C	1:a:144:PRO:HD2	2.38	0.48
1:c:9:ALA:HB2	1:c:135:LEU:HB2	1.95	0.48
1:d:61:GLU:OE1	1:d:65:ARG:NH2	2.46	0.48
1:f:44:PHE:O	1:g:78:TYR:HB3	2.13	0.48
1:m:6:ASN:HB2	1:n:123:PHE:CZ	2.48	0.48
1:n:33:LYS:O	1:n:34:TYR:HB2	2.12	0.48
1:n:49:PRO:HG3	1:n:83:TRP:CZ2	2.48	0.48
1:D:142:ASP:O	1:D:145:VAL:HG12	2.13	0.48
1:F:76:SER:HB3	1:F:104:ARG:NH1	2.27	0.48
1:I:32:GLY:N	1:I:131:PRO:HB3	2.25	0.48
1:P:55:PHE:HE1	1:P:149:VAL:HA	1.78	0.48
1:T:115:PHE:CE1	1:T:120:GLY:HA2	2.48	0.48
1:W:141:ASN:HA	1:X:137:GLN:HG2	1.94	0.48
1:a:96:MET:HE2	1:a:96:MET:HA	1.95	0.48
1:e:38:PHE:HE2	1:e:52:ILE:HG22	1.77	0.48
1:f:5:PRO:C	1:f:7:ARG:H	2.21	0.48
1:f:124:ARG:HB3	1:f:141:ASN:HB2	1.95	0.48
1:k:65:ARG:HG2	1:k:160:GLN:HE22	1.77	0.48
1:k:137:GLN:HE21	1:l:147:ARG:NH2	2.10	0.48
1:F:38:PHE:HB3	1:F:126:LEU:HG	1.94	0.48
1:G:126:LEU:O	1:G:139:THR:HG22	2.13	0.48
1:I:135:LEU:HD23	1:I:135:LEU:H	1.78	0.48
1:K:137:GLN:HB3	1:K:159:PHE:CE2	2.49	0.48
1:L:137:GLN:HB2	1:L:159:PHE:CE2	2.49	0.48
1:M:40:TYR:O	1:M:122:ALA:HB3	2.14	0.48
1:P:15:GLN:NE2	1:P:24:GLU:HG2	2.27	0.48
1:P:136:ARG:O	1:P:137:GLN:HB2	2.13	0.48
1:V:59:VAL:HA	1:V:62:PHE:HD2	1.78	0.48
1:V:71:ALA:O	1:V:72:CYS:HB3	2.13	0.48
1:a:98:ILE:O	1:a:100:LEU:HD22	2.14	0.48
1:h:88:ARG:H	1:h:88:ARG:NE	2.04	0.48
1:n:59:VAL:HG12	1:n:62:PHE:HB2	1.93	0.48
1:I:13:LYS:HG2	1:I:26:CYS:HB2	1.95	0.48
1:N:28:LYS:HD3	1:g:58:GLN:HE22	1.78	0.48
1:V:38:PHE:HB3	1:V:126:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:17:VAL:HG13	1:c:22:PHE:CD2	2.48	0.48
1:d:161:PHE:O	1:d:165:HIS:ND1	2.46	0.48
1:f:34:TYR:CD1	1:f:131:PRO:HD3	2.48	0.48
1:f:106:GLN:O	1:f:110:LYS:HD3	2.14	0.48
1:E:124:ARG:HD2	1:E:142:ASP:O	2.13	0.48
1:G:148:SER:OG	1:H:154:ARG:NH1	2.46	0.48
1:H:32:GLY:C	1:H:131:PRO:HB3	2.39	0.48
1:K:30:TYR:CZ	1:K:70:ILE:HD11	2.49	0.48
1:K:105:LYS:O	1:K:106:GLN:HG2	2.13	0.48
1:L:105:LYS:HZ3	1:L:105:LYS:HB2	1.78	0.48
1:P:132:ASN:HB3	1:h:164:LYS:C	2.38	0.48
1:R:120:GLY:HA3	1:S:105:LYS:HD3	1.95	0.48
1:Y:103:ASP:C	1:Y:105:LYS:H	2.22	0.48
1:b:49:PRO:O	1:b:50:THR:OG1	2.22	0.48
1:c:123:PHE:CD2	1:d:5:PRO:HD2	2.48	0.48
1:f:121:ASN:OD1	1:g:104:ARG:NH2	2.46	0.48
1:h:83:TRP:NE1	1:h:91:GLY:O	2.47	0.48
1:j:75:ASP:HA	1:k:104:ARG:NH1	2.28	0.48
1:k:98:ILE:HG12	1:k:99:PRO:HD2	1.96	0.48
1:m:3:LEU:HG	1:m:4:LEU:H	1.79	0.48
1:n:48:PRO:O	1:n:50:THR:N	2.46	0.48
1:B:4:LEU:HB3	1:B:7:ARG:CG	2.42	0.48
1:B:47:VAL:HG23	1:B:49:PRO:HD3	1.95	0.48
1:G:144:PRO:O	1:H:162:VAL:HG11	2.13	0.48
1:L:13[B]:LYS:HE2	1:L:26:CYS:HB2	1.95	0.48
1:L:56:SER:HB3	1:L:98:ILE:HG12	1.95	0.48
1:P:61:GLU:HG2	1:P:153:LEU:HG	1.96	0.48
1:R:37:LEU:HD13	1:R:112:TYR:CE2	2.48	0.48
1:S:46:PHE:H	1:S:48:PRO:HD3	1.78	0.48
1:W:153:LEU:O	1:W:156:LEU:HG	2.13	0.48
1:Z:76:SER:CB	1:Z:104:ARG:HG2	2.34	0.48
1:c:116:ASP:HB3	1:c:123:PHE:CE2	2.49	0.48
1:g:5:PRO:HD2	1:h:123:PHE:CD2	2.49	0.48
1:h:59:VAL:HG11	1:h:97:LYS:HB2	1.95	0.48
1:h:105:LYS:HG3	1:h:106:GLN:HG2	1.95	0.48
1:l:147:ARG:HG3	1:l:147:ARG:HH11	1.78	0.48
1:m:147:ARG:HG3	1:m:147:ARG:HH11	1.78	0.48
1:m:151:GLU:O	1:m:154:ARG:HG3	2.13	0.48
1:I:126:LEU:HB2	1:I:147:ARG:CZ	2.43	0.48
1:K:9:ALA:HB1	1:K:112:TYR:HE1	1.78	0.48
1:L:129:ILE:HG23	1:L:135:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:35:VAL:HG13	1:U:68:GLN:HB2	1.96	0.48
1:U:60:GLU:O	1:U:63:ASN:ND2	2.46	0.48
1:a:162:VAL:HG23	1:a:163:GLU:HG3	1.95	0.48
1:g:145:VAL:HG21	1:h:159:PHE:CE1	2.48	0.48
1:k:123:PHE:HB3	1:k:140:ILE:HD11	1.96	0.48
1:m:52:ILE:HG23	1:m:53:ILE:H	1.79	0.48
1:B:38:PHE:HB2	1:B:147:ARG:NH1	2.25	0.48
1:G:6:ASN:O	1:G:7:ARG:HB3	2.13	0.48
1:H:3:LEU:H	1:H:3:LEU:HD22	1.78	0.48
1:I:8:PRO:HA	1:I:133:GLY:O	2.14	0.48
1:L:52:ILE:HG23	1:L:147:ARG:HH22	1.78	0.48
1:O:47:VAL:N	1:O:49:PRO:HD2	2.29	0.48
1:R:11:GLU:OE1	1:R:27:LEU:HB3	2.13	0.48
1:T:128:ILE:HD13	1:T:137:GLN:HB3	1.96	0.48
1:W:151:GLU:HG3	1:W:154:ARG:HH21	1.79	0.48
1:X:6:ASN:O	1:X:7:ARG:NH1	2.37	0.48
1:Y:46:PHE:HA	1:Y:48:PRO:CD	2.43	0.48
1:c:148:SER:HB3	1:d:151:GLU:OE1	2.14	0.48
1:d:62:PHE:CE2	1:d:69:VAL:HG21	2.49	0.48
1:h:57:ASP:OD2	1:h:58[B]:GLN:HG3	2.13	0.48
1:h:103:ASP:HB2	1:h:108:ILE:HD12	1.95	0.48
1:i:68:GLN:HG3	1:i:70:ILE:HG22	1.96	0.48
1:i:76:SER:HB2	1:i:79:SER:OG	2.13	0.48
1:j:7:ARG:HG3	1:j:8:PRO:HD2	1.96	0.48
1:j:38:PHE:HB3	1:j:71:ALA:HA	1.94	0.48
1:l:35:VAL:O	1:l:128:ILE:HA	2.13	0.48
1:l:62:PHE:CD2	1:l:69:VAL:HG21	2.48	0.48
1:l:80:HIS:HD2	1:l:101:LEU:O	1.97	0.48
1:n:11:GLU:OE2	1:n:28:LYS:N	2.47	0.48
1:I:87:ASP:HB2	1:I:89:LYS:NZ	2.29	0.48
1:J:116:ASP:C	1:J:116:ASP:OD1	2.56	0.48
1:M:29:ASP:HB3	1:d:23:LYS:NZ	2.28	0.48
1:Q:158:ALA:HA	1:Q:161:PHE:HB2	1.95	0.48
1:S:148:SER:OG	1:S:150:ASP:OD2	2.31	0.48
1:U:40:TYR:HA	1:U:147:ARG:HH21	1.79	0.48
1:W:48:PRO:O	1:W:50:THR:N	2.41	0.48
1:W:106:GLN:HB3	1:W:110:LYS:HG2	1.96	0.48
1:b:125:GLY:HA3	1:b:140:ILE:HG23	1.95	0.48
1:c:4:LEU:HA	1:c:5:PRO:HD3	1.64	0.48
1:g:75:ASP:OD1	1:g:80:HIS:HE1	1.97	0.48
1:h:52:ILE:H	1:h:52:ILE:HD13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:39:PHE:H	1:k:125:GLY:CA	2.27	0.48
1:k:138:ILE:O	1:l:140:ILE:N	2.31	0.48
1:n:5:PRO:HG3	1:n:138:ILE:HG12	1.96	0.48
1:n:160:GLN:HA	1:n:164:LYS:NZ	2.28	0.48
1:G:36:VAL:O	1:G:69:VAL:HA	2.13	0.48
1:H:78:TYR:CG	1:I:45:THR:HG22	2.48	0.48
1:K:36:VAL:HG13	1:K:69:VAL:HA	1.94	0.48
1:L:38:PHE:HD1	1:L:38:PHE:H	1.60	0.48
1:Z:38:PHE:O	1:Z:71:ALA:HA	2.14	0.48
1:c:139:THR:HA	1:d:139:THR:HA	1.95	0.48
1:f:20:GLY:O	1:f:81:LEU:HD21	2.14	0.48
1:m:143:LYS:HB2	1:m:143:LYS:HZ3	1.77	0.48
1:n:108:ILE:HG23	1:n:112:TYR:HE2	1.79	0.48
1:A:38:PHE:HA	1:A:126:LEU:N	2.21	0.47
1:D:65:ARG:NH1	1:D:157:ASP:CG	2.72	0.47
1:E:107:GLU:HG3	1:E:108:ILE:HG13	1.97	0.47
1:F:8:PRO:HA	1:F:134:ILE:HA	1.95	0.47
1:H:68:GLN:HG3	1:H:70:ILE:H	1.79	0.47
1:I:16:ALA:HB2	1:I:25:ILE:HG12	1.96	0.47
1:L:84:ASP:OD1	1:L:94:GLY:O	2.32	0.47
1:N:158:ALA:HA	1:N:161:PHE:HD2	1.78	0.47
1:P:38:PHE:HB2	1:P:125:GLY:O	2.14	0.47
1:P:53:ILE:C	1:P:55:PHE:H	2.21	0.47
1:Q:12:PHE:HB2	1:Q:108:ILE:HG23	1.96	0.47
1:S:87:ASP:OD2	1:S:89:LYS:HG2	2.14	0.47
1:T:11:GLU:HG3	1:T:12:PHE:N	2.28	0.47
1:V:72:CYS:HB2	1:V:102:ALA:N	2.29	0.47
1:Y:10:PRO:HD2	1:Y:112:TYR:HE1	1.78	0.47
1:Y:16:ALA:N	1:Y:23:LYS:O	2.45	0.47
1:b:3:LEU:HD11	1:b:10:PRO:HD3	1.96	0.47
1:c:150:ASP:HA	1:c:153:LEU:HD22	1.96	0.47
1:e:154:ARG:HG2	1:e:154:ARG:HH11	1.79	0.47
1:h:73:SER:O	1:h:74:THR:OG1	2.27	0.47
1:h:86:LEU:HB2	1:h:92:GLY:HA3	1.96	0.47
1:m:36:VAL:HG13	1:m:69:VAL:HA	1.96	0.47
1:m:72:CYS:HB2	1:m:101:LEU:HB3	1.95	0.47
1:n:114:VAL:HG23	1:n:123:PHE:HD2	1.79	0.47
1:G:31:ARG:H	1:G:31:ARG:HG2	1.41	0.47
1:H:18:ILE:HG12	1:H:99:PRO:HB3	1.95	0.47
1:H:39:PHE:O	1:H:147:ARG:NH2	2.47	0.47
1:K:121:ASN:OD1	1:T:104:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:67:CYS:SG	1:P:68:GLN:N	2.87	0.47
1:Q:14:GLY:HA3	1:Q:101:LEU:HG	1.96	0.47
1:V:6:ASN:O	1:V:6:ASN:ND2	2.45	0.47
1:Z:128:ILE:HB	1:Z:137:GLN:HB3	1.96	0.47
1:c:47:VAL:HG13	1:c:48:PRO:HD2	1.96	0.47
1:g:103:ASP:OD1	1:g:108:ILE:HG23	2.13	0.47
1:h:55:PHE:CZ	1:h:62:PHE:HE2	2.32	0.47
1:k:18:ILE:HD11	1:k:25:ILE:HG13	1.95	0.47
1:G:109:SER:OG	1:G:115:PHE:HB2	2.15	0.47
1:H:38:PHE:HB2	1:H:147:ARG:HH21	1.79	0.47
1:I:45:THR:OG1	1:I:46:PHE:N	2.45	0.47
1:K:6:ASN:O	1:K:7:ARG:NH1	2.48	0.47
1:K:80:HIS:CE1	1:K:102:ALA:HB2	2.49	0.47
1:L:46:PHE:C	1:L:48:PRO:HD3	2.40	0.47
1:L:135:LEU:HD13	1:L:138:ILE:HD11	1.96	0.47
1:W:136:ARG:HA	1:W:136:ARG:HE	1.78	0.47
1:c:156:LEU:O	1:c:160:GLN:HG2	2.14	0.47
1:d:12:PHE:HD2	1:d:108:ILE:HG13	1.79	0.47
1:j:56:SER:OG	1:j:96:MET:HA	2.14	0.47
1:j:110:LYS:HB3	1:j:115:PHE:CG	2.49	0.47
1:D:97:LYS:H	1:D:97:LYS:HG2	1.46	0.47
1:D:140:ILE:O	1:D:141:ASN:ND2	2.47	0.47
1:E:121:ASN:HB2	1:E:143:LYS:NZ	2.29	0.47
1:F:110:LYS:HB3	1:F:110:LYS:NZ	2.28	0.47
1:H:53:ILE:HB	1:H:93:LEU:HD23	1.95	0.47
1:P:98:ILE:HG13	1:P:99:PRO:HD2	1.97	0.47
1:R:35:VAL:O	1:R:128:ILE:HA	2.14	0.47
1:R:60:GLU:O	1:R:64:SER:HB3	2.15	0.47
1:S:4:LEU:O	1:S:135:LEU:HD13	2.14	0.47
1:W:45:THR:HB	1:W:46:PHE:O	2.15	0.47
1:Z:40:TYR:HB2	1:Z:71:ALA:HB1	1.95	0.47
1:c:34:TYR:CZ	1:c:131:PRO:HD3	2.49	0.47
1:c:124:ARG:HD2	1:c:143:LYS:O	2.14	0.47
1:d:32:GLY:H	1:d:132:ASN:H	1.62	0.47
1:e:124:ARG:NH1	1:e:145:VAL:O	2.47	0.47
1:h:135:LEU:HD21	1:h:138:ILE:HD11	1.97	0.47
1:m:114:VAL:HG12	1:m:123:PHE:HB2	1.95	0.47
1:D:27:LEU:HD22	1:D:31[B]:ARG:HH11	1.77	0.47
1:E:53:ILE:HD11	1:E:93:LEU:HA	1.96	0.47
1:G:4:LEU:O	1:G:7:ARG:NE	2.47	0.47
1:O:151:GLU:CD	1:O:154:ARG:HH11	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:152:THR:HA	1:Q:155:LEU:HD12	1.96	0.47
1:W:135:LEU:HD23	1:W:138:ILE:CD1	2.45	0.47
1:X:6:ASN:C	1:X:7:ARG:HH11	2.22	0.47
1:Y:14:GLY:C	1:Y:25:ILE:HG22	2.39	0.47
1:Y:44:PHE:O	1:Y:46:PHE:HD1	1.97	0.47
1:b:70:ILE:HB	1:b:101:LEU:HD23	1.95	0.47
1:d:51:GLU:CG	1:d:146:GLY:HA3	2.43	0.47
1:i:159:PHE:HE1	1:j:145:VAL:H	1.61	0.47
1:m:53:ILE:HG12	1:m:54:ALA:N	2.28	0.47
1:n:43:ASP:OD1	1:n:80:HIS:HD2	1.97	0.47
1:K:38:PHE:HE1	1:K:69:VAL:HB	1.79	0.47
1:K:78:TYR:HB3	1:T:44:PHE:O	2.15	0.47
1:M:35:VAL:HG12	1:M:68:GLN:HB2	1.95	0.47
1:O:145:VAL:HG21	1:P:159:PHE:CE1	2.48	0.47
1:P:119:ASP:CG	1:P:121:ASN:HD22	2.23	0.47
1:Q:88:ARG:HA	1:Q:92:GLY:O	2.14	0.47
1:U:5:PRO:HD2	1:V:123:PHE:CD2	2.49	0.47
1:U:17:VAL:O	1:U:100:LEU:HB2	2.14	0.47
1:W:34:TYR:CD1	1:W:131:PRO:HD3	2.50	0.47
1:X:9:ALA:HA	1:X:10:PRO:HD3	1.59	0.47
1:Z:38:PHE:HB2	1:Z:125:GLY:O	2.15	0.47
1:a:12:PHE:CE2	1:a:27:LEU:HD12	2.49	0.47
1:c:59:VAL:O	1:c:63:ASN:ND2	2.48	0.47
1:h:44:PHE:CD1	1:i:79:SER:HA	2.50	0.47
1:i:130:ASP:HB3	1:i:134:ILE:O	2.15	0.47
1:k:30:TYR:CD2	1:k:70:ILE:HD11	2.44	0.47
1:B:51:GLU:OE1	1:B:124:ARG:NH2	2.47	0.47
1:C:116:ASP:OD2	1:C:119:ASP:OD2	2.33	0.47
1:C:125:GLY:HA2	1:C:140:ILE:HA	1.97	0.47
1:E:62:PHE:CZ	1:E:149:VAL:HG23	2.49	0.47
1:E:123:PHE:O	1:E:124:ARG:HG3	2.15	0.47
1:H:34:TYR:CD1	1:H:131:PRO:HD3	2.49	0.47
1:H:48:PRO:CG	1:H:49:PRO:HD3	2.39	0.47
1:N:16:ALA:HB2	1:N:101:LEU:CD1	2.45	0.47
1:N:50:THR:O	1:N:52:ILE:N	2.47	0.47
1:P:109:SER:O	1:P:114:VAL:HG23	2.15	0.47
1:Q:18:ILE:HB	1:Q:99:PRO:HG3	1.96	0.47
1:S:154:ARG:HH22	1:T:146:GLY:C	2.22	0.47
1:T:34:TYR:H	1:T:67:CYS:HA	1.79	0.47
1:U:52:ILE:HD13	1:U:93:LEU:HD22	1.96	0.47
1:U:105:LYS:NZ	1:U:107:GLU:HG3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:71:ALA:HB3	1:V:100:LEU:CB	2.45	0.47
1:X:65:ARG:NH1	1:X:157:ASP:OD1	2.48	0.47
1:X:125:GLY:HA2	1:X:140:ILE:HA	1.96	0.47
1:Y:136:ARG:HA	1:Y:136:ARG:CZ	2.45	0.47
1:Z:32:GLY:N	1:Z:131:PRO:O	2.40	0.47
1:Z:36:VAL:HB	1:Z:69:VAL:HA	1.97	0.47
1:Z:44:PHE:O	1:a:78:TYR:HB2	2.15	0.47
1:a:93:LEU:O	1:a:96:MET:HE3	2.15	0.47
1:a:114:VAL:HB	1:a:123:PHE:HB2	1.96	0.47
1:c:7:ARG:NH2	1:d:116:ASP:HB2	2.30	0.47
1:d:0:THR:HB	1:d:1:MET:H	1.40	0.47
1:d:125:GLY:HA3	1:d:140:ILE:HA	1.96	0.47
1:e:36:VAL:HG22	1:e:69:VAL:HA	1.95	0.47
1:h:34:TYR:HA	1:h:131:PRO:HB3	1.96	0.47
1:h:112:TYR:CE2	1:h:127:PHE:HD2	2.33	0.47
1:i:3:LEU:HB2	1:j:2:VAL:HB	1.97	0.47
1:i:128:ILE:HD13	1:i:137:GLN:HB3	1.97	0.47
1:j:76:SER:HA	1:j:104:ARG:HG2	1.95	0.47
1:j:77:GLN:H	1:j:77:GLN:HG2	1.37	0.47
1:j:88:ARG:HD2	1:j:94:GLY:HA3	1.96	0.47
1:j:116:ASP:HB3	1:j:119:ASP:CB	2.44	0.47
1:j:128:ILE:HB	1:j:137:GLN:HB3	1.96	0.47
1:l:17:VAL:HG11	1:l:81:LEU:HD13	1.96	0.47
1:B:75:ASP:HA	1:C:104:ARG:NH2	2.29	0.47
1:C:58:GLN:HE21	1:C:149:VAL:HG21	1.80	0.47
1:E:114:VAL:HA	1:F:4:LEU:HD11	1.95	0.47
1:I:73:SER:OG	1:I:80:HIS:NE2	2.44	0.47
1:J:41:PRO:HB3	1:J:143:LYS:HZ3	1.79	0.47
1:M:55:PHE:HE2	1:M:69:VAL:HG21	1.80	0.47
1:N:16:ALA:HB2	1:N:101:LEU:HD12	1.97	0.47
1:N:86:LEU:HB3	1:N:91:GLY:HA3	1.96	0.47
1:Q:129:ILE:HD12	1:Q:130:ASP:N	2.30	0.47
1:S:138:ILE:HB	1:T:140:ILE:CG2	2.45	0.47
1:U:40:TYR:HA	1:U:147:ARG:NH2	2.30	0.47
1:d:163:GLU:HB2	1:d:164:LYS:NZ	2.30	0.47
1:f:78:TYR:HB3	1:g:44:PHE:O	2.14	0.47
1:h:68:GLN:O	1:h:69:VAL:HG12	2.15	0.47
1:i:28:LYS:HA	1:i:31:ARG:HH12	1.80	0.47
1:j:45:THR:HG23	1:k:78:TYR:CD1	2.49	0.47
1:m:16:ALA:HB3	1:m:23:LYS:O	2.14	0.47
1:A:31:ARG:HH11	1:A:31:ARG:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:TYR:CE1	1:H:131:PRO:HD3	2.50	0.47
1:M:11:GLU:HA	1:M:27:LEU:HD13	1.96	0.47
1:N:149:VAL:O	1:N:153:LEU:HB2	2.14	0.47
1:P:38:PHE:HE1	1:P:69:VAL:HG22	1.80	0.47
1:U:77:GLN:HA	1:U:102:ALA:HB2	1.96	0.47
1:V:25:ILE:HG12	1:V:101:LEU:HD11	1.97	0.47
1:V:38:PHE:HB2	1:V:147:ARG:HH21	1.80	0.47
1:V:126:LEU:HG	1:V:147:ARG:HG2	1.95	0.47
1:g:24:GLU:O	1:g:25:ILE:HG23	2.14	0.47
1:h:88:ARG:HG2	1:h:89:LYS:N	2.29	0.47
1:l:52:ILE:HD12	1:l:96:MET:HE1	1.97	0.47
1:n:36:VAL:HG22	1:n:128:ILE:HD13	1.97	0.47
1:B:132:ASN:ND2	1:g:164:LYS:HB2	2.29	0.47
1:C:138:ILE:HD12	1:D:140:ILE:HD12	1.96	0.47
1:D:161:PHE:C	1:D:164:LYS:HZ2	2.23	0.47
1:L:39:PHE:O	1:L:147:ARG:NH2	2.35	0.47
1:L:143:LYS:HZ2	1:L:143:LYS:CB	2.28	0.47
1:L:151:GLU:HA	1:L:154:ARG:HB3	1.97	0.47
1:L:159:PHE:HA	1:L:162:VAL:HG12	1.96	0.47
1:Q:4:LEU:O	1:Q:135:LEU:HD23	2.14	0.47
1:T:39:PHE:N	1:T:147:ARG:HH22	2.13	0.47
1:Z:104:ARG:CZ	1:a:74:THR:HB	2.45	0.47
1:a:38:PHE:CE1	1:a:40:TYR:HB3	2.50	0.47
1:i:159:PHE:CD1	1:j:144:PRO:HG2	2.49	0.47
1:B:16:ALA:HB2	1:B:101:LEU:HD23	1.97	0.46
1:C:5:PRO:HB2	1:D:142:ASP:HB3	1.96	0.46
1:D:78:TYR:HB3	1:E:44:PHE:HB2	1.97	0.46
1:E:28:LYS:HD3	1:E:31:ARG:HH12	1.79	0.46
1:E:62:PHE:HZ	1:E:149:VAL:HG23	1.81	0.46
1:E:123:PHE:HZ	1:F:7:ARG:NH1	2.13	0.46
1:K:69:VAL:HG23	1:K:99:PRO:HD2	1.97	0.46
1:L:2:VAL:HG22	1:L:3:LEU:N	2.29	0.46
1:P:74:THR:HG22	1:P:103:ASP:OD2	2.14	0.46
1:P:129:ILE:HG12	1:P:130:ASP:H	1.79	0.46
1:Q:128:ILE:O	1:Q:137:GLN:HB3	2.14	0.46
1:U:34:TYR:CE1	1:U:131:PRO:HD3	2.50	0.46
1:X:149:VAL:O	1:X:152:THR:HG23	2.14	0.46
1:X:161:PHE:HD2	1:X:165:HIS:HB2	1.81	0.46
1:Y:43:ASP:O	1:Y:83:TRP:CD2	2.67	0.46
1:a:118[B]:GLU:OE2	1:b:7:ARG:NH1	2.45	0.46
1:a:140:ILE:HD11	1:b:138:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:105:LYS:H	1:e:105:LYS:HG2	1.55	0.46
1:f:163:GLU:H	1:f:163:GLU:HG3	1.57	0.46
1:g:24:GLU:C	1:g:25:ILE:HG13	2.40	0.46
1:i:13:LYS:HG2	1:i:14:GLY:H	1.79	0.46
1:j:30:TYR:O	1:j:33:LYS:HG3	2.15	0.46
1:j:45:THR:HG22	1:j:46:PHE:HB2	1.97	0.46
1:C:32:GLY:HA2	1:C:131:PRO:HB3	1.97	0.46
1:C:106:GLN:C	1:C:108:ILE:H	2.22	0.46
1:E:115:PHE:CG	1:E:116:ASP:N	2.83	0.46
1:F:67:CYS:SG	1:F:68:GLN:N	2.88	0.46
1:L:124:ARG:NH1	1:L:145:VAL:O	2.49	0.46
1:M:43:ASP:HB2	1:M:75:ASP:OD1	2.16	0.46
1:Q:61:GLU:O	1:Q:64:SER:N	2.43	0.46
1:U:103:ASP:OD2	1:U:106:GLN:HA	2.16	0.46
1:V:118:GLU:OE1	1:V:118:GLU:N	2.45	0.46
1:W:16:ALA:HB2	1:W:25:ILE:HD11	1.97	0.46
1:Z:103:ASP:HB3	1:Z:108:ILE:HG12	1.97	0.46
1:a:76:SER:O	1:a:80:HIS:ND1	2.47	0.46
1:a:128:ILE:HG21	1:a:159:PHE:CE2	2.49	0.46
1:b:36:VAL:HG13	1:b:69:VAL:HA	1.97	0.46
1:C:41:PRO:HG3	1:C:143:LYS:HZ2	1.80	0.46
1:C:87:ASP:O	1:C:92:GLY:N	2.44	0.46
1:F:78:TYR:CD1	1:F:81:LEU:HD21	2.50	0.46
1:G:70:ILE:HG21	1:G:101:LEU:HD23	1.97	0.46
1:H:45:THR:O	1:H:48:PRO:HD2	2.16	0.46
1:H:137:GLN:HB2	1:H:159:PHE:CE2	2.49	0.46
1:I:87:ASP:HB2	1:I:89:LYS:HZ2	1.79	0.46
1:M:18:ILE:HG21	1:M:23:LYS:HD2	1.97	0.46
1:O:88:ARG:NH1	1:O:95:HIS:H	2.14	0.46
1:S:93:LEU:HB2	1:S:96:MET:HE1	1.97	0.46
1:U:36:VAL:HB	1:U:69:VAL:HG22	1.97	0.46
1:W:140:ILE:HB	1:X:138:ILE:CG1	2.43	0.46
1:X:20:GLY:HA2	1:X:81:LEU:HD21	1.96	0.46
1:Z:81:LEU:HG	1:Z:85:ASN:OD1	2.16	0.46
1:Z:104:ARG:HG3	1:a:121:ASN:OD1	2.14	0.46
1:h:98:ILE:HA	1:h:99:PRO:HD3	1.81	0.46
1:i:36:VAL:HG23	1:i:128:ILE:HG13	1.97	0.46
1:A:52:ILE:HA	1:A:55:PHE:HD2	1.80	0.46
1:A:159:PHE:CE1	1:B:145:VAL:HG21	2.49	0.46
1:E:106:GLN:O	1:E:110:LYS:HG2	2.15	0.46
1:J:74:THR:HG21	1:J:121:ASN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:103:ASP:CG	1:J:108:ILE:HG12	2.41	0.46
1:J:125:GLY:HA3	1:J:140:ILE:HA	1.97	0.46
1:J:142:ASP:OD1	1:J:144:PRO:HD2	2.15	0.46
1:U:33:LYS:HZ3	1:U:68:GLN:CG	2.05	0.46
1:U:154:ARG:NE	1:V:148:SER:OG	2.39	0.46
1:V:65:ARG:HH12	1:V:153:LEU:HG	1.81	0.46
1:W:116:ASP:OD1	1:X:7:ARG:NH2	2.48	0.46
1:a:52:ILE:HG23	1:a:53:ILE:HG13	1.98	0.46
1:b:65:ARG:H	1:b:65:ARG:HG2	1.55	0.46
1:b:97:LYS:HE2	1:b:97:LYS:HB3	1.79	0.46
1:c:124:ARG:HD3	1:c:146:GLY:HA2	1.96	0.46
1:d:51:GLU:HB3	1:d:147:ARG:NH1	2.30	0.46
1:m:70:ILE:HD13	1:m:99:PRO:HB2	1.98	0.46
1:A:31:ARG:O	1:A:33:LYS:N	2.49	0.46
1:C:50:THR:HG23	1:C:52:ILE:HG13	1.96	0.46
1:D:22:PHE:CZ	1:D:81:LEU:HG	2.50	0.46
1:D:43:ASP:OD1	1:D:80:HIS:CD2	2.69	0.46
1:E:5:PRO:HB3	1:E:136:ARG:O	2.16	0.46
1:F:126:LEU:HB2	1:F:147:ARG:HD2	1.96	0.46
1:G:96:MET:HE2	1:G:98:ILE:HB	1.98	0.46
1:H:74:THR:HA	1:H:103:ASP:OD1	2.16	0.46
1:I:48:PRO:HG2	1:I:49:PRO:HD2	1.96	0.46
1:K:51:GLU:HG3	1:K:52:ILE:H	1.80	0.46
1:L:112:TYR:HB3	1:L:127:PHE:HE2	1.81	0.46
1:Q:39:PHE:CZ	1:Q:114:VAL:HG21	2.50	0.46
1:R:101:LEU:HD23	1:R:102:ALA:N	2.31	0.46
1:S:11:GLU:HG3	1:S:27:LEU:HD22	1.96	0.46
1:U:65:ARG:NH1	1:U:157:ASP:OD1	2.49	0.46
1:W:28:LYS:HZ3	1:W:28:LYS:CB	2.27	0.46
1:X:73:SER:HB3	1:X:80:HIS:NE2	2.29	0.46
1:Y:52:ILE:HB	1:Y:93:LEU:HD11	1.97	0.46
1:Y:71:ALA:O	1:Y:100:LEU:HA	2.15	0.46
1:b:124:ARG:NH1	1:b:147:ARG:NH2	2.64	0.46
1:d:75:ASP:O	1:d:102:ALA:HB1	2.15	0.46
1:i:100:LEU:HD13	1:i:100:LEU:H	1.81	0.46
1:l:15:GLN:HB3	1:l:102:ALA:HB3	1.98	0.46
1:m:30:TYR:CZ	1:m:70:ILE:HD11	2.51	0.46
1:n:53:ILE:HG12	1:n:54:ALA:H	1.80	0.46
1:C:53:ILE:H	1:C:53:ILE:HD13	1.80	0.46
1:H:15:GLN:HG3	1:H:22:PHE:HB3	1.96	0.46
1:I:65:ARG:O	1:I:66:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:LYS:HB3	1:I:110:LYS:NZ	2.30	0.46
1:J:36:VAL:N	1:J:68:GLN:O	2.28	0.46
1:L:39:PHE:CE1	1:L:114:VAL:HG21	2.50	0.46
1:N:37:LEU:HD22	1:N:70:ILE:HB	1.97	0.46
1:N:104:ARG:HH22	1:O:42:ALA:HA	1.80	0.46
1:O:124:ARG:HB3	1:O:141:ASN:HB3	1.97	0.46
1:P:145:VAL:HG22	1:P:146:GLY:N	2.31	0.46
1:S:108:ILE:HA	1:S:111:ALA:HB3	1.98	0.46
1:a:148:SER:OG	1:b:155:LEU:HD11	2.16	0.46
1:b:124:ARG:HH12	1:b:147:ARG:NH2	2.13	0.46
1:c:36:VAL:HG13	1:c:68:GLN:O	2.15	0.46
1:c:87:ASP:HA	1:c:93:LEU:O	2.15	0.46
1:e:136:ARG:O	1:e:137:GLN:HB2	2.14	0.46
1:g:5:PRO:C	1:g:7:ARG:H	2.24	0.46
1:k:128:ILE:HG22	1:k:136:ARG:HB2	1.97	0.46
1:l:50:THR:C	1:l:52:ILE:H	2.24	0.46
1:l:163:GLU:H	1:l:163:GLU:HG3	1.67	0.46
1:A:40:TYR:CZ	1:A:73:SER:HB2	2.50	0.46
1:B:11:GLU:HA	1:B:27:LEU:HD21	1.98	0.46
1:B:120:GLY:HA3	1:C:104:ARG:O	2.16	0.46
1:C:11:GLU:OE2	1:C:27:LEU:HD22	2.16	0.46
1:F:5:PRO:C	1:F:7:ARG:H	2.24	0.46
1:H:44:PHE:HA	1:H:83:TRP:NE1	2.31	0.46
1:K:128:ILE:O	1:K:135:LEU:HD12	2.15	0.46
1:O:11:GLU:OE1	1:O:28:LYS:HB2	2.14	0.46
1:P:74:THR:HG22	1:P:103:ASP:HB3	1.98	0.46
1:P:119:ASP:HB3	1:P:121:ASN:H	1.81	0.46
1:P:145:VAL:HG22	1:P:146:GLY:H	1.81	0.46
1:Q:63:ASN:HD21	1:Q:98:ILE:HG22	1.81	0.46
1:R:38:PHE:CE2	1:R:52:ILE:HD12	2.51	0.46
1:S:41:PRO:HD3	1:S:124:ARG:NH1	2.30	0.46
1:Y:50:THR:H	1:Y:53:ILE:CG2	2.24	0.46
1:a:147:ARG:NH1	1:a:147:ARG:HG3	2.31	0.46
1:c:22:PHE:CZ	1:c:81:LEU:HD22	2.51	0.46
1:d:22:PHE:CE2	1:d:77:GLN:HB2	2.49	0.46
1:f:69:VAL:O	1:f:98:ILE:HG23	2.15	0.46
1:h:41:PRO:HD3	1:h:124:ARG:HD2	1.98	0.46
1:i:130:ASP:HB2	1:i:136:ARG:HH11	1.80	0.46
1:l:61:GLU:HB3	1:l:153:LEU:HD21	1.97	0.46
1:A:73:SER:HB3	1:A:80:HIS:HE1	1.81	0.46
1:C:97:LYS:HB3	1:C:97:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ASP:HB3	1:D:136:ARG:HD2	1.98	0.46
1:F:28:LYS:HG2	1:F:31:ARG:NH2	2.27	0.46
1:I:136:ARG:HH22	1:J:144:PRO:CG	2.25	0.46
1:L:41:PRO:HD3	1:L:124:ARG:HB2	1.96	0.46
1:M:110:LYS:HD3	1:M:115:PHE:CD1	2.50	0.46
1:O:71:ALA:O	1:O:101:LEU:N	2.35	0.46
1:R:83:TRP:CZ3	1:R:93:LEU:HD13	2.51	0.46
1:T:116:ASP:HB3	1:T:123:PHE:CE2	2.50	0.46
1:T:154:ARG:NH1	1:T:158:ALA:HB2	2.30	0.46
1:Z:42:ALA:HB1	1:a:78:TYR:CE1	2.50	0.46
1:b:127:PHE:HE1	1:b:140:ILE:HG12	1.81	0.46
1:c:51:GLU:OE2	1:c:146:GLY:HA3	2.16	0.46
1:c:85:ASN:HA	1:c:95:HIS:CE1	2.51	0.46
1:d:84:ASP:O	1:d:94:GLY:N	2.42	0.46
1:h:74:THR:HG22	1:h:103:ASP:HB3	1.98	0.46
1:h:79:SER:OG	1:i:75:ASP:OD1	2.32	0.46
1:j:45:THR:CG2	1:j:46:PHE:HB2	2.46	0.46
1:B:12:PHE:CE1	1:B:27:LEU:HB3	2.51	0.46
1:C:114:VAL:HG12	1:C:123:PHE:H	1.81	0.46
1:C:140:ILE:HB	1:D:138:ILE:HB	1.97	0.46
1:M:112:TYR:HB3	1:M:127:PHE:CZ	2.51	0.46
1:N:82:ALA:HB2	1:O:44:PHE:CG	2.51	0.46
1:O:60:GLU:HA	1:O:63:ASN:OD1	2.15	0.46
1:Q:51:GLU:O	1:Q:52:ILE:HG22	2.16	0.46
1:Q:93:LEU:HD11	1:Q:96:MET:HG2	1.98	0.46
1:U:154:ARG:HE	1:V:148:SER:HG	1.62	0.46
1:V:3:LEU:HD21	1:V:10:PRO:HG2	1.98	0.46
1:W:74:THR:HG21	1:W:121:ASN:HA	1.98	0.46
1:Y:53:ILE:HD11	1:Y:88:ARG:NH2	2.25	0.46
1:Y:53:ILE:HA	1:Y:56:SER:HB3	1.98	0.46
1:Y:89:LYS:HB3	1:Y:89:LYS:HZ3	1.81	0.46
1:a:123:PHE:CE2	1:b:5:PRO:HD2	2.50	0.46
1:e:56:SER:OG	1:e:96:MET:HG3	2.15	0.46
1:f:127:PHE:CD1	1:f:138:ILE:HD13	2.51	0.46
1:h:38:PHE:HD2	1:h:147:ARG:NH1	2.12	0.46
1:h:148:SER:O	1:h:152:THR:OG1	2.33	0.46
1:k:86:LEU:CB	1:k:92:GLY:HA3	2.45	0.46
1:B:53:ILE:HD13	1:B:53:ILE:HA	1.86	0.46
1:E:36:VAL:HA	1:E:127:PHE:O	2.16	0.46
1:E:148:SER:H	1:F:154:ARG:NH2	2.14	0.46
1:K:70:ILE:HA	1:K:99:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:ARG:NH2	1:M:75:ASP:OD1	2.49	0.46
1:O:35:VAL:O	1:O:128:ILE:HD12	2.16	0.46
1:R:110:LYS:HG3	1:R:115:PHE:CD2	2.51	0.46
1:R:149:VAL:O	1:R:152:THR:OG1	2.28	0.46
1:S:70:ILE:HG23	1:S:99:PRO:HB2	1.97	0.46
1:X:127:PHE:CD1	1:X:138:ILE:HG22	2.51	0.46
1:c:145:VAL:HG11	1:d:159:PHE:CE1	2.51	0.46
1:d:15:GLN:NE2	1:d:24:GLU:OE1	2.49	0.46
1:e:110:LYS:HB2	1:e:110:LYS:HZ3	1.81	0.46
1:f:157:ASP:O	1:f:161:PHE:HB3	2.16	0.46
1:l:14:GLY:O	1:l:24:GLU:HA	2.16	0.46
1:E:140:ILE:HD12	1:F:5:PRO:HG2	1.97	0.45
1:I:65:ARG:NH1	1:I:153:LEU:HD21	2.27	0.45
1:I:113:GLY:O	1:J:4:LEU:HD21	2.16	0.45
1:J:49:PRO:HA	1:J:50:THR:HA	1.42	0.45
1:K:32:GLY:C	1:K:131:PRO:HB3	2.41	0.45
1:K:51:GLU:OE1	1:K:146:GLY:HA3	2.16	0.45
1:O:106:GLN:O	1:O:110:LYS:HG2	2.16	0.45
1:S:121:ASN:HB2	1:S:143:LYS:NZ	2.30	0.45
1:T:63:ASN:HA	1:T:66:ASN:O	2.16	0.45
1:U:50:THR:OG1	1:U:51:GLU:N	2.48	0.45
1:V:44:PHE:H	1:V:83:TRP:NE1	2.14	0.45
1:V:75:ASP:OD1	1:W:104:ARG:NH1	2.40	0.45
1:Y:163:GLU:HG3	1:Y:164:LYS:N	2.28	0.45
1:c:5:PRO:HD2	1:d:123:PHE:CE2	2.51	0.45
1:g:159:PHE:O	1:g:163:GLU:HG3	2.17	0.45
1:i:34:TYR:CZ	1:i:131:PRO:HD3	2.51	0.45
1:A:149:VAL:O	1:A:152:THR:OG1	2.30	0.45
1:D:37:LEU:HB3	1:D:127:PHE:CD1	2.51	0.45
1:D:66:ASN:HB3	1:D:67:CYS:H	1.29	0.45
1:G:144:PRO:O	1:H:162:VAL:HG21	2.17	0.45
1:I:138:ILE:HB	1:J:140:ILE:HG22	1.97	0.45
1:J:51:GLU:C	1:J:53:ILE:N	2.75	0.45
1:K:105:LYS:HD2	1:K:107:GLU:OE1	2.16	0.45
1:O:40:TYR:HH	1:O:80:HIS:CD2	2.33	0.45
1:P:32:GLY:N	1:P:131:PRO:O	2.50	0.45
1:S:12:PHE:CE2	1:S:27:LEU:HD12	2.52	0.45
1:S:15:GLN:O	1:S:101:LEU:HB2	2.16	0.45
1:V:67:CYS:SG	1:V:68:GLN:N	2.89	0.45
1:X:148:SER:O	1:X:152:THR:HG22	2.17	0.45
1:Y:38:PHE:CZ	1:Y:52:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:25:ILE:HG13	1:Z:26:CYS:H	1.82	0.45
1:Z:48:PRO:HA	1:Z:49:PRO:HD3	1.80	0.45
1:a:136:ARG:NE	1:a:136:ARG:HA	2.31	0.45
1:a:151:GLU:OE2	1:a:154:ARG:NH1	2.49	0.45
1:i:84:ASP:OD2	1:i:100:LEU:HD11	2.16	0.45
1:j:143:LYS:HB2	1:j:143:LYS:HE2	1.83	0.45
1:m:144:PRO:HG2	1:n:162:VAL:HG21	1.98	0.45
1:A:105:LYS:O	1:A:106:GLN:HG2	2.16	0.45
1:B:42:ALA:HB2	1:B:121:ASN:ND2	2.31	0.45
1:C:164:LYS:HZ3	1:C:165:HIS:HB2	1.80	0.45
1:D:37:LEU:HG	1:D:70:ILE:CG2	2.46	0.45
1:E:119:ASP:O	1:E:121:ASN:ND2	2.49	0.45
1:E:138:ILE:HB	1:F:140:ILE:CG1	2.46	0.45
1:G:47:VAL:N	1:G:48:PRO:HD3	2.31	0.45
1:I:33:LYS:HB2	1:I:33:LYS:NZ	2.32	0.45
1:K:73:SER:O	1:K:102:ALA:HA	2.16	0.45
1:M:1:MET:HG2	1:M:2:VAL:N	2.32	0.45
1:M:9:ALA:HA	1:M:10:PRO:HD3	1.83	0.45
1:Q:70:ILE:HB	1:Q:101:LEU:HD13	1.99	0.45
1:T:128:ILE:O	1:T:135:LEU:HD12	2.16	0.45
1:X:19:ASN:HD21	1:X:97:LYS:HG2	1.82	0.45
1:d:18:ILE:HB	1:d:23:LYS:NZ	2.31	0.45
1:h:112:TYR:CE2	1:h:127:PHE:HB2	2.51	0.45
1:i:4:LEU:HD11	1:j:116:ASP:HB2	1.98	0.45
1:l:78:TYR:H	1:l:81:LEU:HB3	1.82	0.45
1:B:55:PHE:CZ	1:B:149:VAL:HG12	2.51	0.45
1:D:96:MET:HG2	1:D:98:ILE:HG12	1.98	0.45
