



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:17 am GMT

PDB ID : 3MKA
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome with propetide
and an T1A mutation at beta-subunit
Authors : Li, D.; Li, H.
Deposited on : 2010-04-14
Resolution : 2.51 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

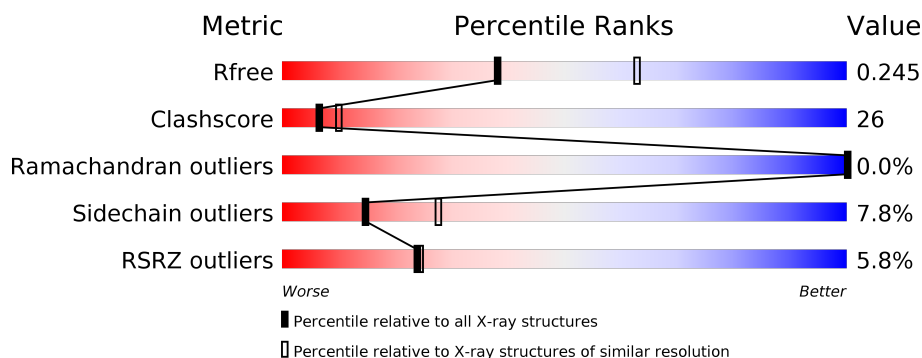
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1	248	<div> <div>12%</div> <div> <div></div> <div>54%</div> <div>29%</div> <div>•</div> <div>12%</div> </div> </div>
1	A	248	<div> <div>5%</div> <div> <div></div> <div>49%</div> <div>38%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	248	<div> <div>7%</div> <div> <div></div> <div>53%</div> <div>31%</div> <div>5%</div> <div>11%</div> </div> </div>
1	D	248	<div> <div>8%</div> <div> <div></div> <div>54%</div> <div>31%</div> <div>5%</div> <div>10%</div> </div> </div>
1	F	248	<div> <div>8%</div> <div> <div></div> <div>54%</div> <div>31%</div> <div>•</div> <div>11%</div> </div> </div>
1	I	248	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>27%</div> <div>5%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	248	
1	M	248	
1	O	248	
1	Q	248	
1	S	248	
1	U	248	
1	W	248	
1	Y	248	
2	2	291	
2	C	291	
2	E	291	
2	G	291	
2	H	291	
2	J	291	
2	L	291	
2	N	291	
2	P	291	
2	R	291	
2	T	291	
2	V	291	
2	X	291	
2	Z	291	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49801 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1713	1078	310	322	3			
1	B	220	Total	C	N	O	S	0	0	0
			1695	1064	308	320	3			
1	D	222	Total	C	N	O	S	0	0	0
			1717	1082	310	322	3			
1	F	221	Total	C	N	O	S	0	0	0
			1706	1073	309	321	3			
1	I	217	Total	C	N	O	S	0	0	0
			1680	1055	305	317	3			
1	K	221	Total	C	N	O	S	0	0	0
			1705	1072	309	321	3			
1	M	224	Total	C	N	O	S	0	0	0
			1730	1090	312	325	3			
1	O	218	Total	C	N	O	S	0	0	0
			1675	1049	306	317	3			
1	Q	222	Total	C	N	O	S	0	0	0
			1716	1081	310	322	3			
1	S	219	Total	C	N	O	S	0	0	0
			1686	1058	307	318	3			
1	U	221	Total	C	N	O	S	0	0	0
			1706	1073	309	321	3			
1	W	221	Total	C	N	O	S	0	0	0
			1710	1078	309	320	3			
1	Y	224	Total	C	N	O	S	0	0	0
			1730	1090	312	325	3			
1	1	219	Total	C	N	O	S	0	0	0
			1693	1065	307	318	3			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	250	Total	C	N	O	S	0	0	0
			1853	1165	320	363	5			
2	E	248	Total	C	N	O	S	0	0	0
			1834	1153	317	359	5			
2	G	251	Total	C	N	O	S	0	0	0
			1858	1168	321	364	5			
2	H	249	Total	C	N	O	S	0	0	0
			1844	1159	319	361	5			
2	J	252	Total	C	N	O	S	0	0	0
			1863	1170	322	366	5			
2	L	251	Total	C	N	O	S	0	0	0
			1857	1167	321	364	5			
2	N	252	Total	C	N	O	S	0	0	0
			1863	1170	322	366	5			
2	P	250	Total	C	N	O	S	0	0	0
			1853	1165	320	363	5			
2	R	246	Total	C	N	O	S	0	0	0
			1822	1145	315	357	5			
2	T	250	Total	C	N	O	S	0	0	0
			1854	1165	320	364	5			
2	V	249	Total	C	N	O	S	0	0	0
			1843	1158	319	361	5			
2	X	249	Total	C	N	O	S	0	0	0
			1848	1162	319	362	5			
2	Z	245	Total	C	N	O	S	0	0	0
			1817	1142	314	356	5			
2	2	246	Total	C	N	O	S	0	0	0
			1829	1150	316	358	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	301	ALA	THR	ENGINEERED	UNP O33245
E	301	ALA	THR	ENGINEERED	UNP O33245
G	301	ALA	THR	ENGINEERED	UNP O33245
H	301	ALA	THR	ENGINEERED	UNP O33245
J	301	ALA	THR	ENGINEERED	UNP O33245
L	301	ALA	THR	ENGINEERED	UNP O33245
N	301	ALA	THR	ENGINEERED	UNP O33245
P	301	ALA	THR	ENGINEERED	UNP O33245
R	301	ALA	THR	ENGINEERED	UNP O33245
T	301	ALA	THR	ENGINEERED	UNP O33245
V	301	ALA	THR	ENGINEERED	UNP O33245
X	301	ALA	THR	ENGINEERED	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	301	ALA	THR	ENGINEERED	UNP O33245
2	301	ALA	THR	ENGINEERED	UNP O33245

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	2	Total O 2 2	0	0
3	C	3	Total O 3 3	0	0
3	D	3	Total O 3 3	0	0
3	E	1	Total O 1 1	0	0
3	F	4	Total O 4 4	0	0
3	G	13	Total O 13 13	0	0
3	H	3	Total O 3 3	0	0
3	I	2	Total O 2 2	0	0
3	J	3	Total O 3 3	0	0
3	K	4	Total O 4 4	0	0
3	L	2	Total O 2 2	0	0
3	M	5	Total O 5 5	0	0
3	N	4	Total O 4 4	0	0
3	O	1	Total O 1 1	0	0
3	P	5	Total O 5 5	0	0
3	R	1	Total O 1 1	0	0
3	S	3	Total O 3 3	0	0

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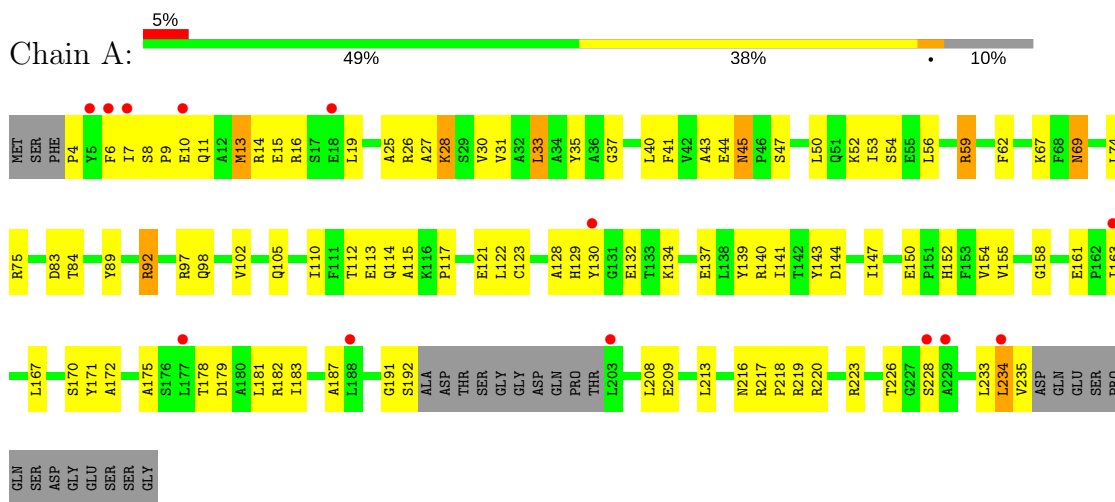
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	3	Total 3	O 3	0	0
3	U	2	Total 2	O 2	0	0
3	V	4	Total 4	O 4	0	0
3	W	6	Total 6	O 6	0	0
3	X	2	Total 2	O 2	0	0
3	Y	6	Total 6	O 6	0	0
3	Z	5	Total 5	O 5	0	0
3	2	5	Total 5	O 5	0	0
3	1	3	Total 3	O 3	0	0

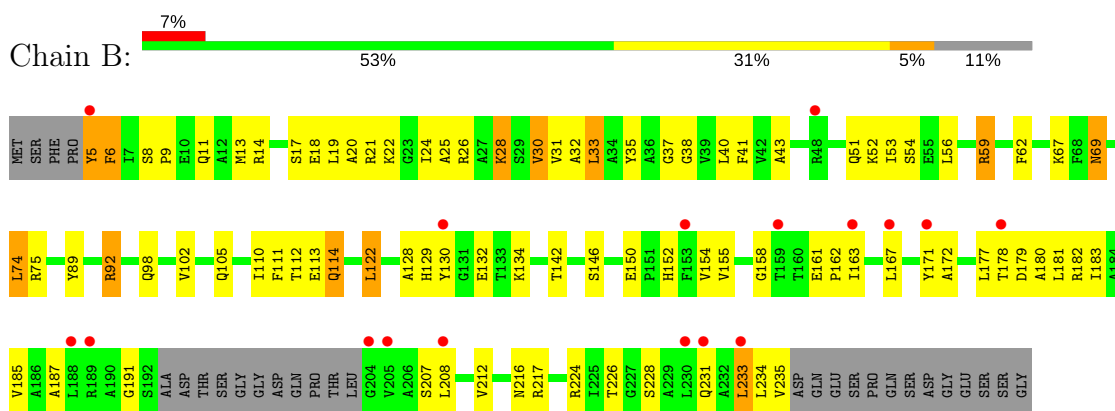
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

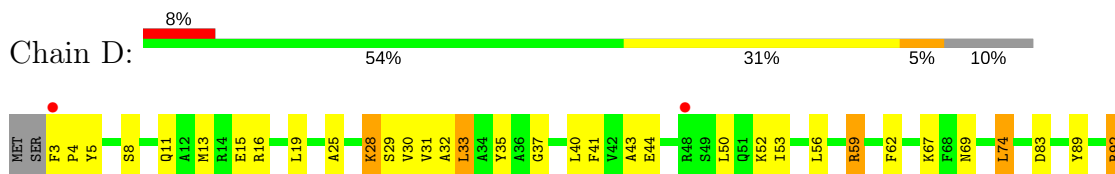
• Molecule 1: Proteasome subunit alpha

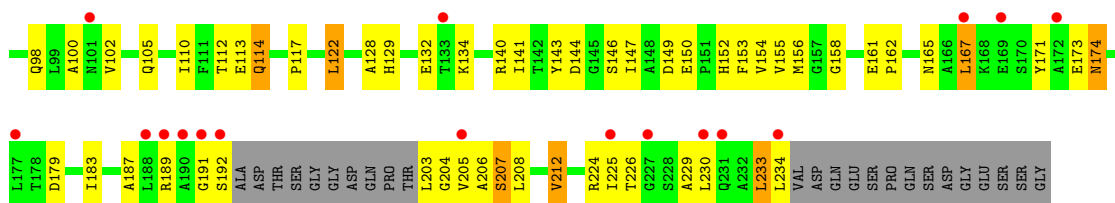


• Molecule 1: Proteasome subunit alpha

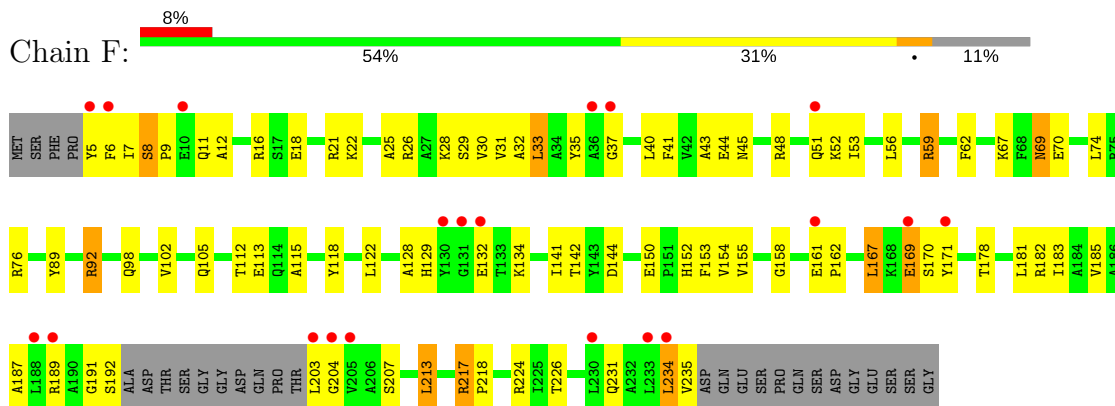


• Molecule 1: Proteasome subunit alpha

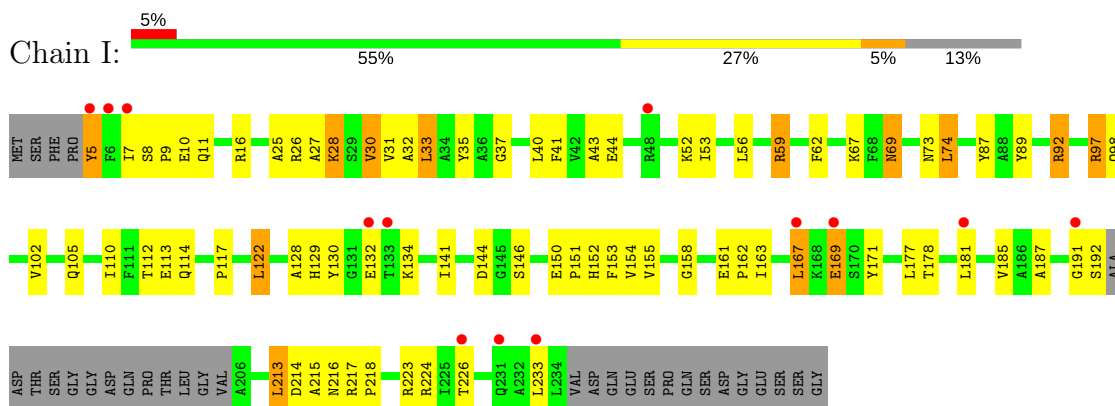




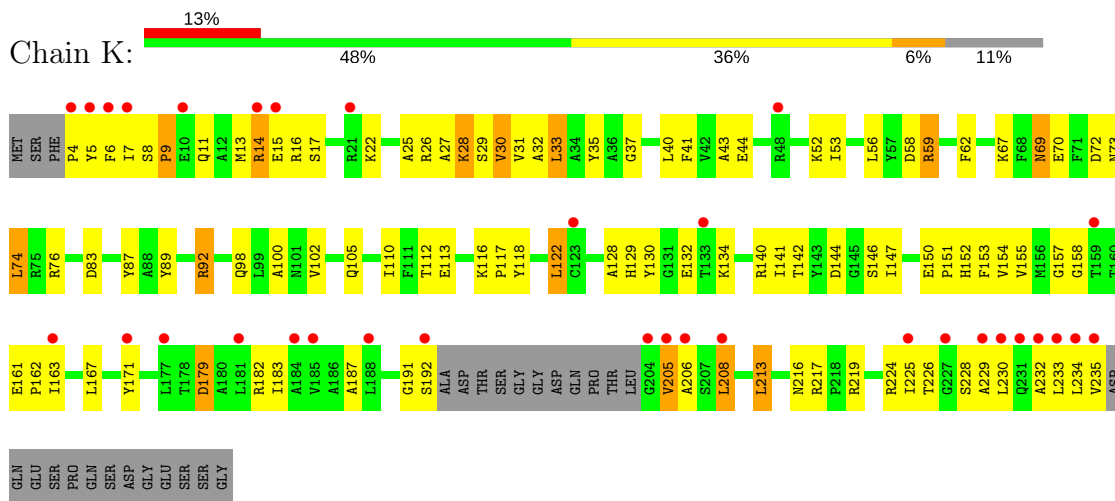
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



Chain M:

Sequence logo for Chain M. The y-axis represents information content in bits. The x-axis shows positions 1 to 300. A color scale at the top indicates conservation levels: 5% (red), 56% (yellow), 29% (light yellow), 5% (orange), and 10% (grey). Amino acids are labeled at the bottom of the logo.

Chain O:

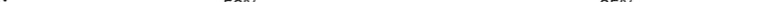
10% 51% 33% 12%

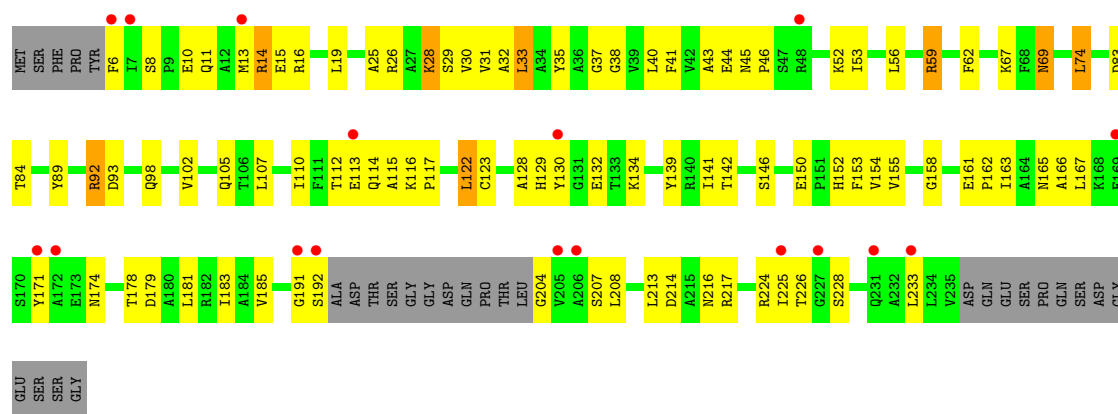
Label	Color
SER	Grey
ASP	Grey
GLY	Grey
GLU	Grey
SER	Grey
SER	Grey
GLY	Grey
E169	Red
S170	Red
Y171	Red
S176	Green
I177	Green
T178	Green
D179	Green
A180	Green
L181	Green
R182	Green
L183	Green
A184	Green
V185	Green
L188	Red
R189	Red
A190	Red
G191	Red
S192	Red
ALA	Grey
ASP	Grey
THR	Grey
SER	Grey
GLY	Grey
GLY	Grey
ASP	Green
GLN	Green
PRO	Green
THR	Green
LEU	Green
G204	Green
V205	Green
A206	Green
S207	Red
L208	Green
L213	Green
R216	Red
R217	Red
P218	Green
R224	Green
T225	Red
T226	Green
A229	Red
L230	Red
Q231	Green
A232	Green
L233	Red
L234	Red
V235	Red
ASP	Grey
GLN	Grey
GLU	Grey
SER	Grey
PRO	Grey
V238	Red
D83	Yellow
Y87	Yellow
R92	Orange
D93	Orange
Q98	Yellow
V102	Yellow
Q105	Yellow
T110	Yellow
F111	Green
T112	Green
E113	Green
Q114	Yellow
A115	Yellow
K116	Yellow
L122	Orange
A128	Yellow
H129	Yellow
Y130	Green
G131	Green
A132	Green
T133	Green
K134	Yellow
Y139	Yellow
R140	Green
I141	Green
T142	Green
Y143	Green
D144	Yellow
G145	Yellow
S146	Yellow
I147	Green
A148	Green
D149	Yellow
E150	Yellow
P151	Yellow
H152	Yellow
F153	Yellow
V154	Yellow
V155	Yellow
R156	Green
G157	Yellow
G158	Yellow
E161	Yellow
P162	Yellow
T163	Yellow
A164	Yellow
N165	Yellow
A166	Green
L167	Yellow
V168	Yellow
S29	Yellow
V30	Yellow
V31	Yellow
A32	Yellow
L33	Yellow
A34	Green
Y35	Yellow
A36	Yellow
G37	Yellow
G38	Green
V39	Green
L40	Yellow
F41	Yellow
V42	Yellow
A43	Yellow
E44	Green
R48	Yellow
Q51	Orange
K52	Yellow
F53	Yellow
S54	Yellow
E55	Green
L56	Green
R59	Orange
F62	Yellow
K67	Yellow
F68	Green
N69	Orange
L74	Orange

Chain Q:

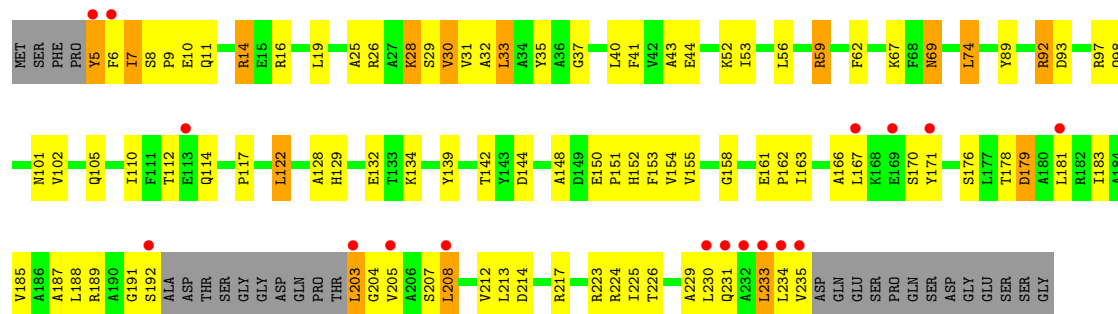
6% 48% 36% 6% 10%

MET SER F3 P4 Y5 F6 I7 S8 P9 E10 Q11 A12 E15 R16 L19 A25 R26 A27 K28 S29 V30 V31 L33 A34 Y35 A36 G37 L40 F41 V42 A43 E44 S47 R48 K52 I53 L56 R59 F62 K67 F68 N69 L74 D83 Y87 I88 Y89 R92 Q98 V102 Q105 I110 F111 T112 E113 Q114 A115 K116 P117 L122 C123 A128 H129 Y130 G131 E132 T133 K134 R135 Y139 L140 I141 T142 Y143 D144 E150 P151 H152 F153 V154 V155 G158 E161 P162 I163 L167 K168 E169 Y170 A172 E173 N174 A175 S176 L177 T178 D179 A180 L181 R182 I183 A184 V185 A186 A187 L188 R189 A190 G191 S192 A194 ASP THR SER GLY ASP GLN PRO THR LEU G204 V205 L208 E209 V210 A211 V212 L213 D214 A215 N216 R217 P218 R224 I225 T226 G227 S228 A229 L230 Q231 A232 L233 L234 V235 ASP GLN GLU SER PRO

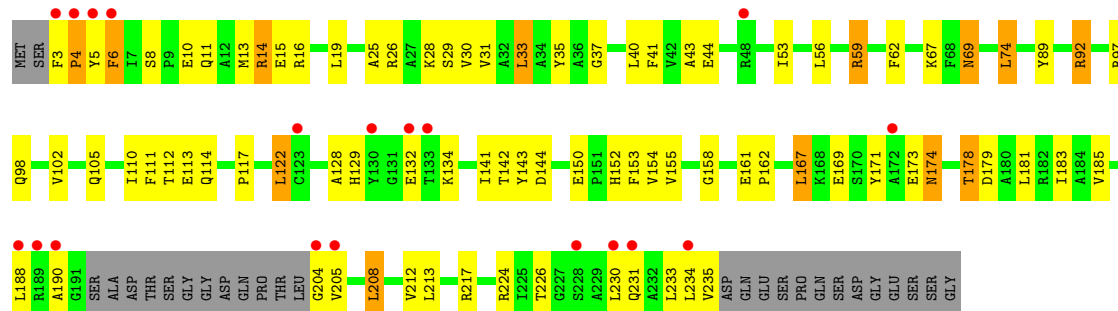
Chain S:  7% 50% 35% 12%



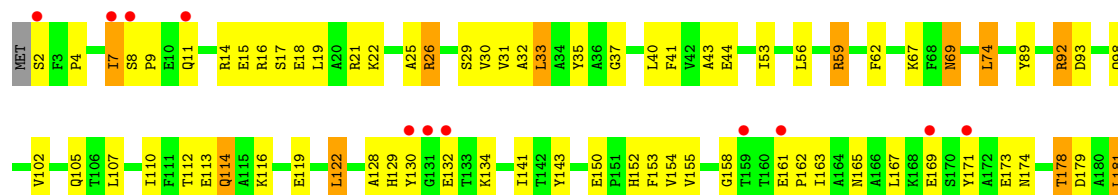
• Molecule 1: Proteasome subunit alpha

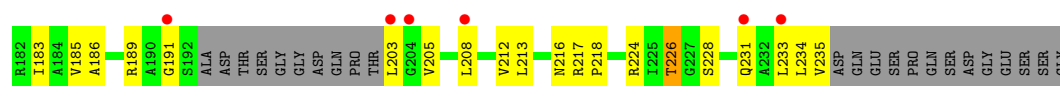


• Molecule 1: Proteasome subunit alpha

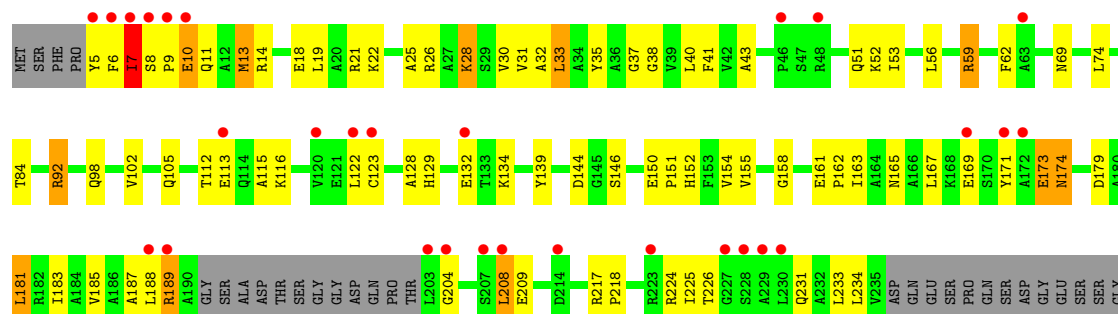


• Molecule 1: Proteasome subunit alpha

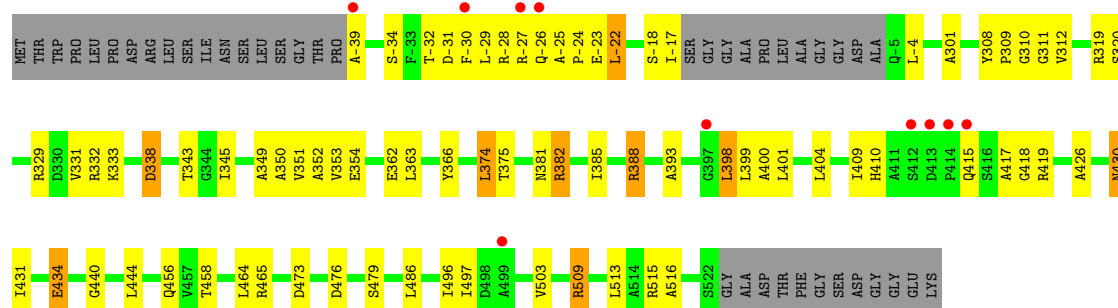




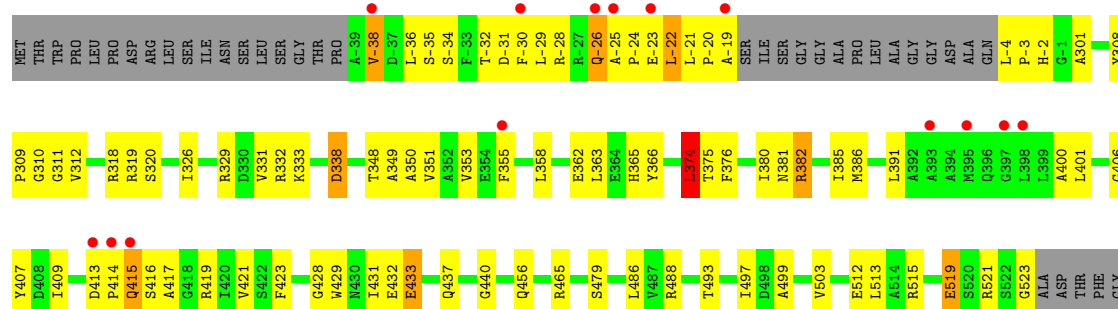
• Molecule 1: Proteasome subunit alpha



• Molecule 2: Proteasome subunit beta

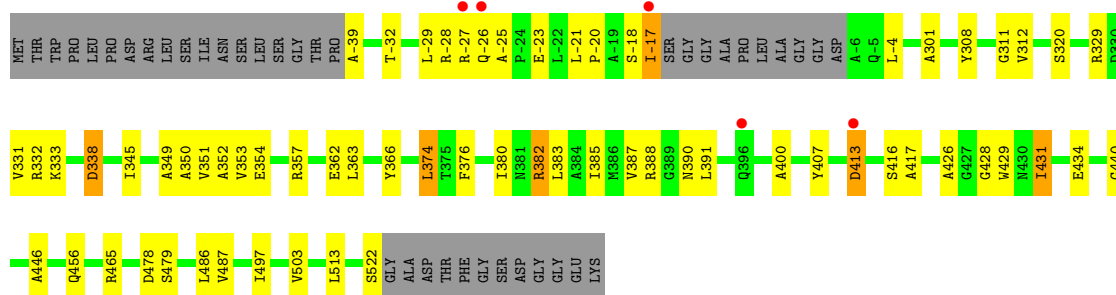


• Molecule 2: Proteasome subunit beta

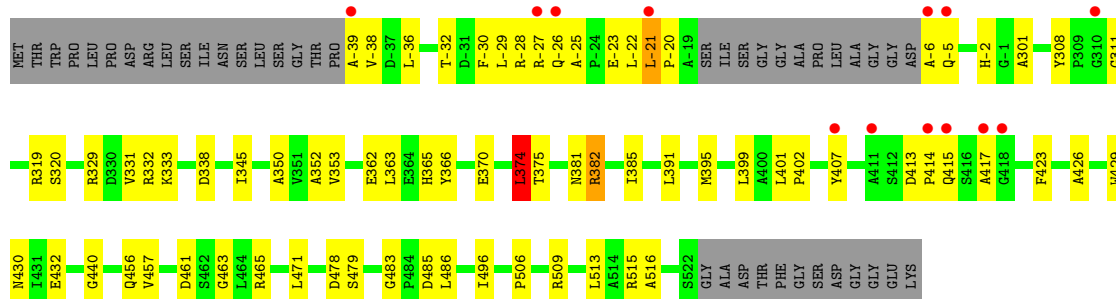


• Molecule 2: Proteasome subunit beta

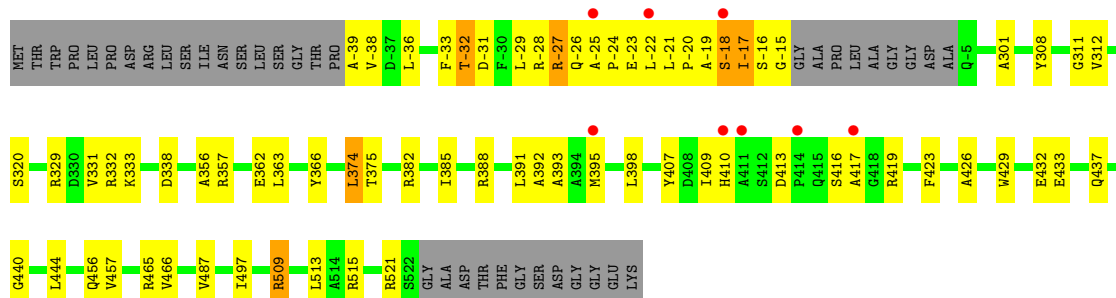




- Molecule 2: Proteasome subunit beta



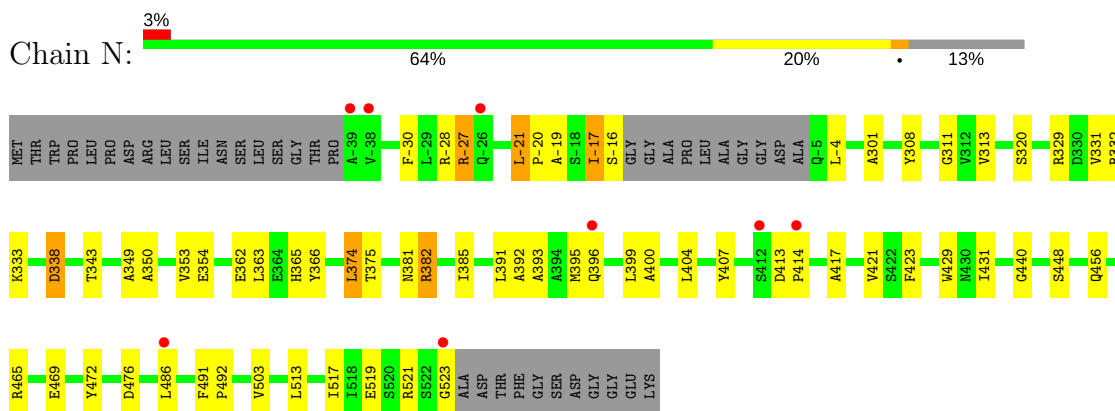
- Molecule 2: Proteasome subunit beta



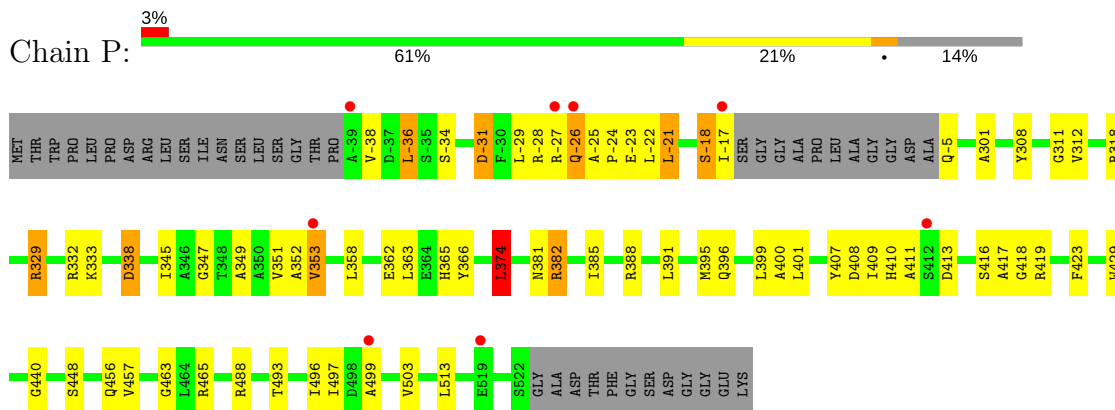
- Molecule 2: Proteasome subunit beta



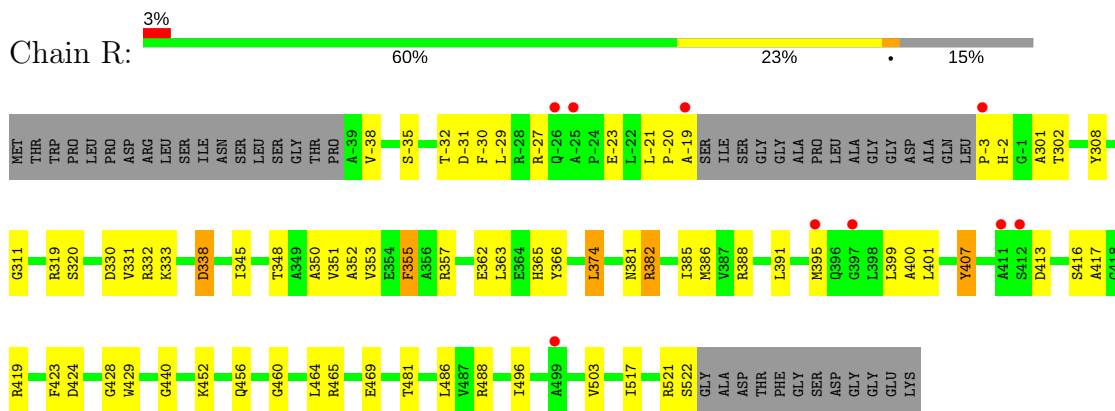
- Molecule 2: Proteasome subunit beta



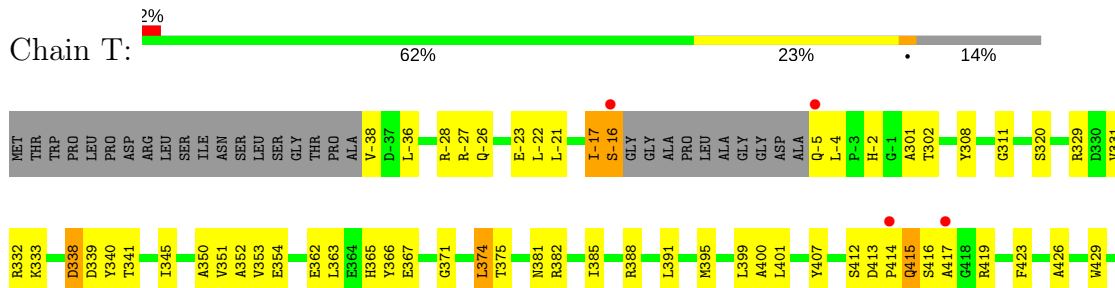
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