1:G:4:LEU:HD13	1:H:123:PHE:HE1	1.80	0.45
1:J:51:GLU:O	1:J:53:ILE:N	2.49	0.45
1:K:87:ASP:N	1:K:87:ASP:OD1	2.48	0.45
1:M:59:VAL:HG12	1:M:63:ASN:HD22	1.81	0.45
1:M:142:ASP:HA	1:N:5:PRO:HG2	1.98	0.45
1:M:159:PHE:O	1:M:163:GLU:HG2	2.17	0.45
1:U:50:THR:O	1:U:52:ILE:HD12	2.17	0.45
1:W:30:TYR:CD2	1:W:35:VAL:HG11	2.51	0.45
1:X:40:TYR:HA	1:X:124:ARG:HB3	1.98	0.45
1:X:112:TYR:HB3	1:X:127:PHE:CE2	2.48	0.45
1:a:74:THR:O	1:a:104:ARG:HA	2.17	0.45
1:b:47:VAL:HG23	1:b:48:PRO:HD2	1.97	0.45
1:c:80:HIS:CD2	1:c:100:LEU:HB3	2.51	0.45
1:c:127:PHE:HD2	1:c:138:ILE:HG13	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:13:LYS:HE3	1:k:13:LYS:HB3	1.78	0.45
1:k:88:ARG:HE	1:k:94:GLY:HA2	1.81	0.45
1:k:98:ILE:HG22	1:k:100:LEU:HD22	1.97	0.45
1:B:46:PHE:HD1	1:B:46:PHE:H	1.62	0.45
1:H:77:GLN:CG	1:H:102:ALA:HB3	2.46	0.45
1:H:130:ASP:HB3	1:H:136:ARG:HH11	1.80	0.45
1:T:137:GLN:HB2	1:T:159:PHE:HE2	1.82	0.45
1:U:134:ILE:HD11	1:U:136:ARG:NH1	2.32	0.45
1:g:25:ILE:HG21	1:g:30:TYR:CZ	2.51	0.45
1:h:60:GLU:CD	1:h:63:ASN:HD21	2.25	0.45
1:l:74:THR:HG23	1:l:109:SER:OG	2.17	0.45
1:A:36:VAL:HB	1:A:128:ILE:HD12	1.98	0.45
1:C:7:ARG:NH1	1:D:116:ASP:OD1	2.50	0.45
1:H:101:LEU:HD22	1:H:102:ALA:H	1.82	0.45
1:I:37:LEU:HD23	1:I:70:ILE:HD11	1.99	0.45
1:K:34:TYR:CD2	1:K:131:PRO:HD3	2.51	0.45
1:L:19:ASN:ND2	1:L:96:MET:O	2.50	0.45
1:N:36:VAL:HG23	1:N:127:PHE:O	2.16	0.45
1:Q:41:PRO:HD3	1:Q:124:ARG:HB2	1.99	0.45
1:R:45:THR:O	1:R:46:PHE:HB2	2.16	0.45
1:X:75:ASP:OD1	1:Y:79:SER:OG	2.30	0.45
1:X:158:ALA:O	1:X:162:VAL:HG13	2.17	0.45
1:Y:8:PRO:HA	1:Y:134:ILE:HA	1.98	0.45
1:Y:18:ILE:HD12	1:Y:98:ILE:O	2.17	0.45
1:Z:36:VAL:O	1:Z:36:VAL:HG12	2.17	0.45
1:c:80:HIS:O	1:c:84:ASP:HB2	2.16	0.45
1:h:56:SER:HA	1:h:96:MET:HG3	1.99	0.45
1:h:163:GLU:HG3	1:h:164:LYS:N	2.31	0.45
1:j:28:LYS:O	1:j:31:ARG:HG2	2.16	0.45
1:n:70:ILE:O	1:n:100:LEU:HA	2.16	0.45
1:A:6:ASN:HB3	1:A:7:ARG:HH21	1.82	0.45
1:A:123:PHE:HE2	1:B:4:LEU:HG	1.82	0.45
1:B:38:PHE:HE1	1:B:52:ILE:HD12	1.80	0.45
1:C:67:CYS:SG	1:C:68:GLN:N	2.90	0.45
1:D:104:ARG:HB3	1:D:105:LYS:H	1.49	0.45
1:G:9:ALA:O	1:G:11:GLU:N	2.50	0.45
1:G:27:LEU:HG	1:G:31:ARG:HD3	1.98	0.45
1:I:36:VAL:HB	1:I:69:VAL:CA	2.43	0.45
1:J:41:PRO:HD3	1:J:124:ARG:HG2	1.99	0.45
1:J:67:CYS:SG	1:J:156:LEU:HG	2.57	0.45
1:M:1:MET:HG3	1:N:3:LEU:N	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:93:LEU:HD22	1:M:93:LEU:H	1.81	0.45
1:P:18:ILE:HG12	1:P:99:PRO:HA	1.99	0.45
1:P:75:ASP:HB3	1:P:79:SER:OG	2.17	0.45
1:P:106:GLN:HB2	1:P:115:PHE:CE1	2.51	0.45
1:T:14:GLY:O	1:T:24:GLU:HG3	2.17	0.45
1:T:27:LEU:HG	1:T:31:ARG:HH22	1.81	0.45
1:T:93:LEU:HD11	1:T:96:MET:HE2	1.97	0.45
1:V:62:PHE:HZ	1:V:149:VAL:HG13	1.80	0.45
1:Y:74:THR:HA	1:Y:103:ASP:HB3	1.98	0.45
1:g:74:THR:HA	1:g:103:ASP:HB3	1.98	0.45
1:j:34:TYR:CD2	1:j:160:GLN:HB3	2.52	0.45
1:k:93:LEU:HB3	1:k:96:MET:SD	2.56	0.45
1:m:65:ARG:NH1	1:m:157:ASP:OD1	2.50	0.45
1:m:89:LYS:HE2	1:m:89:LYS:HB3	1.84	0.45
1:m:125:GLY:HA2	1:m:140:ILE:HG13	1.98	0.45
1:C:65:ARG:NH1	1:C:153:LEU:HG	2.22	0.45
1:D:137:GLN:NE2	1:D:139:THR:OG1	2.44	0.45
1:G:74:THR:HG22	1:G:104:ARG:HH21	1.81	0.45
1:H:116:ASP:HB2	1:H:123:PHE:CE1	2.52	0.45
1:L:16:ALA:O	1:L:22:PHE:HA	2.17	0.45
1:M:143:LYS:HD3	1:M:143:LYS:HA	1.87	0.45
1:O:80:HIS:CD2	1:O:100:LEU:HB3	2.52	0.45
1:Q:3:LEU:HD12	1:Q:138:ILE:HG12	1.99	0.45
1:R:75:ASP:HA	1:S:104:ARG:NH1	2.32	0.45
1:R:125:GLY:HA2	1:R:147:ARG:HH21	1.82	0.45
1:U:127:PHE:HB3	1:U:135:LEU:HD11	1.97	0.45
1:Z:56:SER:HB2	1:Z:96:MET:SD	2.56	0.45
1:Z:95:HIS:O	1:Z:96:MET:HE2	2.16	0.45
1:f:58:GLN:HG2	1:f:149:VAL:HG21	1.99	0.45
1:g:34:TYR:HA	1:g:129:ILE:O	2.17	0.45
1:h:51:GLU:OE1	1:h:146:GLY:HA2	2.16	0.45
1:i:34:TYR:CE1	1:i:131:PRO:HD3	2.52	0.45
1:A:6:ASN:HB3	1:A:7:ARG:NH2	2.31	0.45
1:A:12:PHE:CE2	1:A:27:LEU:HD12	2.52	0.45
1:C:21:GLU:O	1:C:22:PHE:HB2	2.16	0.45
1:E:139:THR:HG23	1:F:139:THR:HG23	1.99	0.45
1:I:130:ASP:OD2	1:I:131:PRO:HD2	2.17	0.45
1:K:76:SER:HB3	1:K:77:GLN:H	1.55	0.45
1:M:38:PHE:HB2	1:M:71:ALA:HB1	1.99	0.45
1:M:39:PHE:HB2	1:M:122:ALA:CB	2.47	0.45
1:M:46:PHE:O	1:M:50:THR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:15:GLN:O	1:O:101:LEU:HD13	2.17	0.45
1:O:74:THR:HA	1:O:103:ASP:O	2.17	0.45
1:V:97:LYS:HZ2	1:V:97:LYS:CB	2.29	0.45
1:Z:72:CYS:HA	1:Z:101:LEU:O	2.17	0.45
1:a:124:ARG:HG3	1:a:143:LYS:HA	1.99	0.45
1:d:47:VAL:HB	1:d:83:TRP:CH2	2.49	0.45
1:f:47:VAL:HG13	1:f:47:VAL:O	2.17	0.45
1:k:32:GLY:O	1:k:33:LYS:HB2	2.16	0.45
1:k:137:GLN:CG	1:l:147:ARG:HH22	2.30	0.45
1:m:123:PHE:HB3	1:m:124:ARG:H	1.54	0.45
1:m:163:GLU:CD	1:m:163:GLU:H	2.23	0.45
1:D:89:LYS:HD2	1:D:90:SER:N	2.32	0.45
1:F:2:VAL:HG22	1:F:3:LEU:N	2.32	0.45
1:H:115:PHE:HE1	1:H:120:GLY:HA2	1.82	0.45
1:L:41:PRO:HD3	1:L:124:ARG:HE	1.81	0.45
1:L:136:ARG:HD3	1:L:159:PHE:CG	2.52	0.45
1:P:34:TYR:N	1:P:131:PRO:HA	2.32	0.45
1:Q:98:ILE:HD13	1:Q:98:ILE:H	1.82	0.45
1:U:50:THR:O	1:U:52:ILE:N	2.47	0.45
1:Z:46:PHE:HD1	1:Z:47:VAL:N	2.15	0.45
1:b:79:SER:HA	1:c:44:PHE:HD2	1.82	0.45
1:b:121:ASN:OD1	1:c:104:ARG:HG3	2.16	0.45
1:d:36:VAL:HB	1:d:128:ILE:HD13	1.98	0.45
1:h:4:LEU:O	1:h:135:LEU:HD23	2.17	0.45
1:h:127:PHE:CE1	1:h:138:ILE:HG23	2.52	0.45
1:i:40:TYR:HE2	1:i:43:ASP:HA	1.82	0.45
1:j:17:VAL:HG21	1:j:80:HIS:CB	2.47	0.45
1:n:59:VAL:HB	1:n:60:GLU:H	1.45	0.45
1:C:103:ASP:OD2	1:C:106:GLN:HA	2.17	0.44
1:H:73:SER:C	1:H:75:ASP:H	2.25	0.44
1:M:6:ASN:OD1	1:M:136:ARG:NH1	2.50	0.44
1:O:36:VAL:CG2	1:O:126:LEU:HD21	2.47	0.44
1:V:41:PRO:O	1:V:73:SER:HB2	2.17	0.44
1:W:107:GLU:O	1:W:110:LYS:HG3	2.17	0.44
1:b:76:SER:HB3	1:b:104:ARG:HD3	2.00	0.44
1:b:164:LYS:HG3	1:b:165:HIS:ND1	2.32	0.44
1:l:72:CYS:SG	1:l:108:ILE:HG13	2.57	0.44
1:A:23:LYS:O	1:A:25:ILE:HG23	2.17	0.44
1:D:30:TYR:CE1	1:D:68:GLN:HG3	2.52	0.44
1:E:107:GLU:HG3	1:E:108:ILE:H	1.82	0.44
1:H:104:ARG:HD2	1:H:104:ARG:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:ALA:HB3	1:M:44:PHE:O	2.18	0.44
1:O:44:PHE:CE1	1:O:83:TRP:HA	2.52	0.44
1:O:154:ARG:HG3	1:O:155:LEU:N	2.32	0.44
1:P:30:TYR:HD1	1:P:33:LYS:HG3	1.82	0.44
1:P:61:GLU:HA	1:P:65:ARG:HH11	1.83	0.44
1:Q:52:ILE:HD13	1:Q:147:ARG:NH2	2.32	0.44
1:S:105:LYS:NZ	1:S:105:LYS:N	2.59	0.44
1:V:34:TYR:CD1	1:V:131:PRO:HD3	2.51	0.44
1:W:7:ARG:O	1:W:134:ILE:HA	2.16	0.44
1:W:50:THR:OG1	1:W:51:GLU:N	2.51	0.44
1:b:46:PHE:HB3	1:b:47:VAL:CB	2.47	0.44
1:e:52:ILE:H	1:e:52:ILE:HD13	1.82	0.44
1:e:140:ILE:N	1:f:138:ILE:O	2.31	0.44
1:f:16:ALA:O	1:f:22:PHE:HA	2.17	0.44
1:f:17:VAL:HG21	1:f:80:HIS:HB2	1.99	0.44
1:i:52:ILE:HG21	1:i:124:ARG:HH12	1.82	0.44
1:j:17:VAL:N	1:j:100:LEU:O	2.44	0.44
1:k:13:LYS:HZ2	1:k:26:CYS:HB3	1.80	0.44
1:m:74:THR:HA	1:m:103:ASP:O	2.18	0.44
1:n:137:GLN:HB2	1:n:159:PHE:HE2	1.82	0.44
1:G:31:ARG:HE	1:G:133:GLY:HA3	1.82	0.44
1:G:154:ARG:HH12	1:G:158:ALA:CB	2.31	0.44
1:H:124:ARG:HD2	1:H:147:ARG:NH1	2.32	0.44
1:K:148:SER:O	1:K:152:THR:OG1	2.22	0.44
1:N:22:PHE:CZ	1:N:77:GLN:HB3	2.51	0.44
1:N:41:PRO:HD3	1:N:124:ARG:HD3	1.99	0.44
1:Q:73:SER:HB3	1:Q:80:HIS:CE1	2.52	0.44
1:R:28:LYS:O	1:R:31:ARG:HD3	2.18	0.44
1:S:5:PRO:HG2	1:T:141:ASN:O	2.18	0.44
1:S:83:TRP:NE1	1:S:92:GLY:HA2	2.32	0.44
1:T:38:PHE:HB2	1:T:147:ARG:CZ	2.48	0.44
1:X:104:ARG:NH2	1:Y:74:THR:HG23	2.33	0.44
1:Y:38:PHE:HB2	1:Y:147:ARG:NH2	2.32	0.44
1:a:40:TYR:H	1:a:124:ARG:HA	1.83	0.44
1:b:145:VAL:HG12	1:b:146:GLY:N	2.32	0.44
1:e:23:LYS:HE2	1:e:23:LYS:O	2.16	0.44
1:e:104:ARG:HH12	1:n:120:GLY:C	2.26	0.44
1:j:5:PRO:C	1:j:7:ARG:H	2.26	0.44
1:j:130:ASP:OD2	1:j:136:ARG:NH2	2.51	0.44
1:k:33:LYS:HG2	1:k:66:ASN:HA	1.98	0.44
1:l:28:LYS:HD2	1:l:31:ARG:HH11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:147:ARG:HH11	1:m:147:ARG:CG	2.29	0.44
1:G:38:PHE:HD1	1:G:69:VAL:HG12	1.82	0.44
1:H:11:GLU:HA	1:H:27:LEU:HD22	1.98	0.44
1:P:134:ILE:CD1	1:P:136:ARG:HH12	2.30	0.44
1:Q:9:ALA:HA	1:Q:10:PRO:HD3	1.86	0.44
1:Q:56:SER:HB3	1:Q:93:LEU:HD22	1.99	0.44
1:T:93:LEU:HD22	1:T:94:GLY:O	2.18	0.44
1:U:51:GLU:OE2	1:U:124:ARG:CZ	2.65	0.44
1:U:78:TYR:HB3	1:d:44:PHE:CB	2.42	0.44
1:V:73:SER:OG	1:V:74:THR:N	2.51	0.44
1:W:65:ARG:HH11	1:W:153:LEU:HD12	1.83	0.44
1:X:137:GLN:HB2	1:X:159:PHE:HE2	1.81	0.44
1:X:164:LYS:HB3	1:X:164:LYS:HZ2	1.80	0.44
1:Z:94:GLY:O	1:Z:95:HIS:CG	2.71	0.44
1:a:147:ARG:HG3	1:a:147:ARG:HH11	1.82	0.44
1:e:12:PHE:CE2	1:e:27:LEU:HG	2.52	0.44
1:e:125:GLY:HA2	1:e:140:ILE:HA	2.00	0.44
1:h:112:TYR:OH	1:h:129:ILE:HG22	2.18	0.44
1:i:116:ASP:HB2	1:i:123:PHE:CE2	2.51	0.44
1:k:16:ALA:O	1:k:22:PHE:HA	2.17	0.44
1:l:145:VAL:HG13	1:l:146:GLY:N	2.29	0.44
1:m:124:ARG:HB2	1:m:141:ASN:H	1.83	0.44
1:C:4:LEU:HB3	1:D:123:PHE:HE2	1.82	0.44
1:E:34:TYR:HB3	1:E:35:VAL:H	1.60	0.44
1:G:64:SER:HB2	1:G:65:ARG:CZ	2.47	0.44
1:H:12:PHE:CE2	1:H:27:LEU:HD13	2.52	0.44
1:J:110:LYS:HG2	1:J:115:PHE:CG	2.53	0.44
1:K:6:ASN:C	1:K:7:ARG:NH1	2.76	0.44
1:M:55:PHE:CD1	1:M:149:VAL:HG22	2.52	0.44
1:N:159:PHE:O	1:N:163:GLU:HG2	2.17	0.44
1:R:74:THR:O	1:R:74:THR:OG1	2.30	0.44
1:R:104:ARG:HH22	1:S:74:THR:HG22	1.82	0.44
1:R:129:ILE:HG22	1:R:130:ASP:H	1.83	0.44
1:T:161:PHE:HD1	1:T:162:VAL:N	2.15	0.44
1:V:74:THR:OG1	1:V:121:ASN:HA	2.17	0.44
1:Y:156:LEU:O	1:Y:160:GLN:HG2	2.16	0.44
1:a:127:PHE:HE2	1:a:138:ILE:HG23	1.82	0.44
1:c:84:ASP:HA	1:c:93:LEU:HD11	1.98	0.44
1:f:104:ARG:NH2	1:g:75:ASP:HB3	2.31	0.44
1:g:32:GLY:N	1:g:131:PRO:O	2.29	0.44
1:g:51:GLU:OE1	1:g:146:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:34:TYR:HA	1:j:131:PRO:HD3	1.98	0.44
1:j:37:LEU:HD11	1:j:127:PHE:HB2	1.99	0.44
1:l:33:LYS:HE2	1:l:33:LYS:HB3	1.85	0.44
1:m:65:ARG:HD3	1:m:65:ARG:N	2.32	0.44
1:D:52:ILE:HD11	1:D:147:ARG:NH2	2.30	0.44
1:D:164:LYS:HD3	1:D:164:LYS:H	1.82	0.44
1:E:34:TYR:CD1	1:E:131:PRO:HD3	2.52	0.44
1:F:6:ASN:ND2	1:F:6:ASN:O	2.50	0.44
1:F:75:ASP:HA	1:G:104:ARG:HH12	1.83	0.44
1:H:42:ALA:HB2	1:I:104:ARG:NH2	2.33	0.44
1:K:6:ASN:HD22	1:L:143:LYS:NZ	2.15	0.44
1:Q:3:LEU:HB3	1:Q:112:TYR:HB2	1.99	0.44
1:S:128:ILE:HD11	1:S:152:THR:HG23	1.99	0.44
1:U:34:TYR:HA	1:U:129:ILE:O	2.17	0.44
1:V:104:ARG:HD2	1:V:104:ARG:HA	1.79	0.44
1:W:114:VAL:HG21	1:W:123:PHE:H	1.82	0.44
1:W:124:ARG:HB2	1:W:141:ASN:HB2	1.99	0.44
1:c:59:VAL:HA	1:c:62:PHE:HD1	1.82	0.44
1:d:147:ARG:HH11	1:d:147:ARG:HB2	1.82	0.44
1:e:142:ASP:OD1	1:e:143:LYS:HD2	2.18	0.44
1:i:124:ARG:O	1:i:141:ASN:HB2	2.17	0.44
1:k:15:GLN:HA	1:k:23:LYS:O	2.17	0.44
1:k:80:HIS:CD2	1:k:100:LEU:HB3	2.52	0.44
1:m:61:GLU:HB2	1:m:153:LEU:HD21	1.99	0.44
1:D:13:LYS:HB2	1:D:13:LYS:HZ3	1.82	0.44
1:E:129:ILE:HD13	1:E:135:LEU:HD13	2.00	0.44
1:F:119:ASP:C	1:F:121:ASN:H	2.25	0.44
1:H:115:PHE:CE1	1:H:120:GLY:HA2	2.53	0.44
1:J:75:ASP:HB2	1:J:80:HIS:CE1	2.52	0.44
1:K:38:PHE:CZ	1:K:71:ALA:HB2	2.52	0.44
1:M:13:LYS:HB3	1:M:13:LYS:HE3	1.69	0.44
1:N:3:LEU:HD23	1:N:3:LEU:HA	1.86	0.44
1:P:34:TYR:HD1	1:P:131:PRO:HG3	1.81	0.44
1:S:164:LYS:HG2	1:S:165:HIS:N	2.33	0.44
1:U:50:THR:C	1:U:52:ILE:H	2.26	0.44
1:W:2:VAL:HG13	1:W:3:LEU:N	2.32	0.44
1:Z:47:VAL:HB	1:Z:48:PRO:HA	2.00	0.44
1:a:38:PHE:CE2	1:a:147:ARG:NH1	2.86	0.44
1:b:119:ASP:HB3	1:b:143:LYS:NZ	2.33	0.44
1:c:73:SER:OG	1:c:74:THR:N	2.50	0.44
1:d:35:VAL:HG22	1:d:129:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:68:GLN:HG3	1:d:70:ILE:HG23	2.00	0.44
1:e:93:LEU:HB3	1:e:94:GLY:H	1.60	0.44
1:h:126:LEU:HB3	1:h:139:THR:HB	1.99	0.44
1:k:38:PHE:HA	1:k:126:LEU:H	1.82	0.44
1:A:31:ARG:HG3	1:A:31:ARG:NH1	2.33	0.44
1:B:47:VAL:HB	1:B:48:PRO:CD	2.45	0.44
1:C:32:GLY:N	1:C:131:PRO:O	2.51	0.44
1:E:32:GLY:HA2	1:E:131:PRO:HB3	1.99	0.44
1:I:113:GLY:HA3	1:J:2:VAL:HG21	1.99	0.44
1:M:1:MET:HG3	1:N:3:LEU:HB2	1.99	0.44
1:M:129:ILE:HG13	1:M:135:LEU:HD23	1.99	0.44
1:P:76:SER:HB2	1:P:79:SER:OG	2.18	0.44
1:Q:22:PHE:HZ	1:Q:77:GLN:HB3	1.83	0.44
1:Q:136:ARG:HB3	1:Q:159:PHE:CE2	2.49	0.44
1:Q:137:GLN:NE2	1:Q:139:THR:OG1	2.45	0.44
1:T:124:ARG:HG3	1:T:147:ARG:NH1	2.32	0.44
1:T:137:GLN:HB2	1:T:159:PHE:CE2	2.51	0.44
1:U:16:ALA:O	1:U:22:PHE:HA	2.18	0.44
1:U:143:LYS:HA	1:U:143:LYS:HD2	1.77	0.44
1:X:49:PRO:O	1:X:52:ILE:HG23	2.17	0.44
1:X:141:ASN:ND2	1:X:145:VAL:HG13	2.33	0.44
1:b:2:VAL:HG13	1:b:3:LEU:N	2.30	0.44
1:b:37:LEU:HD13	1:b:39:PHE:HE1	1.81	0.44
1:b:37:LEU:HD22	1:b:112:TYR:CE2	2.53	0.44
1:e:7:ARG:NH2	1:f:118:GLU:OE2	2.50	0.44
1:e:104:ARG:NH2	1:n:74:THR:HB	2.32	0.44
1:h:31[A]:ARG:HA	1:h:131:PRO:HB2	1.98	0.44
1:m:119:ASP:OD1	1:m:119:ASP:N	2.51	0.44
1:A:74:THR:HG23	1:J:104:ARG:HH11	1.81	0.44
1:B:104:ARG:HH22	1:C:104:ARG:HH22	1.65	0.44
1:C:119:ASP:HB2	1:C:121:ASN:OD1	2.18	0.44
1:D:11:GLU:OE2	1:D:31[B]:ARG:NH2	2.51	0.44
1:D:37:LEU:O	1:D:126:LEU:HA	2.17	0.44
1:G:11:GLU:H	1:G:11:GLU:HG2	1.53	0.44
1:I:77:GLN:CD	1:I:77:GLN:H	2.23	0.44
1:S:33:LYS:NZ	1:S:67:CYS:N	2.64	0.44
1:T:126:LEU:HD13	1:T:139:THR:HB	2.00	0.44
1:W:41:PRO:HG3	1:W:143:LYS:HE2	1.98	0.44
1:W:162:VAL:HG23	1:W:163:GLU:N	2.33	0.44
1:a:135:LEU:HD22	1:a:138:ILE:HD11	2.00	0.44
1:e:107:GLU:HG3	1:e:108:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PRO:HB3	1:B:121:ASN:HB3	2.00	0.43
1:D:67:CYS:HB2	1:D:68:GLN:H	1.45	0.43
1:E:11:GLU:OE2	1:E:26:CYS:HB3	2.17	0.43
1:E:39:PHE:HB2	1:E:125:GLY:H	1.83	0.43
1:H:104:ARG:NH2	1:I:74:THR:HG23	2.31	0.43
1:H:127:PHE:HB3	1:H:135:LEU:HD21	1.99	0.43
1:O:114:VAL:HG11	1:O:125:GLY:HA3	1.98	0.43
1:Q:124:ARG:HD2	1:Q:143:LYS:O	2.18	0.43
1:U:44:PHE:H	1:U:83:TRP:NE1	2.15	0.43
1:X:27:LEU:HG	1:X:28:LYS:N	2.32	0.43
1:X:96:MET:C	1:X:98:ILE:H	2.25	0.43
1:b:105:LYS:H	1:b:105:LYS:HD2	1.83	0.43
1:c:80:HIS:HD2	1:c:100:LEU:HB3	1.83	0.43
1:d:96:MET:HB2	1:d:100:LEU:HD11	2.00	0.43
1:h:86:LEU:HD12	1:h:90:SER:OG	2.18	0.43
1:j:18:ILE:HD12	1:j:99:PRO:HG3	2.00	0.43
1:k:34:TYR:HB2	1:k:67:CYS:HA	1.99	0.43
1:k:116:ASP:OD1	1:k:117:GLU:N	2.51	0.43
1:n:6:ASN:H	1:n:136:ARG:H	1.65	0.43
1:B:43:ASP:OD2	1:B:83:TRP:CE3	2.71	0.43
1:D:121:ASN:HB2	1:D:143:LYS:NZ	2.33	0.43
1:H:129:ILE:HG13	1:H:130:ASP:O	2.17	0.43
1:H:146:GLY:C	1:H:147:ARG:HD3	2.43	0.43
1:J:59:VAL:HG11	1:J:98:ILE:HG21	2.00	0.43
1:J:60:GLU:HG3	1:J:97:LYS:HZ3	1.82	0.43
1:J:136:ARG:HB3	1:J:159:PHE:CE1	2.53	0.43
1:L:74:THR:O	1:L:104:ARG:HD3	2.18	0.43
1:L:129:ILE:O	1:L:130:ASP:HB2	2.18	0.43
1:T:66:ASN:HB3	1:T:67:CYS:H	1.49	0.43
1:V:69:VAL:O	1:V:70:ILE:HG12	2.18	0.43
1:Y:37:LEU:HD13	1:Y:70:ILE:HD12	2.00	0.43
1:d:58:GLN:HG3	1:d:61:GLU:HB2	2.00	0.43
1:i:75:ASP:O	1:i:76:SER:OG	2.30	0.43
1:k:76:SER:HA	1:k:104:ARG:HB2	2.00	0.43
1:n:53:ILE:HD12	1:n:88:ARG:HG2	2.00	0.43
1:C:38:PHE:CE1	1:C:69:VAL:HG23	2.45	0.43
1:F:46:PHE:CZ	1:G:78:TYR:HE1	2.36	0.43
1:G:12:PHE:HE2	1:G:25:ILE:HG12	1.84	0.43
1:J:33:LYS:HE2	1:J:33:LYS:HB3	1.81	0.43
1:L:39:PHE:CZ	1:L:114:VAL:HG21	2.53	0.43
1:N:106:GLN:HB3	1:N:110:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:71:ALA:HB3	1:P:100:LEU:HD12	1.98	0.43
1:P:128:ILE:HD11	1:P:136:ARG:O	2.18	0.43
1:S:139:THR:HG23	1:T:139:THR:OG1	2.18	0.43
1:S:151:GLU:OE1	1:T:151:GLU:HB2	2.18	0.43
1:U:48:PRO:HA	1:U:49:PRO:HD3	1.49	0.43
1:U:159:PHE:HE1	1:V:145:VAL:HG11	1.83	0.43
1:Y:62:PHE:HB3	1:Y:67:CYS:SG	2.59	0.43
1:Z:17:VAL:HG11	1:Z:81:LEU:HD13	2.00	0.43
1:c:128:ILE:O	1:c:136:ARG:N	2.47	0.43
1:d:4:LEU:CD1	1:d:7:ARG:HH12	2.30	0.43
1:d:154:ARG:HH12	1:d:155:LEU:CD2	2.31	0.43
1:g:112:TYR:OH	1:g:129:ILE:HD11	2.18	0.43
1:h:154:ARG:NH1	1:h:155:LEU:HB3	2.34	0.43
1:i:163:GLU:HG3	1:i:164:LYS:H	1.82	0.43
1:j:56:SER:HB2	1:j:96:MET:HG3	1.99	0.43
1:k:130:ASP:CG	1:k:132:ASN:HD22	2.22	0.43
1:k:145:VAL:HG22	1:l:162:VAL:HG11	1.99	0.43
1:l:12:PHE:HB2	1:l:108:ILE:HG22	2.00	0.43
1:n:58:GLN:HE21	1:n:58:GLN:HB2	1.68	0.43
1:A:115:PHE:CE2	1:A:117:GLU:OE1	2.71	0.43
1:H:39:PHE:HB3	1:H:122:ALA:HB1	2.00	0.43
1:M:38:PHE:CE2	1:M:126:LEU:HB3	2.53	0.43
1:M:141:ASN:HA	1:N:137:GLN:OE1	2.18	0.43
1:N:65:ARG:HB2	1:N:156:LEU:HD23	2.00	0.43
1:O:62:PHE:HA	1:O:65:ARG:HG2	1.99	0.43
1:P:13:LYS:CE	1:P:26:CYS:HB2	2.48	0.43
1:R:141:ASN:HB2	1:R:147:ARG:NH2	2.32	0.43
1:S:113:GLY:O	1:T:2:VAL:HG11	2.18	0.43
1:T:51:GLU:CD	1:T:147:ARG:HB3	2.43	0.43
1:U:123:PHE:O	1:U:124:ARG:HB2	2.18	0.43
1:V:89:LYS:HD2	1:V:90:SER:H	1.83	0.43
1:V:160:GLN:O	1:V:164:LYS:HG2	2.17	0.43
1:W:128:ILE:HD13	1:W:137:GLN:HG2	2.01	0.43
1:Z:35:VAL:N	1:Z:129:ILE:HG22	2.33	0.43
1:Z:145:VAL:HG12	1:Z:146:GLY:H	1.84	0.43
1:b:128:ILE:HG23	1:b:137:GLN:HB3	1.99	0.43
1:c:72:CYS:HA	1:c:101:LEU:HB3	1.99	0.43
1:d:31:ARG:HH11	1:d:31:ARG:CG	2.31	0.43
1:e:119:ASP:O	1:e:121:ASN:ND2	2.51	0.43
1:f:50:THR:HB	1:f:52:ILE:HG22	2.00	0.43
1:f:65:ARG:HD2	1:f:160:GLN:HE22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:73:SER:HB3	1:g:80:HIS:HE1	1.84	0.43
1:h:9:ALA:N	1:h:133:GLY:O	2.51	0.43
1:l:58:GLN:HB3	1:l:62:PHE:CD2	2.53	0.43
1:C:40:TYR:HA	1:C:124:ARG:HG2	1.99	0.43
1:C:124:ARG:HB3	1:C:147:ARG:NH1	2.25	0.43
1:G:38:PHE:CA	1:G:126:LEU:H	2.24	0.43
1:G:46:PHE:CG	1:G:47:VAL:N	2.86	0.43
1:G:80:HIS:CD2	1:G:100:LEU:HB3	2.47	0.43
1:H:56:SER:O	1:H:97:LYS:HD3	2.18	0.43
1:L:30:TYR:CD1	1:L:33[B]:LYS:HE2	2.53	0.43
1:N:52:ILE:HD12	1:N:52:ILE:H	1.84	0.43
1:N:97:LYS:O	1:N:98:ILE:HG23	2.18	0.43
1:P:2:VAL:HB	1:P:4:LEU:HG	1.99	0.43
1:R:66:ASN:O	1:R:67:CYS:HB2	2.19	0.43
1:V:110:LYS:HE2	1:V:110:LYS:HB3	1.80	0.43
1:X:11:GLU:HB3	1:X:27:LEU:CD2	2.44	0.43
1:Z:4:LEU:HA	1:Z:5:PRO:HD3	1.84	0.43
1:Z:43:ASP:OD1	1:Z:43:ASP:N	2.51	0.43
1:Z:73:SER:HB3	1:Z:80:HIS:HE2	1.84	0.43
1:c:124:ARG:HG3	1:c:143:LYS:HA	2.01	0.43
1:c:128:ILE:HG12	1:c:137:GLN:HG2	2.01	0.43
1:g:141:ASN:HD22	1:g:145:VAL:HG12	1.84	0.43
1:j:86:LEU:HB3	1:j:92:GLY:HA3	2.00	0.43
1:j:115:PHE:CE1	1:j:122:ALA:HB2	2.53	0.43
1:l:154:ARG:HD3	1:l:155:LEU:HD22	2.00	0.43
1:n:33:LYS:HB3	1:n:66:ASN:O	2.18	0.43
1:A:141:ASN:HB3	1:A:145:VAL:CG1	2.49	0.43
1:B:12:PHE:CD1	1:B:27:LEU:HD22	2.54	0.43
1:K:126:LEU:O	1:K:139:THR:HG23	2.19	0.43
1:M:126:LEU:O	1:M:126:LEU:HD12	2.18	0.43
1:N:21:GLU:OE1	1:N:21:GLU:HA	2.18	0.43
1:N:163:GLU:HG3	1:N:164:LYS:H	1.83	0.43
1:O:137:GLN:HG2	1:P:141:ASN:HA	2.00	0.43
1:R:115:PHE:C	1:R:115:PHE:CD1	2.96	0.43
1:b:47:VAL:HG23	1:b:48:PRO:CD	2.49	0.43
1:c:41:PRO:HB3	1:c:143:LYS:HE3	1.99	0.43
1:d:84:ASP:OD2	1:d:100:LEU:HD21	2.18	0.43
1:i:104:ARG:HA	1:i:104:ARG:HD2	1.78	0.43
1:j:74:THR:HG21	1:j:122:ALA:H	1.84	0.43
1:l:108:ILE:H	1:l:108:ILE:HD13	1.84	0.43
1:m:4:LEU:HB3	1:n:123:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:HB3	1:A:80:HIS:CE1	2.54	0.43
1:C:5:PRO:HD2	1:D:123:PHE:CD2	2.54	0.43
1:C:61:GLU:O	1:C:65:ARG:HD3	2.19	0.43
1:D:37:LEU:HG	1:D:70:ILE:HG21	2.00	0.43
1:D:116:ASP:HB2	1:D:123:PHE:CZ	2.54	0.43
1:E:162:VAL:HG11	1:F:144:PRO:CB	2.49	0.43
1:J:12:PHE:HB2	1:J:108:ILE:CG2	2.49	0.43
1:K:12:PHE:O	1:K:12:PHE:HD1	2.01	0.43
1:L:151:GLU:OE1	1:L:155:LEU:HD21	2.19	0.43
1:M:75:ASP:C	1:M:104:ARG:HB2	2.44	0.43
1:N:128:ILE:CG2	1:N:136:ARG:HB2	2.40	0.43
1:O:59:VAL:HG11	1:O:97:LYS:HB2	2.01	0.43
1:Q:16:ALA:HA	1:Q:100:LEU:O	2.18	0.43
1:R:129:ILE:HG22	1:R:130:ASP:N	2.33	0.43
1:S:89:LYS:HG3	1:S:90:SER:H	1.83	0.43
1:V:11:GLU:OE1	1:V:28:LYS:NZ	2.40	0.43
1:V:62:PHE:O	1:V:67:CYS:HB3	2.19	0.43
1:V:128:ILE:HG12	1:V:129:ILE:N	2.31	0.43
1:X:47:VAL:HG13	1:X:49:PRO:HB3	2.00	0.43
1:X:128:ILE:O	1:X:135:LEU:HD12	2.18	0.43
1:Z:145:VAL:HG12	1:Z:146:GLY:N	2.34	0.43
1:a:66:ASN:HB3	1:a:67:CYS:H	1.65	0.43
1:b:71:ALA:HB3	1:b:100:LEU:HD13	2.00	0.43
1:c:4:LEU:HD22	1:d:123:PHE:HE2	1.83	0.43
1:e:48:PRO:N	1:e:49:PRO:HD3	2.33	0.43
1:f:17:VAL:HG21	1:f:80:HIS:CB	2.49	0.43
1:f:134:ILE:HD11	1:f:136:ARG:HH12	1.83	0.43
1:m:17:VAL:HG22	1:m:22:PHE:CD1	2.53	0.43
1:n:16:ALA:O	1:n:23:LYS:N	2.51	0.43
1:B:126:LEU:HB2	1:B:147:ARG:NH1	2.33	0.43
1:E:5:PRO:HG2	1:F:141:ASN:O	2.18	0.43
1:G:9:ALA:HB2	1:G:135:LEU:HD12	2.00	0.43
1:L:34:TYR:CE1	1:L:131:PRO:HD3	2.54	0.43
1:M:16:ALA:O	1:M:22:PHE:HA	2.18	0.43
1:O:62:PHE:O	1:O:67:CYS:HB2	2.19	0.43
1:P:74:THR:HA	1:P:103:ASP:HB3	2.00	0.43
1:R:50:THR:O	1:R:50:THR:HG22	2.18	0.43
1:V:7:ARG:H	1:V:7:ARG:HG2	1.67	0.43
1:V:80:HIS:HB3	1:V:100:LEU:HG	2.00	0.43
1:Y:4:LEU:HD11	1:Z:115:PHE:O	2.18	0.43
1:Y:18:ILE:HG13	1:Y:100:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:62:PHE:HA	1:Y:65:ARG:HH21	1.84	0.43
1:Z:44:PHE:CD2	1:a:79:SER:HA	2.53	0.43
1:b:37:LEU:HD11	1:b:127:PHE:CG	2.54	0.43
1:b:73:SER:C	1:b:75:ASP:H	2.26	0.43
1:b:108:ILE:HD12	1:b:108:ILE:H	1.83	0.43
1:b:126:LEU:O	1:b:139:THR:HG22	2.19	0.43
1:f:75:ASP:N	1:f:75:ASP:OD1	2.52	0.43
1:i:118:GLU:OE1	1:i:118:GLU:N	2.42	0.43
1:k:157:ASP:O	1:k:161:PHE:HB3	2.19	0.43
1:l:45:THR:HG22	1:l:47:VAL:CG2	2.45	0.43
1:n:13:LYS:NZ	1:n:13:LYS:HB2	2.26	0.43
1:A:3:LEU:HB2	1:A:4:LEU:H	1.51	0.43
1:C:74:THR:HG21	1:C:121:ASN:HA	2.01	0.43
1:E:52:ILE:HB	1:E:53:ILE:H	1.60	0.43
1:G:65:ARG:HG2	1:G:66:ASN:N	2.34	0.43
1:H:15:GLN:O	1:H:16:ALA:HB2	2.18	0.43
1:P:11:GLU:HG3	1:P:27:LEU:HB3	2.01	0.43
1:P:34:TYR:CE2	1:P:156:LEU:HD21	2.53	0.43
1:R:37:LEU:HG	1:R:70:ILE:HB	2.00	0.43
1:R:145:VAL:HG12	1:R:146:GLY:N	2.34	0.43
1:S:8:PRO:HA	1:S:134:ILE:HA	2.01	0.43
1:T:39:PHE:HB3	1:T:122:ALA:HB1	2.01	0.43
1:Z:129:ILE:HG13	1:Z:135:LEU:HA	2.01	0.43
1:c:16:ALA:HB2	1:c:102:ALA:HB2	2.00	0.43
1:d:36:VAL:HG13	1:d:69:VAL:HG22	2.00	0.43
1:f:60:GLU:O	1:f:61:GLU:C	2.62	0.43
1:h:52:ILE:HG12	1:h:53:ILE:N	2.34	0.43
1:j:41:PRO:HG2	1:j:143:LYS:NZ	2.33	0.43
1:j:59:VAL:HA	1:j:62:PHE:HD2	1.83	0.43
1:j:109:SER:HB2	1:j:115:PHE:CE1	2.54	0.43
1:m:104:ARG:O	1:m:106:GLN:NE2	2.48	0.43
1:A:159:PHE:O	1:A:163:GLU:HG2	2.18	0.43
1:B:4:LEU:HD12	1:B:4:LEU:HA	1.93	0.43
1:C:98:ILE:H	1:C:98:ILE:HG13	1.78	0.43
1:C:135:LEU:HD11	1:C:138:ILE:HG13	2.00	0.43
1:M:28:LYS:HE2	1:M:28:LYS:HB3	1.85	0.43
1:P:33:LYS:HB3	1:P:66:ASN:ND2	2.33	0.43
1:W:39:PHE:H	1:W:147:ARG:NH1	2.14	0.43
1:a:103:ASP:OD1	1:a:105:LYS:N	2.47	0.43
1:c:88:ARG:NE	1:c:94:GLY:H	2.17	0.43
1:c:93:LEU:HD12	1:c:95:HIS:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:12:PHE:HD1	1:d:12:PHE:O	2.02	0.43
1:f:59:VAL:O	1:f:60:GLU:HB2	2.19	0.43
1:g:43:ASP:OD1	1:g:75:ASP:OD1	2.37	0.43
1:h:55:PHE:O	1:h:59:VAL:HB	2.19	0.43
1:h:151:GLU:HG3	1:h:154:ARG:NH1	2.34	0.43
1:i:44:PHE:HD1	1:i:44:PHE:HA	1.75	0.43
1:m:4:LEU:HB2	1:m:7:ARG:HE	1.83	0.43
1:A:36:VAL:HG13	1:A:69:VAL:HG23	2.01	0.42
1:B:9:ALA:HA	1:B:10:PRO:HD3	1.82	0.42
1:B:53:ILE:HD13	1:B:56:SER:HB3	2.00	0.42
1:D:155:LEU:O	1:D:159:PHE:HB2	2.19	0.42
1:E:61:GLU:O	1:E:65:ARG:HG2	2.19	0.42
1:E:96:MET:HG2	1:E:100:LEU:HD21	2.01	0.42
1:I:50:THR:O	1:I:51:GLU:HB2	2.19	0.42
1:J:65:ARG:HD3	1:J:65:ARG:H	1.83	0.42
1:K:3:LEU:HG	1:L:1:MET:HG3	2.01	0.42
1:L:52:ILE:HG23	1:L:147:ARG:HH12	1.83	0.42
1:M:10:PRO:HD3	1:M:135:LEU:HD11	2.00	0.42
1:U:40:TYR:O	1:U:73:SER:HB3	2.19	0.42
1:V:72:CYS:HB3	1:V:101:LEU:HB2	2.00	0.42
1:Y:70:ILE:HG23	1:Y:99:PRO:HB2	2.01	0.42
1:b:77:GLN:HG3	1:b:102:ALA:HB2	2.00	0.42
1:b:137:GLN:HG2	1:b:138:ILE:N	2.32	0.42
1:c:106:GLN:O	1:c:110:LYS:HB3	2.18	0.42
1:c:145:VAL:HB	1:d:162:VAL:HG11	2.00	0.42
1:d:65:ARG:NH1	1:d:153:LEU:HB3	2.34	0.42
1:h:15:GLN:HB2	1:h:24:GLU:HB3	2.01	0.42
1:n:100:LEU:C	1:n:100:LEU:HD23	2.44	0.42
1:C:97:LYS:H	1:C:97:LYS:HD2	1.83	0.42
1:D:76:SER:HB3	1:D:104:ARG:CZ	2.49	0.42
1:J:12:PHE:CE1	1:J:27:LEU:HG	2.54	0.42
1:L:60:GLU:HA	1:L:63:ASN:OD1	2.19	0.42
1:M:93:LEU:HB2	1:M:96:MET:HE3	2.01	0.42
1:P:129:ILE:HG23	1:P:130:ASP:O	2.19	0.42
1:S:121:ASN:HB2	1:S:143:LYS:HZ1	1.82	0.42
1:T:39:PHE:CG	1:T:114:VAL:HG21	2.55	0.42
1:U:125:GLY:HA3	1:U:139:THR:O	2.19	0.42
1:Z:128:ILE:HG22	1:Z:136:ARG:HB2	2.01	0.42
1:a:37:LEU:HD21	1:a:127:PHE:HB2	2.00	0.42
1:d:49:PRO:HA	1:d:50:THR:CB	2.45	0.42
1:f:98:ILE:HA	1:f:99:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:34:TYR:O	1:h:35:VAL:HG13	2.19	0.42
1:j:79:SER:HA	1:k:44:PHE:HE2	1.83	0.42
1:k:94:GLY:HA3	1:k:96:MET:H	1.83	0.42
1:l:42:ALA:HA	1:m:104:ARG:HH12	1.83	0.42
1:A:110:LYS:NZ	1:A:115:PHE:CZ	2.87	0.42
1:E:3:LEU:N	1:F:2:VAL:HB	2.35	0.42