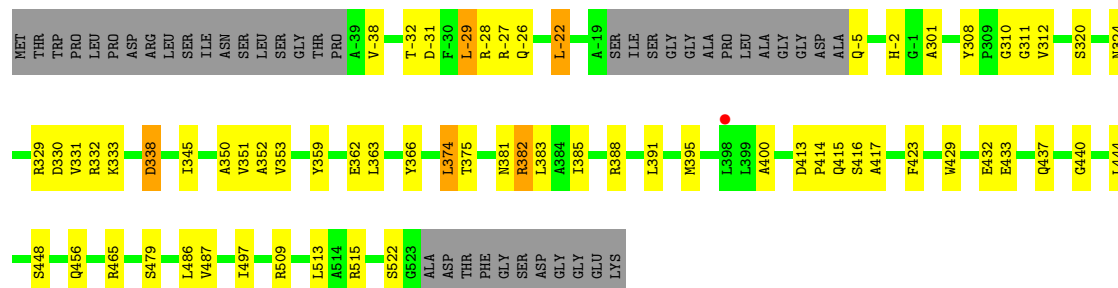
- Molecule 2: Proteasome subunit beta





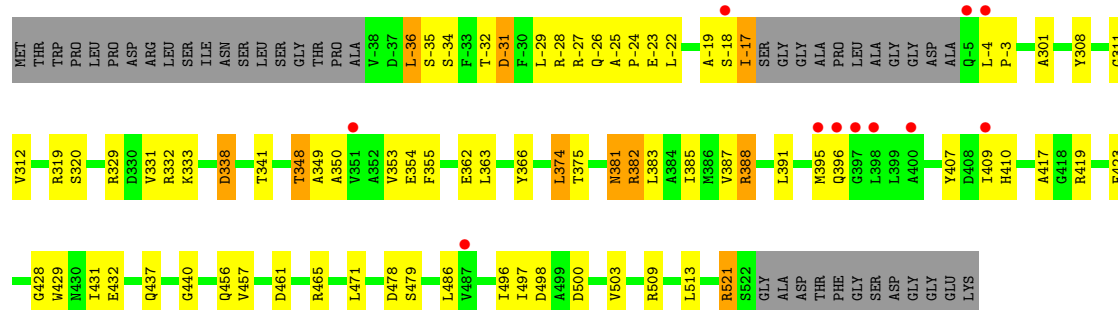
• Molecule 2: Proteasome subunit beta

Chain V: 63% 21% 14%



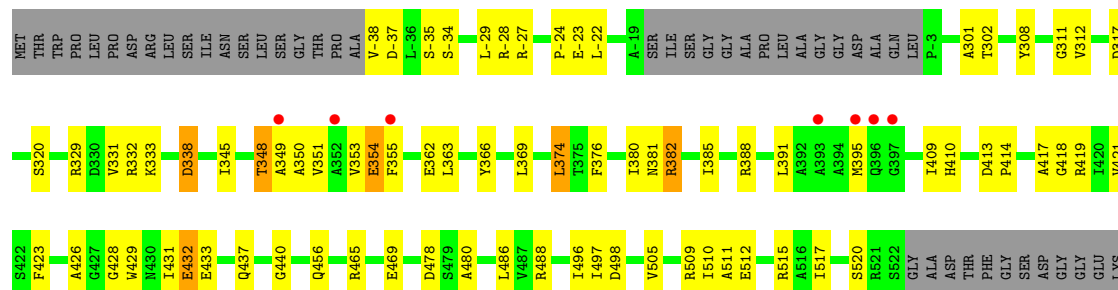
• Molecule 2: Proteasome subunit beta

Chain X: 4% 59% 23% 14%



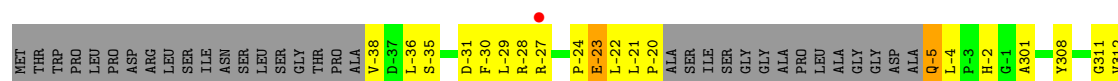
• Molecule 2: Proteasome subunit beta

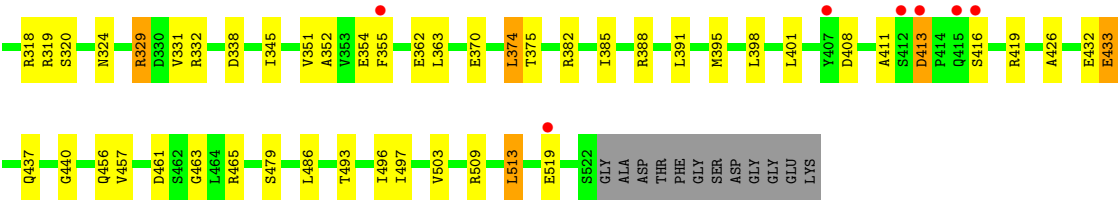
Chain Z: 2% 57% 25% 16%



• Molecule 2: Proteasome subunit beta

Chain 2: 3% 61% 21% 15%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	173.93Å 115.42Å 199.58Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	29.77 – 2.51 35.04 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.77-2.51) 94.0 (35.04-2.51)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.247 0.215 , 0.245	Depositor DCC
R_{free} test set	11793 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49801	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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	1	0.72	0/1720	0.83	0/2325
1	A	0.72	0/1741	0.82	2/2353 (0.1%)
1	B	0.65	0/1722	0.77	0/2327
1	D	0.69	0/1746	0.86	1/2360 (0.0%)
1	F	0.73	0/1733	0.84	2/2342 (0.1%)
1	I	0.72	0/1707	0.86	2/2306 (0.1%)
1	K	0.67	0/1733	0.84	1/2342 (0.0%)
1	M	0.75	0/1759	0.83	1/2378 (0.0%)
1	O	0.66	0/1700	0.84	1/2297 (0.0%)
1	Q	0.69	0/1745	0.81	0/2359
1	S	0.68	0/1712	0.82	1/2313 (0.0%)
1	U	0.71	0/1733	0.84	1/2342 (0.0%)
1	W	0.74	0/1739	0.83	1/2351 (0.0%)
1	Y	0.69	0/1759	0.82	2/2378 (0.1%)
2	2	0.79	0/1858	0.87	0/2520
2	C	0.84	0/1882	0.84	1/2553 (0.0%)
2	E	0.74	0/1863	0.84	2/2527 (0.1%)
2	G	0.86	1/1887 (0.1%)	0.86	2/2560 (0.1%)
2	H	0.84	0/1872	0.88	3/2538 (0.1%)
2	J	0.79	0/1892	0.84	1/2566 (0.0%)
2	L	0.74	0/1886	0.84	2/2558 (0.1%)
2	N	0.80	1/1892 (0.1%)	0.85	0/2566
2	P	0.72	0/1882	0.84	2/2553 (0.1%)
2	R	0.71	0/1851	0.83	1/2510 (0.0%)
2	T	0.82	0/1883	0.84	0/2554
2	V	0.82	0/1872	0.86	0/2539
2	X	0.80	0/1877	0.85	1/2546 (0.0%)
2	Z	0.79	0/1846	0.86	1/2503 (0.0%)
All	All	0.75	2/50492 (0.0%)	0.84	31/68366 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	446	ALA	CA-CB	-5.78	1.40	1.52
2	N	313	VAL	CB-CG1	-5.39	1.41	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	213	LEU	N-CA-C	-5.97	94.87	111.00
1	S	213	LEU	N-CA-C	-5.95	94.93	111.00
1	Y	213	LEU	N-CA-C	-5.92	95.00	111.00
2	L	488	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	I	213	LEU	N-CA-C	-5.86	95.19	111.00
1	M	76	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	F	76	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	G	357	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	Y	165	ASN	O-C-N	-5.80	113.42	122.70
2	P	374	LEU	CA-CB-CG	5.51	127.98	115.30
2	Z	488	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	E	-38	VAL	N-CA-C	-5.47	96.24	111.00
2	X	521	ARG	NE-CZ-NH1	-5.45	117.57	120.30
2	H	-36	LEU	O-C-N	-5.38	114.08	122.70
1	F	213	LEU	N-CA-C	-5.37	96.50	111.00
2	P	488	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	I	97	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	E	374	LEU	CA-CB-CG	5.25	127.37	115.30
1	U	213	LEU	N-CA-C	-5.23	96.89	111.00
1	W	213	LEU	N-CA-C	-5.22	96.90	111.00
2	C	388	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	G	338	ASP	CB-CG-OD1	5.19	122.97	118.30
2	R	488	ARG	NE-CZ-NH1	-5.19	117.71	120.30
2	J	356	ALA	O-C-N	-5.15	114.46	122.70
1	O	213	LEU	N-CA-C	-5.11	97.19	111.00
1	A	97	ARG	NE-CZ-NH2	-5.09	117.76	120.30
2	H	319	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	L	388	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	213	LEU	N-CA-C	-5.03	97.42	111.00
1	D	140	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	H	374	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1	1693	0	1688	133	0
1	A	1713	0	1713	132	0
1	B	1695	0	1685	124	0
1	D	1717	0	1712	138	0
1	F	1706	0	1705	89	0
1	I	1680	0	1673	99	0
1	K	1705	0	1702	149	0
1	M	1730	0	1726	112	0
1	O	1675	0	1676	104	0
1	Q	1716	0	1710	145	0
1	S	1686	0	1685	102	0
1	U	1706	0	1705	150	0
1	W	1710	0	1705	125	0
1	Y	1730	0	1726	91	0
2	2	1829	0	1824	64	0
2	C	1853	0	1850	104	0
2	E	1834	0	1829	94	0
2	G	1858	0	1855	76	0
2	H	1844	0	1841	106	0
2	J	1863	0	1858	85	0
2	L	1857	0	1853	101	0
2	N	1863	0	1858	73	0
2	P	1853	0	1850	98	0
2	R	1822	0	1815	84	0
2	T	1854	0	1850	74	0
2	V	1843	0	1837	73	0
2	X	1848	0	1845	95	0
2	Z	1817	0	1810	82	0
3	1	3	0	0	3	0
3	2	5	0	0	0	0
3	A	6	0	0	3	0
3	B	2	0	0	0	0
3	C	3	0	0	1	0
3	D	3	0	0	1	0
3	E	1	0	0	0	0
3	F	4	0	0	1	0
3	G	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	3	0	0	1	0
3	I	2	0	0	1	0
3	J	3	0	0	1	0
3	K	4	0	0	0	0
3	L	2	0	0	1	0
3	M	5	0	0	5	0
3	N	4	0	0	0	0
3	O	1	0	0	1	0
3	P	5	0	0	0	0
3	R	1	0	0	0	0
3	S	3	0	0	0	0
3	T	3	0	0	0	0
3	U	2	0	0	0	0
3	V	4	0	0	1	0
3	W	6	0	0	0	0
3	X	2	0	0	0	0
3	Y	6	0	0	1	0
3	Z	5	0	0	0	0
All	All	49801	0	49586	2615	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (2615) 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:Q:35:TYR:CE1	1:Q:37:GLY:HA3	1.51	1.43
1:O:35:TYR:CE1	1:O:37:GLY:HA3	1.56	1.40
2:H:407:TYR:CE1	2:H:417:ALA:HB3	1.59	1.36
1:S:35:TYR:CE1	1:S:37:GLY:HA3	1.56	1.36
1:B:35:TYR:CE1	1:B:37:GLY:HA3	1.60	1.35
1:Y:35:TYR:CE1	1:Y:37:GLY:HA3	1.63	1.32
1:D:35:TYR:CE1	1:D:37:GLY:HA3	1.64	1.31
1:Q:152:HIS:HB3	1:Q:171:TYR:CE1	1.66	1.31
1:A:35:TYR:CZ	1:A:37:GLY:HA3	1.67	1.28
1:U:35:TYR:CE1	1:U:37:GLY:HA3	1.70	1.27
1:D:229:ALA:O	1:D:233:LEU:HD13	1.34	1.26
1:D:230:LEU:O	1:D:234:LEU:HD13	1.35	1.26
1:M:7:ILE:HG21	1:W:5:TYR:CD2	1.71	1.25
1:Y:181:LEU:O	1:Y:181:LEU:HD12	1.35	1.25
2:L:407:TYR:CE1	2:L:417:ALA:HB3	1.70	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:413:ASP:OD1	2:L:414:PRO:HD2	1.36	1.24
1:D:3:PHE:CE1	1:F:6:PHE:CZ	2.27	1.22
2:G:456:GLN:NE2	2:G:465:ARG:HH22	1.35	1.22
1:D:207:SER:C	1:D:208:LEU:HD12	1.56	1.22
1:K:5:TYR:CD1	1:M:11:GLN:HG3	1.74	1.21
2:2:413:ASP:OD1	2:2:416:SER:HB2	1.40	1.21
1:K:35:TYR:CE1	1:K:37:GLY:HA3	1.73	1.20
1:B:35:TYR:CZ	1:B:37:GLY:HA3	1.77	1.20
1:W:173:GLU:C	1:W:174:ASN:HD22	1.45	1.18
1:D:207:SER:O	1:D:208:LEU:HD12	1.44	1.18
2:N:-17:ILE:CD1	2:N:392:ALA:HB3	1.74	1.18
2:H:-27:ARG:HG2	2:H:-26:GLN:OE1	1.39	1.18
2:N:413:ASP:OD1	2:N:414:PRO:HD2	1.40	1.18
1:A:7:ILE:O	1:B:5:TYR:HB3	1.42	1.18
1:B:178:THR:HG23	1:B:233:LEU:HD23	1.21	1.17
1:F:35:TYR:CE1	1:F:37:GLY:HA3	1.79	1.17
1:I:35:TYR:CE1	1:I:37:GLY:HA3	1.80	1.15
2:R:301:ALA:HB2	2:R:333:LYS:HZ3	1.01	1.14
1:Y:35:TYR:CE1	1:Y:37:GLY:CA	2.30	1.14
2:X:301:ALA:HB2	2:X:333:LYS:HZ3	1.07	1.14
1:O:35:TYR:CE1	1:O:37:GLY:CA	2.30	1.13
2:T:426:ALA:HB2	2:2:-4:LEU:HD21	1.26	1.13
1:B:35:TYR:CE1	1:B:37:GLY:CA	2.30	1.13
1:D:35:TYR:CE1	1:D:37:GLY:CA	2.30	1.13
2:R:456:GLN:NE2	2:R:465:ARG:HH22	1.44	1.13
2:E:362:GLU:OE2	2:E:382:ARG:HD3	1.46	1.13
1:Q:35:TYR:CE1	1:Q:37:GLY:CA	2.30	1.13
1:S:35:TYR:CE1	1:S:37:GLY:CA	2.30	1.13
2:H:407:TYR:CE1	2:H:417:ALA:CB	2.31	1.12
2:H:-6:ALA:N	2:H:-5:GLN:HB3	1.38	1.12
2:T:415:GLN:N	2:T:415:GLN:HE21	1.45	1.12
1:B:40:LEU:HD12	1:B:212:VAL:HG12	1.31	1.12
1:D:8:SER:HB3	1:D:11:GLN:HG2	1.22	1.11
2:E:-28:ARG:O	2:E:-24:PRO:HG3	1.49	1.11
2:L:456:GLN:NE2	2:L:465:ARG:HH22	1.47	1.11
2:R:-31:ASP:O	2:R:-27:ARG:HD3	1.49	1.11
2:V:456:GLN:NE2	2:V:465:ARG:HH22	1.47	1.10
1:M:7:ILE:HG21	1:W:5:TYR:CE2	1.86	1.10
1:O:163:ILE:O	1:O:167:LEU:HG	1.51	1.10
2:C:-18:SER:HB2	2:C:393:ALA:HB2	1.25	1.09
1:O:51:GLN:H	1:O:51:GLN:NE2	1.49	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:8:SER:CB	1:1:11:GLN:HE21	1.64	1.09
2:T:-17:ILE:O	2:T:-16:SER:HB2	1.47	1.09
1:Q:181:LEU:O	1:Q:185:VAL:HG23	1.49	1.09
1:A:110:ILE:HG23	1:A:114:GLN:HG3	1.13	1.09
1:U:179:ASP:O	1:U:183:ILE:HG13	1.53	1.09
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.34	1.08
2:N:-17:ILE:HD13	2:N:392:ALA:HB3	1.15	1.08
1:W:181:LEU:O	1:W:185:VAL:HG23	1.53	1.08
1:D:3:PHE:CZ	1:F:6:PHE:HZ	1.70	1.08
1:U:35:TYR:CE1	1:U:37:GLY:CA	2.36	1.07
1:1:167:LEU:CD1	1:1:187:ALA:CB	2.33	1.07
2:G:456:GLN:HE22	2:G:465:ARG:NH2	1.51	1.07
1:U:217:ARG:HD2	1:U:223:ARG:HD2	1.28	1.07
2:Z:301:ALA:CB	2:Z:333:LYS:HZ3	1.68	1.06
1:A:35:TYR:CE1	1:A:37:GLY:HA3	1.89	1.06
2:T:456:GLN:NE2	2:T:465:ARG:HH22	1.51	1.06
1:B:234:LEU:O	1:B:235:VAL:HG23	1.51	1.06
1:D:3:PHE:HE1	1:F:6:PHE:CE2	1.73	1.06
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.37	1.06
1:M:7:ILE:HD13	1:W:5:TYR:CD2	1.90	1.06
2:Z:301:ALA:HB2	2:Z:333:LYS:NZ	1.69	1.06
1:Y:35:TYR:CZ	1:Y:37:GLY:HA3	1.91	1.05
2:H:456:GLN:NE2	2:H:465:ARG:HH22	1.53	1.05
1:K:35:TYR:CZ	1:K:37:GLY:HA3	1.92	1.05
1:O:234:LEU:O	1:O:234:LEU:HD13	1.55	1.05
2:N:308:TYR:CZ	2:N:311:GLY:HA3	1.89	1.05
2:Z:301:ALA:HB2	2:Z:333:LYS:HZ3	0.90	1.05
1:1:8:SER:OG	1:1:11:GLN:HG2	1.56	1.05
2:H:-23:GLU:HG2	2:P:-28:ARG:HH21	1.21	1.05
1:W:110:ILE:HG23	1:W:114:GLN:HG3	1.34	1.05
1:I:181:LEU:O	1:I:185:VAL:HG23	1.56	1.04
2:C:456:GLN:NE2	2:C:465:ARG:HH22	1.53	1.04
1:K:4:PRO:HB3	1:W:5:TYR:CD1	1.92	1.04
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.39	1.04
1:U:8:SER:HB3	1:1:5:TYR:HB3	1.04	1.04
1:K:35:TYR:CE1	1:K:37:GLY:CA	2.39	1.04
2:R:456:GLN:HE22	2:R:465:ARG:NH2	1.55	1.03
1:A:45:ASN:HD21	1:A:52:LYS:HD3	1.14	1.03
2:L:-25:ALA:HB1	2:L:-22:LEU:CD2	1.87	1.03
1:D:189:ARG:HH12	1:D:203:LEU:N	1.55	1.03
1:K:30:VAL:HG13	1:K:43:ALA:HB2	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:348:THR:HB	2:Z:351:VAL:HG23	1.40	1.03
1:D:3:PHE:CE1	1:F:6:PHE:HZ	1.68	1.03
1:O:35:TYR:CZ	1:O:37:GLY:HA3	1.93	1.03
2:V:301:ALA:HB2	2:V:333:LYS:HZ3	1.20	1.02
2:R:301:ALA:CB	2:R:333:LYS:HZ3	1.72	1.02
2:Z:301:ALA:CB	2:Z:333:LYS:NZ	2.22	1.02
1:M:7:ILE:HD13	1:W:5:TYR:HD2	1.12	1.02
1:A:7:ILE:HD12	1:A:11:GLN:HG3	1.41	1.02
1:U:97:ARG:HH22	1:U:101:ASN:HD22	1.08	1.02
1:D:3:PHE:HE1	1:F:6:PHE:CZ	1.70	1.01
2:V:456:GLN:HE22	2:V:465:ARG:NH2	1.58	1.01
2:E:407:TYR:CE1	2:E:417:ALA:HB3	1.95	1.01
2:L:-25:ALA:HB1	2:L:-22:LEU:HD23	1.02	1.01
2:X:301:ALA:HB2	2:X:333:LYS:NZ	1.74	1.01
2:H:-6:ALA:N	2:H:-5:GLN:CB	2.18	1.01
1:K:152:HIS:HB3	1:K:171:TYR:CE2	1.96	1.01
1:W:3:PHE:N	1:W:4:PRO:HA	1.76	1.01
2:E:456:GLN:NE2	2:E:465:ARG:HH22	1.56	1.00
1:O:7:ILE:N	1:U:7:ILE:HD12	1.75	1.00
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.42	1.00
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.43	1.00
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.44	1.00
2:C:301:ALA:HB2	2:C:333:LYS:HE2	1.43	0.99
2:T:413:ASP:OD1	2:T:414:PRO:HD2	1.62	0.99
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.44	0.99
1:I:181:LEU:HD12	1:I:181:LEU:O	1.60	0.99
2:L:456:GLN:HE22	2:L:465:ARG:NH2	1.60	0.99
1:O:179:ASP:O	1:O:183:ILE:HG13	1.61	0.99
1:B:178:THR:HG23	1:B:233:LEU:CD2	1.90	0.99
1:D:207:SER:C	1:D:208:LEU:CD1	2.30	0.99
1:Y:234:LEU:O	1:Y:235:VAL:HG23	1.63	0.99
2:L:-26:GLN:HA	2:L:-26:GLN:OE1	1.63	0.98
2:N:308:TYR:CE1	2:N:311:GLY:HA3	1.98	0.98
1:U:35:TYR:CZ	1:U:37:GLY:HA3	1.98	0.98
2:E:301:ALA:HB2	2:E:333:LYS:HE2	1.40	0.98
2:N:301:ALA:HB2	2:N:333:LYS:HZ3	1.29	0.98
1:U:112:THR:HG21	3:I:250:HOH:O	1.62	0.98
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.45	0.97
2:C:456:GLN:HE22	2:C:465:ARG:NH2	1.62	0.97
2:H:456:GLN:HE22	2:H:465:ARG:HH22	1.03	0.97
1:Q:40:LEU:HA	1:Q:212:VAL:HG12	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:ASP:O	1:K:183:ILE:HG13	1.65	0.97
1:U:230:LEU:O	1:U:234:LEU:HD13	1.63	0.97
1:Q:152:HIS:HB3	1:Q:171:TYR:HE1	1.25	0.97
1:Q:35:TYR:CZ	1:Q:37:GLY:HA3	1.98	0.97
1:K:6:PHE:HB3	1:Q:4:PRO:HG3	1.45	0.97
2:T:456:GLN:HE22	2:T:465:ARG:NH2	1.63	0.96
1:A:8:SER:HB2	1:A:9:PRO:HD2	1.46	0.96
1:U:167:LEU:HA	1:U:170:SER:OG	1.64	0.96
2:V:301:ALA:HB2	2:V:333:LYS:NZ	1.81	0.96
1:I:179:ASP:O	1:I:183:ILE:HG13	1.65	0.96
1:M:7:ILE:CD1	1:W:5:TYR:HD2	1.78	0.96
2:H:-27:ARG:HE	2:H:-26:GLN:NE2	1.62	0.96
2:L:-25:ALA:CB	2:L:-22:LEU:HD23	1.94	0.96
2:L:407:TYR:CE1	2:L:417:ALA:CB	2.47	0.96
2:X:456:GLN:NE2	2:X:465:ARG:HH22	1.62	0.96
2:J:301:ALA:HB2	2:J:333:LYS:HZ3	1.29	0.96
2:Z:-27:ARG:HH21	2:Z:-27:ARG:HG2	1.30	0.96
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.45	0.96
2:H:456:GLN:HE22	2:H:465:ARG:NH2	1.64	0.95
1:I:35:TYR:CZ	1:I:37:GLY:HA3	2.01	0.95
1:O:181:LEU:O	1:O:185:VAL:HG23	1.64	0.95
2:V:456:GLN:HE22	2:V:465:ARG:HH22	0.98	0.95
1:B:110:ILE:HG23	1:B:114:GLN:HG3	1.45	0.95
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.45	0.95
1:I:35:TYR:CE1	1:I:37:GLY:CA	2.50	0.95
2:E:456:GLN:HE22	2:E:465:ARG:HH22	0.98	0.95
2:G:308:TYR:CZ	2:G:311:GLY:HA3	2.02	0.95
2:Z:456:GLN:NE2	2:Z:465:ARG:HH22	1.64	0.95
1:B:40:LEU:CD1	1:B:212:VAL:HG12	1.97	0.94
2:Z:456:GLN:HE22	2:Z:465:ARG:HH22	1.06	0.94
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.47	0.94
2:C:434:GLU:HA	2:C:434:GLU:OE1	1.67	0.94
2:P:407:TYR:CE2	2:P:499:ALA:HA	2.03	0.94
1:U:229:ALA:O	1:U:233:LEU:HD21	1.64	0.94
2:E:-32:THR:HG23	2:E:362:GLU:OE1	1.65	0.94
2:H:-6:ALA:H1	2:H:-5:GLN:HB3	1.22	0.94
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.48	0.94
2:X:308:TYR:CZ	2:X:311:GLY:HA3	2.02	0.94
2:Z:350:ALA:O	2:Z:353:VAL:HG12	1.67	0.94
1:I:110:ILE:HG23	1:I:114:GLN:HG3	1.50	0.94
2:N:-17:ILE:HD13	2:N:392:ALA:CB	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:152:HIS:HB3	1:M:171:TYR:CE2	2.03	0.94
2:H:-6:ALA:H3	2:H:-5:GLN:HB3	1.30	0.94
1:O:51:GLN:HE21	1:O:51:GLN:N	1.67	0.93
1:1:7:ILE:HB	1:1:11:GLN:HG3	1.46	0.93
2:J:-39:ALA:HA	2:T:-26:GLN:OE1	1.69	0.93
2:X:456:GLN:HE22	2:X:465:ARG:HH22	1.15	0.93
2:Z:348:THR:CB	2:Z:351:VAL:HG23	1.98	0.93
1:B:178:THR:HA	1:B:233:LEU:HD21	1.50	0.93
1:1:18:GLU:OE1	1:1:22:LYS:HE2	1.66	0.93
1:Y:35:TYR:CE1	1:Y:37:GLY:N	2.36	0.93
1:D:173:GLU:HG2	1:D:174:ASN:OD1	1.69	0.93
1:S:110:ILE:HG23	1:S:114:GLN:HG3	1.51	0.93
2:X:521:ARG:HH11	2:X:521:ARG:HG2	1.34	0.93
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.51	0.92
2:P:308:TYR:CZ	2:P:311:GLY:HA3	2.05	0.92
1:S:35:TYR:HE1	1:S:37:GLY:HA3	1.33	0.92
1:U:181:LEU:HD21	1:U:234:LEU:CD1	1.99	0.92
1:U:8:SER:CB	1:1:5:TYR:HB3	1.97	0.92
1:1:8:SER:CB	1:1:11:GLN:NE2	2.33	0.92
2:J:-17:ILE:HD12	2:J:392:ALA:HB3	1.51	0.92
1:K:16:ARG:HB3	1:K:117:PRO:HG2	1.49	0.92
1:A:35:TYR:CZ	1:A:37:GLY:CA	2.51	0.92
1:K:179:ASP:OD1	1:K:183:ILE:HD11	1.69	0.92
1:O:51:GLN:HE21	1:O:51:GLN:H	1.04	0.92
1:A:19:LEU:HD12	1:B:9:PRO:HB2	1.51	0.92
2:C:409:ILE:HG13	2:C:410:HIS:ND1	1.85	0.92
1:S:15:GLU:OE2	1:1:9:PRO:HD2	1.69	0.92
1:U:214:ASP:HB3	1:U:217:ARG:HG3	1.50	0.91
2:P:407:TYR:CE1	2:P:417:ALA:HB3	2.05	0.91
2:2:-28:ARG:HG2	2:2:-21:LEU:CD1	2.00	0.91
2:E:456:GLN:HE22	2:E:465:ARG:NH2	1.68	0.91
2:N:-21:LEU:HD12	2:N:-20:PRO:HD3	1.49	0.91
1:D:15:GLU:OE2	1:K:8:SER:HB2	1.70	0.91
1:D:35:TYR:HE1	1:D:37:GLY:HA3	1.22	0.91
2:G:362:GLU:OE2	2:G:382:ARG:HD3	1.69	0.91
1:1:8:SER:N	1:1:11:GLN:HE21	1.67	0.91
2:C:-39:ALA:N	2:J:-26:GLN:CD	2.24	0.91
1:Y:181:LEU:C	1:Y:181:LEU:HD12	1.82	0.91
1:Y:179:ASP:O	1:Y:183:ILE:HG13	1.69	0.91
2:G:391:LEU:O	2:G:391:LEU:HD12	1.71	0.91
1:K:4:PRO:HB3	1:W:5:TYR:CG	2.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:413:ASP:HB3	2:G:416:SER:OG	1.69	0.90
1:K:25:ALA:O	1:K:158:GLY:HA2	1.71	0.90
1:A:11:GLN:HE22	1:A:14:ARG:NH2	1.69	0.90
1:D:3:PHE:N	1:D:4:PRO:HD3	1.84	0.90
1:O:8:SER:OG	1:O:11:GLN:HB3	1.71	0.90
2:J:308:TYR:CZ	2:J:311:GLY:HA3	2.06	0.90
2:L:301:ALA:HB2	2:L:333:LYS:HZ3	1.34	0.90
1:U:35:TYR:CE1	1:U:37:GLY:N	2.40	0.90
2:X:382:ARG:HH21	2:X:385:ILE:CD1	1.83	0.90
2:G:301:ALA:HB2	2:G:333:LYS:HZ3	1.33	0.90
2:T:-28:ARG:HB2	2:T:-28:ARG:CZ	2.00	0.90
2:H:413:ASP:OD1	2:H:414:PRO:HD2	1.72	0.90
2:P:465:ARG:HA	2:P:513:LEU:HD21	1.53	0.90
2:T:415:GLN:HE21	2:T:415:GLN:CA	1.84	0.90
1:1:167:LEU:CD1	1:1:187:ALA:HB2	2.01	0.90
1:1:8:SER:HB3	1:1:11:GLN:HE21	1.36	0.89
2:E:413:ASP:HB2	2:E:416:SER:OG	1.72	0.89
1:S:35:TYR:CZ	1:S:37:GLY:HA3	2.07	0.89
1:F:35:TYR:CE1	1:F:37:GLY:CA	2.55	0.89
2:R:301:ALA:HB2	2:R:333:LYS:NZ	1.86	0.89
1:Y:35:TYR:CD1	1:Y:37:GLY:N	2.41	0.89
2:T:308:TYR:CZ	2:T:311:GLY:HA3	2.08	0.89
1:M:7:ILE:CG2	1:W:5:TYR:CE2	2.55	0.89
2:R:456:GLN:HE22	2:R:465:ARG:HH22	0.91	0.89
2:J:487:VAL:HG13	2:R:522:SER:O	1.71	0.89
1:U:8:SER:HB3	1:1:5:TYR:CB	2.00	0.89
1:W:35:TYR:CE1	1:W:37:GLY:HA3	2.07	0.89
2:X:521:ARG:CG	2:X:521:ARG:HH11	1.86	0.89
1:D:35:TYR:CD1	1:D:37:GLY:N	2.41	0.89
2:R:301:ALA:CB	2:R:333:LYS:NZ	2.35	0.89
2:G:-21:LEU:HG	2:G:-20:PRO:HD2	1.53	0.89
2:X:-17:ILE:HG12	2:X:-17:ILE:O	1.71	0.89
1:B:181:LEU:O	1:B:185:VAL:HG23	1.71	0.89
2:G:-18:SER:O	2:G:-17:ILE:HB	1.71	0.88
2:J:301:ALA:HB2	2:J:333:LYS:NZ	1.88	0.88
2:E:308:TYR:CZ	2:E:311:GLY:HA3	2.08	0.88
1:1:18:GLU:CD	1:1:21:ARG:HH21	1.76	0.88
1:A:35:TYR:CE1	1:A:37:GLY:CA	2.56	0.88
1:B:35:TYR:CE1	1:B:37:GLY:N	2.41	0.88
2:X:301:ALA:CB	2:X:333:LYS:NZ	2.35	0.88
1:K:35:TYR:CE1	1:K:37:GLY:N	2.42	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:415:GLN:HA	2:E:415:GLN:HE21	1.36	0.88
1:Q:35:TYR:HE1	1:Q:37:GLY:HA3	1.39	0.87
1:M:35:TYR:CE1	1:M:37:GLY:HA3	2.08	0.87
2:N:456:GLN:NE2	2:N:465:ARG:HH22	1.71	0.87
1:K:6:PHE:HB3	1:Q:4:PRO:CG	2.04	0.87
1:A:45:ASN:HD21	1:A:52:LYS:CD	1.86	0.87
1:O:19:LEU:C	1:O:19:LEU:HD23	1.94	0.87
1:Q:171:TYR:CD2	1:Q:172:ALA:N	2.43	0.87
1:K:4:PRO:HB3	1:W:5:TYR:CE1	2.10	0.86
1:1:35:TYR:CZ	1:1:37:GLY:HA3	2.09	0.86
2:X:331:VAL:HG13	2:X:349:ALA:HB2	1.55	0.86
1:1:8:SER:H	1:1:11:GLN:NE2	1.71	0.86
1:Q:152:HIS:CB	1:Q:171:TYR:CE1	2.57	0.86
1:U:231:GLN:HE22	1:U:235:VAL:HG21	1.40	0.86
2:V:301:ALA:CB	2:V:333:LYS:NZ	2.38	0.86
1:W:174:ASN:N	1:W:174:ASN:HD22	1.73	0.86
2:R:308:TYR:CZ	2:R:311:GLY:HA3	2.10	0.86
1:D:208:LEU:N	1:D:208:LEU:CD1	2.38	0.86
2:J:426:ALA:HB2	2:T:-4:LEU:HD21	1.55	0.86
1:1:8:SER:HB3	1:1:11:GLN:NE2	1.91	0.86
1:B:178:THR:HA	1:B:233:LEU:CD2	2.05	0.86
1:B:22:LYS:O	1:B:26:ARG:HG3	1.75	0.86
1:U:35:TYR:CD1	1:U:37:GLY:N	2.44	0.86
2:C:456:GLN:HE22	2:C:465:ARG:HH22	0.87	0.85
1:K:234:LEU:HD13	1:K:234:LEU:C	1.96	0.85
1:D:35:TYR:CE1	1:D:37:GLY:N	2.43	0.85
2:X:383:LEU:O	2:X:387:VAL:HG23	1.77	0.85
2:2:-28:ARG:HG2	2:2:-21:LEU:HD11	1.56	0.85
2:J:308:TYR:CE1	2:J:311:GLY:HA3	2.11	0.85
1:U:217:ARG:CD	1:U:223:ARG:HD2	2.07	0.85
2:T:415:GLN:CA	2:T:415:GLN:NE2	2.40	0.85
1:B:35:TYR:CD1	1:B:37:GLY:N	2.44	0.85
2:L:-24:PRO:HD2	2:L:-23:GLU:OE2	1.77	0.85
2:X:-17:ILE:HA	2:X:396:GLN:OE1	1.77	0.85
1:Y:110:ILE:HG23	1:Y:114:GLN:HG3	1.57	0.85
1:B:179:ASP:O	1:B:183:ILE:HG13	1.76	0.85
2:E:407:TYR:CE1	2:E:417:ALA:CB	2.60	0.85
2:H:407:TYR:HE1	2:H:417:ALA:HB3	1.34	0.85
1:1:167:LEU:HD13	1:1:187:ALA:CB	2.07	0.84
1:U:181:LEU:HD21	1:U:234:LEU:HD12	1.59	0.84
2:V:308:TYR:CZ	2:V:311:GLY:HA3	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:155:VAL:CG2	1:O:167:LEU:CD1	2.56	0.84
1:O:35:TYR:CD1	1:O:37:GLY:N	2.44	0.84
1:1:167:LEU:HD13	1:1:187:ALA:HB1	1.58	0.84
1:S:35:TYR:CD1	1:S:37:GLY:N	2.45	0.84
2:T:456:GLN:HE22	2:T:465:ARG:HH22	0.87	0.84
2:X:509:ARG:HG3	2:X:509:ARG:HH11	1.43	0.84
2:L:456:GLN:HE22	2:L:465:ARG:HH22	0.86	0.84
2:X:382:ARG:NH2	2:X:385:ILE:HD13	1.92	0.84
1:W:173:GLU:C	1:W:174:ASN:ND2	2.30	0.83
2:P:-26:GLN:HA	2:P:-26:GLN:OE1	1.77	0.83
1:O:155:VAL:CG2	1:O:167:LEU:HD11	2.09	0.83
1:Y:181:LEU:O	1:Y:185:VAL:HG23	1.76	0.83
2:P:-27:ARG:NH1	2:P:-26:GLN:HE21	1.77	0.83
1:Q:25:ALA:O	1:Q:158:GLY:HA2	1.79	0.83
2:Z:456:GLN:HE22	2:Z:465:ARG:NH2	1.77	0.83
2:X:382:ARG:NH2	2:X:385:ILE:CD1	2.42	0.83
1:A:110:ILE:CG2	1:A:114:GLN:HG3	2.06	0.82
1:M:7:ILE:CG2	1:W:5:TYR:CD2	2.60	0.82
1:I:114:GLN:HA	1:I:114:GLN:HE21	1.41	0.82
1:F:33:LEU:HD12	1:F:33:LEU:O	1.80	0.82
1:Q:40:LEU:HD12	1:Q:212:VAL:CG1	2.09	0.82
1:A:7:ILE:HD12	1:A:11:GLN:CG	2.10	0.82
1:S:25:ALA:O	1:S:158:GLY:HA2	1.79	0.82
1:F:203:LEU:N	1:F:234:LEU:HD11	1.94	0.82
1:B:5:TYR:HE2	1:O:11:GLN:HE22	1.27	0.82
2:E:-36:LEU:HD12	2:E:-31:ASP:OD2	1.80	0.82
2:N:301:ALA:HB2	2:N:333:LYS:NZ	1.93	0.82
1:O:155:VAL:HG21	1:O:167:LEU:CD1	2.09	0.82
1:O:8:SER:HG	1:O:11:GLN:HB3	1.42	0.82
2:H:407:TYR:CZ	2:H:417:ALA:CB	2.62	0.82
1:D:8:SER:HB3	1:D:11:GLN:CG	2.09	0.81
1:U:112:THR:CG2	3:1:250:HOH:O	2.22	0.81
1:K:4:PRO:HG3	1:W:5:TYR:CB	2.09	0.81
1:K:4:PRO:HG3	1:W:5:TYR:CG	2.15	0.81
1:F:25:ALA:O	1:F:158:GLY:HA2	1.80	0.81
1:A:6:PHE:HB3	1:B:5:TYR:HB2	1.62	0.81
2:L:301:ALA:HB2	2:L:333:LYS:NZ	1.95	0.81
2:X:362:GLU:OE2	2:X:382:ARG:HD3	1.81	0.81
2:N:456:GLN:HE22	2:N:465:ARG:NH2	1.79	0.81
1:K:152:HIS:CD2	1:K:171:TYR:HE2	1.96	0.81
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:ND2	1:A:52:LYS:HD3	1.96	0.81
1:S:14:ARG:HB2	1:S:14:ARG:NH2	1.96	0.81
2:Z:362:GLU:OE2	2:Z:382:ARG:HD3	1.80	0.81
2:2:456:GLN:HE22	2:2:465:ARG:HH22	1.28	0.81
2:T:426:ALA:CB	2:2:-4:LEU:HD21	2.09	0.81
1:I:129:HIS:HE1	3:I:250:HOH:O	1.63	0.81
2:C:-39:ALA:N	2:J:-26:GLN:NE2	2.29	0.81
1:Y:59:ARG:HD2	1:Y:129:HIS:HA	1.63	0.81
1:U:25:ALA:O	1:U:158:GLY:HA2	1.82	0.80
2:C:-18:SER:HB2	2:C:393:ALA:CB	2.08	0.80
1:A:15:GLU:OE1	1:B:9:PRO:HD2	1.82	0.80
1:A:59:ARG:HD2	1:A:129:HIS:HA	1.64	0.80
1:Q:59:ARG:HD2	1:Q:129:HIS:HA	1.62	0.80
2:Z:511:ALA:HB1	2:Z:515:ARG:NH2	1.97	0.80
1:B:152:HIS:CD2	1:B:171:TYR:HE2	2.00	0.80
2:C:-26:GLN:HB3	2:H:-39:ALA:HB3	1.62	0.80
2:G:-26:GLN:HA	2:G:-26:GLN:OE1	1.82	0.80
2:H:-5:GLN:NE2	2:H:-2:HIS:NE2	2.29	0.80
1:O:35:TYR:CE1	1:O:37:GLY:N	2.50	0.80
2:R:-31:ASP:O	2:R:-27:ARG:CD	2.30	0.80
2:L:354:GLU:CA	2:L:354:GLU:OE1	2.30	0.80
1:M:41:PHE:HB3	1:M:53:ILE:HD13	1.64	0.80
2:P:-27:ARG:NH1	2:P:-26:GLN:NE2	2.30	0.80
2:R:362:GLU:OE2	2:R:382:ARG:HD3	1.81	0.80
2:T:-17:ILE:O	2:T:-16:SER:CB	2.30	0.80
2:G:456:GLN:NE2	2:G:465:ARG:NH2	2.20	0.80
2:T:413:ASP:OD1	2:T:414:PRO:CD	2.30	0.80
1:D:33:LEU:HD12	1:D:33:LEU:O	1.81	0.80
1:F:59:ARG:HD2	1:F:129:HIS:HA	1.62	0.80
2:L:-27:ARG:NH1	2:L:-26:GLN:NE2	2.30	0.80
1:U:97:ARG:NH2	1:U:101:ASN:HD22	1.78	0.80
2:X:-17:ILE:CG1	2:X:-17:ILE:O	2.30	0.80
1:M:7:ILE:HG21	1:W:5:TYR:HD2	1.27	0.80
1:U:97:ARG:HH22	1:U:101:ASN:ND2	1.77	0.80
1:U:59:ARG:HD2	1:U:129:HIS:HA	1.64	0.80
2:X:331:VAL:HG13	2:X:349:ALA:CB	2.11	0.80
1:M:218:PRO:HG2	3:M:249:HOH:O	1.82	0.80
2:P:-27:ARG:NE	2:P:-26:GLN:NE2	2.30	0.80
2:2:308:TYR:CZ	2:2:311:GLY:HA3	2.16	0.79
2:C:-32:THR:HG23	2:C:362:GLU:OE1	1.82	0.79
2:E:-28:ARG:O	2:E:-24:PRO:CG	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:230:LEU:O	1:Q:234:LEU:CD1	2.30	0.79
2:E:415:GLN:CA	2:E:415:GLN:HE21	1.95	0.79
1:K:4:PRO:CB	1:W:5:TYR:CD2	2.65	0.79
2:X:382:ARG:HH21	2:X:385:ILE:HD13	1.47	0.79
1:U:233:LEU:H	1:U:233:LEU:HD23	1.46	0.79
2:G:301:ALA:HB2	2:G:333:LYS:NZ	1.96	0.79
1:Q:191:GLY:O	1:Q:192:SER:HB2	1.81	0.79
1:K:35:TYR:CD1	1:K:37:GLY:N	2.51	0.79
2:E:407:TYR:CE2	2:E:499:ALA:HA	2.18	0.79
2:G:-32:THR:HG23	2:G:362:GLU:OE1	1.83	0.79
1:S:115:ALA:HB1	1:U:6:PHE:HZ	1.47	0.79
1:1:8:SER:OG	1:1:11:GLN:CG	2.30	0.79
2:C:434:GLU:CA	2:C:434:GLU:OE1	2.30	0.79
2:L:-18:SER:O	2:L:-17:ILE:CG2	2.30	0.79
1:A:7:ILE:O	1:B:5:TYR:CB	2.27	0.79
1:W:205:VAL:HG21	1:W:231:GLN:HA	1.64	0.79
1:A:11:GLN:NE2	1:A:14:ARG:NH2	2.30	0.79
2:H:413:ASP:OD1	2:H:414:PRO:CD	2.30	0.79
2:L:354:GLU:HA	2:L:354:GLU:OE1	1.81	0.79
1:Y:234:LEU:O	1:Y:235:VAL:CG2	2.30	0.79
2:G:413:ASP:CB	2:G:416:SER:OG	2.30	0.79
2:H:-27:ARG:NE	2:H:-26:GLN:NE2	2.30	0.79
1:Q:234:LEU:O	1:Q:235:VAL:CG2	2.30	0.79
2:X:456:GLN:HE22	2:X:465:ARG:NH2	1.81	0.79
1:1:18:GLU:OE1	1:1:22:LYS:CE	2.30	0.78
2:G:456:GLN:HE22	2:G:465:ARG:HH22	0.81	0.78
2:C:-39:ALA:H2	2:J:-26:GLN:CD	1.85	0.78
1:Y:169:GLU:OE1	1:Y:169:GLU:HA	1.83	0.78
1:F:169:GLU:OE1	1:F:169:GLU:HA	1.84	0.78
2:Z:308:TYR:CZ	2:Z:311:GLY:HA3	2.19	0.78
1:D:173:GLU:CG	1:D:174:ASN:OD1	2.30	0.78
2:E:415:GLN:HA	2:E:415:GLN:NE2	1.98	0.78
1:O:150:GLU:HG3	1:O:154:VAL:HG22	1.64	0.78
2:T:415:GLN:HA	2:T:415:GLN:NE2	1.97	0.78
1:1:8:SER:N	1:1:11:GLN:NE2	2.30	0.78
1:1:218:PRO:HG2	3:1:249:HOH:O	1.83	0.78
2:C:351:VAL:HG12	2:C:400:ALA:HB2	1.66	0.78
1:D:205:VAL:HG23	1:D:206:ALA:N	1.97	0.78
1:S:114:GLN:HA	1:S:114:GLN:HE21	1.46	0.78
2:L:308:TYR:CZ	2:L:311:GLY:HA3	2.18	0.78
1:Q:153:PHE:CD2	1:Q:171:TYR:HD1	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:59:ARG:HD2	1:S:129:HIS:HA	1.66	0.78
1:U:229:ALA:O	1:U:233:LEU:CD2	2.30	0.78
1:K:4:PRO:CB	1:W:5:TYR:CG	2.67	0.78
1:F:169:GLU:OE1	1:F:169:GLU:CA	2.30	0.78
2:G:308:TYR:CE1	2:G:311:GLY:HA3	2.18	0.78
1:Y:25:ALA:O	1:Y:158:GLY:HA2	1.83	0.78
2:Z:301:ALA:HB1	2:Z:333:LYS:HZ2	1.49	0.78
2:Z:348:THR:HB	2:Z:351:VAL:CG2	2.12	0.78
1:1:59:ARG:HD2	1:1:129:HIS:HA	1.65	0.78
2:2:456:GLN:NE2	2:2:465:ARG:HH22	1.79	0.78
1:B:35:TYR:CZ	1:B:37:GLY:CA	2.59	0.78
1:D:3:PHE:CZ	1:F:6:PHE:CZ	2.61	0.78
1:Q:35:TYR:CD1	1:Q:37:GLY:N	2.51	0.78
2:H:308:TYR:CZ	2:H:311:GLY:HA3	2.18	0.78
1:B:5:TYR:CE2	1:O:11:GLN:NE2	2.51	0.78
2:E:-4:LEU:O	2:E:-2:HIS:HD2	1.65	0.78
1:1:8:SER:CA	1:1:11:GLN:HE21	1.97	0.78
1:A:35:TYR:CE1	1:A:37:GLY:N	2.53	0.77
2:H:-27:ARG:HG2	2:H:-26:GLN:CD	2.04	0.77
1:K:33:LEU:CD1	1:K:40:LEU:HB3	2.14	0.77
2:E:349:ALA:O	2:E:353:VAL:HG12	1.83	0.77
2:P:349:ALA:O	2:P:353:VAL:HG12	1.83	0.77
1:D:150:GLU:HG3	1:D:154:VAL:HG22	1.64	0.77
1:Q:171:TYR:CE2	1:Q:172:ALA:O	2.37	0.77
2:E:-28:ARG:CZ	2:E:-21:LEU:HD23	2.14	0.77
2:E:-24:PRO:O	2:E:-21:LEU:HB2	1.84	0.77
2:L:-35:SER:HB3	2:L:369:LEU:HD12	1.65	0.77
1:O:234:LEU:C	1:O:234:LEU:HD13	2.03	0.77
1:B:234:LEU:O	1:B:235:VAL:CG2	2.30	0.77
1:M:163:ILE:HD11	1:M:191:GLY:HA3	1.65	0.77
1:M:186:ALA:HA	1:M:189:ARG:CZ	2.13	0.77
1:U:11:GLN:HG2	1:1:5:TYR:CE1	2.20	0.77
1:B:59:ARG:HD2	1:B:129:HIS:HA	1.67	0.77
1:I:25:ALA:O	1:I:158:GLY:HA2	1.84	0.77
2:J:301:ALA:CB	2:J:333:LYS:NZ	2.48	0.77
1:M:16:ARG:HB3	1:M:16:ARG:NH1	2.00	0.77
1:B:25:ALA:O	1:B:158:GLY:HA2	1.84	0.77
1:K:5:TYR:CD1	1:M:11:GLN:CG	2.63	0.77
1:W:174:ASN:ND2	1:W:174:ASN:N	2.30	0.77
1:Q:181:LEU:O	1:Q:185:VAL:CG2	2.32	0.77
1:D:59:ARG:HD2	1:D:129:HIS:HA	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:-27:ARG:NE	2:H:-26:GLN:CD	2.39	0.76
1:O:59:ARG:HD2	1:O:129:HIS:HA	1.67	0.76
2:P:-28:ARG:HG2	2:P:-21:LEU:HD21	1.66	0.76
2:Z:301:ALA:HB1	2:Z:333:LYS:NZ	1.99	0.76
1:S:35:TYR:CE1	1:S:37:GLY:N	2.53	0.76
1:B:178:THR:CA	1:B:233:LEU:HD21	2.15	0.76
2:J:362:GLU:OE2	2:J:382:ARG:HD3	1.86	0.76
1:B:40:LEU:CD1	1:B:212:VAL:CG1	2.62	0.76
1:K:13:MET:O	1:K:17:SER:HB2	1.86	0.76
2:C:362:GLU:OE2	2:C:382:ARG:HD3	1.84	0.76
2:N:456:GLN:HE22	2:N:465:ARG:HH22	1.29	0.76
1:B:163:ILE:HG12	1:B:191:GLY:HA3	1.66	0.76
2:H:-23:GLU:HG2	2:P:-28:ARG:NH2	2.00	0.76
2:H:-27:ARG:CG	2:H:-26:GLN:OE1	2.30	0.76
1:K:6:PHE:O	1:Q:4:PRO:HD3	1.86	0.76
2:N:413:ASP:OD1	2:N:414:PRO:CD	2.30	0.76
1:O:178:THR:HG23	1:O:233:LEU:O	1.86	0.76
1:Q:171:TYR:CD2	1:Q:171:TYR:C	2.56	0.76
1:D:15:GLU:OE2	1:K:9:PRO:HD2	1.85	0.76
2:G:-21:LEU:CG	2:G:-20:PRO:HD2	2.14	0.76
2:P:362:GLU:OE2	2:P:382:ARG:HD3	1.86	0.76
1:D:50:LEU:CD1	1:K:147:ILE:HG23	2.16	0.75
2:P:-27:ARG:CZ	2:P:-26:GLN:NE2	2.48	0.75
1:1:173:GLU:CG	1:1:174:ASN:OD1	2.34	0.75
1:W:59:ARG:HD2	1:W:129:HIS:HA	1.68	0.75
2:H:-32:THR:HG23	2:H:362:GLU:OE1	1.87	0.75
2:L:-26:GLN:CA	2:L:-26:GLN:OE1	2.34	0.75
1:D:50:LEU:HD11	1:K:147:ILE:HG23	1.66	0.75
1:K:33:LEU:HD11	1:K:40:LEU:HB3	1.68	0.75
2:C:-26:GLN:HB3	2:H:-39:ALA:CB	2.16	0.75
1:U:207:SER:O	1:U:208:LEU:HD12	1.86	0.75
1:I:59:ARG:HD2	1:I:129:HIS:HA	1.68	0.75
2:N:301:ALA:CB	2:N:333:LYS:NZ	2.49	0.75
1:Q:230:LEU:O	1:Q:234:LEU:HD13	1.86	0.75
2:N:362:GLU:OE2	2:N:382:ARG:HD3	1.86	0.75
1:A:8:SER:HB2	1:A:9:PRO:CD	2.17	0.75
2:L:301:ALA:CB	2:L:333:LYS:NZ	2.50	0.75
1:1:25:ALA:O	1:1:158:GLY:HA2	1.86	0.74
1:A:33:LEU:CD1	1:A:40:LEU:HB3	2.17	0.74
2:P:-27:ARG:HG2	2:P:-26:GLN:OE1	1.87	0.74
1:Q:191:GLY:O	1:Q:192:SER:CB	2.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:348:THR:CB	2:Z:351:VAL:CG2	2.65	0.74
2:H:-23:GLU:CG	2:P:-28:ARG:HH21	1.98	0.74
1:K:234:LEU:HD13	1:K:234:LEU:O	1.88	0.74
1:O:10:GLU:O	1:O:14:ARG:HG3	1.88	0.74
1:W:15:GLU:OE2	1:Y:9:PRO:HG2	1.87	0.74
1:K:205:VAL:HG12	1:K:206:ALA:N	2.02	0.74
1:D:41:PHE:HB3	1:D:53:ILE:HD13	1.70	0.74
1:Q:171:TYR:CE2	1:Q:172:ALA:C	2.61	0.74
1:1:167:LEU:HD11	1:1:187:ALA:CB	2.16	0.74
2:R:-27:ARG:N	2:R:-27:ARG:HD2	2.00	0.74
1:W:16:ARG:NH1	1:W:117:PRO:HD3	2.03	0.74
2:J:433:GLU:HA	2:J:433:GLU:OE1	1.87	0.74
1:Q:234:LEU:N	1:Q:234:LEU:HD12	2.00	0.74
2:C:-18:SER:CB	2:C:393:ALA:HB2	2.11	0.74
1:U:150:GLU:HG3	1:U:154:VAL:HG22	1.68	0.74
1:D:11:GLN:O	1:D:15:GLU:HG3	1.87	0.73
1:U:181:LEU:HD21	1:U:234:LEU:HD11	1.69	0.73
1:A:179:ASP:O	1:A:183:ILE:HG12	1.88	0.73
2:L:362:GLU:OE2	2:L:382:ARG:HD3	1.88	0.73
2:N:513:LEU:O	2:N:517:ILE:HG13	1.88	0.73
1:1:150:GLU:HG3	1:1:154:VAL:HG22	1.69	0.73
1:F:189:ARG:HH21	1:F:203:LEU:CD2	2.00	0.73
2:J:-28:ARG:NH2	2:T:-23:GLU:OE2	2.21	0.73
2:J:-17:ILE:HD12	2:J:392:ALA:CB	2.16	0.73
1:A:41:PHE:HB3	1:A:53:ILE:HD13	1.71	0.73
2:C:-26:GLN:CD	2:H:-39:ALA:HB1	2.09	0.73
1:Q:234:LEU:O	1:Q:235:VAL:HG23	1.88	0.73
2:G:-39:ALA:HB1	2:X:-26:GLN:OE1	1.88	0.73
1:1:33:LEU:CD1	1:1:40:LEU:HB3	2.18	0.73
1:O:35:TYR:HE1	1:O:37:GLY:HA3	1.45	0.73
1:1:152:HIS:CD2	1:1:171:TYR:HE2	2.07	0.73
1:O:19:LEU:HD23	1:O:19:LEU:O	1.89	0.73
2:P:301:ALA:HB2	2:P:333:LYS:HZ3	1.54	0.73
1:Q:112:THR:HG22	1:Q:113:GLU:OE2	1.89	0.73
1:A:35:TYR:OH	1:A:37:GLY:HA3	1.89	0.73
1:D:179:ASP:O	1:D:183:ILE:HG13	1.88	0.73
1:D:205:VAL:CG2	1:D:206:ALA:N	2.51	0.73
2:G:332:ARG:HB2	2:G:332:ARG:NH1	2.03	0.73
2:J:456:GLN:NE2	2:J:465:ARG:HH22	1.87	0.73
2:L:413:ASP:HB3	2:L:416:SER:OG	1.89	0.73
1:Y:41:PHE:HB3	1:Y:53:ILE:HD13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:382:ARG:NH2	2:E:385:ILE:HD13	2.02	0.73
1:K:142:THR:OG1	1:K:144:ASP:HB3	1.89	0.73
2:P:-18:SER:O	2:P:-17:ILE:HB	1.87	0.73
2:C:409:ILE:HD11	2:C:410:HIS:HE1	1.53	0.72
2:P:-28:ARG:CG	2:P:-21:LEU:HD21	2.20	0.72
2:P:465:ARG:CA	2:P:513:LEU:HD21	2.20	0.72
2:N:301:ALA:CB	2:N:333:LYS:HZ3	1.99	0.72
2:P:-28:ARG:HG2	2:P:-21:LEU:CD2	2.19	0.72
1:K:59:ARG:HD2	1:K:129:HIS:HA	1.68	0.72
2:E:308:TYR:CE1	2:E:311:GLY:HA3	2.25	0.72
1:F:150:GLU:HG3	1:F:154:VAL:HG22	1.71	0.72
2:G:-18:SER:O	2:G:-17:ILE:CB	2.38	0.72
2:J:409:ILE:HG13	2:J:410:HIS:ND1	2.04	0.72
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.70	0.72
2:N:519:GLU:O	2:N:523:GLY:N	2.22	0.72
1:O:14:ARG:O	1:O:18:GLU:HG2	1.90	0.72
1:W:150:GLU:HG3	1:W:154:VAL:HG22	1.72	0.72
1:I:35:TYR:CE1	1:I:37:GLY:HA3	2.24	0.72
2:2:413:ASP:OD1	2:2:416:SER:CB	2.30	0.72
2:J:465:ARG:NH1	2:J:465:ARG:HB3	2.04	0.72
1:M:154:VAL:HA	3:M:250:HOH:O	1.90	0.72
1:F:5:TYR:HD1	1:W:11:GLN:HE22	1.37	0.72
1:W:3:PHE:N	1:W:4:PRO:CA	2.51	0.72
1:S:115:ALA:HB1	1:U:6:PHE:CZ	2.25	0.72
2:X:509:ARG:NH1	2:X:509:ARG:HG3	2.01	0.72
2:C:-31:ASP:O	2:C:-27:ARG:HG3	1.90	0.72
1:F:33:LEU:HD11	1:F:40:LEU:HB3	1.72	0.72
1:Y:35:TYR:HE1	1:Y:37:GLY:HA3	1.49	0.72
1:K:152:HIS:CB	1:K:171:TYR:CE2	2.72	0.72
1:K:33:LEU:HD12	1:K:33:LEU:H	1.54	0.72
1:M:16:ARG:HH11	1:M:16:ARG:HB3	1.55	0.72
2:P:-26:GLN:CA	2:P:-26:GLN:OE1	2.38	0.72
1:O:41:PHE:HB3	1:O:53:ILE:HD13	1.72	0.71
2:T:362:GLU:OE2	2:T:382:ARG:HD3	1.89	0.71
2:C:409:ILE:CG1	2:C:410:HIS:ND1	2.53	0.71
2:H:362:GLU:OE2	2:H:382:ARG:HD3	1.90	0.71
2:L:-38:VAL:HG21	2:N:-30:PHE:HE2	1.55	0.71
1:Q:178:THR:HG23	1:Q:233:LEU:O	1.90	0.71
1:Q:234:LEU:H	1:Q:234:LEU:CD1	2.03	0.71
1:I:35:TYR:CE1	1:I:37:GLY:N	2.57	0.71
1:I:150:GLU:HG3	1:I:154:VAL:HG22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:41:PHE:HB3	1:1:53:ILE:HD13	1.72	0.71
2:2:-28:ARG:CG	2:2:-21:LEU:HD11	2.21	0.71
1:I:35:TYR:CD1	1:I:37:GLY:N	2.59	0.71
2:N:-21:LEU:HD12	2:N:-20:PRO:CD	2.20	0.71
1:S:214:ASP:OD1	1:S:216:ASN:N	2.23	0.71
1:U:179:ASP:O	1:U:183:ILE:CG1	2.37	0.71
1:D:35:TYR:CZ	1:D:37:GLY:HA3	2.21	0.71
1:F:11:GLN:HA	1:F:11:GLN:OE1	1.89	0.71
2:X:350:ALA:O	2:X:353:VAL:HG12	1.91	0.71
2:R:-30:PHE:HZ	2:Z:-38:VAL:CG2	2.04	0.71
1:1:167:LEU:HD12	1:1:187:ALA:HB2	1.70	0.71
2:H:-27:ARG:HE	2:H:-26:GLN:CD	1.94	0.71
1:Q:153:PHE:HD2	1:Q:171:TYR:HD1	1.38	0.71
1:B:33:LEU:HD11	1:B:40:LEU:HB3	1.72	0.71
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.72	0.71
1:K:72:ASP:O	1:K:76:ARG:HG3	1.90	0.71
1:S:179:ASP:O	1:S:183:ILE:HG13	1.91	0.71
1:U:217:ARG:HD2	1:U:223:ARG:CD	2.15	0.71
2:V:362:GLU:OE2	2:V:382:ARG:HD3	1.91	0.71
2:Z:308:TYR:CE1	2:Z:311:GLY:HA3	2.25	0.71
1:Q:171:TYR:C	1:Q:171:TYR:HD2	1.94	0.70
1:1:33:LEU:HD11	1:1:40:LEU:HB3	1.73	0.70
1:A:178:THR:O	1:A:182:ARG:HG3	1.91	0.70
1:I:191:GLY:O	1:I:192:SER:C	2.30	0.70
1:U:176:SER:OG	1:U:179:ASP:CG	2.30	0.70
1:U:41:PHE:HB3	1:U:53:ILE:HD13	1.71	0.70
1:1:181:LEU:C	1:1:181:LEU:HD12	2.11	0.70
1:B:182:ARG:HG3	1:B:183:ILE:N	2.05	0.70
2:C:409:ILE:HD11	2:C:410:HIS:CE1	2.27	0.70
1:D:173:GLU:C	1:D:174:ASN:OD1	2.30	0.70
1:K:150:GLU:HG3	1:K:154:VAL:HG22	1.73	0.70
1:B:152:HIS:HB3	1:B:171:TYR:CE2	2.26	0.70
1:B:33:LEU:CD1	1:B:40:LEU:HB3	2.22	0.70
1:K:35:TYR:CZ	1:K:37:GLY:CA	2.68	0.70
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.73	0.70
1:I:167:LEU:HD13	1:I:187:ALA:HB2	1.74	0.70
1:Q:173:GLU:C	1:Q:174:ASN:OD1	2.30	0.70
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.74	0.70
1:W:6:PHE:N	1:W:6:PHE:CD1	2.59	0.70
2:2:362:GLU:OE2	2:2:382:ARG:HD3	1.92	0.70
1:A:15:GLU:HB3	1:B:9:PRO:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:332:ARG:NH1	2:H:332:ARG:HB2	2.07	0.70
1:K:152:HIS:CG	1:K:171:TYR:HE2	2.09	0.70
2:L:332:ARG:HB2	2:L:332:ARG:NH1	2.07	0.70
2:N:332:ARG:HB2	2:N:332:ARG:NH1	2.07	0.70
2:T:338:ASP:OD1	2:T:338:ASP:C	2.29	0.70
2:T:415:GLN:N	2:T:415:GLN:NE2	2.30	0.70
1:U:7:ILE:HA	1:1:6:PHE:HA	1.73	0.70
1:B:17:SER:O	1:B:21:ARG:HG3	1.91	0.70
1:M:7:ILE:CG2	1:W:5:TYR:HE2	2.02	0.70
1:O:234:LEU:CD1	1:O:234:LEU:C	2.60	0.70
2:P:465:ARG:HG3	2:P:513:LEU:HD11	1.74	0.70
1:M:35:TYR:CZ	1:M:37:GLY:HA3	2.27	0.70
1:1:173:GLU:C	1:1:174:ASN:OD1	2.30	0.69
2:G:332:ARG:HB2	2:G:332:ARG:HH11	1.56	0.69
1:I:169:GLU:OE1	1:I:169:GLU:CA	2.41	0.69
2:C:375:THR:HG21	1:I:92:ARG:HB3	1.73	0.69
2:H:-27:ARG:HH11	2:H:-26:GLN:HE21	1.40	0.69
2:L:413:ASP:OD1	2:L:414:PRO:CD	2.30	0.69
2:V:-26:GLN:HE22	2:2:-38:VAL:H1	1.40	0.69
2:2:-31:ASP:OD1	2:2:-27:ARG:NH2	2.26	0.69
1:A:121:GLU:OE2	1:A:140:ARG:HD2	1.92	0.69
1:Q:35:TYR:CE1	1:Q:37:GLY:N	2.61	0.69
1:W:25:ALA:O	1:W:158:GLY:HA2	1.92	0.69
1:U:207:SER:O	1:U:208:LEU:CD1	2.40	0.69
1:U:7:ILE:HG13	1:U:8:SER:N	2.06	0.69
2:X:301:ALA:CB	2:X:333:LYS:HZ3	1.92	0.69
1:O:155:VAL:HG21	1:O:167:LEU:HD12	1.74	0.69
2:P:351:VAL:HG12	2:P:400:ALA:HB2	1.72	0.69
2:R:345:ILE:HB	2:R:352:ALA:HB1	1.73	0.69
1:S:150:GLU:HG3	1:S:154:VAL:HG22	1.75	0.69
1:W:112:THR:HG22	1:W:113:GLU:OE2	1.92	0.69
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.75	0.69
2:P:-17:ILE:HG22	2:P:-17:ILE:O	1.91	0.69
1:Q:110:ILE:HG23	1:Q:114:GLN:HG3	1.73	0.69
1:A:7:ILE:C	1:B:5:TYR:HB3	2.13	0.69
2:G:301:ALA:CB	2:G:333:LYS:NZ	2.55	0.69
1:M:112:THR:HG22	1:M:113:GLU:OE2	1.93	0.69
2:Z:-37:ASP:OD1	2:Z:-35:SER:N	2.25	0.69
1:A:191:GLY:O	1:A:192:SER:HB2	1.93	0.69
1:M:3:PHE:HD1	1:M:4:PRO:HD2	1.58	0.69
2:P:332:ARG:HB2	2:P:332:ARG:NH1	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:-39:ALA:HB1	2:X:-26:GLN:HB3	1.73	0.69
2:E:-30:PHE:CE1	2:E:-26:GLN:HG3	2.28	0.69
1:F:33:LEU:CD1	1:F:33:LEU:O	2.40	0.69
2:R:301:ALA:HB1	2:R:333:LYS:NZ	2.07	0.69
2:T:486:LEU:HG	2:T:515:ARG:HH12	1.57	0.69
1:B:150:GLU:HG3	1:B:154:VAL:HG22	1.74	0.69
1:B:28:LYS:NZ	1:B:52:LYS:HE3	2.09	0.69
1:D:3:PHE:N	1:D:4:PRO:CD	2.56	0.69
1:D:83:ASP:OD2	2:E:365:HIS:ND1	2.20	0.69
2:J:456:GLN:HE22	2:J:465:ARG:HH22	1.38	0.69
2:V:332:ARG:HB2	2:V:332:ARG:NH1	2.07	0.69
2:2:332:ARG:HB2	2:2:332:ARG:NH1	2.07	0.68
2:X:479:SER:HB2	2:2:479:SER:HB2	1.75	0.68
1:D:167:LEU:HD13	1:D:187:ALA:HB2	1.74	0.68
1:D:40:LEU:HA	1:D:212:VAL:HG12	1.74	0.68
1:M:59:ARG:HD2	1:M:129:HIS:HA	1.73	0.68
1:Q:153:PHE:HD2	1:Q:171:TYR:CD1	2.11	0.68
1:S:152:HIS:HB3	1:S:171:TYR:CE2	2.28	0.68
1:Q:89:TYR:CD1	2:Z:374:LEU:HD11	2.28	0.68
1:A:4:PRO:HB3	1:B:11:GLN:OE1	1.93	0.68
2:L:-18:SER:O	2:L:-17:ILE:HG22	1.91	0.68
1:O:51:GLN:N	1:O:51:GLN:NE2	2.30	0.68
1:F:167:LEU:HD13	1:F:187:ALA:HB2	1.76	0.68
1:1:112:THR:HG22	1:1:113:GLU:OE2	1.91	0.68
1:1:128:ALA:HB2	1:1:134:LYS:HB3	1.76	0.68
1:1:165:ASN:O	1:1:169:GLU:HG2	1.93	0.68
1:A:112:THR:HG22	1:A:113:GLU:OE2	1.94	0.68
2:E:407:TYR:HE1	2:E:417:ALA:HB3	1.57	0.68
1:U:16:ARG:NH1	1:U:117:PRO:HD3	2.09	0.68
2:J:-21:LEU:HD12	2:J:-20:PRO:HD2	1.75	0.68
1:K:179:ASP:OD1	1:K:179:ASP:C	2.31	0.68
2:L:407:TYR:CZ	2:L:417:ALA:CB	2.75	0.68
1:M:231:GLN:O	1:M:235:VAL:HG12	1.93	0.68
1:A:89:TYR:CD1	2:P:374:LEU:HD11	2.27	0.68
1:U:231:GLN:HE22	1:U:235:VAL:CG2	2.06	0.68
2:L:301:ALA:CB	2:L:333:LYS:HZ3	2.05	0.68
1:Q:150:GLU:HG3	1:Q:154:VAL:HG22	1.75	0.68
1:Q:40:LEU:CD1	1:Q:212:VAL:CG1	2.72	0.68
1:Y:112:THR:HG22	1:Y:113:GLU:OE2	1.94	0.68
1:1:8:SER:H	1:1:11:GLN:CG	2.07	0.68
1:F:33:LEU:CD1	1:F:40:LEU:HB3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:233:LEU:HD23	1:U:233:LEU:N	2.08	0.68
1:O:7:ILE:N	1:U:7:ILE:CD1	2.54	0.68
1:Y:163:ILE:HG12	1:Y:191:GLY:HA3	1.75	0.68
1:I:31:VAL:HG12	1:I:155:VAL:HG22	1.75	0.68
2:P:351:VAL:CG1	2:P:400:ALA:HB2	2.23	0.68
2:R:332:ARG:HB2	2:R:332:ARG:NH1	2.09	0.68
2:J:-38:VAL:HG11	1:S:84:THR:HG21	1.75	0.68
2:E:-19:ALA:HB2	2:R:388:ARG:HD2	1.76	0.67
2:H:-29:LEU:HD22	2:H:-22:LEU:HD12	1.76	0.67
2:J:456:GLN:HE22	2:J:465:ARG:NH2	1.91	0.67
2:P:301:ALA:HB2	2:P:333:LYS:NZ	2.09	0.67
1:U:28:LYS:CE	1:U:28:LYS:H	2.07	0.67
1:I:87:TYR:O	2:J:357:ARG:NH1	2.26	0.67
1:K:110:ILE:HG21	1:K:118:TYR:CD1	2.29	0.67
2:R:350:ALA:HB2	2:Z:428:GLY:HA3	1.76	0.67
2:2:-31:ASP:O	2:2:-27:ARG:HG3	1.95	0.67
1:B:178:THR:CG2	1:B:233:LEU:HD23	2.12	0.67
1:Q:234:LEU:N	1:Q:234:LEU:CD1	2.57	0.67
1:Y:181:LEU:HD12	1:Y:185:VAL:HG23	1.76	0.67
1:A:33:LEU:HD11	1:A:40:LEU:HB3	1.77	0.67
1:D:35:TYR:HD1	1:D:37:GLY:H	1.39	0.67
2:H:483:GLY:HA2	3:H:60:HOH:O	1.95	0.67
1:M:150:GLU:HG3	1:M:154:VAL:HG22	1.75	0.67
1:S:15:GLU:OE2	1:1:9:PRO:CD	2.41	0.67
1:U:5:TYR:HB2	1:1:7:ILE:O	1.94	0.67
2:2:-20:PRO:HB3	2:2:354:GLU:OE1	1.95	0.67
1:D:112:THR:HG22	1:D:113:GLU:OE2	1.95	0.67
2:P:332:ARG:HB2	2:P:332:ARG:HH11	1.59	0.67
1:U:188:LEU:HD23	1:U:188:LEU:C	2.15	0.67
2:Z:432:GLU:HG3	2:Z:437:GLN:HB2	1.77	0.67
2:J:301:ALA:CB	2:J:333:LYS:HZ3	2.06	0.67
1:Q:40:LEU:HD12	1:Q:212:VAL:HG12	1.77	0.67
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.76	0.67
1:D:191:GLY:O	1:D:192:SER:CB	2.42	0.67
1:U:181:LEU:CD2	1:U:234:LEU:HD12	2.24	0.67
2:V:301:ALA:CB	2:V:333:LYS:HZ3	1.97	0.67
1:K:4:PRO:CG	1:W:5:TYR:CG	2.78	0.67
1:O:25:ALA:O	1:O:158:GLY:HA2	1.95	0.67
1:S:33:LEU:HD12	1:S:33:LEU:O	1.95	0.67
1:D:189:ARG:NH1	1:D:203:LEU:N	2.36	0.67
2:Z:-27:ARG:NH2	2:Z:-27:ARG:HG2	2.04	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:456:GLN:HE22	2:2:465:ARG:NH2	1.93	0.66
1:I:28:LYS:H	1:I:28:LYS:CE	2.09	0.66
1:O:234:LEU:HD12	1:O:235:VAL:HG23	1.77	0.66
1:W:35:TYR:CZ	1:W:37:GLY:HA3	2.29	0.66
1:D:11:GLN:HE22	1:Q:5:TYR:H	1.41	0.66
1:W:33:LEU:O	1:W:33:LEU:HD12	1.94	0.66
2:C:308:TYR:OH	2:C:496:ILE:HD11	1.94	0.66
1:D:191:GLY:O	1:D:192:SER:HB2	1.94	0.66
1:M:25:ALA:O	1:M:158:GLY:HA2	1.96	0.66
2:T:338:ASP:OD1	2:T:340:TYR:N	2.29	0.66
2:G:-21:LEU:HD12	2:G:-20:PRO:HD3	1.78	0.66
1:O:155:VAL:HG21	1:O:167:LEU:HD11	1.74	0.66
2:T:332:ARG:NH1	2:T:332:ARG:HB2	2.10	0.66
2:T:301:ALA:HB2	2:T:333:LYS:HE3	1.76	0.66
1:Y:173:GLU:HG3	1:Y:174:ASN:OD1	1.95	0.66
1:U:5:TYR:HB3	1:1:9:PRO:HD3	1.76	0.66
1:B:31:VAL:HG12	1:B:155:VAL:HG22	1.76	0.66
2:C:417:ALA:O	2:C:419:ARG:NH1	2.29	0.66
2:G:350:ALA:O	2:G:353:VAL:HG12	1.96	0.66
1:K:182:ARG:NH2	1:K:234:LEU:O	2.28	0.66
1:Y:2:SER:O	1:Y:4:PRO:HD3	1.95	0.66
1:A:4:PRO:HG3	1:B:11:GLN:HG2	1.77	0.66
1:U:170:SER:HB2	1:U:183:ILE:CG2	2.26	0.66
1:K:141:ILE:HD12	1:K:141:ILE:N	2.11	0.66
2:P:465:ARG:HA	2:P:513:LEU:CD2	2.26	0.66
2:Z:332:ARG:NH1	2:Z:332:ARG:HB2	2.11	0.66
1:I:167:LEU:HD13	1:I:187:ALA:CB	2.26	0.66
1:K:5:TYR:CG	1:M:11:GLN:HG3	2.30	0.66
1:M:167:LEU:HD13	1:M:187:ALA:HB2	1.78	0.66
2:G:522:SER:HB3	2:V:487:VAL:HG13	1.77	0.66
2:E:-26:GLN:OE1	2:E:-26:GLN:CA	2.44	0.65
2:E:362:GLU:OE2	2:E:382:ARG:CD	2.36	0.65
2:H:332:ARG:HB2	2:H:332:ARG:HH11	1.62	0.65
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.77	0.65
1:A:150:GLU:HG3	1:A:154:VAL:HG22	1.78	0.65
1:F:112:THR:HG22	1:F:113:GLU:OE2	1.95	0.65
2:R:469:GLU:HG3	2:R:517:ILE:HD13	1.78	0.65
2:X:301:ALA:CB	2:X:333:LYS:HZ2	2.08	0.65
1:A:9:PRO:CG	1:O:15:GLU:HB3	2.26	0.65
2:H:407:TYR:CE1	2:H:417:ALA:HB1	2.30	0.65
1:O:112:THR:HG22	1:O:113:GLU:OE2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:10:GLU:HG3	1:W:14:ARG:HH12	1.61	0.65
2:X:381:ASN:O	2:X:385:ILE:HG13	1.96	0.65
1:1:161:GLU:N	1:1:162:PRO:HD2	2.11	0.65
1:A:92:ARG:CG	1:A:92:ARG:HH11	2.08	0.65
2:C:308:TYR:CZ	2:C:311:GLY:HA3	2.32	0.65
1:S:214:ASP:C	1:S:214:ASP:OD1	2.33	0.65
2:J:426:ALA:HB2	2:T:-4:LEU:CD2	2.27	0.65
1:F:35:TYR:CD1	1:F:37:GLY:N	2.63	0.65
1:K:116:LYS:NZ	1:K:117:PRO:O	2.30	0.65
2:L:-35:SER:HB3	2:L:369:LEU:CD1	2.26	0.65
1:Q:214:ASP:OD1	1:Q:216:ASN:N	2.30	0.65
1:U:167:LEU:HA	1:U:170:SER:HG	1.61	0.65
1:U:204:GLY:N	1:U:207:SER:OG	2.30	0.65
1:Y:150:GLU:HG3	1:Y:154:VAL:HG22	1.76	0.65
1:1:152:HIS:HB3	1:1:171:TYR:CE2	2.31	0.65
2:C:301:ALA:O	2:C:440:GLY:HA3	1.97	0.65
2:E:-28:ARG:NE	2:E:-21:LEU:CD2	2.59	0.65
1:K:4:PRO:HB2	1:W:5:TYR:CE2	2.31	0.65
1:W:41:PHE:HB3	1:W:53:ILE:HD13	1.77	0.65
2:X:498:ASP:OD1	2:X:500:ASP:N	2.30	0.65
2:L:354:GLU:N	2:L:354:GLU:OE1	2.30	0.65
1:S:181:LEU:O	1:S:185:VAL:HG23	1.95	0.65
1:1:152:HIS:CD2	1:1:171:TYR:CE2	2.84	0.65
1:A:11:GLN:NE2	1:A:14:ARG:HH21	1.92	0.65
2:H:-29:LEU:CD2	2:H:-22:LEU:HD12	2.27	0.65
2:T:338:ASP:OD1	2:T:339:ASP:N	2.30	0.65
2:J:332:ARG:NH1	2:J:332:ARG:HB2	2.12	0.65
1:M:185:VAL:HG12	1:M:189:ARG:NH1	2.12	0.65
2:R:-29:LEU:HB3	2:R:-21:LEU:HD13	1.78	0.65
1:1:10:GLU:N	1:1:10:GLU:OE1	2.30	0.65
2:N:332:ARG:HH11	2:N:332:ARG:HB2	1.62	0.65
1:B:178:THR:CG2	1:B:233:LEU:CD2	2.73	0.64
2:T:345:ILE:HB	2:T:352:ALA:HB1	1.79	0.64
1:U:207:SER:C	1:U:208:LEU:HD13	2.16	0.64
2:E:351:VAL:CG1	2:E:400:ALA:HB2	2.27	0.64
2:T:414:PRO:C	2:T:415:GLN:HE21	2.01	0.64
1:Y:178:THR:CG2	1:Y:233:LEU:O	2.45	0.64
1:1:18:GLU:OE1	1:1:22:LYS:NZ	2.30	0.64
2:J:-29:LEU:O	2:J:-25:ALA:N	2.30	0.64
1:K:26:ARG:NH1	1:K:26:ARG:HB2	2.13	0.64
1:Q:170:SER:O	1:Q:183:ILE:HD13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:416:SER:O	2:2:419:ARG:NH1	2.30	0.64
1:M:7:ILE:CD1	1:W:5:TYR:CD2	2.65	0.64
1:O:35:TYR:CZ	1:O:37:GLY:CA	2.72	0.64
1:Y:18:GLU:OE1	1:Y:21:ARG:NH2	2.30	0.64
1:1:8:SER:OG	1:1:11:GLN:NE2	2.30	0.64
1:F:169:GLU:N	1:F:169:GLU:OE1	2.30	0.64
2:N:-17:ILE:HG12	2:N:393:ALA:HB2	1.79	0.64
2:V:465:ARG:HG3	2:V:513:LEU:HD12	1.78	0.64
1:W:35:TYR:CE1	1:W:37:GLY:CA	2.79	0.64
1:1:18:GLU:OE2	1:1:21:ARG:NH2	2.30	0.64
2:2:301:ALA:O	2:2:440:GLY:HA3	1.98	0.64
2:E:-26:GLN:OE1	2:E:-26:GLN:N	2.30	0.64
1:F:7:ILE:HG21	1:W:8:SER:HB3	1.79	0.64
1:M:12:ALA:O	1:M:16:ARG:HG3	1.97	0.64
2:P:382:ARG:NH2	2:P:385:ILE:HD13	2.13	0.64
1:U:188:LEU:O	1:U:188:LEU:HD23	1.98	0.64
2:G:350:ALA:O	2:G:353:VAL:CG1	2.45	0.64
1:I:130:TYR:CE1	1:I:216:ASN:O	2.51	0.64
2:J:-38:VAL:HG13	2:J:-38:VAL:O	1.97	0.64
1:O:19:LEU:CD2	1:O:19:LEU:C	2.66	0.64
1:U:92:ARG:CG	1:U:92:ARG:HH11	2.11	0.64
2:V:509:ARG:O	2:V:513:LEU:HD23	1.98	0.64
1:Y:181:LEU:C	1:Y:181:LEU:CD1	2.58	0.64
1:D:174:ASN:N	1:D:174:ASN:OD1	2.31	0.64
2:P:382:ARG:HH21	2:P:385:ILE:HD13	1.62	0.64
1:M:7:ILE:CD1	1:W:5:TYR:HB2	2.27	0.64
1:Y:35:TYR:CZ	1:Y:37:GLY:CA	2.71	0.64
2:C:-23:GLU:OE1	2:H:-28:ARG:NE	2.31	0.64
2:L:-18:SER:C	2:L:-17:ILE:HG22	2.18	0.64
2:L:444:LEU:HB2	3:L:46:HOH:O	1.96	0.64
1:S:112:THR:HG22	1:S:113:GLU:OE2	1.98	0.64
1:B:92:ARG:CG	1:B:92:ARG:HH11	2.11	0.64
1:U:11:GLN:CG	1:1:5:TYR:CZ	2.80	0.64
2:C:351:VAL:CG1	2:C:400:ALA:HB2	2.28	0.63
1:I:114:GLN:HA	1:I:114:GLN:NE2	2.12	0.63
1:I:169:GLU:N	1:I:169:GLU:OE1	2.30	0.63
2:J:444:LEU:HB2	3:J:49:HOH:O	1.96	0.63
1:K:16:ARG:HG3	1:M:9:PRO:HG2	1.80	0.63
2:H:413:ASP:OD1	2:H:415:GLN:N	2.30	0.63
2:H:430:ASN:ND2	2:H:432:GLU:OE2	2.31	0.63
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:512:GLU:OE1	2:Z:512:GLU:HA	1.98	0.63
2:C:301:ALA:HB2	2:C:333:LYS:CE	2.24	0.63
1:D:3:PHE:CE1	1:F:6:PHE:CE2	2.64	0.63
1:I:169:GLU:OE1	1:I:169:GLU:HA	1.99	0.63
2:L:-38:VAL:HG21	2:N:-30:PHE:CE2	2.32	0.63
1:O:31:VAL:HG12	1:O:155:VAL:HG22	1.78	0.63
1:D:152:HIS:HB3	1:D:171:TYR:CE2	2.33	0.63
2:X:-3:PRO:HB2	2:X:348:THR:HG23	1.80	0.63
1:I:174:ASN:N	1:I:174:ASN:OD1	2.32	0.63
1:B:152:HIS:CD2	1:B:171:TYR:CE2	2.86	0.63
1:B:179:ASP:O	1:B:182:ARG:HG2	1.98	0.63
1:B:18:GLU:OE2	1:B:21:ARG:NH1	2.30	0.63
1:F:35:TYR:CZ	1:F:37:GLY:HA3	2.30	0.63
2:H:413:ASP:OD1	2:H:413:ASP:C	2.36	0.63
2:L:349:ALA:O	2:L:353:VAL:HG12	1.98	0.63
1:M:35:TYR:CE1	1:M:37:GLY:CA	2.81	0.63
1:D:16:ARG:HH21	1:M:4:PRO:CG	2.12	0.63
1:D:8:SER:CB	1:D:11:GLN:HG2	2.14	0.63
2:R:332:ARG:HB2	2:R:332:ARG:HH11	1.64	0.63
1:U:189:ARG:O	1:U:189:ARG:HG2	1.97	0.63
1:I:28:LYS:NZ	1:I:52:LYS:HE3	2.13	0.63
1:A:92:ARG:HH11	1:A:92:ARG:HG3	1.64	0.63
1:F:181:LEU:O	1:F:185:VAL:HG23	1.98	0.63
2:C:-39:ALA:H1	2:J:-26:GLN:NE2	1.96	0.63
1:Q:169:GLU:OE1	1:Q:169:GLU:HA	1.98	0.63
2:R:-29:LEU:HB3	2:R:-21:LEU:CD1	2.29	0.63
2:T:332:ARG:HH11	2:T:332:ARG:HB2	1.64	0.63
1:Y:205:VAL:HG21	1:Y:231:GLN:OE1	1.99	0.63
2:H:-5:GLN:NE2	2:H:-2:HIS:CD2	2.67	0.63
1:I:214:ASP:OD1	1:I:216:ASN:N	2.30	0.63
2:P:-27:ARG:HE	2:P:-26:GLN:NE2	1.95	0.63
2:P:-27:ARG:HH11	2:P:-26:GLN:NE2	1.95	0.63
2:Z:332:ARG:HH11	2:Z:332:ARG:HB2	1.64	0.63
1:O:141:ILE:N	1:O:141:ILE:HD12	2.14	0.62
1:A:19:LEU:CD1	1:B:9:PRO:HB2	2.28	0.62
1:K:152:HIS:CG	1:K:171:TYR:CE2	2.87	0.62
2:J:413:ASP:OD2	2:J:416:SER:N	2.30	0.62
2:L:-5:GLN:HA	2:L:-5:GLN:NE2	2.14	0.62
1:M:92:ARG:CG	1:M:92:ARG:HH11	2.12	0.62
1:U:8:SER:N	1:I:5:TYR:O	2.32	0.62
2:Z:312:VAL:HG12	2:Z:497:ILE:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:ALA:O	2:E:440:GLY:HA3	1.98	0.62
2:H:413:ASP:OD1	2:H:414:PRO:N	2.31	0.62
1:M:16:ARG:CB	1:M:16:ARG:HH11	2.12	0.62
1:W:10:GLU:HG3	1:W:14:ARG:NH1	2.14	0.62
1:I:128:ALA:HB2	1:I:134:LYS:HB3	1.80	0.62
2:P:407:TYR:HE2	2:P:499:ALA:HA	1.57	0.62
1:Q:234:LEU:C	1:Q:235:VAL:HG23	2.20	0.62
1:K:4:PRO:HB3	1:W:5:TYR:CD2	2.33	0.62
2:X:350:ALA:O	2:X:353:VAL:CG1	2.47	0.62
2:R:-30:PHE:CZ	2:Z:-38:VAL:CG2	2.82	0.62
2:L:-18:SER:O	2:L:-17:ILE:HG23	2.00	0.62
1:Q:152:HIS:HB3	1:Q:171:TYR:CZ	2.31	0.62
1:S:92:ARG:HH11	1:S:92:ARG:CG	2.13	0.62
1:U:128:ALA:HB2	1:U:134:LYS:HB3	1.82	0.62
2:G:-21:LEU:HD12	2:G:-20:PRO:CD	2.29	0.62
2:G:407:TYR:CE1	2:G:417:ALA:HB3	2.34	0.62
1:I:33:LEU:HD12	1:I:33:LEU:O	2.00	0.62
1:K:92:ARG:CG	1:K:92:ARG:HH11	2.12	0.62
1:U:98:GLN:O	1:U:102:VAL:HG23	1.99	0.62
1:Y:178:THR:HG23	1:Y:233:LEU:O	2.00	0.62
1:S:163:ILE:O	1:S:167:LEU:HG	1.99	0.62
2:X:382:ARG:NH2	2:X:385:ILE:HD12	2.15	0.62
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.82	0.62
1:B:9:PRO:O	1:B:13:MET:HB2	2.00	0.62
2:C:-39:ALA:H1	2:J:-26:GLN:CD	1.99	0.62
2:E:351:VAL:HG12	2:E:400:ALA:HB2	1.81	0.62
1:U:35:TYR:HE1	1:U:37:GLY:HA3	1.56	0.62
1:I:19:LEU:O	1:I:19:LEU:HD23	2.00	0.61
1:I:231:GLN:HA	1:I:234:LEU:HD12	1.80	0.61
2:L:-24:PRO:CD	2:L:-23:GLU:OE2	2.47	0.61
1:M:31:VAL:HG12	1:M:155:VAL:HG22	1.82	0.61
2:P:407:TYR:CE2	2:P:499:ALA:CA	2.80	0.61
2:J:-31:ASP:OD2	2:J:-27:ARG:HD3	2.00	0.61
1:Q:163:ILE:HG23	1:Q:187:ALA:O	2.00	0.61
1:A:11:GLN:CD	1:A:14:ARG:HH21	2.02	0.61
1:D:16:ARG:NH1	1:D:117:PRO:HD3	2.15	0.61
1:F:31:VAL:HG12	1:F:155:VAL:HG22	1.81	0.61
1:I:178:THR:HG23	1:I:233:LEU:O	2.01	0.61
1:K:112:THR:HG22	1:K:113:GLU:OE2	2.00	0.61
2:N:301:ALA:CB	2:N:333:LYS:HD3	2.31	0.61
2:P:-23:GLU:HG2	2:P:-22:LEU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:167:LEU:CA	1:U:170:SER:OG	2.46	0.61
2:V:301:ALA:CB	2:V:333:LYS:HD3	2.30	0.61
2:V:332:ARG:HH11	2:V:332:ARG:HB2	1.63	0.61
1:Y:181:LEU:O	1:Y:181:LEU:CD1	2.30	0.61
2:Z:301:ALA:CB	2:Z:333:LYS:HZ2	2.05	0.61
2:2:416:SER:OG	2:2:419:ARG:NH2	2.30	0.61
1:S:141:ILE:HD12	1:S:141:ILE:N	2.14	0.61
1:W:173:GLU:HB3	1:W:174:ASN:ND2	2.15	0.61
2:X:332:ARG:HB2	2:X:332:ARG:NH1	2.15	0.61
1:1:8:SER:H	1:1:11:GLN:CD	2.04	0.61
1:U:93:ASP:OD1	2:2:375:THR:HG23	1.99	0.61
1:B:128:ALA:HB2	1:B:134:LYS:HB3	1.82	0.61