1:M:161:PHE:HA	1:M:164:LYS:NZ	2.34	0.42
1:O:36:VAL:HB	1:O:128:ILE:HD13	2.01	0.42
1:T:2:VAL:HG13	1:T:4:LEU:HD22	2.00	0.42
1:U:76:SER:HB2	1:U:104:ARG:CZ	2.48	0.42
1:V:38:PHE:HB3	1:V:126:LEU:CD2	2.50	0.42
1:a:145:VAL:HG11	1:b:159:PHE:CZ	2.53	0.42
1:b:12:PHE:HB2	1:b:108:ILE:HG13	2.00	0.42
1:b:98:ILE:HA	1:b:99:PRO:HD3	1.81	0.42
1:b:137:GLN:HE22	1:b:155:LEU:HD13	1.83	0.42
1:c:119:ASP:O	1:c:121:ASN:N	2.53	0.42
1:e:34:TYR:O	1:e:67:CYS:HA	2.19	0.42
1:g:15:GLN:HG2	1:g:77:GLN:HB3	2.01	0.42
1:h:44:PHE:HB2	1:i:78:TYR:HB3	2.00	0.42
1:k:4:LEU:HD22	1:l:123:PHE:CZ	2.49	0.42
1:l:36:VAL:HG22	1:l:69:VAL:HA	2.01	0.42
1:l:76:SER:HB2	1:l:102:ALA:HB1	2.00	0.42
1:m:124:ARG:HG3	1:m:141:ASN:HB2	2.02	0.42
1:n:119:ASP:C	1:n:121:ASN:H	2.27	0.42
1:n:137:GLN:HB2	1:n:159:PHE:CE2	2.55	0.42
1:D:72:CYS:SG	1:D:73:SER:N	2.93	0.42
1:D:74:THR:HG23	1:D:122:ALA:HB2	2.01	0.42
1:E:88:ARG:NE	1:E:94:GLY:HA3	2.35	0.42
1:F:128:ILE:O	1:F:135:LEU:HD12	2.19	0.42
1:K:63:ASN:CG	1:K:64:SER:H	2.28	0.42
1:R:123:PHE:O	1:R:124:ARG:HB2	2.18	0.42
1:W:38:PHE:CD2	1:W:71:ALA:HB2	2.55	0.42
1:Y:38:PHE:HZ	1:Y:52:ILE:HG12	1.84	0.42
1:Z:2:VAL:HG22	1:Z:3:LEU:N	2.33	0.42
1:b:84:ASP:HA	1:b:93:LEU:CD1	2.49	0.42
1:c:37:LEU:HD12	1:c:39:PHE:CE1	2.54	0.42
1:e:5:PRO:C	1:e:7:ARG:H	2.26	0.42
1:f:61:GLU:HA	1:f:64:SER:OG	2.19	0.42
1:g:142:ASP:CG	1:g:143:LYS:H	2.28	0.42
1:h:31[B]:ARG:HA	1:h:131:PRO:HB2	1.99	0.42
1:i:27:LEU:O	1:i:31:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:38:PHE:O	1:j:72:CYS:N	2.53	0.42
1:j:159:PHE:O	1:j:163:GLU:HG2	2.20	0.42
1:l:81:LEU:O	1:l:84:ASP:HB2	2.20	0.42
1:A:17:VAL:HG23	1:A:80:HIS:HB2	2.01	0.42
1:A:58:GLN:OE1	1:A:61:GLU:HB2	2.19	0.42
1:D:37:LEU:HB3	1:D:127:PHE:CE1	2.54	0.42
1:D:72:CYS:HA	1:D:101:LEU:O	2.19	0.42
1:F:11:GLU:OE2	1:F:27:LEU:HB3	2.20	0.42
1:F:97:LYS:H	1:F:97:LYS:HD2	1.84	0.42
1:F:119:ASP:O	1:G:104:ARG:HG2	2.19	0.42
1:G:12:PHE:HB2	1:G:108:ILE:HD12	2.01	0.42
1:H:98:ILE:O	1:H:100:LEU:HD12	2.19	0.42
1:J:0:THR:HB	1:J:1:MET:H	1.66	0.42
1:K:53:ILE:HG23	1:K:88:ARG:HD3	2.02	0.42
1:N:3:LEU:HD21	1:N:10:PRO:HD3	2.01	0.42
1:O:145:VAL:HG12	1:O:146:GLY:N	2.35	0.42
1:R:120:GLY:CA	1:S:105:LYS:HD3	2.49	0.42
1:V:22:PHE:CE1	1:V:77:GLN:HB3	2.55	0.42
1:V:123:PHE:O	1:V:124:ARG:HD2	2.19	0.42
1:W:3:LEU:C	1:W:4:LEU:HD12	2.43	0.42
1:b:50:THR:H	1:b:52:ILE:HG12	1.83	0.42
1:d:56:SER:O	1:d:59:VAL:HG13	2.19	0.42
1:e:148:SER:HB3	1:f:154:ARG:CZ	2.50	0.42
1:e:151:GLU:OE1	1:e:154:ARG:NH1	2.51	0.42
1:k:112:TYR:HB3	1:k:114:VAL:CG2	2.49	0.42
1:n:117:GLU:O	1:n:120:GLY:N	2.50	0.42
1:C:149:VAL:O	1:C:152:THR:OG1	2.28	0.42
1:F:3:LEU:H	1:F:3:LEU:HD22	1.84	0.42
1:F:74:THR:HG23	1:F:103:ASP:HB2	2.01	0.42
1:G:130:ASP:CG	1:G:132:ASN:H	2.27	0.42
1:K:6:ASN:ND2	1:L:142:ASP:HB2	2.34	0.42
1:K:128:ILE:HG22	1:K:136:ARG:HB2	2.01	0.42
1:M:62:PHE:O	1:M:67:CYS:HB3	2.20	0.42
1:M:84:ASP:O	1:M:94:GLY:HA2	2.19	0.42
1:P:6:ASN:H	1:P:136:ARG:HB3	1.85	0.42
1:P:49:PRO:O	1:P:52:ILE:HG13	2.20	0.42
1:Q:39:PHE:CE1	1:Q:114:VAL:HG21	2.55	0.42
1:R:38:PHE:HE2	1:R:52:ILE:HD12	1.83	0.42
1:U:33:LYS:HB2	1:U:33:LYS:HE3	1.75	0.42
1:U:36:VAL:O	1:U:37:LEU:C	2.62	0.42
1:V:18:ILE:HB	1:V:23:LYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:33:LYS:HG2	1:Z:66:ASN:HB3	2.02	0.42
1:b:53:ILE:HD11	1:b:88:ARG:NH2	2.35	0.42
1:c:68:GLN:OE1	1:c:70:ILE:HG23	2.19	0.42
1:d:134:ILE:HD11	1:d:136:ARG:HH22	1.84	0.42
1:e:86:LEU:HG	1:e:87:ASP:H	1.85	0.42
1:h:42:ALA:CB	1:i:104:ARG:HH22	2.33	0.42
1:h:45:THR:OG1	1:h:46:PHE:N	2.52	0.42
1:n:18:ILE:HD13	1:n:99:PRO:HD3	2.00	0.42
1:A:40:TYR:CE2	1:A:73:SER:HB2	2.55	0.42
1:A:96:MET:HE3	1:A:98:ILE:HB	2.02	0.42
1:B:31:ARG:HH11	1:B:133:GLY:HA3	1.80	0.42
1:C:100:LEU:H	1:C:100:LEU:HD23	1.85	0.42
1:C:130:ASP:HB2	1:C:136:ARG:HG2	2.00	0.42
1:F:114:VAL:HB	1:F:123:PHE:H	1.84	0.42
1:G:33:LYS:O	1:G:131:PRO:HA	2.19	0.42
1:H:40:TYR:CE1	1:H:73:SER:HB2	2.55	0.42
1:J:66:ASN:HB3	1:J:67:CYS:H	1.62	0.42
1:L:37:LEU:HD22	1:L:37:LEU:HA	1.84	0.42
1:O:159:PHE:O	1:O:162:VAL:HG22	2.20	0.42
1:P:86:LEU:O	1:P:94:GLY:HA2	2.20	0.42
1:P:130:ASP:OD1	1:P:133:GLY:N	2.38	0.42
1:X:124:ARG:HD2	1:X:145:VAL:O	2.19	0.42
1:Z:124:ARG:HB3	1:Z:147:ARG:HG3	2.02	0.42
1:a:3:LEU:HD23	1:a:3:LEU:HA	1.78	0.42
1:b:128:ILE:HG13	1:b:136:ARG:HB2	2.01	0.42
1:e:107:GLU:HG3	1:e:108:ILE:HG13	2.01	0.42
1:f:14:GLY:O	1:f:24:GLU:HA	2.19	0.42
1:f:123:PHE:CD2	1:f:143:LYS:HG2	2.54	0.42
1:h:70:ILE:HD11	1:h:101:LEU:HD21	2.01	0.42
1:h:129:ILE:HG13	1:h:130:ASP:N	2.33	0.42
1:m:152:THR:HA	1:m:155:LEU:HB2	2.01	0.42
1:B:31:ARG:HH12	1:B:133:GLY:HA3	1.80	0.42
1:B:127:PHE:CE2	1:B:138:ILE:HG23	2.54	0.42
1:C:5:PRO:HD2	1:D:123:PHE:CE2	2.55	0.42
1:I:76:SER:HA	1:I:104:ARG:HD3	2.01	0.42
1:K:89:LYS:HG3	1:K:90:SER:H	1.85	0.42
1:L:47:VAL:N	1:L:48:PRO:HD3	2.35	0.42
1:M:1:MET:HB2	1:N:2:VAL:HA	2.00	0.42
1:N:104:ARG:HD2	1:O:120:GLY:O	2.20	0.42
1:Q:72:CYS:O	1:Q:80:HIS:NE2	2.35	0.42
1:S:34:TYR:HB2	1:S:66:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:127:PHE:HA	1:W:138:ILE:HD13	2.01	0.42
1:X:6:ASN:HB3	1:X:7:ARG:NH1	2.35	0.42
1:Z:81:LEU:HD12	1:Z:84:ASP:HB3	2.01	0.42
1:Z:105:LYS:HZ3	1:Z:105:LYS:HB2	1.84	0.42
1:e:81:LEU:HD13	1:e:81:LEU:HA	1.89	0.42
1:e:104:ARG:HH12	1:n:121:ASN:N	2.16	0.42
1:f:38:PHE:HE2	1:f:52:ILE:CG1	2.29	0.42
1:h:35:VAL:HG23	1:h:129:ILE:HG23	2.01	0.42
1:i:55:PHE:CE2	1:i:147:ARG:HB2	2.54	0.42
1:k:9:ALA:HA	1:k:10:PRO:HD3	1.87	0.42
1:m:36:VAL:HG13	1:m:69:VAL:HG13	2.01	0.42
1:m:147:ARG:HB3	1:m:147:ARG:CZ	2.48	0.42
1:C:25:ILE:O	1:C:25:ILE:HG23	2.19	0.42
1:C:140:ILE:O	1:D:137:GLN:HG2	2.20	0.42
1:E:151:GLU:HG2	1:F:151:GLU:HG2	2.02	0.42
1:F:38:PHE:O	1:F:71:ALA:HA	2.19	0.42
1:H:51:GLU:O	1:H:54:ALA:HB3	2.20	0.42
1:K:75:ASP:HA	1:K:104:ARG:NE	2.30	0.42
1:L:18:ILE:N	1:L:20:GLY:H	2.17	0.42
1:M:18:ILE:HG13	1:M:19:ASN:N	2.30	0.42
1:N:104:ARG:HH11	1:O:121:ASN:HA	1.85	0.42
1:P:39:PHE:CD2	1:P:72:CYS:HB3	2.55	0.42
1:S:17:VAL:HB	1:S:100:LEU:HB2	2.01	0.42
1:Y:25:ILE:HG21	1:Y:101:LEU:HB3	2.02	0.42
1:d:0:THR:C	1:d:2:VAL:H	2.26	0.42
1:d:52:ILE:HB	1:d:93:LEU:HD21	2.00	0.42
1:e:104:ARG:NH1	1:n:121:ASN:HA	2.31	0.42
1:f:109:SER:HB3	1:f:115:PHE:HB2	2.01	0.42
1:j:67:CYS:HB2	1:j:156:LEU:CD2	2.50	0.42
1:k:51:GLU:H	1:k:51:GLU:HG3	1.61	0.42
1:n:116:ASP:HB2	1:n:122:ALA:C	2.45	0.42
1:A:31:ARG:C	1:A:33:LYS:H	2.28	0.42
1:I:4:LEU:HD22	1:J:123:PHE:CE2	2.55	0.42
1:K:67:CYS:SG	1:K:68:GLN:N	2.93	0.42
1:L:51:GLU:OE2	1:L:146:GLY:HA3	2.20	0.42
1:P:130:ASP:HB3	1:P:133:GLY:HA2	2.01	0.42
1:Q:39:PHE:O	1:Q:40:TYR:HB3	2.20	0.42
1:U:50:THR:OG1	1:U:53:ILE:HG13	2.20	0.42
1:W:9:ALA:HA	1:W:10:PRO:HD3	1.93	0.42
1:W:154:ARG:NH2	1:X:148:SER:HB2	2.34	0.42
1:X:104:ARG:NE	1:Y:121:ASN:OD1	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:126:LEU:HB3	1:a:139:THR:CG2	2.50	0.42
1:b:8:PRO:O	1:b:135:LEU:N	2.53	0.42
1:c:130:ASP:CG	1:c:132:ASN:H	2.28	0.42
1:e:18:ILE:N	1:e:23:LYS:NZ	2.66	0.42
1:e:74:THR:HG21	1:e:121:ASN:HA	2.01	0.42
1:e:124:ARG:O	1:e:147:ARG:HD3	2.20	0.42
1:f:11:GLU:HA	1:f:27:LEU:HD12	2.01	0.42
1:i:3:LEU:HD22	1:j:1:MET:HB3	2.01	0.42
1:i:147:ARG:H	1:i:147:ARG:HE	1.66	0.42
1:j:73:SER:HB3	1:j:80:HIS:CE1	2.55	0.42
1:F:116:ASP:C	1:F:118:GLU:H	2.28	0.41
1:G:3:LEU:HB2	1:H:2:VAL:HB	2.02	0.41
1:J:96:MET:HE3	1:J:98:ILE:HG13	2.01	0.41
1:N:36:VAL:HB	1:N:128:ILE:HD13	2.02	0.41
1:Q:140:ILE:HG23	1:R:138:ILE:HB	2.02	0.41
1:R:74:THR:HG23	1:S:104:ARG:NH2	2.34	0.41
1:T:137:GLN:NE2	1:T:139:THR:HG1	2.16	0.41
1:U:3:LEU:HD23	1:U:3:LEU:HA	1.84	0.41
1:V:39:PHE:CD2	1:V:114:VAL:HG21	2.55	0.41
1:V:104:ARG:HG3	1:W:119:ASP:O	2.20	0.41
1:W:162:VAL:HG23	1:W:163:GLU:OE1	2.20	0.41
1:Y:46:PHE:HA	1:Y:47:VAL:C	2.45	0.41
1:Y:153:LEU:O	1:Y:157:ASP:OD2	2.38	0.41
1:a:67:CYS:SG	1:a:68:GLN:N	2.93	0.41
1:a:162:VAL:HG23	1:a:163:GLU:N	2.34	0.41
1:b:34:TYR:HB2	1:b:66:ASN:O	2.19	0.41
1:b:97:LYS:H	1:b:97:LYS:HG2	1.65	0.41
1:e:50:THR:O	1:e:50:THR:HG22	2.20	0.41
1:e:76:SER:HB3	1:e:104:ARG:HD3	2.01	0.41
1:k:115:PHE:CG	1:k:116:ASP:N	2.88	0.41
1:n:55:PHE:CE2	1:n:149:VAL:HG22	2.55	0.41
1:B:21:GLU:HA	1:B:21:GLU:OE1	2.20	0.41
1:E:34:TYR:O	1:E:35:VAL:HB	2.20	0.41
1:I:53:ILE:HD11	1:I:93:LEU:HD22	2.02	0.41
1:J:37:LEU:HD13	1:J:70:ILE:HD12	2.02	0.41
1:J:141:ASN:HB3	1:J:142:ASP:H	1.68	0.41
1:Q:13:LYS:HA	1:Q:26:CYS:HB3	2.02	0.41
1:Q:44:PHE:HB3	1:Q:83:TRP:CD1	2.55	0.41
1:Q:56:SER:OG	1:Q:93:LEU:HB2	2.21	0.41
1:R:77:GLN:HG3	1:R:78:TYR:H	1.86	0.41
1:T:48:PRO:HB2	1:T:50:THR:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:140:ILE:HB	1:V:138:ILE:HB	2.03	0.41
1:V:112:TYR:HD1	1:V:112:TYR:HA	1.64	0.41
1:X:3:LEU:HD22	1:X:3:LEU:HA	1.84	0.41
1:Z:88:ARG:NH2	1:Z:95:HIS:O	2.52	0.41
1:a:115:PHE:HD2	1:a:117:GLU:OE2	2.03	0.41
1:d:97:LYS:HE3	1:d:97:LYS:HB2	1.87	0.41
1:d:136:ARG:NE	1:d:136:ARG:HA	2.35	0.41
1:f:86:LEU:O	1:f:94:GLY:N	2.50	0.41
1:j:97:LYS:H	1:j:97:LYS:HG2	1.53	0.41
1:j:108:ILE:HG12	1:j:109:SER:N	2.35	0.41
1:k:28:LYS:HA	1:k:31:ARG:NH1	2.35	0.41
1:m:155:LEU:HD23	1:n:145:VAL:HG21	2.02	0.41
1:n:163:GLU:HG3	1:n:164:LYS:HG3	2.02	0.41
1:B:76:SER:HB3	1:B:104:ARG:HE	1.85	0.41
1:H:49:PRO:HB3	1:H:52:ILE:HG13	2.02	0.41
1:H:67:CYS:SG	1:H:68:GLN:N	2.94	0.41
1:K:22:PHE:O	1:K:23:LYS:HB2	2.20	0.41
1:K:88:ARG:HA	1:K:92:GLY:O	2.21	0.41
1:K:123:PHE:CD2	1:L:4:LEU:HD22	2.55	0.41
1:M:31:ARG:O	1:M:131:PRO:HA	2.20	0.41
1:M:153:LEU:O	1:M:156:LEU:HG	2.20	0.41
1:P:40:TYR:O	1:P:73:SER:HA	2.20	0.41
1:S:130:ASP:HB3	1:S:133:GLY:O	2.21	0.41
1:T:13:LYS:HA	1:T:25:ILE:O	2.20	0.41
1:T:50:THR:HB	1:T:51:GLU:H	1.50	0.41
1:T:160:GLN:HG2	1:T:161:PHE:N	2.33	0.41
1:U:5:PRO:C	1:U:7:ARG:H	2.28	0.41
1:U:12:PHE:HE1	1:U:25:ILE:HB	1.85	0.41
1:U:149:VAL:O	1:U:153:LEU:HB2	2.20	0.41
1:V:119:ASP:HB2	1:V:121:ASN:HD21	1.84	0.41
1:X:79:SER:HA	1:Y:44:PHE:CD2	2.55	0.41
1:Y:93:LEU:HD13	1:Y:93:LEU:HA	1.84	0.41
1:a:96:MET:HB2	1:a:100:LEU:HD21	2.03	0.41
1:c:17:VAL:HG13	1:c:22:PHE:CG	2.56	0.41
1:d:49:PRO:HB2	1:d:52:ILE:H	1.84	0.41
1:f:32:GLY:C	1:f:131:PRO:HB3	2.45	0.41
1:f:39:PHE:HB2	1:f:125:GLY:N	2.34	0.41
1:f:141:ASN:HB3	1:f:145:VAL:HG13	2.02	0.41
1:f:147:ARG:NH1	1:f:147:ARG:HB2	2.35	0.41
1:k:76:SER:HB3	1:k:79:SER:HB2	2.02	0.41
1:m:27:LEU:HG	1:m:31:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASP:HB2	1:D:80:HIS:NE2	2.34	0.41
1:E:104:ARG:HG3	1:E:105:LYS:N	2.35	0.41
1:F:130:ASP:CG	1:F:134:ILE:HG12	2.45	0.41
1:F:137:GLN:HE21	1:F:137:GLN:HB3	1.65	0.41
1:G:36:VAL:CG1	1:G:69:VAL:HG22	2.48	0.41
1:H:126:LEU:HB3	1:H:139:THR:HG23	2.03	0.41
1:J:73:SER:O	1:J:102:ALA:HB1	2.20	0.41
1:J:143:LYS:NZ	1:J:143:LYS:HB3	2.36	0.41
1:P:46:PHE:CE1	1:P:47:VAL:HG23	2.55	0.41
1:P:70:ILE:HA	1:P:99:PRO:HG2	2.02	0.41
1:P:143:LYS:HD3	1:P:143:LYS:HA	1.95	0.41
1:U:77:GLN:H	1:U:77:GLN:HG3	1.36	0.41
1:W:34:TYR:CE1	1:W:131:PRO:HD3	2.56	0.41
1:W:73:SER:HB3	1:W:80:HIS:NE2	2.35	0.41
1:W:101:LEU:HD23	1:W:102:ALA:N	2.35	0.41
1:Y:22:PHE:CZ	1:Y:77:GLN:HB3	2.53	0.41
1:Z:38:PHE:HD1	1:Z:38:PHE:H	1.68	0.41
1:Z:41:PRO:HD3	1:Z:147:ARG:HH12	1.85	0.41
1:c:154:ARG:NH1	1:d:148:SER:HB3	2.35	0.41
1:g:73:SER:HB3	1:g:80:HIS:CE1	2.55	0.41
1:h:32:GLY:H	1:h:131:PRO:HB2	1.86	0.41
1:B:4:LEU:HB3	1:B:7:ARG:HG3	2.02	0.41
1:D:3:LEU:C	1:D:4:LEU:HD12	2.45	0.41
1:G:24:GLU:O	1:G:24:GLU:HG3	2.20	0.41
1:G:74:THR:HG22	1:G:104:ARG:NH2	2.36	0.41
1:I:83:TRP:CD2	1:I:93:LEU:HG	2.55	0.41
1:K:7:ARG:HG3	1:K:8:PRO:HD2	2.03	0.41
1:K:124:ARG:HA	1:K:147:ARG:NH2	2.36	0.41
1:L:45:THR:C	1:L:47:VAL:N	2.78	0.41
1:N:65:ARG:CB	1:N:156:LEU:HD23	2.51	0.41
1:P:34:TYR:CD1	1:P:131:PRO:HG3	2.56	0.41
1:Q:44:PHE:HD2	1:Q:83:TRP:CD1	2.38	0.41
1:Q:84:ASP:CG	1:Q:96:MET:HB2	2.45	0.41
1:R:50:THR:HG23	1:R:53:ILE:HG13	2.01	0.41
1:S:4:LEU:HB2	1:S:7:ARG:HD2	2.03	0.41
1:X:33:LYS:HB2	1:X:34:TYR:HB2	2.02	0.41
1:Y:18:ILE:HG21	1:Y:98:ILE:O	2.20	0.41
1:Y:139:THR:CG2	1:Z:139:THR:HG23	2.50	0.41
1:Z:112:TYR:HB3	1:Z:127:PHE:CE2	2.56	0.41
1:b:93:LEU:HD13	1:b:96:MET:CG	2.50	0.41
1:d:157:ASP:O	1:d:161:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:153:LEU:O	1:e:157:ASP:OD2	2.38	0.41
1:f:105:LYS:HG2	1:g:118:GLU:O	2.21	0.41
1:f:164:LYS:NZ	1:f:165:HIS:CE1	2.89	0.41
1:g:118:GLU:OE1	1:g:118:GLU:N	2.41	0.41
1:i:136:ARG:HD3	1:i:159:PHE:CD2	2.55	0.41
1:j:9:ALA:H	1:j:133:GLY:C	2.21	0.41
1:j:76:SER:OG	1:j:104:ARG:NH1	2.53	0.41
1:k:39:PHE:HA	1:k:72:CYS:O	2.20	0.41
1:m:118:GLU:OE1	1:m:118:GLU:N	2.51	0.41
1:B:4:LEU:HB3	1:B:7:ARG:HG2	2.02	0.41
1:K:39:PHE:CE2	1:K:114:VAL:HG21	2.56	0.41
1:K:72:CYS:CB	1:K:101:LEU:HB3	2.50	0.41
1:K:115:PHE:HA	1:K:122:ALA:HA	2.01	0.41
1:N:75:ASP:OD2	1:O:79:SER:OG	2.33	0.41
1:O:127:PHE:CE1	1:O:138:ILE:HG23	2.55	0.41
1:P:19:ASN:O	1:P:19:ASN:ND2	2.53	0.41
1:Q:63:ASN:N	1:Q:63:ASN:OD1	2.53	0.41
1:R:56:SER:O	1:R:59:VAL:HG13	2.21	0.41
1:R:58:GLN:O	1:R:61:GLU:HG3	2.20	0.41
1:T:41:PRO:CB	1:T:143:LYS:HZ2	2.26	0.41
1:X:39:PHE:HB2	1:X:125:GLY:H	1.85	0.41
1:X:41:PRO:HG3	1:X:143:LYS:HZ2	1.85	0.41
1:Z:56:SER:HB2	1:Z:96:MET:HE3	2.01	0.41
1:b:8:PRO:O	1:b:9:ALA:HB2	2.21	0.41
1:d:151:GLU:O	1:d:155:LEU:HG	2.21	0.41
1:d:163:GLU:HB2	1:d:164:LYS:HZ3	1.86	0.41
1:g:76:SER:HA	1:g:104:ARG:HD3	2.02	0.41
1:g:128:ILE:O	1:g:135:LEU:HD12	2.21	0.41
1:j:128:ILE:CG2	1:j:136:ARG:HB3	2.49	0.41
1:m:15:GLN:HG3	1:m:24:GLU:HB2	2.02	0.41
1:E:11:GLU:HG2	1:E:27:LEU:CB	2.48	0.41
1:E:37:LEU:HD12	1:E:127:PHE:HD2	1.85	0.41
1:G:64:SER:HB2	1:G:65:ARG:HH12	1.82	0.41
1:I:71:ALA:HB3	1:I:100:LEU:HD23	2.03	0.41
1:P:164:LYS:O	1:P:165:HIS:ND1	2.54	0.41
1:Q:10:PRO:HD2	1:Q:112:TYR:CD2	2.56	0.41
1:R:34:TYR:N	1:R:34:TYR:CD1	2.86	0.41
1:S:74:THR:HA	1:S:103:ASP:O	2.20	0.41
1:U:12:PHE:O	1:U:26:CYS:HA	2.21	0.41
1:U:147:ARG:O	1:U:148:SER:OG	2.36	0.41
1:V:39:PHE:HB2	1:V:124:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:45:THR:OG1	1:V:46:PHE:HD1	2.04	0.41
1:Y:149:VAL:O	1:Y:153:LEU:HD22	2.21	0.41
1:Z:39:PHE:CE2	1:Z:109:SER:HA	2.56	0.41
1:Z:41:PRO:O	1:a:104:ARG:NH2	2.44	0.41
1:a:44:PHE:HA	1:a:83:TRP:CE2	2.55	0.41
1:a:116:ASP:C	1:a:118[B]:GLU:H	2.28	0.41
1:a:145:VAL:HG23	1:b:162:VAL:HG21	2.03	0.41
1:d:55:PHE:HD1	1:d:149:VAL:HG22	1.84	0.41
1:f:13[A]:LYS:HZ1	1:f:24:GLU:HG2	1.85	0.41
1:h:78:TYR:HB3	1:i:44:PHE:HB3	2.01	0.41
1:i:145:VAL:HB	1:j:159:PHE:CE1	2.56	0.41
1:l:78:TYR:O	1:l:82:ALA:HB3	2.21	0.41
1:l:103:ASP:HA	1:l:108:ILE:HD11	2.02	0.41
1:l:126:LEU:HB3	1:l:139:THR:HB	2.01	0.41
1:l:127:PHE:CD1	1:l:138:ILE:HG13	2.55	0.41
1:A:58:GLN:HE22	1:A:61:GLU:HG3	1.86	0.41
1:C:114:VAL:HG13	1:C:123:PHE:HB2	2.02	0.41
1:D:65:ARG:HH11	1:D:157:ASP:CG	2.18	0.41
1:F:44:PHE:HB2	1:G:78:TYR:HB3	2.01	0.41
1:G:56:SER:CB	1:G:96:MET:HG3	2.51	0.41
1:H:59:VAL:HG12	1:H:69:VAL:HG21	2.03	0.41
1:H:124:ARG:HD2	1:H:147:ARG:HH11	1.85	0.41
1:K:89:LYS:HB2	1:K:89:LYS:HE3	1.73	0.41
1:M:2:VAL:HG13	1:M:3:LEU:N	2.36	0.41
1:M:34:TYR:OH	1:M:163:GLU:OE2	2.38	0.41
1:N:47:VAL:HG11	1:N:51:GLU:OE2	2.20	0.41
1:O:110:LYS:HG2	1:O:110:LYS:H	1.60	0.41
1:S:13:LYS:HB3	1:S:13:LYS:HZ2	1.85	0.41
1:S:110:LYS:HD3	1:S:115:PHE:CD2	2.55	0.41
1:U:96:MET:HB3	1:U:100:LEU:HD11	2.03	0.41
1:U:105:LYS:HB3	1:U:105:LYS:NZ	2.35	0.41
1:V:2:VAL:HG22	1:V:3:LEU:N	2.36	0.41
1:V:42:ALA:O	1:V:73:SER:OG	2.26	0.41
1:W:66:ASN:HD22	1:W:66:ASN:HA	1.71	0.41
1:Z:46:PHE:HD1	1:Z:47:VAL:H	1.68	0.41
1:a:116:ASP:C	1:a:118[A]:GLU:H	2.28	0.41
1:d:36:VAL:HA	1:d:127:PHE:O	2.19	0.41
1:d:164:LYS:H	1:d:164:LYS:HE2	1.85	0.41
1:e:49:PRO:O	1:e:50:THR:OG1	2.31	0.41
1:e:50:THR:HA	1:e:53:ILE:CG1	2.49	0.41
1:h:50:THR:OG1	1:h:54:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:11:GLU:HG2	1:i:27:LEU:HD12	2.02	0.41
1:l:28:LYS:HA	1:l:31:ARG:CZ	2.51	0.41
1:l:136:ARG:HA	1:l:136:ARG:HD2	1.76	0.41
1:m:71:ALA:O	1:m:101:LEU:N	2.54	0.41
1:n:130:ASP:CG	1:n:134:ILE:HB	2.45	0.41
1:A:5:PRO:C	1:A:7:ARG:H	2.29	0.41
1:A:78:TYR:CZ	1:J:45:THR:HG23	2.55	0.41
1:A:78:TYR:HA	1:A:81:LEU:HB2	2.02	0.41
1:A:106:GLN:O	1:A:109:SER:OG	2.38	0.41
1:B:104:ARG:HG2	1:C:119:ASP:O	2.21	0.41
1:D:54:ALA:O	1:D:58[B]:GLN:HG2	2.21	0.41
1:D:107:GLU:HG3	1:D:108:ILE:N	2.36	0.41
1:E:65:ARG:NH1	1:E:153:LEU:HD22	2.36	0.41
1:E:140:ILE:HD13	1:E:141:ASN:N	2.35	0.41
1:G:4:LEU:HB3	1:H:123:PHE:CE1	2.56	0.41
1:G:123:PHE:CZ	1:H:6:ASN:HB2	2.56	0.41
1:H:130:ASP:CB	1:H:136:ARG:HH11	2.33	0.41
1:H:142:ASP:HB3	1:H:144:PRO:HD2	2.03	0.41
1:I:53:ILE:HA	1:I:96:MET:HE1	2.02	0.41
1:K:52:ILE:H	1:K:52:ILE:HD12	1.86	0.41
1:L:15:GLN:O	1:L:102:ALA:N	2.53	0.41
1:M:11:GLU:OE2	1:M:31:ARG:NH2	2.54	0.41
1:N:28:LYS:HD3	1:g:58:GLN:NE2	2.36	0.41
1:N:110:LYS:HE2	1:N:110:LYS:HB3	1.84	0.41
1:O:89:LYS:H	1:O:89:LYS:HG3	1.66	0.41
1:P:62:PHE:O	1:P:67:CYS:HB3	2.21	0.41
1:P:83:TRP:HB3	1:P:93:LEU:HB2	2.02	0.41
1:P:128:ILE:O	1:P:135:LEU:HG	2.20	0.41
1:P:153:LEU:HD13	1:P:153:LEU:HA	1.86	0.41
1:Q:57:ASP:O	1:Q:59:VAL:HG23	2.21	0.41
1:R:62:PHE:CA	1:R:67:CYS:HB3	2.51	0.41
1:R:130:ASP:HB2	1:R:136:ARG:HH11	1.86	0.41
1:R:147:ARG:HD3	1:R:147:ARG:HA	1.83	0.41
1:S:93:LEU:HD12	1:S:93:LEU:O	2.21	0.41
1:S:128:ILE:HG12	1:S:137:GLN:HG2	2.02	0.41
1:S:135:LEU:HD23	1:S:135:LEU:HA	1.95	0.41
1:T:109:SER:CB	1:T:115:PHE:HB2	2.50	0.41
1:W:86:LEU:HB2	1:W:92:GLY:HA3	2.03	0.41
1:X:16:ALA:HA	1:X:100:LEU:O	2.20	0.41
1:X:34:TYR:HB3	1:X:35:VAL:H	1.61	0.41
1:Y:73:SER:C	1:Y:75:ASP:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:113:GLY:O	1:Z:4:LEU:HD11	2.21	0.41
1:Y:130:ASP:HB3	1:Y:136:ARG:HD2	2.03	0.41
1:Z:74:THR:HB	1:a:104:ARG:HD2	2.02	0.41
1:a:22:PHE:HD1	1:a:22:PHE:HA	1.75	0.41
1:a:87:ASP:OD2	1:a:90:SER:OG	2.36	0.41
1:b:75:ASP:HA	1:c:104:ARG:CZ	2.51	0.41
1:c:25:ILE:O	1:c:27:LEU:N	2.54	0.41
1:c:74:THR:OG1	1:c:75:ASP:N	2.49	0.41
1:c:105:LYS:HB3	1:c:107:GLU:OE1	2.21	0.41
1:d:18:ILE:HB	1:d:23:LYS:HZ2	1.86	0.41
1:e:40:TYR:CZ	1:e:73:SER:HB2	2.56	0.41
1:e:68:GLN:O	1:e:70:ILE:HD12	2.21	0.41
1:f:25:ILE:HG22	1:f:26:CYS:H	1.85	0.41
1:f:39:PHE:CD1	1:f:72:CYS:HB3	2.56	0.41
1:g:84:ASP:HA	1:g:93:LEU:HB2	2.02	0.41
1:g:109:SER:HB3	1:g:114:VAL:O	2.21	0.41
1:h:9:ALA:HA	1:h:10:PRO:HD3	1.80	0.41
1:i:37:LEU:O	1:i:127:PHE:N	2.39	0.41
1:j:3:LEU:HB3	1:j:135:LEU:HD21	2.01	0.41
1:k:124:ARG:NH1	1:k:146:GLY:HA2	2.35	0.41
1:l:12:PHE:O	1:l:26:CYS:HA	2.21	0.41
1:l:32:GLY:HA2	1:l:131:PRO:HB3	2.03	0.41
1:A:151:GLU:CB	1:B:151:GLU:HG3	2.42	0.41
1:D:114:VAL:CG2	1:D:115:PHE:H	2.27	0.41
1:F:125:GLY:HA2	1:F:140:ILE:HA	2.03	0.41
1:H:104:ARG:NH2	1:I:121:ASN:OD1	2.54	0.41
1:L:5:PRO:HB3	1:L:136:ARG:HA	2.02	0.41
1:M:41:PRO:O	1:M:121:ASN:ND2	2.54	0.41
1:M:48:PRO:HG2	1:M:49:PRO:HD3	2.03	0.41
1:P:30:TYR:CZ	1:P:68:GLN:HB2	2.55	0.41
1:P:75:ASP:O	1:P:76:SER:OG	2.28	0.41
1:S:87:ASP:HA	1:S:94:GLY:HA2	2.03	0.41
1:S:136:ARG:HG3	1:T:142:ASP:CB	2.50	0.41
1:T:156:LEU:O	1:T:160:GLN:HB3	2.21	0.41
1:Z:3:LEU:HD13	1:Z:4:LEU:N	2.36	0.41
1:a:33:LYS:HG2	1:a:66:ASN:HD22	1.86	0.41
1:c:37:LEU:HD22	1:c:37:LEU:HA	1.86	0.41
1:j:3:LEU:HD23	1:j:3:LEU:HA	1.85	0.41
1:k:108:ILE:O	1:k:112:TYR:HB2	2.20	0.41
1:l:33:LYS:HD2	1:l:66:ASN:OD1	2.21	0.41
1:m:65:ARG:NH2	1:m:153:LEU:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:39:PHE:CB	1:n:124:ARG:HA	2.45	0.41
1:C:5:PRO:HG2	1:D:142:ASP:HB3	2.02	0.40
1:C:130:ASP:CG	1:C:131:PRO:HD2	2.46	0.40
1:E:40:TYR:CZ	1:E:73:SER:HB2	2.56	0.40
1:F:18:ILE:C	1:F:20:GLY:N	2.79	0.40
1:F:47:VAL:O	1:F:49:PRO:HD3	2.21	0.40
1:H:86:LEU:HB3	1:H:92:GLY:HA3	2.03	0.40
1:K:6:ASN:ND2	1:L:143:LYS:NZ	2.69	0.40
1:K:58:GLN:HE22	1:K:61:GLU:HG3	1.86	0.40
1:L:52:ILE:HD11	1:L:124:ARG:CZ	2.51	0.40
1:L:104:ARG:HD2	1:M:120:GLY:HA3	2.02	0.40
1:M:25:ILE:CG1	1:M:101:LEU:HD21	2.50	0.40
1:M:55:PHE:CE2	1:M:69:VAL:HG21	2.56	0.40
1:O:62:PHE:O	1:O:67:CYS:N	2.50	0.40
1:P:164:LYS:HE3	1:P:164:LYS:HB3	1.70	0.40
1:R:10:PRO:HD2	1:R:112:TYR:CE1	2.57	0.40
1:T:72:CYS:SG	1:T:103:ASP:HB2	2.61	0.40
1:V:43:ASP:HB2	1:V:75:ASP:OD2	2.20	0.40
1:V:44:PHE:H	1:V:83:TRP:HE1	1.69	0.40
1:X:38:PHE:CE1	1:X:71:ALA:HB2	2.56	0.40
1:X:43:ASP:OD2	1:X:80:HIS:CD2	2.70	0.40
1:b:46:PHE:HB3	1:b:47:VAL:CA	2.51	0.40
1:b:117:GLU:H	1:b:117:GLU:CD	2.29	0.40
1:e:74:THR:O	1:e:104:ARG:HA	2.21	0.40
1:g:41:PRO:HD3	1:g:124:ARG:HH12	1.82	0.40
1:i:53:ILE:HD12	1:i:93:LEU:O	2.21	0.40
1:k:37:LEU:HD11	1:k:127:PHE:CD2	2.56	0.40
1:l:62:PHE:CG	1:l:69:VAL:HG21	2.57	0.40
1:m:11:GLU:OE2	1:m:28:LYS:HG2	2.20	0.40
1:n:13:LYS:HB2	1:n:13:LYS:HE3	1.69	0.40
1:G:137:GLN:NE2	1:G:139:THR:HB	2.35	0.40
1:H:16:ALA:HB2	1:H:25:ILE:HG12	2.03	0.40
1:M:38:PHE:HE2	1:M:147:ARG:HH11	1.68	0.40
1:U:98:ILE:O	1:U:100:LEU:HD12	2.21	0.40
1:V:163:GLU:H	1:V:163:GLU:CD	2.29	0.40
1:a:93:LEU:HD13	1:a:96:MET:HG3	2.01	0.40
1:f:39:PHE:HB2	1:f:125:GLY:H	1.86	0.40
1:f:137:GLN:HE21	1:f:155:LEU:HD13	1.86	0.40
1:i:159:PHE:CZ	1:j:142:ASP:HB3	2.56	0.40
1:j:76:SER:HB2	1:j:79:SER:HB2	2.03	0.40
1:k:56:SER:HB3	1:k:96:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:88:ARG:HA	1:k:92:GLY:O	2.21	0.40
1:l:127:PHE:CE1	1:l:138:ILE:HG13	2.57	0.40
1:m:159:PHE:HD1	1:m:159:PHE:HA	1.78	0.40
1:A:70:ILE:HG13	1:A:99:PRO:O	2.22	0.40
1:E:136:ARG:HD3	1:E:136:ARG:HA	1.89	0.40
1:H:70:ILE:HG12	1:H:99:PRO:HB2	2.03	0.40
1:M:114:VAL:O	1:M:123:PHE:HB2	2.21	0.40
1:M:142:ASP:OD2	1:N:136:ARG:HA	2.21	0.40
1:O:145:VAL:HG21	1:P:159:PHE:CD1	2.57	0.40
1:Q:12:PHE:O	1:Q:26:CYS:HB2	2.21	0.40
1:Q:137:GLN:HG3	1:Q:138:ILE:N	2.36	0.40
1:S:52:ILE:HG12	1:S:53:ILE:HG13	2.03	0.40
1:T:116:ASP:OD1	1:T:119:ASP:HB2	2.21	0.40
1:U:34:TYR:O	1:U:35:VAL:C	2.64	0.40
1:U:73:SER:O	1:U:103:ASP:HB3	2.22	0.40
1:X:81:LEU:O	1:X:85:ASN:HB2	2.21	0.40
1:X:86:LEU:HB3	1:X:92:GLY:HA3	2.03	0.40
1:X:98:ILE:O	1:X:100:LEU:HD22	2.21	0.40
1:Y:9:ALA:HA	1:Y:10:PRO:HD3	1.92	0.40
1:a:18:ILE:HD13	1:a:99:PRO:HA	2.03	0.40
1:b:37:LEU:HA	1:b:70:ILE:HG12	2.03	0.40
1:b:105:LYS:HE2	1:b:105:LYS:HB3	1.94	0.40
1:g:69:VAL:O	1:g:99:PRO:HD2	2.22	0.40
1:h:40:TYR:HA	1:h:41:PRO:HD3	1.93	0.40
1:k:16:ALA:HB3	1:k:101:LEU:HA	2.02	0.40
1:l:65:ARG:NH1	1:l:157:ASP:OD1	2.53	0.40
1:m:128:ILE:HB	1:m:137:GLN:HB3	2.02	0.40
1:n:52:ILE:HD12	1:n:93:LEU:HD11	2.03	0.40
1:A:124:ARG:HA	1:A:147:ARG:NH1	2.36	0.40
1:D:119:ASP:CG	1:D:143:LYS:NZ	2.70	0.40
1:E:61:GLU:O	1:E:65:ARG:NH1	2.54	0.40
1:G:40:TYR:HA	1:G:41:PRO:HD3	1.81	0.40
1:H:37:LEU:HD21	1:H:39:PHE:CZ	2.56	0.40
1:I:80:HIS:HB3	1:I:100:LEU:HD13	2.02	0.40
1:J:101:LEU:HD22	1:J:102:ALA:H	1.86	0.40
1:L:5:PRO:HA	1:L:135:LEU:HD12	2.04	0.40
1:M:22:PHE:CE1	1:M:77:GLN:HB3	2.56	0.40
1:N:144:PRO:HG2	1:N:145:VAL:HG22	2.03	0.40
1:O:116:ASP:OD2	1:O:119:ASP:N	2.50	0.40
1:S:124:ARG:HH11	1:S:124:ARG:HA	1.86	0.40
1:U:40:TYR:HA	1:U:41:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:56:SER:HB2	1:U:97:LYS:N	2.31	0.40
1:Z:40:TYR:HE1	1:Z:43:ASP:CG	2.29	0.40
1:Z:98:ILE:HA	1:Z:99:PRO:HD3	1.76	0.40
1:c:23:LYS:HE3	1:c:23:LYS:HB3	1.87	0.40
1:d:7:ARG:HA	1:d:8:PRO:HD3	1.72	0.40
1:d:137:GLN:HE22	1:d:139:THR:HB	1.87	0.40
1:f:71:ALA:O	1:f:101:LEU:HD23	2.22	0.40
1:f:97:LYS:HA	1:f:97:LYS:HD3	1.85	0.40
1:g:49:PRO:HA	1:g:50:THR:HA	1.67	0.40
1:g:110:LYS:HE2	1:g:115:PHE:CE2	2.57	0.40
1:h:129:ILE:HA	1:h:135:LEU:HD12	2.04	0.40
1:i:27:LEU:HA	1:i:30:TYR:CD2	2.56	0.40
1:k:123:PHE:O	1:k:124:ARG:HG3	2.22	0.40
1:n:122:ALA:O	1:n:143:LYS:HE2	2.22	0.40
1:A:124:ARG:HB2	1:A:141:ASN:H	1.85	0.40
1:D:104:ARG:C	1:D:106:GLN:N	2.80	0.40
1:E:75:ASP:HB3	1:E:79:SER:OG	2.21	0.40
1:F:127:PHE:CE2	1:F:138:ILE:HG23	2.56	0.40
1:F:130:ASP:OD1	1:F:134:ILE:HG12	2.22	0.40
1:G:98:ILE:HA	1:G:99:PRO:HD2	1.91	0.40
1:H:59:VAL:HG11	1:H:98:ILE:HG12	2.03	0.40
1:J:125:GLY:C	1:J:147:ARG:HH12	2.29	0.40
1:P:106:GLN:NE2	1:Q:106:GLN:OE1	2.54	0.40
1:R:54:ALA:O	1:R:58:GLN:HG3	2.21	0.40
1:T:160:GLN:HB3	1:T:160:GLN:HE21	1.66	0.40
1:a:17:VAL:HG21	1:a:81:LEU:HB2	2.04	0.40
1:h:33:LYS:HE3	1:h:33:LYS:HB3	1.90	0.40
1:i:4:LEU:HD12	1:i:5:PRO:HD2	2.04	0.40
1:j:33:LYS:C	1:j:131:PRO:HD3	2.46	0.40
1:l:86:LEU:CB	1:l:92:GLY:HA3	2.50	0.40