1:D:230:LEU:O	1:D:234:LEU:CD1	2.30	0.61
1:K:4:PRO:CB	1:W:5:TYR:CE2	2.82	0.61
1:B:177:LEU:HG	1:B:233:LEU:HD11	1.83	0.61
2:E:-23:GLU:OE1	2:E:-23:GLU:HA	2.00	0.61
1:Q:26:ARG:O	1:Q:26:ARG:CG	2.49	0.61
2:R:-29:LEU:HD23	2:R:-21:LEU:CD1	2.31	0.61
1:W:14:ARG:HG2	1:W:14:ARG:HH11	1.64	0.61
1:1:18:GLU:OE1	1:1:21:ARG:NH2	2.31	0.61
1:I:112:THR:HG22	1:I:113:GLU:OE2	2.00	0.61
2:L:332:ARG:HB2	2:L:332:ARG:HH11	1.64	0.61
2:2:391:LEU:O	2:2:395:MET:HG2	1.99	0.61
2:V:433:GLU:OE1	2:V:433:GLU:HA	2.00	0.61
1:B:19:LEU:HD23	1:B:19:LEU:C	2.21	0.61
2:E:-28:ARG:NE	2:E:-21:LEU:HD23	2.16	0.61
1:I:33:LEU:CD1	1:I:40:LEU:HB3	2.31	0.61
2:J:465:ARG:HB3	2:J:465:ARG:HH11	1.66	0.61
1:S:16:ARG:NH1	1:S:117:PRO:HD3	2.16	0.61
2:J:-17:ILE:HB	2:J:393:ALA:HB2	1.81	0.61
1:K:33:LEU:HD12	1:K:33:LEU:N	2.15	0.61
2:X:-18:SER:O	2:X:-17:ILE:C	2.39	0.61
2:X:308:TYR:CE1	2:X:311:GLY:HA3	2.35	0.61
2:H:-29:LEU:O	2:H:-25:ALA:C	2.39	0.60
2:L:301:ALA:CB	2:L:333:LYS:HD3	2.31	0.60
2:L:432:GLU:HG3	2:L:437:GLN:HB2	1.82	0.60
2:P:301:ALA:CB	2:P:333:LYS:NZ	2.64	0.60
1:Y:92:ARG:HH11	1:Y:92:ARG:CG	2.14	0.60
1:F:35:TYR:HE1	1:F:37:GLY:HA3	1.58	0.60
1:Q:114:GLN:HE21	1:Q:114:GLN:HA	1.65	0.60
1:Q:7:ILE:HD11	1:Q:12:ALA:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PHE:HA	1:B:6:PHE:O	2.01	0.60
1:I:59:ARG:NH2	1:I:217:ARG:O	2.34	0.60
2:L:-22:LEU:H	2:L:-22:LEU:HD22	1.65	0.60
1:U:170:SER:HB2	1:U:183:ILE:HG22	1.82	0.60
2:V:456:GLN:NE2	2:V:465:ARG:NH2	2.26	0.60
1:D:233:LEU:N	1:D:233:LEU:CD1	2.64	0.60
1:F:92:ARG:HH11	1:F:92:ARG:CG	2.15	0.60
1:Q:26:ARG:O	1:Q:26:ARG:HG2	2.00	0.60
1:A:128:ALA:HB2	1:A:134:LYS:HB3	1.83	0.60
2:H:485:ASP:OD1	2:H:485:ASP:C	2.39	0.60
1:D:19:LEU:HD12	1:K:9:PRO:HB3	1.81	0.60
2:Z:348:THR:CG2	2:Z:351:VAL:HG23	2.30	0.60
1:B:112:THR:HG22	1:B:113:GLU:OE2	2.01	0.60
1:O:164:ALA:HA	1:O:167:LEU:HD12	1.83	0.60
1:A:31:VAL:HG12	1:A:155:VAL:HG22	1.84	0.60
1:U:28:LYS:H	1:U:28:LYS:HE3	1.67	0.60
2:2:332:ARG:HB2	2:2:332:ARG:HH11	1.67	0.60
1:A:143:TYR:CD1	1:A:144:ASP:N	2.70	0.60
1:M:155:VAL:HG11	1:M:163:ILE:HB	1.81	0.60
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.84	0.60
1:S:128:ALA:HB2	1:S:134:LYS:HB3	1.83	0.60
2:G:382:ARG:NH2	2:G:385:ILE:HD13	2.15	0.60
1:M:110:ILE:HG23	1:M:114:GLN:HG3	1.84	0.60
1:Y:128:ALA:HB2	1:Y:134:LYS:HB3	1.84	0.60
1:I:225:ILE:HG21	1:I:233:LEU:HD12	1.82	0.60
1:D:204:GLY:O	1:D:208:LEU:HD13	2.01	0.60
1:K:234:LEU:C	1:K:234:LEU:CD1	2.69	0.60
1:Q:16:ARG:NH1	1:Q:117:PRO:HD3	2.16	0.60
1:D:31:VAL:HG12	1:D:155:VAL:HG22	1.83	0.59
1:K:31:VAL:HG12	1:K:155:VAL:HG22	1.83	0.59
1:M:141:ILE:N	1:M:141:ILE:HD12	2.17	0.59
1:M:161:GLU:N	1:M:162:PRO:HD2	2.16	0.59
2:T:320:SER:HB2	2:T:331:VAL:HG21	1.84	0.59
1:W:173:GLU:CB	1:W:174:ASN:ND2	2.65	0.59
1:B:33:LEU:HD12	1:B:33:LEU:O	2.02	0.59
2:C:430:ASN:ND2	2:C:431:ILE:C	2.55	0.59
1:F:189:ARG:HH21	1:F:203:LEU:HD23	1.65	0.59
2:J:332:ARG:HH11	2:J:332:ARG:HB2	1.67	0.59
1:M:152:HIS:CD2	1:M:171:TYR:HE2	2.20	0.59
1:Q:177:LEU:HD23	1:Q:233:LEU:HD11	1.83	0.59
1:S:8:SER:HB3	1:S:11:GLN:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:207:SER:C	1:U:208:LEU:CD1	2.70	0.59
1:1:167:LEU:HD11	1:1:187:ALA:HB3	1.84	0.59
2:C:-4:LEU:CD1	2:C:398:LEU:HD11	2.33	0.59
1:I:163:ILE:HD11	1:I:191:GLY:HA3	1.83	0.59
1:K:5:TYR:HD1	1:M:11:GLN:HG3	1.59	0.59
2:L:-20:PRO:O	2:L:-19:ALA:HB3	2.00	0.59
1:Y:31:VAL:HG12	1:Y:155:VAL:HG22	1.84	0.59
1:U:7:ILE:CA	1:1:5:TYR:O	2.51	0.59
2:X:331:VAL:CG1	2:X:349:ALA:HB2	2.30	0.59
2:X:374:LEU:HD11	1:Y:89:TYR:CD1	2.38	0.59
2:Z:-27:ARG:HH21	2:Z:-27:ARG:CG	2.09	0.59
1:A:8:SER:CB	1:A:9:PRO:HD2	2.26	0.59
1:K:4:PRO:HB3	1:W:5:TYR:CZ	2.38	0.59
1:D:92:ARG:CG	1:D:92:ARG:HH11	2.16	0.59
2:E:376:PHE:CE2	2:E:380:ILE:HD11	2.38	0.59
2:N:465:ARG:HB3	2:N:465:ARG:NH1	2.18	0.59
2:P:-17:ILE:O	2:P:-17:ILE:CG2	2.49	0.59
1:B:180:ALA:HA	1:B:183:ILE:HD12	1.85	0.59
1:B:6:PHE:N	1:B:6:PHE:HD2	2.00	0.59
1:I:92:ARG:CG	1:I:92:ARG:HH11	2.15	0.59
2:G:-17:ILE:HD13	2:G:-17:ILE:C	2.23	0.59
2:G:391:LEU:HD12	2:G:391:LEU:C	2.22	0.59
2:J:-38:VAL:O	2:J:-36:LEU:HD22	2.03	0.59
2:H:-30:PHE:HZ	2:P:-38:VAL:HG21	1.68	0.58
1:M:186:ALA:CB	1:M:189:ARG:NH2	2.66	0.58
1:O:11:GLN:HA	1:O:14:ARG:HE	1.67	0.58
1:O:92:ARG:HH11	1:O:92:ARG:CG	2.16	0.58
1:A:13:MET:HE1	1:O:116:LYS:CD	2.33	0.58
1:D:143:TYR:CD1	1:D:144:ASP:N	2.71	0.58
2:H:-27:ARG:NH1	2:H:-26:GLN:HE21	2.01	0.58
1:K:179:ASP:OD1	1:K:183:ILE:CD1	2.47	0.58
1:M:153:PHE:CD1	1:M:167:LEU:HD23	2.37	0.58
2:R:308:TYR:OH	2:R:496:ILE:HD11	2.03	0.58
2:Z:382:ARG:NH2	2:Z:385:ILE:HD13	2.17	0.58
2:J:-28:ARG:HH11	2:J:-21:LEU:HD21	1.67	0.58
1:Y:234:LEU:C	1:Y:235:VAL:HG23	2.23	0.58
2:C:-29:LEU:CD2	2:C:-25:ALA:HB3	2.34	0.58
1:M:98:GLN:O	1:M:102:VAL:HG23	2.03	0.58
2:P:407:TYR:CE1	2:P:417:ALA:CB	2.82	0.58
1:W:33:LEU:O	1:W:33:LEU:CD1	2.51	0.58
1:1:217:ARG:HD2	1:1:218:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:413:ASP:CG	2:T:414:PRO:HD2	2.23	0.58
1:U:205:VAL:HG21	1:U:231:GLN:HB2	1.84	0.58
2:V:301:ALA:CB	2:V:333:LYS:HZ2	2.14	0.58
2:C:319:ARG:HG3	2:C:320:SER:N	2.19	0.58
1:D:161:GLU:H	1:D:161:GLU:CD	2.07	0.58
2:H:391:LEU:O	2:H:395:MET:HG2	2.04	0.58
2:H:461:ASP:OD1	2:H:509:ARG:NH2	2.37	0.58
2:X:301:ALA:HB1	2:X:333:LYS:HZ2	1.68	0.58
2:C:430:ASN:ND2	2:C:430:ASN:C	2.57	0.58
2:G:376:PHE:CE2	2:G:380:ILE:HD11	2.38	0.58
2:L:-22:LEU:N	2:L:-22:LEU:HD22	2.19	0.58
1:Q:171:TYR:HD2	1:Q:172:ALA:N	1.95	0.58
1:Q:234:LEU:O	1:Q:235:VAL:HG22	2.02	0.58
2:V:391:LEU:O	2:V:395:MET:HG2	2.04	0.58
1:Y:98:GLN:O	1:Y:102:VAL:HG23	2.04	0.58
1:A:25:ALA:O	1:A:158:GLY:HA2	2.03	0.58
2:L:-4:LEU:O	2:L:-2:HIS:HD2	1.86	0.58
2:X:432:GLU:HG3	2:X:437:GLN:HB2	1.85	0.58
1:I:163:ILE:HD13	1:I:188:LEU:HD23	1.85	0.58
1:D:33:LEU:CD1	1:D:40:LEU:HB3	2.34	0.58
2:E:301:ALA:CB	2:E:333:LYS:HE2	2.25	0.58
1:S:14:ARG:CZ	1:S:14:ARG:HB2	2.33	0.58
2:Z:496:ILE:HG13	2:Z:505:VAL:CG2	2.34	0.58
1:I:152:HIS:HB3	1:I:171:TYR:CZ	2.39	0.57
1:F:128:ALA:HB2	1:F:134:LYS:HB3	1.86	0.57
1:I:35:TYR:CZ	1:I:37:GLY:CA	2.79	0.57
1:M:11:GLN:OE1	1:M:11:GLN:HA	2.02	0.57
1:A:16:ARG:NH1	1:A:117:PRO:HD3	2.20	0.57
1:B:6:PHE:N	1:B:6:PHE:CD2	2.68	0.57
1:I:28:LYS:HE3	1:I:28:LYS:N	2.18	0.57
2:R:308:TYR:CE2	2:R:311:GLY:HA3	2.39	0.57
1:W:128:ALA:HB2	1:W:134:LYS:HB3	1.86	0.57
2:R:-30:PHE:HZ	2:Z:-38:VAL:HG23	1.68	0.57
1:I:141:ILE:HD12	1:I:141:ILE:N	2.20	0.57
1:D:19:LEU:HD12	1:K:9:PRO:CB	2.33	0.57
2:N:456:GLN:NE2	2:N:465:ARG:NH2	2.42	0.57
1:Y:92:ARG:HH11	1:Y:92:ARG:HG3	1.70	0.57
2:J:432:GLU:HG3	2:J:437:GLN:HB2	1.85	0.57
1:B:20:ALA:O	1:B:24:ILE:HG13	2.03	0.57
1:I:152:HIS:HB3	1:I:171:TYR:CZ	2.40	0.57
1:I:31:VAL:HG12	1:I:155:VAL:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:ARG:HH11	1:1:92:ARG:CG	2.18	0.57
2:E:382:ARG:NH2	2:E:385:ILE:CD1	2.68	0.57
2:T:340:TYR:O	2:T:341:THR:HG22	2.03	0.57
1:A:33:LEU:O	1:A:33:LEU:HD12	2.05	0.57
2:G:-29:LEU:O	2:G:-25:ALA:N	2.36	0.57
1:I:16:ARG:NH1	1:I:117:PRO:HD3	2.20	0.57
1:S:19:LEU:C	1:S:19:LEU:HD23	2.25	0.57
2:Z:511:ALA:HB1	2:Z:515:ARG:HH21	1.69	0.57
2:R:-29:LEU:HD23	2:R:-21:LEU:HD12	1.87	0.57
2:R:-27:ARG:CD	2:R:-27:ARG:N	2.67	0.57
1:U:11:GLN:HG2	1:1:5:TYR:CZ	2.39	0.57
1:W:92:ARG:CG	1:W:92:ARG:HH11	2.17	0.57
2:X:-31:ASP:O	2:X:-27:ARG:HG2	2.05	0.57
2:Z:414:PRO:HA	2:Z:417:ALA:HB2	1.87	0.57
1:A:9:PRO:HG3	1:O:15:GLU:HB3	1.86	0.57
1:B:8:SER:OG	1:B:11:GLN:HB2	2.04	0.57
1:D:33:LEU:HD11	1:D:40:LEU:HB3	1.85	0.57
2:H:-23:GLU:CG	2:P:-28:ARG:NH2	2.63	0.57
1:S:28:LYS:NZ	1:S:52:LYS:HE3	2.20	0.57
2:T:486:LEU:HG	2:T:515:ARG:NH1	2.19	0.57
1:1:152:HIS:CG	1:1:171:TYR:CE2	2.93	0.56
2:2:382:ARG:NH2	2:2:385:ILE:HD13	2.20	0.56
2:H:-27:ARG:HH11	2:H:-26:GLN:NE2	2.02	0.56
2:L:-38:VAL:CG2	2:N:-30:PHE:CE2	2.87	0.56
2:N:469:GLU:HG3	2:N:517:ILE:HG21	1.87	0.56
2:R:301:ALA:HB1	2:R:333:LYS:HZ2	1.68	0.56
1:S:129:HIS:HB2	1:S:132:GLU:CD	2.26	0.56
1:U:231:GLN:HA	1:U:231:GLN:OE1	2.04	0.56
2:V:350:ALA:O	2:V:353:VAL:HG12	2.05	0.56
1:Y:110:ILE:O	1:Y:114:GLN:HB2	2.05	0.56
1:F:45:ASN:N	1:F:207:SER:O	2.33	0.56
2:G:429:TRP:HZ3	2:G:431:ILE:HD12	1.71	0.56
2:V:-26:GLN:NE2	2:2:-38:VAL:H1	2.01	0.56
1:A:13:MET:HE3	1:O:116:LYS:HD2	1.88	0.56
1:K:58:ASP:OD1	1:K:219:ARG:NH1	2.39	0.56
2:N:382:ARG:NH2	2:N:385:ILE:HD13	2.21	0.56
2:T:382:ARG:NH2	2:T:385:ILE:HD13	2.20	0.56
1:B:161:GLU:H	1:B:161:GLU:CD	2.08	0.56
1:D:25:ALA:O	1:D:158:GLY:HA2	2.05	0.56
1:F:129:HIS:HB2	1:F:132:GLU:CD	2.26	0.56
2:2:408:ASP:HB3	2:2:411:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:TYR:HE1	1:I:216:ASN:O	1.88	0.56
1:I:152:HIS:CD2	1:I:171:TYR:CE2	2.92	0.56
1:I:214:ASP:OD1	1:I:214:ASP:C	2.42	0.56
2:P:-18:SER:O	2:P:-17:ILE:CB	2.53	0.56
1:W:141:ILE:HD12	1:W:141:ILE:N	2.21	0.56
1:Y:152:HIS:HB3	1:Y:171:TYR:CZ	2.40	0.56
2:Z:353:VAL:CG1	2:Z:354:GLU:N	2.68	0.56
1:D:13:MET:CE	1:Q:116:LYS:HD2	2.35	0.56
1:I:214:ASP:OD1	1:I:215:ALA:N	2.39	0.56
1:K:98:GLN:O	1:K:102:VAL:HG23	2.05	0.56
2:L:408:ASP:HB3	2:L:411:ALA:HB2	1.88	0.56
2:R:416:SER:O	2:R:419:ARG:NH1	2.38	0.56
2:T:382:ARG:HH21	2:T:385:ILE:HD13	1.70	0.56
1:W:205:VAL:HG13	1:W:230:LEU:HB3	1.87	0.56
1:M:7:ILE:CG2	1:W:5:TYR:HD2	2.12	0.56
1:D:208:LEU:HD13	1:D:208:LEU:N	2.20	0.56
1:Q:173:GLU:CG	1:Q:174:ASN:OD1	2.54	0.56
1:Q:92:ARG:HH11	1:Q:92:ARG:CG	2.19	0.56
1:Y:163:ILE:CG1	1:Y:191:GLY:HA3	2.35	0.56
2:E:-26:GLN:OE1	2:E:-26:GLN:HA	2.05	0.56
2:L:366:TYR:CE2	2:L:374:LEU:HD13	2.41	0.56
2:X:521:ARG:CG	2:X:521:ARG:NH1	2.57	0.56
1:I:225:ILE:HG21	1:I:233:LEU:CD1	2.36	0.56
2:C:312:VAL:HG12	2:C:497:ILE:HB	1.87	0.56
1:D:11:GLN:HE22	1:Q:5:TYR:N	2.03	0.56
1:K:7:ILE:HB	1:K:11:GLN:HG3	1.88	0.56
1:M:128:ALA:HB2	1:M:134:LYS:HB3	1.88	0.56
1:M:186:ALA:HB2	1:M:189:ARG:HH22	1.70	0.56
2:N:382:ARG:HH21	2:N:385:ILE:HD13	1.71	0.56
1:O:217:ARG:HD2	1:O:218:PRO:HD2	1.86	0.56
2:G:479:SER:HB2	2:V:479:SER:HB2	1.87	0.56
2:G:366:TYR:CE2	2:G:374:LEU:HD13	2.41	0.56
2:R:-27:ARG:H	2:R:-27:ARG:HD2	1.68	0.56
1:W:26:ARG:NH1	1:W:26:ARG:HB2	2.20	0.56
1:A:11:GLN:HE22	1:A:14:ARG:HH22	1.50	0.56
2:E:415:GLN:NE2	2:E:415:GLN:CA	2.61	0.56
1:K:70:GLU:HG2	1:K:118:TYR:CE2	2.41	0.56
1:K:87:TYR:O	2:L:357:ARG:NH1	2.36	0.56
1:O:224:ARG:HG2	1:O:224:ARG:HH11	1.70	0.56
1:W:181:LEU:O	1:W:185:VAL:CG2	2.43	0.56
1:A:161:GLU:CD	1:A:161:GLU:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:ILE:CD1	1:I:191:GLY:HA3	2.36	0.55
1:I:33:LEU:HD11	1:I:40:LEU:HB3	1.87	0.55
1:I:92:ARG:HG3	1:I:92:ARG:HH11	1.71	0.55
2:N:301:ALA:O	2:N:440:GLY:HA3	2.06	0.55
2:R:-27:ARG:CD	2:R:-27:ARG:H	2.19	0.55
2:E:-30:PHE:HZ	2:R:-38:VAL:CG2	2.18	0.55
2:R:391:LEU:O	2:R:395:MET:HG2	2.06	0.55
1:U:11:GLN:HG3	1:1:5:TYR:CZ	2.40	0.55
1:B:92:ARG:HG3	1:B:92:ARG:HH11	1.70	0.55
1:I:163:ILE:HG12	1:I:191:GLY:HA3	1.88	0.55
2:L:-4:LEU:O	2:L:-2:HIS:CD2	2.59	0.55
1:M:152:HIS:CB	1:M:171:TYR:CE2	2.85	0.55
1:Q:30:VAL:HG22	1:Q:52:LYS:HZ3	1.71	0.55
2:R:-20:PRO:O	2:R:-19:ALA:HB2	2.05	0.55
1:S:14:ARG:HB2	1:S:14:ARG:HH21	1.71	0.55
2:T:391:LEU:O	2:T:395:MET:HG2	2.07	0.55
1:B:59:ARG:NH2	1:B:217:ARG:O	2.38	0.55
1:F:189:ARG:HH21	1:F:203:LEU:HD21	1.69	0.55
1:F:7:ILE:HD11	1:F:12:ALA:HA	1.87	0.55
1:O:161:GLU:H	1:O:161:GLU:CD	2.10	0.55
1:Q:142:THR:OG1	1:Q:144:ASP:HB3	2.06	0.55
1:U:231:GLN:CA	1:U:231:GLN:OE1	2.53	0.55
1:D:189:ARG:HH12	1:D:203:LEU:CA	2.19	0.55
2:E:-36:LEU:O	2:E:-35:SER:HB2	2.06	0.55
1:O:152:HIS:HD2	1:O:171:TYR:OH	1.90	0.55
2:T:366:TYR:CE2	2:T:374:LEU:HD13	2.40	0.55
1:U:28:LYS:N	1:U:28:LYS:HE3	2.21	0.55
1:B:142:THR:OG1	1:B:146:SER:HB2	2.07	0.55
2:H:301:ALA:O	2:H:440:GLY:HA3	2.06	0.55
1:K:163:ILE:HD11	1:K:191:GLY:HA3	1.88	0.55
1:U:92:ARG:HH11	1:U:92:ARG:HG3	1.70	0.55
2:X:407:TYR:CE1	2:X:417:ALA:HB3	2.42	0.55
2:N:-17:ILE:O	2:N:-16:SER:HB3	2.07	0.55
2:P:-17:ILE:HG21	2:P:396:GLN:OE1	2.06	0.55
1:Q:163:ILE:HG23	1:Q:187:ALA:C	2.26	0.55
1:O:155:VAL:HG22	1:O:167:LEU:HD11	1.87	0.55
2:C:354:GLU:OE1	2:C:354:GLU:HA	2.07	0.55
2:E:310:GLY:HA2	2:E:414:PRO:O	2.07	0.55
2:L:-5:GLN:HA	2:L:-5:GLN:HE21	1.72	0.55
1:O:30:VAL:HG22	1:O:52:LYS:HZ3	1.72	0.55
2:P:407:TYR:HE1	2:P:417:ALA:HB3	1.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:129:HIS:HB2	1:W:132:GLU:CD	2.27	0.55
1:A:122:LEU:CD1	1:A:141:ILE:HB	2.37	0.55
1:D:28:LYS:NZ	1:D:52:LYS:HE3	2.22	0.55
2:H:382:ARG:NH2	2:H:385:ILE:HD13	2.21	0.55
1:I:161:GLU:H	1:I:161:GLU:CD	2.10	0.55
1:I:28:LYS:H	1:I:28:LYS:HE3	1.72	0.55
2:J:515:ARG:HG2	2:J:515:ARG:HH11	1.72	0.55
1:U:7:ILE:HA	1:I:5:TYR:O	2.07	0.55
2:X:391:LEU:O	2:X:395:MET:HG2	2.06	0.55
2:2:-28:ARG:O	2:2:-24:PRO:HG3	2.07	0.55
2:E:-30:PHE:CZ	2:E:-26:GLN:HG3	2.41	0.55
2:E:308:TYR:HB2	2:E:309:PRO:HD2	1.89	0.55
2:E:-30:PHE:HZ	2:R:-38:VAL:HG23	1.71	0.55
1:K:28:LYS:H	1:K:28:LYS:CE	2.20	0.55
2:L:-23:GLU:CD	2:L:-23:GLU:H	2.09	0.55
1:U:89:TYR:CD1	2:2:374:LEU:HD11	2.42	0.55
2:R:456:GLN:NE2	2:R:465:ARG:NH2	2.25	0.54
1:U:224:ARG:HH11	1:U:224:ARG:HG2	1.72	0.54
2:X:332:ARG:HB2	2:X:332:ARG:HH11	1.71	0.54
1:K:28:LYS:NZ	1:K:52:LYS:HE3	2.22	0.54
1:D:16:ARG:NE	1:M:3:PHE:HE1	2.06	0.54
1:O:98:GLN:O	1:O:102:VAL:HG23	2.07	0.54
1:1:13:MET:CE	1:1:13:MET:HA	2.38	0.54
2:2:432:GLU:HG3	2:2:437:GLN:HB2	1.88	0.54
1:M:186:ALA:HB2	1:M:189:ARG:NH2	2.22	0.54
1:W:235:VAL:O	1:W:235:VAL:HG12	2.06	0.54
1:Y:141:ILE:N	1:Y:141:ILE:HD12	2.23	0.54
1:Y:169:GLU:OE1	1:Y:169:GLU:CA	2.54	0.54
1:A:8:SER:CB	1:A:9:PRO:CD	2.83	0.54
2:R:355:PHE:CE2	2:R:386:MET:HE2	2.43	0.54
1:S:161:GLU:CD	1:S:161:GLU:H	2.11	0.54
1:F:129:HIS:HE1	3:F:251:HOH:O	1.90	0.54
2:H:-27:ARG:C	2:H:-26:GLN:OE1	2.45	0.54
1:I:27:ALA:HB1	1:I:28:LYS:CE	2.37	0.54
1:K:234:LEU:O	1:K:235:VAL:C	2.45	0.54
1:O:152:HIS:CD2	1:O:171:TYR:CE2	2.95	0.54
1:O:83:ASP:OD2	2:P:365:HIS:ND1	2.29	0.54
1:S:152:HIS:HB3	1:S:171:TYR:CZ	2.42	0.54
1:W:31:VAL:HG12	1:W:155:VAL:HG22	1.89	0.54
1:W:33:LEU:HD11	1:W:40:LEU:HB3	1.90	0.54
1:A:152:HIS:HB3	1:A:171:TYR:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:430:ASN:ND2	2:C:431:ILE:N	2.55	0.54
1:I:5:TYR:HD1	1:I:5:TYR:N	2.05	0.54
2:N:343:THR:HG22	2:N:404:LEU:HD12	1.89	0.54
2:E:319:ARG:HG3	2:E:320:SER:N	2.21	0.54
1:K:56:LEU:HG	1:K:62:PHE:HB2	1.89	0.54
1:K:76:ARG:NH1	2:L:370:GLU:OE2	2.41	0.54
1:U:31:VAL:HG12	1:U:155:VAL:HG22	1.90	0.54
1:I:8:SER:H	1:I:11:GLN:HG3	1.72	0.54
1:A:13:MET:CE	1:O:116:LYS:CD	2.86	0.54
2:C:-29:LEU:O	2:C:-25:ALA:N	2.40	0.54
2:C:-18:SER:CB	2:C:393:ALA:CB	2.79	0.54
2:J:-16:SER:O	2:J:-15:GLY:C	2.46	0.54
1:Q:35:TYR:CZ	1:Q:37:GLY:CA	2.74	0.54
1:W:205:VAL:HG21	1:W:231:GLN:CA	2.37	0.54
1:Y:161:GLU:H	1:Y:161:GLU:CD	2.11	0.54
1:A:13:MET:HE1	1:O:116:LYS:HD3	1.89	0.54
2:G:382:ARG:NH2	2:G:385:ILE:CD1	2.71	0.54
1:I:129:HIS:HB2	1:I:132:GLU:CD	2.28	0.54
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.90	0.54
1:K:100:ALA:HB1	1:K:147:ILE:HD11	1.90	0.54
1:Q:161:GLU:H	1:Q:161:GLU:CD	2.11	0.54
1:Q:26:ARG:NH1	1:Q:26:ARG:HB2	2.22	0.54
2:T:413:ASP:C	2:T:413:ASP:OD1	2.46	0.54
1:Y:205:VAL:CG2	1:Y:231:GLN:OE1	2.56	0.54
1:I:173:GLU:HG2	1:I:174:ASN:OD1	2.07	0.54
1:D:16:ARG:NH2	1:M:4:PRO:HG3	2.22	0.54
1:I:5:TYR:N	1:I:5:TYR:CD1	2.76	0.54
2:J:-32:THR:HG22	2:J:-31:ASP:N	2.23	0.54
1:D:13:MET:CE	1:Q:19:LEU:HD21	2.38	0.54
1:Y:181:LEU:CD1	1:Y:185:VAL:CG2	2.86	0.54
1:I:8:SER:OG	1:I:11:GLN:CD	2.46	0.53
1:I:19:LEU:HD23	1:I:19:LEU:C	2.28	0.53
1:A:154:VAL:HA	3:A:249:HOH:O	2.07	0.53
1:B:40:LEU:HD13	1:B:212:VAL:CG1	2.38	0.53
1:K:4:PRO:HB2	1:W:5:TYR:CD2	2.43	0.53
1:M:185:VAL:HG12	1:M:189:ARG:HH11	1.73	0.53
1:M:28:LYS:HB3	1:M:44:GLU:HG3	1.90	0.53
1:M:56:LEU:HG	1:M:62:PHE:HB2	1.90	0.53
2:P:-27:ARG:NE	2:P:-26:GLN:CD	2.61	0.53
2:V:509:ARG:O	2:V:513:LEU:CD2	2.56	0.53
2:Z:409:ILE:HG13	2:Z:410:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:-29:LEU:HD23	2:C:-25:ALA:HB3	1.90	0.53
2:E:338:ASP:OD1	2:E:338:ASP:C	2.46	0.53
1:F:98:GLN:O	1:F:102:VAL:HG23	2.08	0.53
2:L:382:ARG:NH2	2:L:385:ILE:HD13	2.23	0.53
2:P:-34:SER:HB3	2:P:-31:ASP:HB2	1.90	0.53
2:P:301:ALA:O	2:P:440:GLY:HA3	2.09	0.53
1:Q:7:ILE:HG21	1:Q:15:GLU:OE1	2.08	0.53
1:S:178:THR:HG23	1:S:233:LEU:O	2.09	0.53
1:F:217:ARG:HD2	1:F:218:PRO:HD2	1.90	0.53
2:G:349:ALA:O	2:G:353:VAL:HG12	2.08	0.53
2:L:-18:SER:C	2:L:-17:ILE:CG2	2.77	0.53
2:V:382:ARG:NH2	2:V:385:ILE:HD13	2.24	0.53
2:X:301:ALA:O	2:X:440:GLY:HA3	2.07	0.53
1:U:11:GLN:CG	1:I:5:TYR:CE1	2.92	0.53
2:H:-6:ALA:H1	2:H:-5:GLN:CB	2.02	0.53
1:Q:234:LEU:H	1:Q:234:LEU:HD12	1.68	0.53
1:A:130:TYR:CD1	1:A:218:PRO:HA	2.43	0.53
1:A:35:TYR:CD1	1:A:37:GLY:N	2.63	0.53
2:E:391:LEU:HD12	2:E:391:LEU:O	2.08	0.53
2:G:-21:LEU:CD1	2:G:-20:PRO:HD2	2.37	0.53
1:I:177:LEU:CD2	1:I:233:LEU:HD21	2.39	0.53
2:L:301:ALA:HB1	2:L:333:LYS:HD3	1.89	0.53
1:S:31:VAL:HG12	1:S:155:VAL:HG22	1.90	0.53
1:W:14:ARG:CG	1:W:14:ARG:HH11	2.21	0.53
1:W:28:LYS:HB3	1:W:44:GLU:HG3	1.89	0.53
2:G:-39:ALA:CB	2:X:-26:GLN:OE1	2.55	0.53
1:A:25:ALA:HB2	3:A:252:HOH:O	2.09	0.53
1:D:167:LEU:O	1:D:171:TYR:N	2.40	0.53
2:G:-26:GLN:CA	2:G:-26:GLN:OE1	2.54	0.53
2:H:382:ARG:HH21	2:H:385:ILE:HD13	1.74	0.53
2:Z:-28:ARG:O	2:Z:-24:PRO:HG3	2.08	0.53
1:D:156:MET:HA	3:D:249:HOH:O	2.08	0.53
1:F:35:TYR:CE1	1:F:37:GLY:N	2.77	0.53
2:L:434:GLU:OE2	2:L:434:GLU:HA	2.09	0.53
1:M:217:ARG:HD2	1:M:218:PRO:HD2	1.91	0.53
1:U:35:TYR:CZ	1:U:37:GLY:CA	2.79	0.53
1:B:19:LEU:O	1:B:19:LEU:HD23	2.08	0.53
2:N:-27:ARG:HG3	2:N:-27:ARG:O	2.08	0.53
2:R:382:ARG:NH2	2:R:385:ILE:HD13	2.24	0.53
1:W:161:GLU:CD	1:W:161:GLU:H	2.12	0.53
2:E:-28:ARG:HB2	2:E:-21:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:TYR:CD1	2:N:374:LEU:HD11	2.44	0.53
1:O:234:LEU:CD1	1:O:234:LEU:O	2.42	0.53
1:S:98:GLN:O	1:S:102:VAL:HG23	2.09	0.53
1:U:40:LEU:HA	1:U:212:VAL:HG12	1.91	0.53
2:V:301:ALA:HB1	2:V:333:LYS:CD	2.39	0.53
1:W:173:GLU:CA	1:W:174:ASN:HD22	2.20	0.53
1:B:35:TYR:OH	1:B:37:GLY:HA3	2.06	0.52
1:I:163:ILE:CG1	1:I:191:GLY:HA3	2.38	0.52
1:I:28:LYS:NZ	1:I:52:LYS:HE3	2.24	0.52
2:J:-17:ILE:CD1	2:J:392:ALA:CB	2.85	0.52
1:M:152:HIS:HB3	1:M:171:TYR:CZ	2.43	0.52
1:U:33:LEU:CD1	1:U:40:LEU:HB3	2.39	0.52
2:V:366:TYR:CE2	2:V:374:LEU:HD13	2.44	0.52
2:X:478:ASP:OD1	2:2:324:ASN:HB3	2.08	0.52
2:C:496:ILE:HG23	2:C:503:VAL:HG23	1.91	0.52
2:L:-38:VAL:CG2	2:N:-30:PHE:CZ	2.92	0.52
2:R:521:ARG:O	2:R:522:SER:CB	2.57	0.52
2:T:340:TYR:C	2:T:341:THR:CG2	2.78	0.52
2:T:416:SER:O	2:T:419:ARG:NH1	2.30	0.52
1:U:110:ILE:O	1:U:114:GLN:HB2	2.09	0.52
1:A:98:GLN:O	1:A:102:VAL:HG23	2.08	0.52
1:B:13:MET:CE	1:B:111:PHE:HE2	2.22	0.52
1:B:129:HIS:HB2	1:B:132:GLU:CD	2.30	0.52
1:B:28:LYS:H	1:B:28:LYS:HE2	1.73	0.52
2:C:464:LEU:O	2:C:464:LEU:HG	2.10	0.52
2:E:423:PHE:CE1	2:E:429:TRP:HB3	2.45	0.52
1:F:92:ARG:HH11	1:F:92:ARG:HG3	1.74	0.52
2:J:413:ASP:HB3	2:J:416:SER:OG	2.10	0.52
1:O:185:VAL:O	1:O:189:ARG:N	2.40	0.52
2:R:301:ALA:O	2:R:440:GLY:HA3	2.08	0.52
1:W:56:LEU:HG	1:W:62:PHE:HB2	1.91	0.52
1:F:161:GLU:H	1:F:161:GLU:CD	2.13	0.52
1:S:130:TYR:CE1	1:S:216:ASN:O	2.62	0.52
2:T:308:TYR:CE2	2:T:311:GLY:HA3	2.43	0.52
1:F:9:PRO:HA	1:W:6:PHE:HE1	1.75	0.52
1:B:74:LEU:HD23	1:B:122:LEU:HD21	1.91	0.52
1:K:92:ARG:HH11	1:K:92:ARG:HG3	1.74	0.52
1:O:92:ARG:HH11	1:O:92:ARG:HG3	1.75	0.52
2:X:428:GLY:CA	2:Z:350:ALA:CB	2.88	0.52
1:I:35:TYR:CZ	1:I:37:GLY:CA	2.87	0.52
1:A:122:LEU:HD12	1:A:141:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:CG	1:A:218:PRO:HA	2.44	0.52
1:D:100:ALA:HB1	1:D:147:ILE:HD11	1.91	0.52
1:F:167:LEU:HD13	1:F:187:ALA:CB	2.40	0.52
2:G:301:ALA:CB	2:G:333:LYS:HZ3	2.10	0.52
1:Q:129:HIS:HB2	1:Q:132:GLU:CD	2.30	0.52
1:U:191:GLY:O	1:U:192:SER:C	2.47	0.52
1:W:15:GLU:CD	1:Y:9:PRO:HG2	2.29	0.52
2:X:428:GLY:HA2	2:Z:350:ALA:CB	2.39	0.52
1:F:170:SER:O	1:F:183:ILE:HD13	2.10	0.52
1:F:30:VAL:HG22	1:F:52:LYS:HZ3	1.75	0.52
1:K:28:LYS:HE3	1:K:28:LYS:N	2.25	0.52
2:L:-23:GLU:HG2	2:L:-22:LEU:HD22	1.91	0.52
2:C:366:TYR:CE2	2:C:374:LEU:HD13	2.44	0.52
2:E:358:LEU:HD23	2:E:386:MET:CE	2.39	0.52
1:B:33:LEU:CD1	1:B:33:LEU:O	2.58	0.52
1:U:181:LEU:O	1:U:185:VAL:HG23	2.09	0.52
1:U:217:ARG:HH11	1:U:223:ARG:HG2	1.75	0.52
1:W:19:LEU:C	1:W:19:LEU:HD23	2.31	0.52
1:1:19:LEU:C	1:1:19:LEU:CD2	2.78	0.52
1:1:51:GLN:HA	1:1:209:GLU:OE2	2.10	0.52
1:A:217:ARG:HH21	1:A:223:ARG:HE	1.58	0.52
2:E:318:ARG:HD3	2:E:493:THR:HG23	1.92	0.52
2:G:-29:LEU:O	2:G:-25:ALA:C	2.49	0.52
1:I:224:ARG:HH11	1:I:224:ARG:HG2	1.75	0.52
2:R:407:TYR:C	2:R:407:TYR:CD2	2.84	0.52
1:S:33:LEU:CD1	1:S:40:LEU:HB3	2.39	0.52
2:X:428:GLY:HA2	2:Z:350:ALA:HB1	1.91	0.52
1:1:92:ARG:HH11	1:1:92:ARG:HG3	1.75	0.51
2:C:338:ASP:OD1	2:C:338:ASP:C	2.49	0.51
1:K:161:GLU:H	1:K:161:GLU:CD	2.12	0.51
1:Q:211:ALA:O	1:Q:212:VAL:HG13	2.09	0.51
1:S:28:LYS:H	1:S:28:LYS:CE	2.23	0.51
1:U:176:SER:HG	1:U:179:ASP:CG	2.11	0.51
2:V:-31:ASP:O	2:V:-27:ARG:HG2	2.10	0.51
1:W:181:LEU:O	1:W:181:LEU:HD12	2.09	0.51
2:X:375:THR:HG23	1:Y:93:ASP:OD1	2.10	0.51
1:1:7:ILE:HB	1:1:11:GLN:CG	2.30	0.51
1:A:6:PHE:HB2	1:B:5:TYR:CD1	2.45	0.51
1:B:92:ARG:HB3	2:H:375:THR:HG21	1.92	0.51
2:E:301:ALA:HB2	2:E:333:LYS:CE	2.29	0.51
2:H:-28:ARG:HB3	2:H:-28:ARG:CZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:-30:PHE:CZ	2:P:-38:VAL:HG21	2.45	0.51
1:Q:27:ALA:HB1	1:Q:28:LYS:HE2	1.92	0.51
1:U:152:HIS:HB3	1:U:171:TYR:CE2	2.45	0.51
1:B:92:ARG:CG	1:B:92:ARG:NH1	2.73	0.51
2:C:332:ARG:HB2	2:C:332:ARG:CZ	2.40	0.51
1:D:92:ARG:HH11	1:D:92:ARG:HG3	1.74	0.51
2:J:509:ARG:HG3	2:J:509:ARG:HH11	1.74	0.51
1:K:129:HIS:HB2	1:K:132:GLU:CD	2.30	0.51
2:L:382:ARG:HH21	2:L:385:ILE:HD13	1.74	0.51
1:Q:171:TYR:HE2	1:Q:172:ALA:C	2.11	0.51
2:T:413:ASP:OD1	2:T:415:GLN:N	2.41	0.51
1:Y:163:ILE:HG12	1:Y:191:GLY:CA	2.41	0.51
2:C:430:ASN:HD22	2:C:430:ASN:C	2.14	0.51
1:D:233:LEU:N	1:D:233:LEU:HD12	2.23	0.51
2:L:407:TYR:HE1	2:L:417:ALA:HB3	1.61	0.51
2:L:382:ARG:HD2	1:M:89:TYR:HE1	1.76	0.51
2:N:366:TYR:CE2	2:N:374:LEU:HD13	2.45	0.51
1:O:152:HIS:HB3	1:O:171:TYR:CZ	2.45	0.51
1:S:15:GLU:HB3	1:1:9:PRO:HG2	1.92	0.51
2:T:407:TYR:CE1	2:T:417:ALA:HB3	2.46	0.51
1:U:225:ILE:HG21	1:U:233:LEU:HD11	1.91	0.51
1:Y:67:LYS:HG2	1:Y:69:ASN:HD21	1.76	0.51
1:B:182:ARG:CG	1:B:183:ILE:N	2.72	0.51
2:G:351:VAL:HG12	2:G:400:ALA:HB2	1.92	0.51
1:S:114:GLN:HA	1:S:114:GLN:NE2	2.21	0.51
2:J:388:ARG:NH1	2:T:-21:LEU:O	2.44	0.51
2:X:-36:LEU:O	2:X:-35:SER:HB2	2.11	0.51
1:A:129:HIS:HB2	1:A:132:GLU:CD	2.31	0.51
2:C:309:PRO:HG2	2:C:458:THR:O	2.10	0.51
1:D:35:TYR:HE1	1:D:37:GLY:CA	1.99	0.51
1:I:152:HIS:CD2	1:I:171:TYR:HE2	2.28	0.51
2:J:-23:GLU:HG3	2:J:-22:LEU:CD1	2.41	0.51
1:U:7:ILE:CB	1:1:5:TYR:O	2.59	0.51
1:U:89:TYR:HE1	2:2:382:ARG:HD2	1.76	0.51
1:W:33:LEU:CD1	1:W:40:LEU:HB3	2.40	0.51
2:N:519:GLU:OE2	2:N:523:GLY:O	2.29	0.51
1:Q:28:LYS:H	1:Q:28:LYS:CE	2.24	0.51
1:S:15:GLU:OE2	1:1:9:PRO:HG2	2.11	0.51
1:S:224:ARG:HG2	1:S:224:ARG:HH11	1.76	0.51
1:W:143:TYR:CD1	1:W:144:ASP:N	2.79	0.51
1:Y:33:LEU:CD1	1:Y:40:LEU:HB3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:-26:GLN:CG	2:H:-39:ALA:CB	2.88	0.51
1:I:163:ILE:HG12	1:I:191:GLY:CA	2.40	0.51
2:J:301:ALA:CB	2:J:333:LYS:HZ2	2.22	0.51
1:Q:28:LYS:NZ	1:Q:52:LYS:HE3	2.26	0.51
1:S:33:LEU:CD1	1:S:33:LEU:O	2.59	0.51
1:W:178:THR:HG23	1:W:233:LEU:HD22	1.93	0.51
2:X:496:ILE:HG22	2:X:503:VAL:HG22	1.92	0.51
1:1:112:THR:O	1:1:112:THR:HG22	2.11	0.51
1:A:26:ARG:NH1	1:A:26:ARG:HB2	2.26	0.51
1:B:152:HIS:CG	1:B:171:TYR:CE2	2.99	0.51
2:C:-34:SER:HB3	2:C:-31:ASP:HB2	1.93	0.51
2:H:350:ALA:O	2:H:353:VAL:HG12	2.11	0.51
2:C:-26:GLN:CB	2:H:-39:ALA:CB	2.89	0.51
2:J:-29:LEU:O	2:J:-25:ALA:C	2.49	0.51
1:K:70:GLU:HB3	1:K:118:TYR:CD2	2.45	0.51
1:D:16:ARG:HH21	1:M:4:PRO:CD	2.24	0.51
1:M:92:ARG:HH11	1:M:92:ARG:HG3	1.74	0.51
2:N:472:TYR:CD2	2:N:521:ARG:NH1	2.79	0.51
1:Q:234:LEU:C	1:Q:235:VAL:CG2	2.79	0.51
2:R:382:ARG:HH21	2:R:385:ILE:HD13	1.75	0.51
1:B:171:TYR:CE1	1:B:172:ALA:O	2.64	0.50
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.93	0.50
2:C:444:LEU:HB2	3:C:69:HOH:O	2.11	0.50
1:K:35:TYR:OH	1:K:37:GLY:HA3	2.09	0.50
2:L:301:ALA:O	2:L:440:GLY:HA3	2.11	0.50
2:P:308:TYR:CE1	2:P:311:GLY:HA3	2.44	0.50
2:R:338:ASP:C	2:R:338:ASP:OD1	2.50	0.50
2:T:340:TYR:O	2:T:341:THR:CG2	2.58	0.50
2:X:-34:SER:OG	2:X:-32:THR:HG22	2.12	0.50
1:D:167:LEU:HD13	1:D:187:ALA:CB	2.40	0.50
1:F:152:HIS:HB3	1:F:171:TYR:CE2	2.46	0.50
1:Q:178:THR:CG2	1:Q:233:LEU:O	2.58	0.50
1:F:141:ILE:N	1:F:141:ILE:HD12	2.25	0.50
2:H:366:TYR:CE2	2:H:374:LEU:HD13	2.46	0.50
1:I:27:ALA:HB1	1:I:28:LYS:HE2	1.93	0.50
1:M:33:LEU:HB3	1:M:153:PHE:HB3	1.92	0.50
2:N:421:VAL:HG22	2:N:431:ILE:HG12	1.93	0.50
2:T:413:ASP:OD1	2:T:414:PRO:N	2.44	0.50
2:X:320:SER:HB2	2:X:331:VAL:HG21	1.94	0.50
1:1:173:GLU:HG3	1:1:174:ASN:OD1	2.09	0.50
1:A:15:GLU:OE1	1:B:8:SER:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASP:OD2	1:D:146:SER:OG	2.30	0.50
2:L:-27:ARG:HH11	2:L:-26:GLN:NE2	2.08	0.50
2:P:391:LEU:O	2:P:395:MET:HG2	2.11	0.50
1:Q:224:ARG:HG2	1:Q:224:ARG:HH11	1.77	0.50
1:W:205:VAL:HG22	1:W:234:LEU:HD12	1.94	0.50
1:A:67:LYS:HG2	1:A:69:ASN:HD21	1.77	0.50
1:F:178:THR:O	1:F:182:ARG:HG3	2.11	0.50
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.94	0.50
2:G:301:ALA:O	2:G:440:GLY:HA3	2.12	0.50
2:G:428:GLY:HA2	2:X:350:ALA:HB1	1.93	0.50
2:H:423:PHE:CE1	2:H:429:TRP:HB3	2.46	0.50
1:K:144:ASP:O	1:K:144:ASP:OD1	2.30	0.50
1:K:29:SER:OG	1:K:157:GLY:O	2.30	0.50
1:M:189:ARG:O	1:M:192:SER:O	2.30	0.50
2:N:407:TYR:CE1	2:N:417:ALA:HB3	2.47	0.50
1:Q:83:ASP:OD2	2:R:365:HIS:ND1	2.24	0.50
1:Y:130:TYR:CE1	1:Y:216:ASN:O	2.64	0.50
2:R:-30:PHE:CZ	2:Z:-38:VAL:HG23	2.45	0.50
1:D:129:HIS:HB2	1:D:132:GLU:CD	2.32	0.50
2:L:-29:LEU:O	2:L:-25:ALA:N	2.41	0.50
2:L:345:ILE:HB	2:L:352:ALA:HB1	1.94	0.50
2:N:343:THR:HG22	2:N:404:LEU:CD1	2.41	0.50
2:H:-23:GLU:HB3	2:P:-28:ARG:NH2	2.26	0.50
1:U:166:ALA:O	1:U:170:SER:OG	2.30	0.50
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.93	0.50
2:V:301:ALA:CB	2:V:333:LYS:CD	2.89	0.50
2:V:413:ASP:OD1	2:V:413:ASP:O	2.30	0.50
1:W:40:LEU:HA	1:W:212:VAL:HG12	1.92	0.50
2:2:-23:GLU:OE1	2:2:-23:GLU:O	2.30	0.50
2:C:345:ILE:HB	2:C:352:ALA:HB1	1.92	0.50
1:D:144:ASP:O	1:D:144:ASP:OD1	2.30	0.50
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.94	0.50
2:G:312:VAL:HG12	2:G:497:ILE:HB	1.94	0.50
1:K:152:HIS:CD2	1:K:171:TYR:CE2	2.88	0.50
1:A:137:GLU:HG2	1:O:48:ARG:HH22	1.76	0.50
1:Q:176:SER:OG	1:Q:179:ASP:OD1	2.30	0.50
1:S:92:ARG:HH11	1:S:92:ARG:HG3	1.75	0.50
1:1:33:LEU:O	1:1:33:LEU:HD12	2.12	0.50
1:1:56:LEU:HG	1:1:62:PHE:HB2	1.93	0.50
1:A:170:SER:OG	1:A:183:ILE:HG23	2.12	0.50
1:D:28:LYS:CE	1:D:28:LYS:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:173:GLU:OE1	1:Q:174:ASN:OD1	2.30	0.50
1:Q:8:SER:HB2	1:Q:9:PRO:CD	2.42	0.50
1:W:110:ILE:HG23	1:W:114:GLN:CG	2.24	0.50
1:1:129:HIS:HB2	1:1:132:GLU:CD	2.32	0.50
1:B:51:GLN:NE2	1:I:97:ARG:NH2	2.60	0.50
2:C:301:ALA:CB	2:C:333:LYS:HE2	2.30	0.50
1:D:110:ILE:HG23	1:D:114:GLN:HG3	1.94	0.50
1:D:40:LEU:HD12	1:D:212:VAL:HG13	1.94	0.50
2:H:-27:ARG:NH1	2:H:-26:GLN:NE2	2.60	0.50
2:L:301:ALA:HB1	2:L:333:LYS:CD	2.42	0.50
2:V:-5:GLN:NE2	2:V:-2:HIS:CE1	2.80	0.50
1:W:152:HIS:HB3	1:W:171:TYR:CE2	2.47	0.50
1:W:204:GLY:O	1:W:208:LEU:HB2	2.12	0.50
2:C:382:ARG:HD2	1:I:89:TYR:CE1	2.47	0.49
1:F:16:ARG:NH2	1:F:115:ALA:O	2.45	0.49
1:I:216:ASN:O	1:I:216:ASN:OD1	2.30	0.49
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.93	0.49
2:Z:345:ILE:N	2:Z:345:ILE:HD12	2.27	0.49
1:1:204:GLY:O	1:1:208:LEU:HB2	2.13	0.49
2:E:-30:PHE:CZ	2:R:-38:VAL:HG23	2.47	0.49
1:F:191:GLY:O	1:F:192:SER:HB3	2.12	0.49
1:K:130:TYR:CE1	1:K:216:ASN:O	2.65	0.49
1:K:130:TYR:HE1	1:K:216:ASN:O	1.95	0.49
1:K:29:SER:H	1:K:44:GLU:CG	2.25	0.49
1:D:16:ARG:NH2	1:M:4:PRO:CG	2.75	0.49
1:U:161:GLU:CD	1:U:161:GLU:H	2.16	0.49
2:Z:331:VAL:HG22	2:Z:349:ALA:HB2	1.93	0.49
1:A:28:LYS:HB2	1:A:52:LYS:NZ	2.27	0.49
1:I:98:GLN:O	1:I:102:VAL:HG23	2.12	0.49
1:K:4:PRO:HG3	1:W:5:TYR:CD2	2.46	0.49
2:L:509:ARG:NH1	2:L:512:GLU:OE1	2.45	0.49
2:P:-27:ARG:O	2:P:-26:GLN:OE1	2.30	0.49
1:S:26:ARG:NH1	1:S:26:ARG:HB2	2.28	0.49
1:Y:130:TYR:HE1	1:Y:216:ASN:O	1.94	0.49
2:C:-28:ARG:HD3	2:J:-23:GLU:OE2	2.12	0.49
1:D:50:LEU:CD1	1:K:147:ILE:CG2	2.89	0.49
2:E:362:GLU:HG2	2:E:382:ARG:HG2	1.95	0.49
2:V:301:ALA:HB2	2:V:333:LYS:CE	2.42	0.49
2:X:350:ALA:C	2:X:353:VAL:HG12	2.33	0.49
1:Y:181:LEU:CD1	1:Y:185:VAL:HG23	2.42	0.49
2:Z:382:ARG:HH21	2:Z:385:ILE:HD13	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:-17:ILE:CG2	2:C:-17:ILE:O	2.60	0.49
2:E:-38:VAL:HG23	2:L:-26:GLN:HB3	1.93	0.49
1:F:33:LEU:CD1	1:F:33:LEU:C	2.80	0.49
2:J:301:ALA:O	2:J:440:GLY:HA3	2.13	0.49
2:P:418:GLY:O	2:P:419:ARG:NH1	2.45	0.49
1:S:83:ASP:OD2	2:T:365:HIS:ND1	2.32	0.49
2:V:338:ASP:OD1	2:V:338:ASP:C	2.50	0.49
2:T:388:ARG:NH1	2:2:-20:PRO:HA	2.28	0.49
1:B:35:TYR:N	1:B:38:GLY:O	2.43	0.49
2:C:434:GLU:O	2:C:434:GLU:OE1	2.30	0.49
2:H:-27:ARG:O	2:H:-26:GLN:OE1	2.30	0.49
1:K:28:LYS:HB3	1:K:44:GLU:HG3	1.94	0.49
1:Q:40:LEU:HD12	1:Q:212:VAL:HG13	1.94	0.49
2:T:366:TYR:CD2	2:T:374:LEU:HD13	2.48	0.49
1:U:92:ARG:CG	1:U:92:ARG:NH1	2.73	0.49
1:W:173:GLU:CB	1:W:174:ASN:HD22	2.24	0.49
1:K:4:PRO:CG	1:W:5:TYR:CD2	2.95	0.49
2:Z:-27:ARG:NH2	2:Z:-27:ARG:CG	2.68	0.49
2:C:382:ARG:NH2	2:C:385:ILE:HD13	2.27	0.49
2:G:345:ILE:HB	2:G:352:ALA:HB1	1.94	0.49
2:P:409:ILE:HG13	2:P:410:HIS:CD2	2.47	0.49
1:U:163:ILE:HG23	1:U:187:ALA:O	2.13	0.49
1:U:191:GLY:O	1:U:192:SER:O	2.30	0.49
1:U:231:GLN:OE1	1:U:231:GLN:O	2.30	0.49
1:Y:181:LEU:HD11	1:Y:185:VAL:CG2	2.42	0.49
1:1:144:ASP:OD2	1:1:146:SER:OG	2.30	0.49
2:2:382:ARG:HH21	2:2:385:ILE:HD13	1.78	0.49
1:A:217:ARG:NH2	1:A:223:ARG:HG2	2.28	0.49
1:O:129:HIS:HB2	1:O:132:GLU:CD	2.33	0.49
1:O:144:ASP:OD1	1:O:146:SER:OG	2.30	0.49
2:P:338:ASP:OD1	2:P:338:ASP:C	2.51	0.49
1:S:35:TYR:CZ	1:S:37:GLY:CA	2.84	0.49
1:U:28:LYS:NZ	1:U:52:LYS:HE3	2.28	0.49
1:Y:129:HIS:HB2	1:Y:132:GLU:CD	2.33	0.49
2:Z:338:ASP:OD1	2:Z:338:ASP:C	2.51	0.49
1:A:144:ASP:OD1	1:A:144:ASP:O	2.30	0.49
2:C:399:LEU:HD12	2:C:400:ALA:H	1.77	0.49
1:D:74:LEU:HD23	1:D:122:LEU:HD21	1.94	0.49
1:D:161:GLU:N	1:D:162:PRO:HD2	2.28	0.49
1:K:179:ASP:OD1	1:K:179:ASP:O	2.30	0.49
1:K:33:LEU:CD1	1:K:33:LEU:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:92:ARG:CG	1:K:92:ARG:NH1	2.74	0.49
1:Q:171:TYR:CD2	1:Q:172:ALA:C	2.86	0.49
1:D:89:TYR:CD1	2:R:374:LEU:HD11	2.48	0.49
1:W:15:GLU:OE2	1:Y:9:PRO:CG	2.61	0.49
1:W:224:ARG:HH11	1:W:224:ARG:HG2	1.78	0.49
2:C:382:ARG:HD2	1:I:89:TYR:HE1	1.76	0.49
1:D:98:GLN:O	1:D:102:VAL:HG23	2.13	0.49
2:G:320:SER:HB2	2:G:331:VAL:HG21	1.93	0.49
2:G:428:GLY:CA	2:X:350:ALA:CB	2.91	0.49
1:K:28:LYS:H	1:K:28:LYS:HE3	1.78	0.49
1:K:35:TYR:HE1	1:K:37:GLY:HA3	1.62	0.49
2:L:338:ASP:OD1	2:L:338:ASP:C	2.51	0.49
1:S:191:GLY:O	1:S:192:SER:O	2.31	0.49
2:G:426:ALA:HB2	2:X:-4:LEU:HD21	1.95	0.49
2:Z:-35:SER:HB3	2:Z:369:LEU:HD12	1.95	0.49
1:A:217:ARG:NH2	1:A:223:ARG:HE	2.11	0.48
2:E:-25:ALA:CB	2:E:-22:LEU:HD22	2.43	0.48
1:F:30:VAL:HG22	1:F:52:LYS:NZ	2.28	0.48
2:J:-31:ASP:OD1	2:J:-27:ARG:NE	2.45	0.48
2:J:382:ARG:NH2	2:J:385:ILE:HD13	2.28	0.48
1:K:11:GLN:O	1:K:15:GLU:HG3	2.13	0.48
1:K:225:ILE:HG21	1:K:233:LEU:HD11	1.96	0.48
1:M:74:LEU:HD23	1:M:122:LEU:HD21	1.94	0.48
2:R:330:ASP:OD2	2:Z:433:GLU:HG3	2.13	0.48
1:S:11:GLN:O	1:S:14:ARG:HG2	2.13	0.48
1:S:59:ARG:NH2	1:S:217:ARG:O	2.39	0.48
1:A:92:ARG:CG	1:A:92:ARG:NH1	2.71	0.48
2:H:407:TYR:CZ	2:H:417:ALA:HB3	2.25	0.48
1:I:144:ASP:OD1	1:I:146:SER:OG	2.30	0.48
2:L:375:THR:HG21	1:M:92:ARG:HB3	1.96	0.48
1:O:161:GLU:O	1:O:165:ASN:HB2	2.14	0.48
2:R:413:ASP:HB3	2:R:416:SER:OG	2.13	0.48
2:T:399:LEU:HD11	2:T:401:LEU:HD13	1.94	0.48
1:U:129:HIS:HB2	1:U:132:GLU:CD	2.34	0.48
1:A:130:TYR:CE1	1:A:216:ASN:O	2.66	0.48
1:A:141:ILE:N	1:A:141:ILE:HD12	2.28	0.48
2:H:338:ASP:C	2:H:338:ASP:OD1	2.51	0.48
1:I:217:ARG:NH2	1:I:223:ARG:HE	2.11	0.48
1:K:67:LYS:HG2	1:K:69:ASN:HD21	1.78	0.48
1:W:142:THR:OG1	1:W:144:ASP:HB3	2.13	0.48
1:I:28:LYS:CE	1:I:28:LYS:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:NH1	1:A:128:ALA:O	2.38	0.48
2:C:419:ARG:HG2	2:C:419:ARG:HH11	1.77	0.48
2:C:308:TYR:CZ	2:C:496:ILE:HD11	2.48	0.48
1:M:155:VAL:N	3:M:250:HOH:O	2.20	0.48
1:O:224:ARG:HG2	1:O:224:ARG:NH1	2.29	0.48
2:V:382:ARG:HH21	2:V:385:ILE:HD13	1.77	0.48
1:Y:67:LYS:HG2	1:Y:69:ASN:ND2	2.29	0.48
1:Y:74:LEU:HD23	1:Y:122:LEU:HD21	1.94	0.48
2:Z:433:GLU:OE1	2:Z:433:GLU:HA	2.13	0.48
2:2:-20:PRO:CB	2:2:354:GLU:OE1	2.60	0.48
1:D:150:GLU:CG	1:D:154:VAL:HG22	2.39	0.48
2:E:382:ARG:HH21	2:E:385:ILE:CD1	2.26	0.48
2:H:308:TYR:CE2	2:H:496:ILE:HD11	2.49	0.48
2:J:366:TYR:CE2	2:J:374:LEU:HD13	2.48	0.48
1:O:153:PHE:CD1	1:O:167:LEU:HD13	2.48	0.48
1:O:92:ARG:HB3	2:V:375:THR:HG21	1.94	0.48
1:Q:92:ARG:HH11	1:Q:92:ARG:HG3	1.77	0.48
2:R:-30:PHE:CZ	2:Z:-38:VAL:HG21	2.48	0.48
2:T:340:TYR:C	2:T:341:THR:HG23	2.33	0.48
1:U:8:SER:HA	1:U:9:PRO:HD2	1.61	0.48
1:Y:224:ARG:HG2	1:Y:224:ARG:HH11	1.78	0.48
1:D:229:ALA:O	1:D:233:LEU:CD1	2.30	0.48
1:K:224:ARG:HH11	1:K:224:ARG:HG2	1.78	0.48
1:K:8:SER:HB2	1:K:9:PRO:HD2	1.95	0.48
1:O:67:LYS:HG2	1:O:69:ASN:HD21	1.78	0.48
2:R:464:LEU:O	2:R:464:LEU:HG	2.13	0.48
1:S:155:VAL:HG21	1:S:167:LEU:HD12	1.96	0.48
1:U:176:SER:OG	1:U:179:ASP:OD1	2.30	0.48
2:N:448:SER:HB3	2:V:448:SER:HB3	1.96	0.48
2:X:366:TYR:CE2	2:X:374:LEU:HD13	2.49	0.48
2:2:461:ASP:OD1	2:2:509:ARG:NH2	2.41	0.48
1:F:22:LYS:HB2	1:F:22:LYS:HE3	1.74	0.48
2:G:-28:ARG:HG2	2:G:-21:LEU:CD2	2.43	0.48
2:G:362:GLU:HG2	2:G:382:ARG:HG2	1.96	0.48
2:H:301:ALA:HB2	2:H:333:LYS:NZ	2.28	0.48
2:T:-2:HIS:C	2:T:-2:HIS:ND1	2.66	0.48
2:V:308:TYR:CE2	2:V:311:GLY:HA3	2.49	0.48
2:X:409:ILE:HG13	2:X:410:HIS:CD2	2.49	0.48
1:Y:40:LEU:HA	1:Y:212:VAL:HG12	1.96	0.48
2:Z:478:ASP:OD1	2:Z:480:ALA:N	2.41	0.48
1:1:98:GLN:O	1:1:102:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:-23:GLU:HG3	2:N:-28:ARG:HD2	1.95	0.48
1:K:83:ASP:OD2	2:L:365:HIS:ND1	2.38	0.48
1:M:167:LEU:HD13	1:M:187:ALA:CB	2.42	0.48
1:D:16:ARG:NE	1:M:3:PHE:CE1	2.82	0.48
1:Q:173:GLU:HG2	1:Q:174:ASN:OD1	2.13	0.48
1:W:152:HIS:HB3	1:W:171:TYR:CZ	2.49	0.48
2:X:461:ASP:OD1	2:X:509:ARG:NH2	2.47	0.48
1:Y:33:LEU:HB3	1:Y:153:PHE:HB3	1.96	0.48
1:B:13:MET:HE1	1:B:111:PHE:HE2	1.79	0.48
1:B:67:LYS:HG2	1:B:69:ASN:HD21	1.78	0.48
1:B:8:SER:HA	1:B:9:PRO:HD2	1.74	0.48
2:C:409:ILE:CD1	2:C:410:HIS:CE1	2.95	0.48
2:E:319:ARG:HD2	2:E:326:ILE:HG12	1.95	0.48
1:I:74:LEU:HD23	1:I:122:LEU:HD21	1.96	0.48
2:J:-28:ARG:NH2	2:T:-23:GLU:CD	2.67	0.48
1:K:30:VAL:HG13	1:K:43:ALA:CB	2.27	0.48
1:D:19:LEU:CD1	1:K:9:PRO:HB3	2.44	0.48
1:Q:214:ASP:C	1:Q:214:ASP:OD1	2.52	0.48
1:U:33:LEU:HB3	1:U:153:PHE:HB3	1.96	0.48
1:W:13:MET:CE	1:W:111:PHE:HE2	2.27	0.48
2:X:486:LEU:N	2:X:486:LEU:CD1	2.77	0.48
1:A:155:VAL:N	3:A:249:HOH:O	2.22	0.48
2:H:301:ALA:HB2	2:H:333:LYS:HZ3	1.77	0.48
1:K:4:PRO:HB3	1:W:5:TYR:CE2	2.48	0.48
2:P:456:GLN:OE1	2:P:465:ARG:NH2	2.44	0.48
1:W:19:LEU:O	1:W:19:LEU:HD23	2.13	0.48
1:Y:56:LEU:HG	1:Y:62:PHE:HB2	1.95	0.48
1:A:123:CYS:HA	1:A:139:TYR:O	2.14	0.47
2:C:515:ARG:O	2:C:516:ALA:C	2.52	0.47
1:F:161:GLU:N	1:F:162:PRO:HD2	2.29	0.47
2:J:509:ARG:NH1	2:J:509:ARG:HG3	2.26	0.47
1:K:167:LEU:HG	1:K:187:ALA:CB	2.44	0.47
2:P:301:ALA:CB	2:P:333:LYS:HD3	2.44	0.47
2:T:301:ALA:O	2:T:440:GLY:HA3	2.14	0.47
1:U:178:THR:HG23	1:U:233:LEU:O	2.14	0.47
2:V:301:ALA:HB1	2:V:333:LYS:HZ2	1.79	0.47
2:Z:469:GLU:HG3	2:Z:517:ILE:HD13	1.95	0.47
1:A:13:MET:CE	1:O:116:LYS:HD2	2.43	0.47
1:K:144:ASP:OD2	1:K:146:SER:OG	2.30	0.47
1:Q:179:ASP:O	1:Q:183:ILE:HG13	2.14	0.47
1:Q:27:ALA:HB1	1:Q:28:LYS:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:308:TYR:CZ	2:R:496:ILE:HD11	2.49	0.47
1:U:203:LEU:HA	1:U:207:SER:OG	2.15	0.47
2:X:338:ASP:OD2	2:X:341:THR:N	2.47	0.47
2:N:399:LEU:HG	2:N:400:ALA:N	2.28	0.47
2:Z:353:VAL:HG13	2:Z:354:GLU:N	2.28	0.47
1:D:16:ARG:CD	1:M:3:PHE:HE1	2.27	0.47
1:F:29:SER:H	1:F:44:GLU:CG	2.28	0.47
1:K:14:ARG:HG3	1:K:14:ARG:HH11	1.79	0.47
1:S:35:TYR:N	1:S:38:GLY:O	2.46	0.47
2:T:375:THR:HG21	1:1:92:ARG:HB3	1.96	0.47
1:1:224:ARG:HG2	1:1:224:ARG:HH11	1.80	0.47
1:B:28:LYS:HZ1	1:B:52:LYS:HE3	1.78	0.47
2:H:301:ALA:CB	2:H:333:LYS:NZ	2.77	0.47
2:N:308:TYR:CE1	2:N:311:GLY:CA	2.87	0.47
2:P:413:ASP:HB3	2:P:416:SER:OG	2.14	0.47
2:R:517:ILE:O	2:R:521:ARG:HG2	2.14	0.47
1:U:224:ARG:NH1	1:U:224:ARG:HG2	2.30	0.47
1:W:173:GLU:HB3	1:W:174:ASN:HD21	1.76	0.47
2:C:-25:ALA:HB1	2:C:-22:LEU:HD22	1.95	0.47
1:D:59:ARG:NH1	1:D:128:ALA:O	2.35	0.47
2:E:421:VAL:HG22	2:E:431:ILE:HG12	1.96	0.47
2:J:312:VAL:HG12	2:J:497:ILE:HB	1.95	0.47
1:K:4:PRO:HG3	1:W:5:TYR:HB2	1.94	0.47
1:Q:7:ILE:CD1	1:Q:12:ALA:HA	2.45	0.47
2:E:-20:PRO:HA	2:R:388:ARG:NH1	2.29	0.47
2:R:407:TYR:C	2:R:407:TYR:HD2	2.18	0.47
2:T:461:ASP:OD1	2:T:509:ARG:NH2	2.47	0.47
2:G:388:ARG:HG3	2:X:-19:ALA:HB2	1.97	0.47
2:X:331:VAL:HG22	2:X:349:ALA:HB2	1.96	0.47
1:B:67:LYS:HG2	1:B:69:ASN:ND2	2.30	0.47
1:D:16:ARG:HH11	1:D:117:PRO:HD3	1.80	0.47
1:F:67:LYS:HG2	1:F:69:ASN:HD21	1.80	0.47
2:H:515:ARG:O	2:H:516:ALA:C	2.53	0.47
2:J:-18:SER:O	2:J:398:LEU:CD1	2.63	0.47
1:K:142:THR:HG1	1:K:144:ASP:HB3	1.76	0.47
2:R:351:VAL:HG12	2:R:400:ALA:HB2	1.96	0.47
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.96	0.47
2:T:-4:LEU:N	2:T:-4:LEU:HD12	2.30	0.47
1:U:179:ASP:N	1:U:179:ASP:OD1	2.48	0.47
1:D:141:ILE:N	1:D:141:ILE:HD12	2.30	0.47
1:F:7:ILE:HD12	1:F:11:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:ARG:HB2	1:I:26:ARG:NH1	2.29	0.47
1:I:5:TYR:N	1:U:5:TYR:HH	2.12	0.47
2:J:407:TYR:CE1	2:J:417:ALA:HB3	2.49	0.47
1:M:154:VAL:CA	3:M:250:HOH:O	2.57	0.47
2:L:-38:VAL:HG23	2:N:-30:PHE:CZ	2.49	0.47
2:P:-27:ARG:C	2:P:-26:GLN:OE1	2.53	0.47
2:G:478:ASP:OD1	2:V:324:ASN:HB3	2.15	0.47
1:Y:19:LEU:O	1:Y:19:LEU:HD23	2.15	0.47
1:Y:92:ARG:CG	1:Y:92:ARG:NH1	2.75	0.47
2:Z:320:SER:HB2	2:Z:331:VAL:HG21	1.96	0.47
2:V:-26:GLN:NE2	2:2:-38:VAL:N	2.63	0.47
2:J:320:SER:HB2	2:J:331:VAL:HG21	1.96	0.47
2:L:320:SER:HB2	2:L:331:VAL:HG21	1.97	0.47
2:N:-17:ILE:O	2:N:396:GLN:OE1	2.33	0.47
2:N:301:ALA:HB1	2:N:333:LYS:HD3	1.95	0.47
1:Q:98:GLN:O	1:Q:102:VAL:HG23	2.15	0.47
1:S:28:LYS:N	1:S:28:LYS:HE3	2.30	0.47
1:U:33:LEU:HD12	1:U:40:LEU:HB3	1.95	0.47
1:U:67:LYS:HG2	1:U:69:ASN:HD21	1.80	0.47
1:I:181:LEU:O	1:I:185:VAL:HG23	2.14	0.47
1:B:5:TYR:HE2	1:O:11:GLN:NE2	2.01	0.47
1:D:167:LEU:HA	1:D:167:LEU:HD12	1.61	0.47
1:F:204:GLY:O	1:F:207:SER:OG	2.30	0.47
2:H:-29:LEU:O	2:H:-25:ALA:N	2.46	0.47
2:L:-29:LEU:HD23	2:L:-21:LEU:CD1	2.44	0.47
2:L:432:GLU:CD	2:L:437:GLN:HE21	2.18	0.47
2:L:448:SER:HB3	2:P:448:SER:HB3	1.97	0.47
1:F:92:ARG:HB3	2:N:375:THR:HG21	1.96	0.47
2:P:457:VAL:HG13	2:P:463:GLY:CA	2.45	0.47
1:Q:172:ALA:HB2	1:Q:183:ILE:HD11	1.97	0.47
2:H:513:LEU:HA	2:H:513:LEU:HD12	1.74	0.47
1:K:11:GLN:HA	1:K:14:ARG:HB2	1.97	0.47
2:P:-23:GLU:OE1	2:V:-28:ARG:NH2	2.47	0.47
1:W:92:ARG:HG3	1:W:92:ARG:HH11	1.79	0.47
1:A:45:ASN:HB2	1:A:209:GLU:HB2	1.97	0.46
2:E:366:TYR:CE2	2:E:374:LEU:HD13	2.50	0.46
2:G:522:SER:HB3	2:V:487:VAL:HA	1.97	0.46
1:I:224:ARG:NH1	1:I:224:ARG:HG2	2.30	0.46
1:K:67:LYS:HG2	1:K:69:ASN:ND2	2.30	0.46
1:M:83:ASP:OD2	2:N:365:HIS:ND1	2.40	0.46
1:O:33:LEU:HD12	1:O:33:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:28:LYS:N	1:Q:28:LYS:HE3	2.30	0.46
2:R:351:VAL:CG1	2:R:400:ALA:HB2	2.44	0.46
2:Z:376:PHE:CE2	2:Z:380:ILE:HD11	2.50	0.46
1:A:33:LEU:HD12	1:A:40:LEU:HB3	1.94	0.46
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.80	0.46
2:C:-30:PHE:HZ	2:H:-38:VAL:HG21	1.80	0.46
1:M:92:ARG:CG	1:M:92:ARG:NH1	2.74	0.46
2:N:350:ALA:O	2:N:353:VAL:HG12	2.16	0.46
2:V:515:ARG:HG2	2:V:515:ARG:HH11	1.80	0.46
2:X:353:VAL:HG13	2:X:354:GLU:N	2.30	0.46
2:X:486:LEU:HD12	2:X:486:LEU:N	2.31	0.46
1:Y:17:SER:HG	1:Y:143:TYR:HH	1.63	0.46
1:A:181:LEU:HD23	1:A:233:LEU:HB3	1.96	0.46
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.97	0.46
2:J:388:ARG:O	2:J:388:ARG:HG2	2.14	0.46
1:Q:161:GLU:N	1:Q:162:PRO:HD2	2.30	0.46
2:X:496:ILE:CG2	2:X:503:VAL:HG22	2.46	0.46
1:A:7:ILE:HD13	1:A:15:GLU:CD	2.35	0.46
1:B:28:LYS:H	1:B:28:LYS:CE	2.28	0.46
2:C:343:THR:HG22	2:C:404:LEU:HD12	1.97	0.46
2:H:332:ARG:HH11	2:H:332:ARG:CB	2.28	0.46
2:J:391:LEU:O	2:J:395:MET:HG2	2.16	0.46
2:L:423:PHE:CE1	2:L:429:TRP:HB3	2.50	0.46
1:O:32:ALA:HA	1:O:40:LEU:O	2.15	0.46
1:Q:167:LEU:O	1:Q:171:TYR:N	2.48	0.46
2:R:319:ARG:CG	2:R:320:SER:N	2.78	0.46
1:S:67:LYS:HG2	1:S:69:ASN:HD21	1.80	0.46
2:V:413:ASP:OD1	2:V:416:SER:OG	2.30	0.46
1:Y:217:ARG:HD2	1:Y:218:PRO:HD2	1.97	0.46
1:Y:217:ARG:CD	1:Y:218:PRO:HD2	2.45	0.46
1:I:10:GLU:CA	1:I:10:GLU:OE1	2.63	0.46
1:I:161:GLU:N	1:I:162:PRO:CD	2.79	0.46
2:E:432:GLU:OE2	2:E:437:GLN:NE2	2.48	0.46
2:H:301:ALA:CB	2:H:333:LYS:HD3	2.45	0.46
2:J:301:ALA:CB	2:J:333:LYS:HD3	2.45	0.46
2:L:382:ARG:HD2	1:M:89:TYR:CE1	2.51	0.46
1:D:13:MET:HE1	1:Q:116:LYS:HD2	1.97	0.46
1:Q:29:SER:H	1:Q:44:GLU:CG	2.28	0.46
1:S:74:LEU:HD23	1:S:122:LEU:HD21	1.97	0.46
1:U:208:LEU:HA	1:U:208:LEU:HD12	1.35	0.46
2:V:-26:GLN:HE22	2:2:-38:VAL:N	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:162:PRO:HB2	1:W:190:ALA:O	2.16	0.46
1:W:179:ASP:O	1:W:183:ILE:HG13	2.15	0.46
1:A:45:ASN:OD1	1:A:209:GLU:OE1	2.34	0.46
1:F:8:SER:O	1:F:11:GLN:CB	2.64	0.46
1:I:26:ARG:CG	1:I:26:ARG:O	2.64	0.46
1:I:30:VAL:HG22	1:I:52:LYS:NZ	2.31	0.46
1:I:67:LYS:HG2	1:I:69:ASN:HD21	1.81	0.46
1:K:229:ALA:O	1:K:233:LEU:HG	2.16	0.46
1:M:144:ASP:OD1	1:M:146:SER:OG	2.30	0.46
2:P:-29:LEU:HD23	2:P:-29:LEU:HA	1.71	0.46
1:Q:114:GLN:HE21	1:Q:114:GLN:CA	2.25	0.46
1:S:123:CYS:HA	1:S:139:TYR:O	2.16	0.46
1:W:29:SER:H	1:W:44:GLU:CG	2.28	0.46
1:F:7:ILE:CG2	1:W:8:SER:HB3	2.46	0.46
2:X:423:PHE:CE1	2:X:429:TRP:HB3	2.51	0.46
2:Z:366:TYR:CE2	2:Z:374:LEU:HD13	2.50	0.46
1:1:28:LYS:N	1:1:28:LYS:HE3	2.30	0.46
1:A:9:PRO:CD	1:O:15:GLU:HB3	2.46	0.46
1:Q:19:LEU:HD23	1:Q:19:LEU:C	2.36	0.46
2:T:350:ALA:O	2:T:353:VAL:HG12	2.16	0.46
2:V:-32:THR:O	2:V:-28:ARG:HG3	2.15	0.46
2:V:486:LEU:N	2:V:486:LEU:CD1	2.79	0.46
2:2:320:SER:HB2	2:2:331:VAL:HG21	1.97	0.46
2:C:409:ILE:HG13	2:C:410:HIS:N	2.31	0.46
1:D:28:LYS:N	1:D:28:LYS:HE3	2.31	0.46
2:E:310:GLY:N	2:E:415:GLN:HA	2.30	0.46
1:F:203:LEU:N	1:F:234:LEU:CD1	2.74	0.46
2:J:-25:ALA:N	2:J:-24:PRO:HD3	2.31	0.46
1:M:26:ARG:HE	1:M:26:ARG:HB2	1.50	0.46
1:M:67:LYS:HG2	1:M:69:ASN:HD21	1.81	0.46
1:O:163:ILE:O	1:O:167:LEU:CG	2.43	0.46
1:O:230:LEU:HD12	1:O:230:LEU:O	2.15	0.46
1:Y:217:ARG:HD3	1:Y:218:PRO:HD3	1.97	0.46
2:2:308:TYR:CE2	2:2:496:ILE:HD11	2.51	0.46
1:B:231:GLN:NE2	1:B:231:GLN:O	2.48	0.46
2:H:-27:ARG:CZ	2:H:-26:GLN:NE2	2.79	0.46
2:H:320:SER:HB2	2:H:331:VAL:HG21	1.98	0.46
2:H:407:TYR:CZ	2:H:417:ALA:HB1	2.46	0.46
1:K:205:VAL:HG22	1:K:230:LEU:HG	1.97	0.46
2:L:332:ARG:CB	2:L:332:ARG:HH11	2.29	0.46
1:M:29:SER:OG	1:M:157:GLY:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:SER:HB3	3:O:249:HOH:O	2.16	0.46
1:Q:176:SER:OG	1:Q:179:ASP:CG	2.54	0.46
2:R:-3:PRO:O	2:R:348:THR:HA	2.16	0.46
2:X:338:ASP:OD2	2:X:341:THR:HG23	2.16	0.46
2:2:-29:LEU:CD2	2:2:-22:LEU:HD12	2.45	0.46
1:A:7:ILE:CD1	1:A:11:GLN:HG3	2.28	0.46
2:C:-17:ILE:O	2:C:-17:ILE:HG23	2.16	0.46
2:C:509:ARG:HG3	2:C:509:ARG:HH11	1.79	0.46
2:P:-25:ALA:N	2:P:-24:PRO:HD3	2.31	0.46
1:S:15:GLU:OE2	1:1:9:PRO:CG	2.63	0.46
2:X:-36:LEU:O	2:X:-35:SER:CB	2.64	0.46
2:V:330:ASP:OD2	2:2:433:GLU:HG3	2.16	0.45
2:C:320:SER:HB2	2:C:331:VAL:HG21	1.98	0.45
1:K:27:ALA:HB1	1:K:28:LYS:CE	2.46	0.45
2:P:351:VAL:HG11	2:P:400:ALA:HB2	1.98	0.45
1:S:142:THR:OG1	1:S:146:SER:HB2	2.16	0.45
1:S:33:LEU:HD11	1:S:40:LEU:HB3	1.97	0.45
2:V:414:PRO:HA	2:V:417:ALA:HB2	1.97	0.45
1:W:74:LEU:HD23	1:W:122:LEU:HD21	1.98	0.45
1:W:205:VAL:CG2	1:W:231:GLN:HA	2.41	0.45
2:Z:-29:LEU:O	2:Z:-28:ARG:C	2.54	0.45
2:Z:496:ILE:HG13	2:Z:505:VAL:HG22	1.97	0.45
1:1:8:SER:O	1:1:11:GLN:CG	2.64	0.45
2:C:479:SER:HB2	2:E:479:SER:HB2	1.98	0.45
1:F:11:GLN:CA	1:F:11:GLN:OE1	2.59	0.45
1:F:92:ARG:NH1	1:F:92:ARG:CG	2.76	0.45
1:F:9:PRO:HA	1:W:6:PHE:CE1	2.50	0.45
2:J:-23:GLU:HG3	2:J:-22:LEU:HD12	1.97	0.45
2:N:301:ALA:HB1	2:N:333:LYS:CD	2.46	0.45
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.97	0.45
2:R:302:THR:OG1	2:R:481:THR:OG1	2.28	0.45
1:W:114:GLN:HE21	1:W:114:GLN:HA	1.82	0.45
1:W:208:LEU:HA	1:W:208:LEU:HD12	1.71	0.45
1:Y:161:GLU:N	1:Y:162:PRO:HD2	2.31	0.45
1:A:130:TYR:HB2	1:A:218:PRO:HA	1.97	0.45
1:B:89:TYR:CD1	2:H:374:LEU:HD11	2.50	0.45
2:H:478:ASP:OD1	2:L:324:ASN:HB3	2.15	0.45
2:H:479:SER:HB2	2:L:479:SER:HB2	1.98	0.45
2:H:506:PRO:HG2	2:H:509:ARG:HB2	1.97	0.45
1:I:28:LYS:HB3	1:I:44:GLU:HG3	1.98	0.45
2:J:423:PHE:CE1	2:J:429:TRP:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:301:ALA:HB2	2:L:333:LYS:CE	2.46	0.45
2:R:407:TYR:CE2	2:R:417:ALA:HB1	2.51	0.45
1:W:205:VAL:O	1:W:205:VAL:HG12	2.15	0.45
2:Z:348:THR:HG21	2:Z:351:VAL:HG23	1.97	0.45
2:Z:423:PHE:CE1	2:Z:429:TRP:HB3	2.52	0.45
2:2:312:VAL:HG12	2:2:497:ILE:HB	1.98	0.45
1:D:173:GLU:CB	1:D:174:ASN:OD1	2.63	0.45
2:G:350:ALA:O	2:G:353:VAL:HG13	2.16	0.45
1:Q:152:HIS:CB	1:Q:171:TYR:HE1	2.08	0.45
1:Q:208:LEU:HD12	1:Q:208:LEU:HA	1.77	0.45
1:Q:7:ILE:HB	1:Q:11:GLN:OE1	2.15	0.45
1:S:92:ARG:CG	1:S:92:ARG:NH1	2.74	0.45
2:T:351:VAL:HG12	2:T:400:ALA:HB2	1.97	0.45
1:1:13:MET:HA	1:1:13:MET:HE2	1.98	0.45
1:1:152:HIS:CB	1:1:171:TYR:CE2	2.98	0.45
1:B:98:GLN:HG2	2:H:370:GLU:OE1	2.16	0.45
2:E:351:VAL:HG11	2:E:400:ALA:HB2	1.98	0.45
2:E:358:LEU:HD23	2:E:386:MET:HE3	1.98	0.45
1:I:213:LEU:HD23	1:I:213:LEU:HA	1.84	0.45
1:M:163:ILE:HG23	1:M:187:ALA:O	2.17	0.45
2:P:366:TYR:CE2	2:P:374:LEU:HD13	2.51	0.45
1:Q:175:ALA:HB1	1:Q:179:ASP:HB2	1.98	0.45
1:U:231:GLN:NE2	1:U:235:VAL:CG2	2.75	0.45
1:K:4:PRO:CB	1:W:5:TYR:CZ	3.00	0.45
1:D:5:TYR:OH	1:Y:7:ILE:O	2.22	0.45
2:H:-21:LEU:HA	2:H:-20:PRO:HD3	1.82	0.45
1:K:208:LEU:HA	1:K:208:LEU:HD12	1.30	0.45
2:L:-17:ILE:HA	2:L:396:GLN:OE1	2.16	0.45
2:N:423:PHE:CE1	2:N:429:TRP:HB3	2.51	0.45
1:Q:172:ALA:HB1	1:Q:175:ALA:HB2	1.99	0.45
2:V:332:ARG:CB	2:V:332:ARG:HH11	2.29	0.45
2:2:-36:LEU:O	2:2:-35:SER:HB2	2.16	0.45
1:B:207:SER:O	1:B:208:LEU:HD12	2.16	0.45
1:A:6:PHE:CB	1:B:5:TYR:HB2	2.40	0.45
2:C:419:ARG:HG2	2:C:419:ARG:NH1	2.32	0.45
1:I:216:ASN:OD1	1:I:216:ASN:C	2.55	0.45
1:K:22:LYS:O	1:K:25:ALA:HB3	2.16	0.45
2:P:401:LEU:HA	2:P:401:LEU:HD12	1.75	0.45
1:Q:130:TYR:CD1	1:Q:218:PRO:HA	2.52	0.45
1:S:130:TYR:HE1	1:S:216:ASN:O	1.99	0.45
1:U:203:LEU:HA	1:U:203:LEU:HD12	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:208:LEU:N	1:U:208:LEU:HD13	2.30	0.45
2:V:509:ARG:CZ	2:V:513:LEU:HD21	2.47	0.45
1:B:187:ALA:O	1:B:191:GLY:N	2.47	0.45
2:G:-4:LEU:N	2:G:-4:LEU:HD22	2.32	0.45
1:I:130:TYR:CD1	1:I:216:ASN:O	2.70	0.45
1:I:161:GLU:N	1:I:162:PRO:HD2	2.32	0.45
1:K:161:GLU:N	1:K:162:PRO:HD2	2.32	0.45
1:K:163:ILE:CD1	1:K:191:GLY:HA3	2.47	0.45
1:M:7:ILE:HG22	1:M:8:SER:N	2.31	0.45
1:O:30:VAL:HG22	1:O:52:LYS:NZ	2.31	0.45
2:P:345:ILE:HB	2:P:352:ALA:HB1	1.99	0.45
1:Q:234:LEU:HD13	1:Q:234:LEU:H	1.79	0.45
2:R:308:TYR:CD1	2:R:460:GLY:N	2.85	0.45
2:C:349:ALA:O	2:C:350:ALA:C	2.54	0.45
1:S:29:SER:H	1:S:44:GLU:CG	2.29	0.45
1:U:40:LEU:HD12	1:U:212:VAL:HG12	1.98	0.45
2:X:-29:LEU:HD23	2:X:-29:LEU:HA	1.77	0.45
2:2:388:ARG:HG3	2:2:426:ALA:O	2.17	0.45
1:B:130:TYR:CE1	1:B:216:ASN:O	2.70	0.45
1:B:181:LEU:HD22	1:B:233:LEU:HD13	1.98	0.45
1:B:234:LEU:C	1:B:235:VAL:HG23	2.29	0.45
2:C:-25:ALA:N	2:C:-24:PRO:HD3	2.32	0.45
2:C:476:ASP:OD1	2:E:488:ARG:NH2	2.50	0.45
1:D:207:SER:C	1:D:208:LEU:HD13	2.31	0.45
1:F:142:THR:OG1	1:F:144:ASP:HB3	2.16	0.45
2:G:-32:THR:O	2:G:-28:ARG:HG3	2.17	0.45
2:R:366:TYR:CE2	2:R:374:LEU:HD13	2.51	0.45
2:2:332:ARG:CB	2:2:332:ARG:HH11	2.30	0.44
1:A:115:ALA:HB3	1:B:112:THR:CG2	2.48	0.44
1:F:231:GLN:O	1:F:235:VAL:HG23	2.18	0.44
1:I:144:ASP:OD2	1:I:144:ASP:O	2.35	0.44
1:K:74:LEU:HD23	1:K:122:LEU:HD21	1.99	0.44
2:L:407:TYR:CD1	2:L:417:ALA:HB3	2.40	0.44
2:N:338:ASP:C	2:N:338:ASP:OD1	2.56	0.44
2:R:-2:HIS:C	2:R:-2:HIS:CD2	2.91	0.44
2:T:351:VAL:CG1	2:T:400:ALA:HB2	2.47	0.44
1:U:188:LEU:C	1:U:188:LEU:CD2	2.85	0.44
2:Z:331:VAL:HG13	2:Z:349:ALA:HA	1.99	0.44
1:A:130:TYR:HE1	1:A:216:ASN:O	2.00	0.44