All (2) 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:N:19:ASN:ND2	1:b:60:GLU:OE2[2_655]	2.06	0.14
1:R:33:LYS:NZ	1:Y:66:ASN:OD1[1_565]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/186 (87%)	132 (82%)	27 (17%)	2 (1%)	10	42
1	B	165/186 (89%)	145 (88%)	18 (11%)	2 (1%)	10	42
1	C	163/186 (88%)	141 (86%)	18 (11%)	4 (2%)	4	28
1	D	164/186 (88%)	148 (90%)	13 (8%)	3 (2%)	6	34
1	E	160/186 (86%)	134 (84%)	20 (12%)	6 (4%)	2	20
1	F	163/186 (88%)	140 (86%)	17 (10%)	6 (4%)	2	21
1	G	161/186 (87%)	135 (84%)	25 (16%)	1 (1%)	21	55
1	H	163/186 (88%)	131 (80%)	25 (15%)	7 (4%)	2	18
1	I	162/186 (87%)	131 (81%)	28 (17%)	3 (2%)	6	33
1	J	164/186 (88%)	144 (88%)	19 (12%)	1 (1%)	21	55
1	K	159/186 (86%)	133 (84%)	23 (14%)	3 (2%)	6	33
1	L	164/186 (88%)	140 (85%)	22 (13%)	2 (1%)	10	42
1	M	163/186 (88%)	137 (84%)	24 (15%)	2 (1%)	10	42
1	N	164/186 (88%)	143 (87%)	20 (12%)	1 (1%)	21	55
1	O	161/186 (87%)	139 (86%)	19 (12%)	3 (2%)	6	33
1	P	163/186 (88%)	134 (82%)	23 (14%)	6 (4%)	2	21
1	Q	154/186 (83%)	118 (77%)	29 (19%)	7 (4%)	2	17
1	R	162/186 (87%)	136 (84%)	25 (15%)	1 (1%)	21	55
1	S	162/186 (87%)	136 (84%)	23 (14%)	3 (2%)	6	33
1	T	164/186 (88%)	141 (86%)	20 (12%)	3 (2%)	6	34
1	U	161/186 (87%)	135 (84%)	21 (13%)	5 (3%)	3	24
1	V	165/186 (89%)	141 (86%)	21 (13%)	3 (2%)	6	34
1	W	163/186 (88%)	132 (81%)	28 (17%)	3 (2%)	6	34
1	X	164/186 (88%)	137 (84%)	23 (14%)	4 (2%)	4	29
1	Y	161/186 (87%)	133 (83%)	26 (16%)	2 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	163/186 (88%)	136 (83%)	25 (15%)	2 (1%)	10	42
1	a	162/186 (87%)	135 (83%)	24 (15%)	3 (2%)	6	33
1	b	163/186 (88%)	133 (82%)	28 (17%)	2 (1%)	10	42
1	c	162/186 (87%)	136 (84%)	23 (14%)	3 (2%)	6	33
1	d	164/186 (88%)	146 (89%)	17 (10%)	1 (1%)	21	55
1	e	160/186 (86%)	134 (84%)	21 (13%)	5 (3%)	3	24
1	f	165/186 (89%)	149 (90%)	14 (8%)	2 (1%)	10	42
1	g	163/186 (88%)	134 (82%)	25 (15%)	4 (2%)	4	28
1	h	163/186 (88%)	136 (83%)	25 (15%)	2 (1%)	10	42
1	i	154/186 (83%)	121 (79%)	31 (20%)	2 (1%)	9	40
1	j	163/186 (88%)	136 (83%)	24 (15%)	3 (2%)	6	34
1	k	162/186 (87%)	136 (84%)	23 (14%)	3 (2%)	6	33
1	l	163/186 (88%)	135 (83%)	23 (14%)	5 (3%)	3	24
1	m	154/186 (83%)	129 (84%)	24 (16%)	1 (1%)	21	55
1	n	164/186 (88%)	125 (76%)	32 (20%)	7 (4%)	2	18
All	All	6481/7440 (87%)	5437 (84%)	916 (14%)	128 (2%)	6	32