1:A:167:LEU:HD13	1:A:187:ALA:HB2	1.99	0.44
2:N:472:TYR:HD2	2:N:521:ARG:NH1	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:408:ASP:HB3	2:P:411:ALA:HB2	1.99	0.44
1:Q:33:LEU:HD11	1:Q:180:ALA:HB1	1.99	0.44
2:E:-30:PHE:CZ	2:R:-38:VAL:CG2	2.99	0.44
1:S:30:VAL:HG22	1:S:52:LYS:HZ3	1.83	0.44
2:J:388:ARG:NH2	2:T:354:GLU:OE2	2.50	0.44
1:A:219:ARG:NH2	1:A:220:ARG:HD2	2.32	0.44
1:B:40:LEU:HD13	1:B:212:VAL:HG11	1.98	0.44
2:C:-29:LEU:HD22	2:C:-25:ALA:HB3	1.99	0.44
2:C:513:LEU:HA	2:C:513:LEU:HD12	1.82	0.44
1:K:232:ALA:HA	1:K:235:VAL:HG23	2.00	0.44
1:Q:211:ALA:O	1:Q:212:VAL:CG1	2.65	0.44
1:S:165:ASN:O	1:S:166:ALA:C	2.53	0.44
2:T:302:THR:OG1	2:T:481:THR:OG1	2.29	0.44
1:U:230:LEU:CD1	1:U:234:LEU:HD11	2.48	0.44
2:Z:388:ARG:HG3	2:Z:426:ALA:O	2.18	0.44
1:I:150:GLU:CG	1:I:154:VAL:HG22	2.45	0.44
1:B:11:GLN:HG3	1:B:14:ARG:NH1	2.32	0.44
2:C:398:LEU:HD12	2:C:398:LEU:HA	1.63	0.44
1:F:18:GLU:OE1	1:F:21:ARG:NE	2.38	0.44
2:H:399:LEU:HD11	2:H:401:LEU:HD13	1.99	0.44
1:I:32:ALA:O	1:I:153:PHE:HA	2.18	0.44
1:M:7:ILE:O	1:M:9:PRO:HD3	2.18	0.44
2:P:-27:ARG:CZ	2:P:-26:GLN:HE21	2.22	0.44
2:P:388:ARG:O	2:P:388:ARG:HG2	2.17	0.44
1:Q:205:VAL:O	1:Q:205:VAL:CG1	2.66	0.44
1:Q:30:VAL:HG22	1:Q:52:LYS:NZ	2.31	0.44
2:Z:418:GLY:O	2:Z:419:ARG:NH1	2.50	0.44
1:I:28:LYS:HZ2	1:I:52:LYS:HE3	1.80	0.44
1:A:19:LEU:O	1:A:19:LEU:HD23	2.18	0.44
2:G:390:ASN:O	2:G:390:ASN:CG	2.56	0.44
2:N:486:LEU:N	2:N:486:LEU:CD1	2.81	0.44
1:O:67:LYS:HG2	1:O:69:ASN:ND2	2.31	0.44
2:P:416:SER:O	2:P:419:ARG:NH1	2.30	0.44
1:Q:92:ARG:CG	1:Q:92:ARG:NH1	2.80	0.44
1:U:231:GLN:NE2	1:U:235:VAL:HG21	2.19	0.44
1:U:67:LYS:HG2	1:U:69:ASN:ND2	2.32	0.44
2:V:310:GLY:H	2:V:415:GLN:HA	1.83	0.44
1:W:161:GLU:N	1:W:162:PRO:HD2	2.32	0.44
1:W:33:LEU:CD1	1:W:33:LEU:C	2.84	0.44
1:W:35:TYR:CE1	1:W:37:GLY:N	2.85	0.44
1:Y:22:LYS:HB3	1:Y:26:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:35:TYR:OH	1:Y:37:GLY:HA3	2.14	0.44
1:B:98:GLN:O	1:B:102:VAL:HG23	2.18	0.44
2:C:399:LEU:HD12	2:C:400:ALA:N	2.32	0.44
2:E:428:GLY:HA3	2:L:350:ALA:HB2	1.99	0.44
1:I:152:HIS:HB3	1:I:171:TYR:CE2	2.52	0.44
1:K:232:ALA:HA	1:K:235:VAL:CG2	2.47	0.44
1:M:59:ARG:NH2	1:M:217:ARG:O	2.46	0.44
1:M:29:SER:H	1:M:44:GLU:CG	2.31	0.44
2:N:-20:PRO:CD	2:N:-19:ALA:H	2.30	0.44
2:C:-29:LEU:O	2:C:-25:ALA:C	2.56	0.44
2:C:308:TYR:CE1	2:C:311:GLY:HA3	2.52	0.44
2:C:382:ARG:HH21	2:C:385:ILE:HD13	1.83	0.44
1:F:28:LYS:HB3	1:F:44:GLU:HG3	1.99	0.44
2:N:320:SER:HB2	2:N:331:VAL:HG21	1.99	0.44
1:U:203:LEU:C	1:U:207:SER:OG	2.56	0.44
2:X:-32:THR:HG23	2:X:-31:ASP:N	2.33	0.44
1:B:30:VAL:HG22	1:B:52:LYS:NZ	2.32	0.44
2:E:486:LEU:N	2:E:486:LEU:CD1	2.80	0.44
2:G:332:ARG:HH11	2:G:332:ARG:CB	2.26	0.44
2:G:374:LEU:HD11	1:W:89:TYR:CD1	2.53	0.44
2:J:-19:ALA:O	2:J:-17:ILE:HG22	2.18	0.44
1:K:152:HIS:HB3	1:K:171:TYR:CZ	2.48	0.44
1:O:11:GLN:HA	1:O:14:ARG:NE	2.32	0.44
2:P:308:TYR:CZ	2:P:496:ILE:HD11	2.53	0.44
2:P:423:PHE:CE1	2:P:429:TRP:HB3	2.53	0.44
2:P:465:ARG:HG3	2:P:513:LEU:CD1	2.45	0.44
1:Q:141:ILE:HD12	1:Q:141:ILE:N	2.33	0.44
1:S:116:LYS:HG2	1:S:116:LYS:HZ2	1.68	0.44
2:T:434:GLU:OE2	2:2:329:ARG:HD2	2.18	0.44
1:U:10:GLU:CG	1:U:14:ARG:NH2	2.81	0.44
1:U:19:LEU:HD23	1:U:19:LEU:C	2.38	0.44
2:V:432:GLU:HG3	2:V:437:GLN:HB2	1.98	0.44
2:X:498:ASP:OD1	2:X:500:ASP:HB2	2.18	0.44
1:Y:167:LEU:HA	1:Y:167:LEU:HD12	1.86	0.44
1:1:33:LEU:H	1:1:33:LEU:HD12	1.83	0.44
2:2:486:LEU:CD1	2:2:486:LEU:N	2.81	0.44
1:A:217:ARG:NH2	1:A:223:ARG:NE	2.65	0.44
1:A:67:LYS:HG2	1:A:69:ASN:ND2	2.33	0.44
2:E:-30:PHE:C	2:E:-30:PHE:CD2	2.91	0.44
2:E:350:ALA:HB2	2:R:428:GLY:HA3	2.00	0.44
2:H:308:TYR:C	2:H:308:TYR:CD1	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:ILE:HG23	1:I:187:ALA:O	2.18	0.44
1:I:217:ARG:NH1	1:I:223:ARG:HG2	2.33	0.44
1:M:116:LYS:NZ	1:M:119:GLU:OE2	2.49	0.44
1:O:161:GLU:N	1:O:162:PRO:HD2	2.33	0.44
1:Q:74:LEU:HD23	1:Q:122:LEU:HD21	2.00	0.44
2:R:350:ALA:O	2:R:353:VAL:HG12	2.18	0.44
1:U:161:GLU:N	1:U:162:PRO:HD2	2.33	0.44
2:G:487:VAL:HG13	2:V:522:SER:HB3	1.99	0.44
1:M:7:ILE:HD13	1:W:5:TYR:HB2	1.97	0.44
2:X:312:VAL:HG12	2:X:497:ILE:HB	1.99	0.44
2:C:388:ARG:O	2:C:388:ARG:HG2	2.18	0.43
2:C:486:LEU:CD1	2:C:486:LEU:N	2.81	0.43
1:D:161:GLU:N	1:D:161:GLU:CD	2.70	0.43
1:D:161:GLU:O	1:D:165:ASN:ND2	2.51	0.43
1:D:92:ARG:CG	1:D:92:ARG:NH1	2.78	0.43
2:H:456:GLN:NE2	2:H:465:ARG:NH2	2.32	0.43
1:K:217:ARG:HD3	1:K:217:ARG:HA	1.73	0.43
1:O:150:GLU:CG	1:O:154:VAL:HG22	2.40	0.43
1:Q:130:TYR:CE1	1:Q:216:ASN:O	2.71	0.43
2:Z:348:THR:OG1	2:Z:351:VAL:HG21	2.17	0.43
1:I:92:ARG:NH1	1:I:92:ARG:CG	2.79	0.43
1:A:234:LEU:O	1:A:235:VAL:HG22	2.18	0.43
2:C:332:ARG:HB2	2:C:332:ARG:NH1	2.34	0.43
1:F:32:ALA:O	1:F:153:PHE:HA	2.17	0.43
1:I:92:ARG:CG	1:I:92:ARG:NH1	2.76	0.43
2:L:301:ALA:CB	2:L:333:LYS:CD	2.96	0.43
1:O:176:SER:OG	1:O:179:ASP:OD2	2.30	0.43
2:P:332:ARG:CB	2:P:332:ARG:HH11	2.27	0.43
1:Q:171:TYR:HE2	1:Q:173:GLU:CA	2.31	0.43
1:Q:29:SER:N	1:Q:44:GLU:OE1	2.49	0.43
1:S:152:HIS:CD2	1:S:171:TYR:HE2	2.35	0.43
2:V:301:ALA:O	2:V:440:GLY:HA3	2.18	0.43
1:Y:33:LEU:HD12	1:Y:40:LEU:HB3	2.00	0.43
1:I:33:LEU:O	1:I:33:LEU:CD1	2.66	0.43
2:2:-4:LEU:O	2:2:-2:HIS:HD2	2.01	0.43
1:A:167:LEU:HD13	1:A:187:ALA:CB	2.48	0.43
1:B:152:HIS:CB	1:B:171:TYR:CE2	2.98	0.43
1:D:67:LYS:HG2	1:D:69:ASN:HD21	1.84	0.43
2:H:401:LEU:HA	2:H:401:LEU:HD12	1.83	0.43
2:J:-22:LEU:HD12	2:J:-22:LEU:N	2.33	0.43
2:E:375:THR:HG21	1:K:92:ARG:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:472:TYR:HD2	2:N:521:ARG:HH12	1.66	0.43
1:Q:8:SER:HB2	1:Q:9:PRO:HD2	2.00	0.43
1:U:205:VAL:HG22	1:U:230:LEU:HG	2.01	0.43
2:V:345:ILE:HB	2:V:352:ALA:HB1	1.99	0.43
2:V:486:LEU:N	2:V:486:LEU:HD12	2.33	0.43
2:G:426:ALA:HB2	2:X:-4:LEU:CD2	2.47	0.43
2:T:-38:VAL:CG2	2:2:-30:PHE:HZ	2.31	0.43
2:C:401:LEU:HA	2:C:401:LEU:HD12	1.84	0.43
1:D:50:LEU:HD13	1:K:147:ILE:CG2	2.49	0.43
1:F:67:LYS:HG2	1:F:69:ASN:ND2	2.32	0.43
2:G:351:VAL:CG1	2:G:400:ALA:HB2	2.48	0.43
1:S:14:ARG:HG3	1:S:15:GLU:N	2.33	0.43
1:S:30:VAL:HG22	1:S:52:LYS:NZ	2.32	0.43
2:V:301:ALA:HB1	2:V:333:LYS:HD3	1.98	0.43
2:Z:-23:GLU:HG3	2:Z:-23:GLU:O	2.17	0.43
2:Z:-35:SER:HB3	2:Z:369:LEU:CD1	2.48	0.43
2:Z:432:GLU:HA	2:Z:432:GLU:OE1	2.17	0.43
2:2:351:VAL:HG21	2:2:398:LEU:HB3	2.00	0.43
2:2:457:VAL:HG22	2:2:463:GLY:HA2	2.00	0.43
2:2:318:ARG:HD3	2:2:493:THR:HG23	2.00	0.43
2:E:401:LEU:HA	2:E:401:LEU:HD12	1.76	0.43
2:H:-21:LEU:HD12	2:H:-21:LEU:HA	1.71	0.43
1:M:129:HIS:HB2	1:M:132:GLU:CD	2.39	0.43
1:M:30:VAL:HG22	1:M:52:LYS:NZ	2.34	0.43
1:Q:172:ALA:CB	1:Q:175:ALA:HB2	2.48	0.43
1:Q:19:LEU:O	1:Q:19:LEU:HD23	2.17	0.43
1:S:116:LYS:HG2	1:S:117:PRO:O	2.19	0.43
1:S:8:SER:HB3	1:S:11:GLN:CG	2.48	0.43
1:D:40:LEU:CD1	1:D:212:VAL:HG13	2.47	0.43
2:G:-21:LEU:HD12	2:G:-21:LEU:HA	1.85	0.43
1:M:161:GLU:CB	1:M:162:PRO:CD	2.97	0.43
2:R:496:ILE:HG23	2:R:503:VAL:HG22	2.00	0.43
1:S:33:LEU:HB3	1:S:153:PHE:HB3	2.01	0.43
1:I:7:ILE:HG12	1:S:6:PHE:O	2.19	0.43
2:T:-4:LEU:CD1	2:T:-4:LEU:N	2.82	0.43
1:W:98:GLN:O	1:W:102:VAL:HG23	2.19	0.43
2:2:338:ASP:OD1	2:2:338:ASP:C	2.57	0.43
2:2:-5:GLN:HB2	2:2:-5:GLN:HE21	1.66	0.43
1:A:234:LEU:C	1:A:235:VAL:HG23	2.38	0.43
1:A:234:LEU:C	1:A:235:VAL:CG2	2.86	0.43
2:C:366:TYR:CD2	2:C:374:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:473:ASP:OD2	2:R:452:LYS:NZ	2.35	0.43
1:D:234:LEU:N	1:D:234:LEU:CD1	2.81	0.43
2:E:320:SER:HB2	2:E:331:VAL:HG21	2.00	0.43
2:G:301:ALA:CB	2:G:333:LYS:HZ2	2.31	0.43
2:J:301:ALA:HB2	2:J:333:LYS:CE	2.49	0.43
2:P:-26:GLN:C	2:P:-24:PRO:HD3	2.39	0.43
1:D:11:GLN:NE2	1:Q:5:TYR:H	2.13	0.43
2:T:-17:ILE:HG12	2:T:-16:SER:H	1.83	0.43
2:X:388:ARG:HB2	2:X:388:ARG:HE	1.41	0.43
1:A:182:ARG:HH12	1:A:235:VAL:HA	1.84	0.43
1:A:170:SER:OG	1:A:183:ILE:CG2	2.67	0.43
2:E:-3:PRO:O	2:E:348:THR:HA	2.19	0.43
2:E:486:LEU:N	2:E:486:LEU:HD12	2.33	0.43
2:H:-6:ALA:HA	2:H:-5:GLN:HB2	1.42	0.43
2:N:301:ALA:CB	2:N:333:LYS:CD	2.96	0.43
1:Q:67:LYS:HG2	1:Q:69:ASN:HD21	1.84	0.43
2:J:374:LEU:HD11	1:S:89:TYR:CD1	2.54	0.43
1:U:150:GLU:CG	1:U:154:VAL:HG22	2.43	0.43
1:U:29:SER:H	1:U:44:GLU:CG	2.31	0.43
2:X:-23:GLU:HG2	2:X:-22:LEU:N	2.34	0.43
2:R:-30:PHE:CE2	2:Z:-38:VAL:HG21	2.53	0.43
2:H:457:VAL:HG13	2:H:463:GLY:CA	2.48	0.43
2:J:308:TYR:CD1	2:J:308:TYR:C	2.91	0.43
1:S:19:LEU:HD23	1:S:19:LEU:O	2.18	0.43
2:T:332:ARG:CB	2:T:332:ARG:HH11	2.30	0.43
2:Z:348:THR:OG1	2:Z:351:VAL:CG2	2.66	0.43
1:I:173:GLU:CB	1:I:174:ASN:OD1	2.66	0.43
1:A:28:LYS:HB2	1:A:52:LYS:HZ2	1.83	0.43
2:C:430:ASN:ND2	2:C:431:ILE:O	2.51	0.43
2:C:-26:GLN:CG	2:H:-39:ALA:HB1	2.49	0.43
2:L:343:THR:HG22	2:L:404:LEU:CD1	2.49	0.43
2:L:523:GLY:O	2:L:524:ALA:HB2	2.19	0.43
1:O:8:SER:HA	1:O:9:PRO:HD2	1.75	0.43
1:Q:172:ALA:HB2	1:Q:183:ILE:CD1	2.48	0.43
1:S:161:GLU:N	1:S:162:PRO:HD2	2.33	0.43
1:S:204:GLY:O	1:S:207:SER:N	2.41	0.43
1:U:204:GLY:O	1:U:207:SER:N	2.35	0.43
2:V:-32:THR:HG22	2:V:-28:ARG:CZ	2.49	0.43
1:Y:116:LYS:NZ	1:Y:119:GLU:OE2	2.42	0.43
1:D:59:ARG:CD	1:D:129:HIS:HA	2.44	0.42
1:D:19:LEU:C	1:D:19:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ILE:HG21	1:D:233:LEU:CD2	2.49	0.42
2:E:406:GLY:O	2:E:419:ARG:N	2.46	0.42
1:F:56:LEU:HD23	1:F:56:LEU:HA	1.89	0.42
2:H:345:ILE:HB	2:H:352:ALA:HB1	2.00	0.42
1:I:33:LEU:CD1	1:I:33:LEU:O	2.65	0.42
1:I:30:VAL:HG22	1:I:52:LYS:HZ3	1.84	0.42
2:J:382:ARG:HH21	2:J:385:ILE:HD13	1.83	0.42
1:K:140:ARG:C	1:K:141:ILE:HD12	2.39	0.42
1:K:32:ALA:O	1:K:153:PHE:HA	2.19	0.42
2:L:464:LEU:O	2:L:464:LEU:HG	2.19	0.42
1:M:12:ALA:O	1:M:16:ARG:CG	2.65	0.42
2:R:423:PHE:CE1	2:R:429:TRP:HB3	2.54	0.42
1:S:174:ASN:HD22	1:S:174:ASN:N	2.16	0.42
2:E:-28:ARG:NH2	2:E:-21:LEU:HD23	2.33	0.42
1:D:3:PHE:HZ	1:F:6:PHE:HZ	1.49	0.42
2:H:-27:ARG:CG	2:H:-26:GLN:CD	2.84	0.42
1:I:150:GLU:HA	1:I:151:PRO:HD3	1.88	0.42
1:Q:173:GLU:O	1:Q:174:ASN:CB	2.66	0.42
1:S:167:LEU:O	1:S:171:TYR:N	2.51	0.42
1:S:32:ALA:O	1:S:153:PHE:HA	2.19	0.42
2:T:423:PHE:CE1	2:T:429:TRP:HB3	2.54	0.42
1:U:28:LYS:HB3	1:U:44:GLU:HG3	2.01	0.42
1:Y:29:SER:H	1:Y:44:GLU:CG	2.32	0.42
1:1:26:ARG:CG	1:1:26:ARG:O	2.66	0.42
1:B:30:VAL:HG13	1:B:43:ALA:CB	2.25	0.42
2:C:417:ALA:O	2:C:419:ARG:HG2	2.19	0.42
1:D:207:SER:O	1:D:208:LEU:CD1	2.38	0.42
1:D:30:VAL:HG22	1:D:52:LYS:NZ	2.34	0.42
1:F:152:HIS:HB3	1:F:171:TYR:CZ	2.54	0.42
1:I:217:ARG:NH2	1:I:223:ARG:NE	2.66	0.42
2:J:-33:PHE:CE1	2:J:-29:LEU:HD13	2.53	0.42
2:N:332:ARG:HH11	2:N:332:ARG:CB	2.30	0.42
1:S:69:ASN:HD22	1:S:69:ASN:H	1.68	0.42
1:U:10:GLU:HG2	1:U:14:ARG:NH2	2.34	0.42
1:U:40:LEU:CD1	1:U:212:VAL:HG12	2.49	0.42
1:Y:19:LEU:HD23	1:Y:19:LEU:C	2.40	0.42
1:A:115:ALA:HB3	1:B:112:THR:HG22	2.01	0.42
1:D:224:ARG:HH11	1:D:224:ARG:HG2	1.84	0.42
2:E:312:VAL:HG12	2:E:497:ILE:HB	2.01	0.42
1:F:150:GLU:CG	1:F:154:VAL:HG22	2.45	0.42
2:C:-4:LEU:HD22	2:H:426:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:506:PRO:O	2:H:509:ARG:HB3	2.19	0.42
1:I:33:LEU:HD12	1:I:40:LEU:HB3	2.01	0.42
2:J:521:ARG:HA	2:J:521:ARG:HD3	1.87	0.42
1:K:16:ARG:HG3	1:M:9:PRO:CG	2.49	0.42
1:O:26:ARG:O	1:O:26:ARG:CG	2.67	0.42
2:N:476:ASP:O	2:P:329:ARG:NH2	2.52	0.42
1:Q:48:ARG:HG2	1:Q:48:ARG:O	2.19	0.42
2:R:399:LEU:HD11	2:R:401:LEU:HD13	2.01	0.42
1:U:32:ALA:HA	1:U:40:LEU:O	2.19	0.42
1:1:8:SER:O	1:1:11:GLN:HG2	2.19	0.42
2:2:308:TYR:CE2	2:2:311:GLY:HA3	2.51	0.42
1:A:234:LEU:O	1:A:235:VAL:CG2	2.68	0.42
1:A:28:LYS:H	1:A:28:LYS:CE	2.32	0.42
2:C:418:GLY:O	2:C:419:ARG:NH1	2.52	0.42
2:J:-17:ILE:CD1	2:J:392:ALA:HB1	2.49	0.42
1:K:213:LEU:HD23	1:K:213:LEU:HA	1.89	0.42
1:M:152:HIS:NE2	1:M:173:GLU:OE2	2.48	0.42
2:N:350:ALA:O	2:N:354:GLU:HG2	2.19	0.42
2:P:-28:ARG:HG2	2:P:-21:LEU:HD23	1.99	0.42
2:P:-17:ILE:HG21	2:P:396:GLN:CD	2.39	0.42
1:U:26:ARG:HB2	1:U:26:ARG:NH1	2.34	0.42
2:V:-29:LEU:HD12	2:V:-29:LEU:HA	1.72	0.42
2:X:-28:ARG:O	2:X:-24:PRO:HG3	2.19	0.42
1:1:10:GLU:O	1:1:14:ARG:HB2	2.20	0.42
1:D:233:LEU:CD1	1:D:233:LEU:H	2.32	0.42
1:D:3:PHE:HE1	1:F:6:PHE:HE2	1.52	0.42
2:E:433:GLU:H	2:E:433:GLU:HG2	1.67	0.42
2:G:-17:ILE:CD1	2:G:-17:ILE:C	2.88	0.42
2:G:486:LEU:CD1	2:G:486:LEU:N	2.82	0.42
2:N:-21:LEU:HG	2:N:-20:PRO:HD2	2.00	0.42
1:O:87:TYR:OH	2:P:358:LEU:HB2	2.20	0.42
1:U:30:VAL:HG22	1:U:52:LYS:NZ	2.35	0.42
2:P:-21:LEU:O	2:V:388:ARG:NH1	2.53	0.42
2:V:415:GLN:OE1	2:V:415:GLN:CA	2.67	0.42
1:1:18:GLU:OE2	1:1:21:ARG:NE	2.52	0.42
2:2:401:LEU:HD12	2:2:401:LEU:HA	1.87	0.42
1:B:150:GLU:CG	1:B:154:VAL:HG22	2.47	0.42
1:D:152:HIS:HB3	1:D:171:TYR:CZ	2.55	0.42
2:H:-23:GLU:HB3	2:P:-28:ARG:HH22	1.83	0.42
2:H:-30:PHE:HZ	2:P:-38:VAL:CG2	2.32	0.42
2:L:376:PHE:CE2	2:L:380:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:-21:LEU:HA	2:T:-21:LEU:HD23	1.72	0.42
2:T:301:ALA:HB2	2:T:333:LYS:CE	2.46	0.42
1:U:74:LEU:HD23	1:U:122:LEU:HD21	2.01	0.42
2:V:423:PHE:CE1	2:V:429:TRP:HB3	2.54	0.42
1:W:150:GLU:CG	1:W:154:VAL:HG22	2.46	0.42
1:Y:217:ARG:HD3	1:Y:218:PRO:CD	2.49	0.42
1:U:89:TYR:CE1	2:2:382:ARG:HD2	2.54	0.42
2:E:-4:LEU:O	2:E:-2:HIS:CD2	2.58	0.42
2:E:515:ARG:O	2:E:519:GLU:HB2	2.19	0.42
1:F:224:ARG:HH11	1:F:224:ARG:HG2	1.85	0.42
2:G:366:TYR:CD2	2:G:374:LEU:HD13	2.55	0.42
1:I:130:TYR:CG	1:I:218:PRO:HA	2.55	0.42
1:I:8:SER:O	1:I:11:GLN:N	2.53	0.42
2:L:308:TYR:CE2	2:L:311:GLY:HA3	2.55	0.42
2:L:-38:VAL:HG12	2:L:-37:ASP:N	2.33	0.42
1:M:35:TYR:N	1:M:38:GLY:O	2.49	0.42
1:O:29:SER:OG	1:O:157:GLY:O	2.37	0.42
1:U:16:ARG:HH11	1:U:117:PRO:HD3	1.85	0.42
1:W:33:LEU:HB3	1:W:153:PHE:HB3	2.01	0.42
2:Z:433:GLU:CA	2:Z:433:GLU:OE1	2.67	0.42
1:A:83:ASP:OD2	2:H:365:HIS:ND1	2.38	0.42
1:B:32:ALA:HA	1:B:40:LEU:O	2.19	0.42
1:D:233:LEU:HD13	1:D:233:LEU:H	1.85	0.42
2:E:407:TYR:CD1	2:E:417:ALA:HB3	2.51	0.42
2:J:457:VAL:CG2	2:J:466:VAL:HG21	2.49	0.42
2:L:-22:LEU:H	2:L:-22:LEU:CD2	2.31	0.42
1:M:155:VAL:C	1:M:156:MET:HG3	2.39	0.42
1:Q:224:ARG:HG2	1:Q:224:ARG:NH1	2.34	0.42
1:U:167:LEU:O	1:U:171:TYR:N	2.38	0.42
1:W:16:ARG:NH2	1:W:114:GLN:O	2.51	0.42
2:X:319:ARG:CG	2:X:320:SER:N	2.82	0.42
2:2:416:SER:O	2:2:419:ARG:CZ	2.68	0.42
2:G:383:LEU:O	2:G:387:VAL:HG23	2.20	0.42
2:H:301:ALA:HB1	2:H:333:LYS:HD3	2.02	0.42
1:K:163:ILE:HG23	1:K:187:ALA:O	2.20	0.42
1:K:191:GLY:O	1:K:192:SER:C	2.58	0.42
1:S:224:ARG:HG2	1:S:224:ARG:NH1	2.34	0.42
1:S:26:ARG:O	1:S:26:ARG:CG	2.68	0.42
1:I:188:LEU:O	1:I:189:ARG:C	2.59	0.41
1:I:35:TYR:CE1	1:I:37:GLY:CA	2.98	0.41
1:A:27:ALA:HB1	1:A:28:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:SER:H	1:D:44:GLU:CG	2.33	0.41
2:E:-28:ARG:CZ	2:E:-21:LEU:CD2	2.90	0.41
2:J:332:ARG:HH11	2:J:332:ARG:CB	2.32	0.41
1:K:26:ARG:CZ	1:K:26:ARG:HB2	2.49	0.41
1:O:164:ALA:O	1:O:167:LEU:HB2	2.20	0.41
1:Q:28:LYS:HB3	1:Q:44:GLU:HG3	2.02	0.41
2:R:521:ARG:O	2:R:522:SER:HB3	2.19	0.41
2:V:320:SER:HB2	2:V:331:VAL:HG21	2.01	0.41
2:X:308:TYR:CE2	2:X:311:GLY:HA3	2.53	0.41
2:2:345:ILE:HB	2:2:352:ALA:HB1	2.01	0.41
1:A:172:ALA:HB3	1:A:175:ALA:HB2	2.03	0.41
2:C:-4:LEU:CD1	2:C:398:LEU:CD1	2.97	0.41
2:E:358:LEU:HD23	2:E:386:MET:HE1	2.01	0.41
2:E:415:GLN:N	2:E:415:GLN:HE21	2.18	0.41
2:E:465:ARG:HG3	2:E:513:LEU:HD11	2.01	0.41
2:L:-32:THR:HG22	2:L:-31:ASP:N	2.36	0.41
2:L:491:PHE:HB3	2:L:492:PRO:HD2	2.02	0.41
1:M:35:TYR:CE1	1:M:37:GLY:N	2.88	0.41
1:O:142:THR:OG1	1:O:144:ASP:HB3	2.20	0.41
2:R:308:TYR:CE2	2:R:311:GLY:C	2.94	0.41
1:S:155:VAL:CG2	1:S:167:LEU:HD12	2.51	0.41
2:T:-36:LEU:HD21	1:1:84:THR:HG22	2.02	0.41
1:U:26:ARG:HG2	1:U:26:ARG:O	2.20	0.41
2:V:-38:VAL:HG13	2:V:-38:VAL:O	2.20	0.41
1:W:14:ARG:NH1	1:W:14:ARG:CG	2.80	0.41
2:X:419:ARG:HH11	2:X:419:ARG:HG2	1.84	0.41
1:Y:226:THR:CG2	3:Y:252:HOH:O	2.68	0.41
2:Z:413:ASP:HA	2:Z:414:PRO:HD2	1.85	0.41
1:A:161:GLU:CD	1:A:161:GLU:N	2.73	0.41
1:A:9:PRO:CD	1:A:10:GLU:H	2.32	0.41
1:B:178:THR:CA	1:B:233:LEU:CD2	2.82	0.41
1:F:8:SER:O	1:F:11:GLN:HB3	2.19	0.41
2:J:-38:VAL:CG1	2:J:-38:VAL:O	2.67	0.41
2:J:419:ARG:HG2	2:J:419:ARG:NH1	2.35	0.41
2:L:-20:PRO:O	2:L:-19:ALA:CB	2.66	0.41
1:M:59:ARG:NH1	1:M:128:ALA:O	2.36	0.41
2:N:391:LEU:O	2:N:395:MET:HG2	2.19	0.41
2:R:521:ARG:HD3	2:R:521:ARG:HA	1.82	0.41
1:S:107:LEU:HD23	1:S:107:LEU:HA	1.94	0.41
1:S:28:LYS:H	1:S:28:LYS:HE3	1.85	0.41
1:U:40:LEU:CD1	1:U:212:VAL:CG1	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:26:ARG:CG	1:U:26:ARG:O	2.68	0.41
2:X:301:ALA:HB1	2:X:333:LYS:NZ	2.24	0.41
1:1:150:GLU:HA	1:1:151:PRO:HD3	1.89	0.41
2:C:310:GLY:HA2	2:C:415:GLN:HA	2.01	0.41
1:D:234:LEU:HD12	1:D:234:LEU:N	2.35	0.41
2:E:521:ARG:C	2:E:523:GLY:H	2.23	0.41
1:I:150:GLU:CG	1:I:154:VAL:HG22	2.44	0.41
1:I:233:LEU:HD12	1:I:233:LEU:HA	1.61	0.41
2:J:419:ARG:HG2	2:J:419:ARG:HH11	1.86	0.41
2:L:-27:ARG:O	2:L:-26:GLN:OE1	2.38	0.41
2:L:453:LEU:HB3	2:L:466:VAL:HG22	2.03	0.41
1:O:110:ILE:HG23	1:O:114:GLN:HG3	2.01	0.41
2:P:347:GLY:HA3	2:P:399:LEU:O	2.21	0.41
2:R:401:LEU:HA	2:R:401:LEU:HD12	1.79	0.41
2:Z:486:LEU:CD1	2:Z:486:LEU:N	2.84	0.41
1:1:8:SER:N	1:1:11:GLN:HG3	2.34	0.41
1:B:28:LYS:CE	1:B:52:LYS:HE3	2.49	0.41
1:F:51:GLN:NE2	1:W:97:ARG:NH2	2.68	0.41
1:K:150:GLU:CG	1:K:154:VAL:HG22	2.47	0.41
1:K:33:LEU:HD13	1:K:33:LEU:O	2.20	0.41
1:K:56:LEU:HD23	1:K:56:LEU:HA	1.88	0.41
1:M:129:HIS:HE1	3:M:253:HOH:O	2.04	0.41
1:U:5:TYR:N	1:U:5:TYR:CD1	2.87	0.41
2:V:388:ARG:O	2:V:388:ARG:HG2	2.20	0.41
1:M:7:ILE:HD11	1:W:5:TYR:HB2	2.02	0.41
1:Y:26:ARG:HB2	1:Y:26:ARG:HE	1.75	0.41
1:A:33:LEU:HD11	1:A:40:LEU:HD23	2.03	0.41
1:A:47:SER:OG	1:A:50:LEU:HG	2.20	0.41
2:P:-21:LEU:HA	2:P:-21:LEU:HD12	1.81	0.41
2:P:-28:ARG:HG3	2:P:-21:LEU:HD21	2.00	0.41
1:Q:10:GLU:OE2	1:Q:10:GLU:HA	2.21	0.41
1:U:150:GLU:HA	1:U:151:PRO:HD3	1.88	0.41
2:X:331:VAL:HG13	2:X:349:ALA:CA	2.50	0.41
1:A:163:ILE:O	1:A:167:LEU:HB2	2.19	0.41
1:A:59:ARG:NH2	1:A:217:ARG:O	2.47	0.41
1:A:54:SER:CB	1:A:75:ARG:HD2	2.51	0.41
1:F:213:LEU:HA	1:F:213:LEU:HD23	1.88	0.41
2:J:375:THR:HG21	1:S:92:ARG:HB3	2.02	0.41
1:K:7:ILE:CD1	1:M:8:SER:HA	2.51	0.41
1:M:174:ASN:OD1	1:M:174:ASN:N	2.54	0.41
1:M:208:LEU:HD12	1:M:208:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:491:PHE:HB3	2:N:492:PRO:HD2	2.02	0.41
1:S:16:ARG:NH2	1:S:114:GLN:O	2.50	0.41
1:W:16:ARG:HH11	1:W:117:PRO:HD3	1.79	0.41
1:Y:107:LEU:HA	1:Y:107:LEU:HD23	1.94	0.41
1:1:8:SER:N	1:1:11:GLN:CG	2.79	0.41
1:A:235:VAL:HG12	1:A:235:VAL:O	2.20	0.41
1:B:11:GLN:HG3	1:B:14:ARG:HH12	1.86	0.41
1:B:161:GLU:N	1:B:162:PRO:HD2	2.35	0.41
2:C:409:ILE:CG1	2:C:410:HIS:CE1	3.04	0.41
1:D:149:ASP:OD2	1:Q:47:SER:OG	2.38	0.41
2:L:308:TYR:OH	2:L:496:ILE:HD11	2.21	0.41
1:M:22:LYS:O	1:M:25:ALA:HB3	2.21	0.41
2:N:486:LEU:HD12	2:N:486:LEU:N	2.35	0.41
1:O:161:GLU:N	1:O:161:GLU:CD	2.74	0.41
2:P:318:ARG:HD3	2:P:493:THR:HG23	2.03	0.41
1:U:8:SER:H	1:1:5:TYR:C	2.23	0.41
2:P:-26:GLN:HB3	2:V:-38:VAL:HG12	2.03	0.41
2:V:444:LEU:HB2	3:V:47:HOH:O	2.19	0.41
1:W:167:LEU:HD12	1:W:167:LEU:HA	1.57	0.41
1:B:35:TYR:HE1	1:B:37:GLY:HA3	1.58	0.41
1:D:32:ALA:O	1:D:153:PHE:HA	2.21	0.41
1:D:28:LYS:H	1:D:28:LYS:HE3	1.86	0.41
1:O:114:GLN:O	1:O:115:ALA:C	2.58	0.41
1:O:150:GLU:HA	1:O:151:PRO:HD3	1.87	0.41
1:Q:233:LEU:HD23	1:Q:233:LEU:HA	1.73	0.41
1:D:11:GLN:CD	1:Q:5:TYR:HD1	2.24	0.41
2:R:-23:GLU:HB2	2:Z:-28:ARG:NH2	2.36	0.41
1:S:8:SER:HB3	1:S:11:GLN:CB	2.51	0.41
2:T:367:GLU:O	2:T:371:GLY:N	2.53	0.41
2:Z:498:ASP:OD1	2:Z:498:ASP:C	2.59	0.41
2:C:388:ARG:HG3	2:C:426:ALA:O	2.21	0.41
2:C:-4:LEU:HD13	2:C:398:LEU:HD11	2.03	0.41
1:M:163:ILE:CD1	1:M:191:GLY:HA3	2.43	0.41
2:N:350:ALA:O	2:N:353:VAL:CG1	2.69	0.41
1:O:59:ARG:NH1	1:O:128:ALA:O	2.39	0.41
2:P:-23:GLU:HG2	2:P:-22:LEU:HG	2.02	0.41
1:S:45:ASN:HA	1:S:46:PRO:HD2	1.89	0.41
1:B:30:VAL:HG22	1:B:52:LYS:HZ3	1.86	0.41
2:E:374:LEU:HD11	1:K:89:TYR:CD1	2.56	0.41
1:F:59:ARG:NH2	1:F:217:ARG:O	2.51	0.41
1:I:67:LYS:HG2	1:I:69:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:ASN:ND2	1:M:105:GLN:NE2	2.70	0.41
1:M:20:ALA:O	1:M:24:ILE:HG13	2.21	0.41
1:O:74:LEU:HD23	1:O:122:LEU:HD21	2.03	0.41
1:O:93:ASP:OD1	2:V:375:THR:HG23	2.21	0.41
2:P:308:TYR:CE2	2:P:496:ILE:HD11	2.56	0.41
2:R:320:SER:HB2	2:R:331:VAL:HG21	2.02	0.41
1:U:234:LEU:N	1:U:234:LEU:CD1	2.84	0.41
2:V:312:VAL:HG12	2:V:497:ILE:HB	2.03	0.41
1:W:15:GLU:OE2	1:Y:9:PRO:HB2	2.21	0.41
2:X:-22:LEU:HD12	2:X:-22:LEU:HA	1.81	0.41
2:X:382:ARG:HH21	2:X:385:ILE:HD12	1.69	0.41
1:1:112:THR:CG2	1:1:112:THR:O	2.69	0.40
1:1:33:LEU:HD12	1:1:40:LEU:HB3	2.00	0.40
1:A:7:ILE:CD1	1:A:15:GLU:CD	2.89	0.40
2:J:515:ARG:HG2	2:J:515:ARG:NH1	2.36	0.40
1:M:152:HIS:CG	1:M:171:TYR:CE2	3.09	0.40
2:N:-20:PRO:CG	2:N:-19:ALA:N	2.84	0.40
1:O:139:TYR:HA	1:O:148:ALA:O	2.20	0.40
1:Q:123:CYS:HA	1:Q:139:TYR:O	2.22	0.40
1:Q:140:ARG:C	1:Q:141:ILE:HD12	2.42	0.40
2:R:424:ASP:C	2:R:424:ASP:OD1	2.59	0.40
1:S:152:HIS:CB	1:S:171:TYR:CE2	3.01	0.40
2:V:351:VAL:HG12	2:V:400:ALA:HB2	2.02	0.40
2:X:496:ILE:HG23	2:X:496:ILE:O	2.21	0.40
1:Y:59:ARG:CD	1:Y:129:HIS:HA	2.44	0.40
1:B:130:TYR:HE1	1:B:216:ASN:O	2.04	0.40
1:B:54:SER:CB	1:B:75:ARG:HD2	2.51	0.40
2:H:471:LEU:HA	2:H:471:LEU:HD12	1.93	0.40
1:I:161:GLU:N	1:I:161:GLU:CD	2.73	0.40
1:K:167:LEU:HA	1:K:167:LEU:HD23	1.58	0.40
2:N:301:ALA:HB2	2:N:333:LYS:CE	2.50	0.40
2:P:312:VAL:HG12	2:P:497:ILE:HB	2.03	0.40
1:Q:161:GLU:CD	1:Q:161:GLU:N	2.74	0.40
1:S:67:LYS:HG2	1:S:69:ASN:ND2	2.36	0.40
1:U:142:THR:OG1	1:U:144:ASP:HB3	2.21	0.40
2:V:359:TYR:CE1	2:V:383:LEU:HB2	2.56	0.40
1:W:10:GLU:CG	1:W:14:ARG:HH12	2.31	0.40
2:X:-25:ALA:N	2:X:-24:PRO:HD3	2.36	0.40
2:X:-32:THR:CG2	2:X:-31:ASP:N	2.84	0.40
2:X:338:ASP:OD2	2:X:341:THR:OG1	2.30	0.40
2:X:350:ALA:HA	2:X:353:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:15:GLU:O	1:Y:19:LEU:N	2.44	0.40
2:Z:301:ALA:O	2:Z:440:GLY:HA3	2.21	0.40
2:Z:391:LEU:O	2:Z:395:MET:HG2	2.21	0.40
1:1:123:CYS:HA	1:1:139:TYR:O	2.22	0.40
1:1:32:ALA:HA	1:1:40:LEU:O	2.21	0.40
1:U:98:GLN:HG2	2:2:370:GLU:OE1	2.22	0.40
1:A:16:ARG:NH2	1:A:114:GLN:O	2.39	0.40
2:C:-4:LEU:CD2	2:H:426:ALA:HB2	2.51	0.40
2:P:-17:ILE:CG2	2:P:396:GLN:OE1	2.68	0.40
1:Q:167:LEU:HD23	1:Q:167:LEU:HA	1.85	0.40
1:Q:87:TYR:O	2:R:357:ARG:NH1	2.54	0.40
1:S:35:TYR:HD1	1:S:37:GLY:H	1.50	0.40
2:V:-22:LEU:HD12	2:V:-22:LEU:HA	1.86	0.40
1:W:11:GLN:O	1:W:15:GLU:HG3	2.21	0.40
2:Z:302:THR:N	2:Z:317:ASP:OD2	2.35	0.40
2:Z:421:VAL:HG22	2:Z:431:ILE:HG12	2.03	0.40
1:U:112:THR:HG23	1:1:115:ALA:HB3	2.03	0.40
2:2:319:ARG:CG	2:2:320:SER:N	2.85	0.40
2:2:513:LEU:HD12	2:2:513:LEU:HA	1.78	0.40
1:A:44:GLU:C	1:A:45:ASN:HD22	2.24	0.40
1:A:4:PRO:HB3	1:B:11:GLN:CD	2.41	0.40
1:B:59:ARG:NH1	1:B:128:ALA:O	2.36	0.40
1:D:189:ARG:O	1:D:192:SER:N	2.55	0.40
2:G:338:ASP:OD1	2:G:338:ASP:C	2.59	0.40
1:K:150:GLU:HA	1:K:151:PRO:HD3	1.86	0.40
1:K:161:GLU:CD	1:K:161:GLU:N	2.75	0.40
1:K:224:ARG:HG2	1:K:224:ARG:NH1	2.36	0.40
2:N:349:ALA:O	2:N:353:VAL:HG12	2.21	0.40
1:O:9:PRO:O	1:O:13:MET:HG2	2.21	0.40
2:P:301:ALA:CB	2:P:333:LYS:HZ3	2.25	0.40
1:A:84:THR:HG22	2:P:-36:LEU:HD11	2.02	0.40
1:Q:173:GLU:O	1:Q:174:ASN:OD1	2.40	0.40
1:Q:40:LEU:HD13	1:Q:212:VAL:HG11	2.03	0.40
2:R:486:LEU:CD1	2:R:486:LEU:N	2.84	0.40
2:J:375:THR:HG23	1:S:93:ASP:OD1	2.21	0.40
2:T:471:LEU:HD12	2:T:471:LEU:HA	1.95	0.40
1:W:67:LYS:HG2	1:W:69:ASN:HD21	1.86	0.40
1:Y:11:GLN:HG2	1:Y:14:ARG:HH12	1.86	0.40
1:Y:186:ALA:O	1:Y:189:ARG:CG	2.70	0.40
1:Y:14:ARG:O	1:Y:18:GLU:HG2	2.21	0.40
1:Y:32:ALA:O	1:Y:153:PHE:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:56:LEU:HD23	1:Y:56:LEU:HA	1.91	0.40
1:1:35:TYR:CE2	1:1:38:GLY:N	2.89	0.40
1:A:33:LEU:O	1:A:33:LEU:CD1	2.69	0.40
1:B:33:LEU:HD12	1:B:40:LEU:HB3	2.01	0.40
1:D:30:VAL:HG22	1:D:52:LYS:HZ3	1.86	0.40
1:D:29:SER:N	1:D:44:GLU:OE1	2.50	0.40
2:E:-29:LEU:O	2:E:-25:ALA:C	2.60	0.40
1:F:70:GLU:HG2	1:F:118:TYR:CZ	2.56	0.40
2:G:353:VAL:HG13	2:G:354:GLU:N	2.36	0.40
2:G:428:GLY:HA2	2:X:350:ALA:CB	2.49	0.40
2:L:509:ARG:HD2	2:L:509:ARG:O	2.22	0.40
1:M:205:VAL:HG23	1:M:234:LEU:CD1	2.51	0.40
1:M:56:LEU:HA	1:M:56:LEU:HD23	1.91	0.40
1:M:67:LYS:HG2	1:M:69:ASN:ND2	2.36	0.40
1:S:225:ILE:HG21	1:S:233:LEU:HD12	2.04	0.40
1:U:139:TYR:HA	1:U:148:ALA:O	2.21	0.40
2:X:457:VAL:HG12	2:X:457:VAL:O	2.20	0.40

There are no symmetry-related clashes.

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	1	215/248 (87%)	204 (95%)	10 (5%)	1 (0%)	32	53
1	A	218/248 (88%)	208 (95%)	10 (5%)	0	100	100
1	B	216/248 (87%)	205 (95%)	11 (5%)	0	100	100
1	D	218/248 (88%)	202 (93%)	16 (7%)	0	100	100
1	F	217/248 (88%)	208 (96%)	9 (4%)	0	100	100
1	I	213/248 (86%)	204 (96%)	9 (4%)	0	100	100
1	K	217/248 (88%)	206 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	220/248 (89%)	215 (98%)	5 (2%)	0	100	100
1	O	214/248 (86%)	202 (94%)	12 (6%)	0	100	100
1	Q	218/248 (88%)	205 (94%)	13 (6%)	0	100	100
1	S	215/248 (87%)	202 (94%)	13 (6%)	0	100	100
1	U	217/248 (88%)	203 (94%)	14 (6%)	0	100	100
1	W	217/248 (88%)	205 (94%)	11 (5%)	1 (0%)	32	53
1	Y	220/248 (89%)	212 (96%)	8 (4%)	0	100	100
2	2	242/291 (83%)	241 (100%)	1 (0%)	0	100	100
2	C	246/291 (84%)	241 (98%)	5 (2%)	0	100	100
2	E	244/291 (84%)	239 (98%)	5 (2%)	0	100	100
2	G	247/291 (85%)	246 (100%)	1 (0%)	0	100	100
2	H	244/291 (84%)	239 (98%)	5 (2%)	0	100	100
2	J	248/291 (85%)	245 (99%)	3 (1%)	0	100	100
2	L	247/291 (85%)	240 (97%)	6 (2%)	1 (0%)	38	59
2	N	248/291 (85%)	244 (98%)	4 (2%)	0	100	100
2	P	246/291 (84%)	244 (99%)	2 (1%)	0	100	100
2	R	242/291 (83%)	240 (99%)	2 (1%)	0	100	100
2	T	246/291 (84%)	243 (99%)	3 (1%)	0	100	100
2	V	245/291 (84%)	244 (100%)	1 (0%)	0	100	100
2	X	245/291 (84%)	244 (100%)	1 (0%)	0	100	100
2	Z	241/291 (83%)	240 (100%)	1 (0%)	0	100	100
All	All	6466/7546 (86%)	6271 (97%)	192 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	4	PRO
2	L	-19	ALA
1	1	7	ILE