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	E	34	TYR
1	E	106	GLN
1	F	19	ASN
1	H	69	VAL
1	H	142	ASP
1	I	69	VAL
1	L	36	VAL
1	O	69	VAL
1	P	34	TYR
1	Q	34	TYR
1	Q	52	ILE
1	U	53	ILE
1	W	52	ILE
1	Z	19	ASN
1	e	50	THR
1	g	35	VAL

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Mol	Chain	Res	Type
1	g	142	ASP
1	k	52	ILE
1	l	74	THR
1	A	32	GLY
1	E	35	VAL
1	E	52	ILE
1	H	46	PHE
1	H	123	PHE
1	O	70	ILE
1	P	35	VAL
1	P	137	GLN
1	Q	134	ILE
1	U	50	THR
1	V	70	ILE
1	X	54	ALA
1	X	140	ILE
1	Y	18	ILE
1	Y	69	VAL
1	Z	18	ILE
1	c	6	ASN
1	h	35	VAL
1	i	90	SER
1	j	69	VAL
1	n	31	ARG
1	C	17	VAL
1	C	31	ARG
1	C	107	GLU
1	E	46	PHE
1	F	45	THR
1	H	16	ALA
1	I	70	ILE
1	S	134	ILE
1	S	136	ARG
1	T	46	PHE
1	U	51	GLU
1	a	52	ILE
1	e	49	PRO
1	e	137	GLN
1	f	123	PHE
1	g	52	ILE
1	G	11	GLU
1	J	52	ILE

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Mol	Chain	Res	Type
1	K	46	PHE
1	Q	59	VAL
1	S	45	THR
1	T	11	GLU
1	W	72	CYS
1	a	67	CYS
1	j	121	ASN
1	l	73	SER
1	l	104	ARG
1	m	52	ILE
1	n	53	ILE
1	n	59	VAL
1	C	25	ILE
1	D	105	LYS
1	F	18	ILE
1	F	163	GLU
1	L	19	ASN
1	M	143	LYS
1	N	75	ASP
1	T	6	ASN
1	V	71	ALA
1	V	102	ALA
1	X	35	VAL
1	X	53	ILE
1	f	59	VAL
1	l	31	ARG
1	n	115	PHE
1	n	116	ASP
1	B	3	LEU
1	D	70	ILE
1	H	114	VAL
1	P	106	GLN
1	e	93	LEU
1	E	120	GLY
1	R	114	VAL
1	a	35	VAL
1	b	9	ALA
1	b	41	PRO
1	c	5	PRO
1	g	25	ILE
1	k	114	VAL
1	B	4	LEU

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Mol	Chain	Res	Type
1	H	25	ILE
1	P	114	VAL
1	Q	35	VAL
1	U	69	VAL
1	d	69	VAL
1	h	69	VAL
1	k	35	VAL
1	n	133	GLY
1	K	114	VAL
1	M	144	PRO
1	Q	40	TYR
1	e	70	ILE
1	i	140	ILE
1	D	114	VAL
1	F	52	ILE
1	I	41	PRO
1	K	70	ILE
1	O	18	ILE
1	P	145	VAL
1	Q	36	VAL
1	U	52	ILE
1	W	134	ILE
1	c	114	VAL
1	j	114	VAL
1	l	47	VAL
1	n	41	PRO
1	F	2	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/162 (88%)	121 (85%)	21 (15%)	3	17
1	B	146/162 (90%)	130 (89%)	16 (11%)	6	27
1	C	144/162 (89%)	125 (87%)	19 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	145/162 (90%)	126 (87%)	19 (13%)	4	21
1	E	141/162 (87%)	126 (89%)	15 (11%)	6	28
1	F	144/162 (89%)	124 (86%)	20 (14%)	3	20
1	G	142/162 (88%)	114 (80%)	28 (20%)	1	8
1	H	144/162 (89%)	114 (79%)	30 (21%)	1	6
1	I	143/162 (88%)	123 (86%)	20 (14%)	3	19
1	J	145/162 (90%)	123 (85%)	22 (15%)	3	17
1	K	140/162 (86%)	112 (80%)	28 (20%)	1	7
1	L	145/162 (90%)	112 (77%)	33 (23%)	1	5
1	M	144/162 (89%)	125 (87%)	19 (13%)	4	21
1	N	145/162 (90%)	117 (81%)	28 (19%)	1	8
1	O	142/162 (88%)	120 (84%)	22 (16%)	2	16
1	P	144/162 (89%)	118 (82%)	26 (18%)	2	10
1	Q	137/162 (85%)	107 (78%)	30 (22%)	1	6
1	R	143/162 (88%)	126 (88%)	17 (12%)	5	24
1	S	143/162 (88%)	121 (85%)	22 (15%)	2	16
1	T	145/162 (90%)	123 (85%)	22 (15%)	3	17
1	U	142/162 (88%)	118 (83%)	24 (17%)	2	13
1	V	146/162 (90%)	119 (82%)	27 (18%)	1	9
1	W	144/162 (89%)	116 (81%)	28 (19%)	1	8
1	X	145/162 (90%)	123 (85%)	22 (15%)	3	17
1	Y	142/162 (88%)	117 (82%)	25 (18%)	2	11
1	Z	144/162 (89%)	118 (82%)	26 (18%)	2	10
1	a	143/162 (88%)	117 (82%)	26 (18%)	2	10
1	b	144/162 (89%)	124 (86%)	20 (14%)	3	20
1	c	143/162 (88%)	112 (78%)	31 (22%)	1	6
1	d	145/162 (90%)	121 (83%)	24 (17%)	2	13
1	e	141/162 (87%)	114 (81%)	27 (19%)	1	8
1	f	146/162 (90%)	114 (78%)	32 (22%)	1	6
1	g	144/162 (89%)	117 (81%)	27 (19%)	1	9
1	h	144/162 (89%)	119 (83%)	25 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	137/162 (85%)	99 (72%)	38 (28%)	0	3
1	j	144/162 (89%)	119 (83%)	25 (17%)	2	11
1	k	143/162 (88%)	116 (81%)	27 (19%)	1	9
1	l	144/162 (89%)	113 (78%)	31 (22%)	1	6
1	m	137/162 (85%)	115 (84%)	22 (16%)	2	14
1	n	145/162 (90%)	126 (87%)	19 (13%)	4	21
All	All	5727/6480 (88%)	4744 (83%)	983 (17%)	2	12

All (983) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	LEU
1	A	7	ARG
1	A	31	ARG
1	A	36	VAL
1	A	58	GLN
1	A	59	VAL
1	A	74	THR
1	A	77	GLN
1	A	81	LEU
1	A	84	ASP
1	A	93	LEU
1	A	101	LEU
1	A	105	LYS
1	A	114	VAL
1	A	124	ARG
1	A	134	ILE
1	A	139	THR
1	A	140	ILE
1	A	154	ARG
1	A	163	GLU
1	B	6	ASN
1	B	13[A]	LYS
1	B	13[B]	LYS
1	B	18	ILE
1	B	25	ILE
1	B	53	ILE
1	B	58	GLN
1	B	59	VAL

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Mol	Chain	Res	Type
1	B	75	ASP
1	B	81	LEU
1	B	83	TRP
1	B	86	LEU
1	B	93	LEU
1	B	104	ARG
1	B	134	ILE
1	B	154	ARG
1	C	17	VAL
1	C	47	VAL
1	C	51	GLU
1	C	53	ILE
1	C	58	GLN
1	C	61	GLU
1	C	65	ARG
1	C	69	VAL
1	C	93	LEU
1	C	97	LYS
1	C	98	ILE
1	C	100	LEU
1	C	104	ARG
1	C	119	ASP
1	C	121	ASN
1	C	123	PHE
1	C	126	LEU
1	C	155	LEU
1	C	164	LYS
1	D	7	ARG
1	D	13	LYS
1	D	17	VAL
1	D	24	GLU
1	D	25	ILE
1	D	27	LEU
1	D	52	ILE
1	D	69	VAL
1	D	88	ARG
1	D	93	LEU
1	D	96	MET
1	D	97	LYS
1	D	104	ARG
1	D	127	PHE
1	D	147	ARG

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Mol	Chain	Res	Type
1	D	151	GLU
1	D	155	LEU
1	D	159	PHE
1	D	164	LYS
1	E	4	LEU
1	E	7	ARG
1	E	25	ILE
1	E	33	LYS
1	E	35	VAL
1	E	46	PHE
1	E	47	VAL
1	E	52	ILE
1	E	60	GLU
1	E	105	LYS
1	E	106	GLN
1	E	135	LEU
1	E	140	ILE
1	E	147	ARG
1	E	161	PHE
1	F	3	LEU
1	F	18	ILE
1	F	22	PHE
1	F	35	VAL
1	F	46	PHE
1	F	47	VAL
1	F	58	GLN
1	F	65	ARG
1	F	69	VAL
1	F	93	LEU
1	F	97	LYS
1	F	106	GLN
1	F	110	LYS
1	F	123	PHE
1	F	130	ASP
1	F	136	ARG
1	F	137	GLN
1	F	139	THR
1	F	161	PHE
1	F	163	GLU
1	G	7	ARG
1	G	22	PHE
1	G	24	GLU

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Mol	Chain	Res	Type
1	G	25	ILE
1	G	31	ARG
1	G	36	VAL
1	G	40	TYR
1	G	43	ASP
1	G	45	THR
1	G	47	VAL
1	G	52	ILE
1	G	57	ASP
1	G	59	VAL
1	G	69	VAL
1	G	77	GLN
1	G	83	TRP
1	G	89	LYS
1	G	97	LYS
1	G	101	LEU
1	G	105	LYS
1	G	114	VAL
1	G	124	ARG
1	G	130	ASP
1	G	147	ARG
1	G	153	LEU
1	G	156	LEU
1	G	159	PHE
1	G	164	LYS
1	H	1	MET
1	H	2	VAL
1	H	3	LEU
1	H	7	ARG
1	H	24	GLU
1	H	33	LYS
1	H	37	LEU
1	H	47	VAL
1	H	50	THR
1	H	53	ILE
1	H	65	ARG
1	H	69	VAL
1	H	70	ILE
1	H	72	CYS
1	H	74	THR
1	H	75	ASP
1	H	87	ASP

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Mol	Chain	Res	Type
1	H	93	LEU
1	H	95	HIS
1	H	97	LYS
1	H	105	LYS
1	H	114	VAL
1	H	129	ILE
1	H	135	LEU
1	H	136	ARG
1	H	141	ASN
1	H	147	ARG
1	H	153	LEU
1	H	159	PHE
1	H	164	LYS
1	I	6	ASN
1	I	19	ASN
1	I	21	GLU
1	I	33	LYS
1	I	37	LEU
1	I	47	VAL
1	I	61	GLU
1	I	74	THR
1	I	75	ASP
1	I	77	GLN
1	I	89	LYS
1	I	97	LYS
1	I	98	ILE
1	I	105	LYS
1	I	110	LYS
1	I	114	VAL
1	I	128	ILE
1	I	130	ASP
1	I	149	VAL
1	I	154	ARG
1	J	1	MET
1	J	11	GLU
1	J	27	LEU
1	J	29	ASP
1	J	46	PHE
1	J	50	THR
1	J	52	ILE
1	J	55	PHE
1	J	65	ARG

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Mol	Chain	Res	Type
1	J	67	CYS
1	J	70	ILE
1	J	84	ASP
1	J	88	ARG
1	J	116	ASP
1	J	135	LEU
1	J	140	ILE
1	J	141	ASN
1	J	143	LYS
1	J	145	VAL
1	J	152	THR
1	J	154	ARG
1	J	163	GLU
1	K	3	LEU
1	K	12	PHE
1	K	27	LEU
1	K	34	TYR
1	K	37	LEU
1	K	45	THR
1	K	47	VAL
1	K	58	GLN
1	K	59	VAL
1	K	60	GLU
1	K	69	VAL
1	K	77	GLN
1	K	87	ASP
1	K	95	HIS
1	K	96	MET
1	K	108	ILE
1	K	112	TYR
1	K	114	VAL
1	K	123	PHE
1	K	130	ASP
1	K	132	ASN
1	K	137	GLN
1	K	138	ILE
1	K	139	THR
1	K	143	LYS
1	K	147	ARG
1	K	153	LEU
1	K	156	LEU
1	L	17	VAL

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Mol	Chain	Res	Type
1	L	21	GLU
1	L	28	LYS
1	L	31	ARG
1	L	33[A]	LYS
1	L	33[B]	LYS
1	L	35	VAL
1	L	36	VAL
1	L	37	LEU
1	L	38	PHE
1	L	39	PHE
1	L	40	TYR
1	L	43	ASP
1	L	47	VAL
1	L	62	PHE
1	L	63	ASN
1	L	65	ARG
1	L	69	VAL
1	L	93	LEU
1	L	95	HIS
1	L	97	LYS
1	L	100	LEU
1	L	104	ARG
1	L	105	LYS
1	L	106	GLN
1	L	126	LEU
1	L	128	ILE
1	L	143	LYS
1	L	145	VAL
1	L	147	ARG
1	L	154	ARG
1	L	155	LEU
1	L	160	GLN
1	M	21	GLU
1	M	36	VAL
1	M	45	THR
1	M	47	VAL
1	M	75	ASP
1	M	93	LEU
1	M	97	LYS
1	M	98	ILE
1	M	100	LEU
1	M	114	VAL

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Mol	Chain	Res	Type
1	M	117	GLU
1	M	121	ASN
1	M	128	ILE
1	M	138	ILE
1	M	147	ARG
1	M	150	ASP
1	M	155	LEU
1	M	159	PHE
1	M	161	PHE
1	N	12	PHE
1	N	13	LYS
1	N	18	ILE
1	N	35	VAL
1	N	36	VAL
1	N	37	LEU
1	N	47	VAL
1	N	51	GLU
1	N	60	GLU
1	N	74	THR
1	N	83	TRP
1	N	89	LYS
1	N	96	MET
1	N	97	LYS
1	N	100	LEU
1	N	104	ARG
1	N	112	TYR
1	N	123	PHE
1	N	135	LEU
1	N	141	ASN
1	N	142	ASP
1	N	145	VAL
1	N	147	ARG
1	N	149	VAL
1	N	151	GLU
1	N	159	PHE
1	N	161	PHE
1	N	165	HIS
1	O	18	ILE
1	O	25	ILE
1	O	29	ASP
1	O	36	VAL
1	O	37	LEU

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Mol	Chain	Res	Type
1	O	50	THR
1	O	51	GLU
1	O	55	PHE
1	O	60	GLU
1	O	67	CYS
1	O	70	ILE
1	O	78	TYR
1	O	80	HIS
1	O	89	LYS
1	O	104	ARG
1	O	110	LYS
1	O	123	PHE
1	O	135	LEU
1	O	140	ILE
1	O	147	ARG
1	O	153	LEU
1	O	154	ARG
1	P	17	VAL
1	P	22	PHE
1	P	30	TYR
1	P	35	VAL
1	P	37	LEU
1	P	46	PHE
1	P	53	ILE
1	P	58	GLN
1	P	60	GLU
1	P	65	ARG
1	P	75	ASP
1	P	83	TRP
1	P	85	ASN
1	P	98	ILE
1	P	104	ARG
1	P	105	LYS
1	P	106	GLN
1	P	114	VAL
1	P	119	ASP
1	P	123	PHE
1	P	127	PHE
1	P	130	ASP
1	P	147	ARG
1	P	150	ASP
1	P	153	LEU

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Mol	Chain	Res	Type
1	P	160	GLN
1	Q	7	ARG
1	Q	11	GLU
1	Q	17	VAL
1	Q	21	GLU
1	Q	22	PHE
1	Q	37	LEU
1	Q	55	PHE
1	Q	62	PHE
1	Q	68	GLN
1	Q	69	VAL
1	Q	75	ASP
1	Q	80	HIS
1	Q	83	TRP
1	Q	93	LEU
1	Q	96	MET
1	Q	98	ILE
1	Q	100	LEU
1	Q	105	LYS
1	Q	112	TYR
1	Q	114	VAL
1	Q	119	ASP
1	Q	121	ASN
1	Q	123	PHE
1	Q	129	ILE
1	Q	134	ILE
1	Q	135	LEU
1	Q	138	ILE
1	Q	145	VAL
1	Q	150	ASP
1	Q	153	LEU
1	R	17	VAL
1	R	27	LEU
1	R	40	TYR
1	R	45	THR
1	R	55	PHE
1	R	61	GLU
1	R	74	THR
1	R	89	LYS
1	R	98	ILE
1	R	108	ILE
1	R	114	VAL

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Mol	Chain	Res	Type
1	R	116	ASP
1	R	118	GLU
1	R	123	PHE
1	R	135	LEU
1	R	143	LYS
1	R	153	LEU
1	S	22	PHE
1	S	24	GLU
1	S	26	CYS
1	S	27	LEU
1	S	31	ARG
1	S	37	LEU
1	S	51	GLU
1	S	52	ILE
1	S	53	ILE
1	S	74	THR
1	S	88	ARG
1	S	96	MET
1	S	101	LEU
1	S	104	ARG
1	S	105	LYS
1	S	114	VAL
1	S	124	ARG
1	S	147	ARG
1	S	150	ASP
1	S	160	GLN
1	S	162	VAL
1	S	164	LYS
1	T	3	LEU
1	T	21	GLU
1	T	25	ILE
1	T	47	VAL
1	T	50	THR
1	T	53	ILE
1	T	70	ILE
1	T	75	ASP
1	T	86	LEU
1	T	93	LEU
1	T	100	LEU
1	T	101	LEU
1	T	123	PHE
1	T	126	LEU

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Mol	Chain	Res	Type
1	T	130	ASP
1	T	145	VAL
1	T	151	GLU
1	T	155	LEU
1	T	157	ASP
1	T	159	PHE
1	T	160	GLN
1	T	161	PHE
1	U	21	GLU
1	U	28	LYS
1	U	35	VAL
1	U	37	LEU
1	U	43	ASP
1	U	47	VAL
1	U	50	THR
1	U	53	ILE
1	U	57	ASP
1	U	58	GLN
1	U	60	GLU
1	U	63	ASN
1	U	65	ARG
1	U	72	CYS
1	U	77	GLN
1	U	83	TRP
1	U	87	ASP
1	U	89	LYS
1	U	98	ILE
1	U	105	LYS
1	U	123	PHE
1	U	141	ASN
1	U	145	VAL
1	U	160	GLN
1	V	6	ASN
1	V	7	ARG
1	V	18	ILE
1	V	27	LEU
1	V	28	LYS
1	V	36	VAL
1	V	37	LEU
1	V	38	PHE
1	V	43	ASP
1	V	59	VAL

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Mol	Chain	Res	Type
1	V	61	GLU
1	V	65	ARG
1	V	74	THR
1	V	86	LEU
1	V	89	LYS
1	V	97	LYS
1	V	112	TYR
1	V	119	ASP
1	V	121	ASN
1	V	124	ARG
1	V	128	ILE
1	V	129	ILE
1	V	137	GLN
1	V	147	ARG
1	V	161	PHE
1	V	163	GLU
1	V	165	HIS
1	W	1	MET
1	W	11	GLU
1	W	15	GLN
1	W	18	ILE
1	W	25	ILE
1	W	28	LYS
1	W	33	LYS
1	W	35	VAL
1	W	37	LEU
1	W	57	ASP
1	W	65	ARG
1	W	66	ASN
1	W	72	CYS
1	W	77	GLN
1	W	84	ASP
1	W	95	HIS
1	W	96	MET
1	W	105	LYS
1	W	110	LYS
1	W	114	VAL
1	W	126	LEU
1	W	129	ILE
1	W	130	ASP
1	W	137	GLN
1	W	139	THR

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Mol	Chain	Res	Type
1	W	143	LYS
1	W	153	LEU
1	W	160	GLN
1	X	2	VAL
1	X	3	LEU
1	X	11	GLU
1	X	17	VAL
1	X	23	LYS
1	X	25	ILE
1	X	45	THR
1	X	52	ILE
1	X	57	ASP
1	X	59	VAL
1	X	72	CYS
1	X	85	ASN
1	X	86	LEU
1	X	93	LEU
1	X	95	HIS
1	X	101	LEU
1	X	104	ARG
1	X	106	GLN
1	X	138	ILE
1	X	152	THR
1	X	156	LEU
1	X	161	PHE
1	Y	7	ARG
1	Y	17	VAL
1	Y	18	ILE
1	Y	22	PHE
1	Y	24	GLU
1	Y	35	VAL
1	Y	68	GLN
1	Y	74	THR
1	Y	77	GLN
1	Y	80	HIS
1	Y	83	TRP
1	Y	89	LYS
1	Y	97	LYS
1	Y	100	LEU
1	Y	101	LEU
1	Y	108	ILE
1	Y	118	GLU

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Mol	Chain	Res	Type
1	Y	124	ARG
1	Y	126	LEU
1	Y	147	ARG
1	Y	151	GLU
1	Y	153	LEU
1	Y	156	LEU
1	Y	161	PHE
1	Y	164	LYS
1	Z	21	GLU
1	Z	23	LYS
1	Z	29	ASP
1	Z	31	ARG
1	Z	35	VAL
1	Z	38	PHE
1	Z	55	PHE
1	Z	58	GLN
1	Z	65	ARG
1	Z	67	CYS
1	Z	68	GLN
1	Z	69	VAL
1	Z	70	ILE
1	Z	78	TYR
1	Z	80	HIS
1	Z	86	LEU
1	Z	93	LEU
1	Z	98	ILE
1	Z	100	LEU
1	Z	101	LEU
1	Z	104	ARG
1	Z	105	LYS
1	Z	140	ILE
1	Z	143	LYS
1	Z	153	LEU
1	Z	163	GLU
1	a	22	PHE
1	a	29	ASP
1	a	36	VAL
1	a	37	LEU
1	a	43	ASP
1	a	65	ARG
1	a	68	GLN
1	a	69	VAL

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Mol	Chain	Res	Type
1	a	70	ILE
1	a	73	SER
1	a	77	GLN
1	a	81	LEU
1	a	86	LEU
1	a	95	HIS
1	a	97	LYS
1	a	98	ILE
1	a	101	LEU
1	a	108	ILE
1	a	116	ASP
1	a	119	ASP
1	a	134	ILE
1	a	136	ARG
1	a	140	ILE
1	a	143	LYS
1	a	145	VAL
1	a	163	GLU
1	b	3	LEU
1	b	18	ILE
1	b	28	LYS
1	b	29	ASP
1	b	35	VAL
1	b	47	VAL
1	b	60	GLU
1	b	65	ARG
1	b	70	ILE
1	b	105	LYS
1	b	107	GLU
1	b	123	PHE
1	b	124	ARG
1	b	128	ILE
1	b	130	ASP
1	b	139	THR
1	b	140	ILE
1	b	143	LYS
1	b	154	ARG
1	b	164	LYS
1	c	13	LYS
1	c	17	VAL
1	c	23	LYS
1	c	27	LEU

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Mol	Chain	Res	Type
1	c	28	LYS
1	c	34	TYR
1	c	36	VAL
1	c	37	LEU
1	c	38	PHE
1	c	47	VAL
1	c	52	ILE
1	c	57	ASP
1	c	58	GLN
1	c	63	ASN
1	c	69	VAL
1	c	97	LYS
1	c	98	ILE
1	c	103	ASP
1	c	108	ILE
1	c	110	LYS
1	c	114	VAL
1	c	118	GLU
1	c	130	ASP
1	c	134	ILE
1	c	137	GLN
1	c	143	LYS
1	c	145	VAL
1	c	147	ARG
1	c	153	LEU
1	c	155	LEU
1	c	161	PHE
1	d	0	THR
1	d	2	VAL
1	d	7	ARG
1	d	12	PHE
1	d	31	ARG
1	d	36	VAL
1	d	37	LEU
1	d	46	PHE
1	d	51	GLU
1	d	53	ILE
1	d	70	ILE
1	d	75	ASP
1	d	88	ARG
1	d	89	LYS
1	d	97	LYS

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Mol	Chain	Res	Type
1	d	126	LEU
1	d	129	ILE
1	d	134	ILE
1	d	136	ARG
1	d	147	ARG
1	d	152	THR
1	d	160	GLN
1	d	161	PHE
1	d	164	LYS
1	e	11	GLU
1	e	17	VAL
1	e	22	PHE
1	e	23	LYS
1	e	31	ARG
1	e	35	VAL
1	e	52	ILE
1	e	60	GLU
1	e	65	ARG
1	e	75	ASP
1	e	85	ASN
1	e	87	ASP
1	e	88	ARG
1	e	89	LYS
1	e	95	HIS
1	e	96	MET
1	e	97	LYS
1	e	104	ARG
1	e	110	LYS
1	e	118	GLU
1	e	135	LEU
1	e	136	ARG
1	e	139	THR
1	e	143	LYS
1	e	154	ARG
1	e	155	LEU
1	e	160	GLN
1	f	3	LEU
1	f	12	PHE
1	f	13[A]	LYS
1	f	13[B]	LYS
1	f	17	VAL
1	f	18	ILE

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Mol	Chain	Res	Type
1	f	25	ILE
1	f	27	LEU
1	f	28	LYS
1	f	33[A]	LYS
1	f	33[B]	LYS
1	f	36	VAL
1	f	50	THR
1	f	52	ILE
1	f	67	CYS
1	f	69	VAL
1	f	77	GLN
1	f	81	LEU
1	f	89	LYS
1	f	101	LEU
1	f	110	LYS
1	f	118	GLU
1	f	126	LEU
1	f	137	GLN
1	f	138	ILE
1	f	140	ILE
1	f	149	VAL
1	f	154	ARG
1	f	161	PHE
1	f	162	VAL
1	f	163	GLU
1	f	164	LYS
1	g	2	VAL
1	g	4	LEU
1	g	15	GLN
1	g	25	ILE
1	g	29	ASP
1	g	33	LYS
1	g	36	VAL
1	g	37	LEU
1	g	47	VAL
1	g	60	GLU
1	g	63	ASN
1	g	77	GLN
1	g	84	ASP
1	g	89	LYS
1	g	108	ILE
1	g	112	TYR

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Mol	Chain	Res	Type
1	g	119	ASP
1	g	123	PHE
1	g	132	ASN
1	g	138	ILE
1	g	141	ASN
1	g	148	SER
1	g	155	LEU
1	g	156	LEU
1	g	159	PHE
1	g	161	PHE
1	g	164	LYS
1	h	7	ARG
1	h	15	GLN
1	h	19	ASN
1	h	25	ILE
1	h	35	VAL
1	h	38	PHE
1	h	40	TYR
1	h	46	PHE
1	h	52	ILE
1	h	57	ASP
1	h	63	ASN
1	h	70	ILE
1	h	84	ASP
1	h	88	ARG
1	h	96	MET
1	h	104	ARG
1	h	114	VAL
1	h	121	ASN
1	h	129	ILE
1	h	140	ILE
1	h	141	ASN
1	h	147	ARG
1	h	152	THR
1	h	153	LEU
1	h	154	ARG
1	i	19	ASN
1	i	23	LYS
1	i	25	ILE
1	i	27	LEU
1	i	33	LYS
1	i	34	TYR

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Mol	Chain	Res	Type
1	i	36	VAL
1	i	39	PHE
1	i	44	PHE
1	i	52	ILE
1	i	53	ILE
1	i	57	ASP
1	i	61	GLU
1	i	63	ASN
1	i	66	ASN
1	i	70	ILE
1	i	74	THR
1	i	80	HIS
1	i	81	LEU
1	i	86	LEU
1	i	87	ASP
1	i	88	ARG
1	i	89	LYS
1	i	98	ILE
1	i	100	LEU
1	i	101	LEU
1	i	115	PHE
1	i	121	ASN
1	i	123	PHE
1	i	130	ASP
1	i	137	GLN
1	i	138	ILE
1	i	140	ILE
1	i	145	VAL
1	i	147	ARG
1	i	149	VAL
1	i	156	LEU
1	i	157	ASP
1	j	11	GLU
1	j	12	PHE
1	j	13	LYS
1	j	33	LYS
1	j	50	THR
1	j	69	VAL
1	j	70	ILE
1	j	74	THR
1	j	77	GLN
1	j	83	TRP

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Mol	Chain	Res	Type
1	j	89	LYS
1	j	97	LYS
1	j	98	ILE
1	j	104	ARG
1	j	108	ILE
1	j	112	TYR
1	j	114	VAL
1	j	123	PHE
1	j	124	ARG
1	j	126	LEU
1	j	145	VAL
1	j	149	VAL
1	j	153	LEU
1	j	154	ARG
1	j	155	LEU
1	k	3	LEU
1	k	7	ARG
1	k	17	VAL
1	k	30	TYR
1	k	35	VAL
1	k	38	PHE
1	k	47	VAL
1	k	50	THR
1	k	65	ARG
1	k	67	CYS
1	k	69	VAL
1	k	81	LEU
1	k	83	TRP
1	k	95	HIS
1	k	96	MET
1	k	98	ILE
1	k	112	TYR
1	k	114	VAL
1	k	126	LEU
1	k	140	ILE
1	k	143	LYS
1	k	147	ARG
1	k	150	ASP
1	k	152	THR
1	k	154	ARG
1	k	156	LEU
1	k	163	GLU

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Mol	Chain	Res	Type
1	l	3	LEU
1	l	7	ARG
1	l	26	CYS
1	l	31	ARG
1	l	35	VAL
1	l	38	PHE
1	l	52	ILE
1	l	53	ILE
1	l	57	ASP
1	l	62	PHE
1	l	74	THR
1	l	75	ASP
1	l	80	HIS
1	l	93	LEU
1	l	97	LYS
1	l	101	LEU
1	l	108	ILE
1	l	114	VAL
1	l	117	GLU
1	l	118	GLU
1	l	121	ASN
1	l	123	PHE
1	l	128	ILE
1	l	129	ILE
1	l	137	GLN
1	l	138	ILE
1	l	147	ARG
1	l	156	LEU
1	l	160	GLN
1	l	161	PHE
1	l	163	GLU
1	m	4	LEU
1	m	6	ASN
1	m	7	ARG
1	m	21	GLU
1	m	25	ILE
1	m	36	VAL
1	m	37	LEU
1	m	53	ILE
1	m	61	GLU
1	m	65	ARG
1	m	74	THR

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Mol	Chain	Res	Type
1	m	96	MET
1	m	98	ILE
1	m	100	LEU
1	m	101	LEU
1	m	112	TYR
1	m	114	VAL
1	m	135	LEU
1	m	143	LYS
1	m	147	ARG
1	m	156	LEU
1	m	163	GLU
1	n	3	LEU
1	n	7	ARG
1	n	13	LYS
1	n	17	VAL
1	n	22	PHE
1	n	47	VAL
1	n	52	ILE
1	n	55	PHE
1	n	58	GLN
1	n	59	VAL
1	n	75	ASP
1	n	77	GLN
1	n	88	ARG
1	n	89	LYS
1	n	118	GLU
1	n	119	ASP
1	n	130	ASP
1	n	141	ASN
1	n	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	19	ASN
1	A	121	ASN
1	A	141	ASN
1	B	15	GLN
1	B	95	HIS
1	B	132	ASN
1	B	160	GLN

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Mol	Chain	Res	Type
1	C	121	ASN
1	C	141	ASN
1	E	6	ASN
1	E	80	HIS
1	F	6	ASN
1	F	77	GLN
1	G	63	ASN
1	G	80	HIS
1	G	106	GLN
1	G	137	GLN
1	H	63	ASN
1	H	68	GLN
1	H	121	ASN
1	H	165	HIS
1	I	132	ASN
1	J	141	ASN
1	K	6	ASN
1	K	19	ASN
1	K	58	GLN
1	K	137	GLN
1	L	19	ASN
1	L	95	HIS
1	M	77	GLN
1	M	141	ASN
1	N	19	ASN
1	N	66	ASN
1	N	68	GLN
1	N	77	GLN
1	O	58	GLN
1	O	68	GLN
1	P	58	GLN
1	Q	68	GLN
1	Q	121	ASN
1	R	68	GLN
1	R	80	HIS
1	T	15	GLN
1	T	77	GLN
1	U	68	GLN
1	U	80	HIS
1	V	58	GLN
1	W	19	ASN
1	W	66	ASN

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Mol	Chain	Res	Type
1	W	132	ASN
1	X	63	ASN
1	X	77	GLN
1	X	165	HIS
1	Z	68	GLN
1	Z	77	GLN
1	Z	132	ASN
1	a	63	ASN
1	a	68	GLN
1	b	58	GLN
1	b	68	GLN
1	b	85	ASN
1	b	121	ASN
1	c	132	ASN
1	c	137	GLN
1	d	77	GLN
1	d	95	HIS
1	d	106	GLN
1	d	132	ASN
1	e	68	GLN
1	e	106	GLN
1	f	58	GLN
1	f	95	HIS
1	f	165	HIS
1	g	68	GLN
1	g	77	GLN
1	g	80	HIS
1	h	63	ASN
1	i	58	GLN
1	i	66	ASN
1	i	68	GLN
1	i	85	ASN
1	i	106	GLN
1	i	132	ASN
1	j	58	GLN
1	j	160	GLN
1	k	6	ASN
1	k	19	ASN
1	k	80	HIS
1	k	137	GLN
1	k	165	HIS
1	l	137	GLN

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Mol	Chain	Res	Type
1	m	15	GLN
1	m	58	GLN
1	m	77	GLN
1	m	85	ASN
1	m	132	ASN
1	n	58	GLN
1	n	141	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	163/186 (87%)	-1.46	0 100 100	110, 111, 112, 112	0
1	B	165/186 (88%)	-1.42	0 100 100	67, 111, 112, 112	2 (1%)
1	C	165/186 (88%)	-1.49	0 100 100	110, 111, 111, 112	0
1	D	164/186 (88%)	-1.49	0 100 100	64, 111, 111, 112	2 (1%)
1	E	162/186 (87%)	-1.43	0 100 100	110, 111, 111, 112	0
1	F	165/186 (88%)	-1.46	0 100 100	110, 111, 112, 112	0
1	G	162/186 (87%)	-1.45	0 100 100	67, 111, 112, 112	1 (0%)
1	H	165/186 (88%)	-1.43	0 100 100	110, 111, 112, 112	0
1	I	163/186 (87%)	-1.43	0 100 100	66, 111, 112, 112	1 (0%)
1	J	166/186 (89%)	-1.44	0 100 100	110, 111, 112, 112	0
1	K	161/186 (86%)	-1.44	0 100 100	110, 111, 112, 112	0
1	L	164/186 (88%)	-1.40	0 100 100	67, 111, 112, 112	2 (1%)
1	M	165/186 (88%)	-1.43	0 100 100	110, 111, 112, 112	0
1	N	164/186 (88%)	-1.39	0 100 100	64, 111, 112, 112	2 (1%)
1	O	163/186 (87%)	-1.38	0 100 100	110, 111, 112, 112	0
1	P	165/186 (88%)	-1.42	0 100 100	110, 111, 112, 112	0
1	Q	157/186 (84%)	-1.39	0 100 100	67, 111, 112, 112	1 (0%)
1	R	164/186 (88%)	-1.46	0 100 100	110, 111, 112, 112	0
1	S	163/186 (87%)	-1.50	0 100 100	67, 111, 111, 112	1 (0%)
1	T	166/186 (89%)	-1.48	0 100 100	109, 111, 111, 112	0
1	U	163/186 (87%)	-1.48	0 100 100	110, 111, 112, 112	0
1	V	165/186 (88%)	-1.43	0 100 100	67, 111, 112, 112	2 (1%)
1	W	165/186 (88%)	-1.48	0 100 100	109, 111, 111, 112	0
1	X	164/186 (88%)	-1.45	0 100 100	64, 111, 111, 112	2 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	163/186 (87%)	-1.40	0	100 100	110, 111, 112, 112 0
1	Z	165/186 (88%)	-1.43	0	100 100	103, 111, 112, 112 0
1	a	163/186 (87%)	-1.44	0	100 100	66, 111, 112, 112 1 (0%)
1	b	165/186 (88%)	-1.44	0	100 100	110, 111, 112, 112 0
1	c	163/186 (87%)	-1.38	0	100 100	67, 111, 112, 113 1 (0%)
1	d	166/186 (89%)	-1.42	0	100 100	110, 111, 112, 112 0
1	e	162/186 (87%)	-1.46	0	100 100	110, 111, 111, 112 0
1	f	165/186 (88%)	-1.46	0	100 100	67, 111, 111, 112 2 (1%)
1	g	165/186 (88%)	-1.46	0	100 100	110, 111, 112, 112 0
1	h	163/186 (87%)	-1.41	0	100 100	64, 111, 112, 113 2 (1%)
1	i	158/186 (84%)	-1.44	0	100 100	110, 111, 112, 112 0
1	j	165/186 (88%)	-1.41	0	100 100	109, 111, 112, 112 0
1	k	163/186 (87%)	-1.39	0	100 100	67, 111, 112, 112 1 (0%)
1	l	165/186 (88%)	-1.43	0	100 100	110, 111, 112, 112 0
1	m	157/186 (84%)	-1.33	0	100 100	67, 111, 112, 112 1 (0%)
1	n	166/186 (89%)	-1.45	0	100 100	110, 111, 112, 112 0
All	All	6543/7440 (87%)	-1.43	0	100 100	64, 111, 112, 113 24 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.