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	1	168/192 (88%)	150 (89%)	18 (11%)	8	15
1	A	171/192 (89%)	157 (92%)	14 (8%)	13	25
1	B	168/192 (88%)	152 (90%)	16 (10%)	10	19
1	D	171/192 (89%)	157 (92%)	14 (8%)	13	25
1	F	170/192 (88%)	155 (91%)	15 (9%)	12	22
1	I	167/192 (87%)	151 (90%)	16 (10%)	10	18
1	K	170/192 (88%)	154 (91%)	16 (9%)	10	19
1	M	173/192 (90%)	157 (91%)	16 (9%)	11	20
1	O	167/192 (87%)	153 (92%)	14 (8%)	13	24
1	Q	171/192 (89%)	152 (89%)	19 (11%)	7	13
1	S	168/192 (88%)	154 (92%)	14 (8%)	13	25
1	U	170/192 (88%)	153 (90%)	17 (10%)	9	17
1	W	170/192 (88%)	153 (90%)	17 (10%)	9	17
1	Y	173/192 (90%)	155 (90%)	18 (10%)	8	15
2	2	186/216 (86%)	175 (94%)	11 (6%)	23	42
2	C	188/216 (87%)	176 (94%)	12 (6%)	20	38
2	E	185/216 (86%)	168 (91%)	17 (9%)	11	20
2	G	188/216 (87%)	177 (94%)	11 (6%)	23	42
2	H	186/216 (86%)	178 (96%)	8 (4%)	33	58
2	J	189/216 (88%)	179 (95%)	10 (5%)	26	48
2	L	188/216 (87%)	175 (93%)	13 (7%)	18	34
2	N	189/216 (88%)	178 (94%)	11 (6%)	23	43
2	P	188/216 (87%)	174 (93%)	14 (7%)	16	30
2	R	184/216 (85%)	175 (95%)	9 (5%)	29	52
2	T	189/216 (88%)	176 (93%)	13 (7%)	18	34
2	V	186/216 (86%)	178 (96%)	8 (4%)	33	58
2	X	188/216 (87%)	173 (92%)	15 (8%)	14	27
2	Z	184/216 (85%)	169 (92%)	15 (8%)	13	25
All	All	4995/5712 (87%)	4604 (92%)	391 (8%)	15	28

All (391) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	28	LYS
1	A	33	LEU
1	A	45	ASN
1	A	59	ARG
1	A	69	ASN
1	A	74	LEU
1	A	92	ARG
1	A	105	GLN
1	A	147	ILE
1	A	208	LEU
1	A	226	THR
1	A	228	SER
1	A	234	LEU
1	B	5	TYR
1	B	6	PHE
1	B	28	LYS
1	B	30	VAL
1	B	33	LEU
1	B	59	ARG
1	B	69	ASN
1	B	74	LEU
1	B	92	ARG
1	B	105	GLN
1	B	114	GLN
1	B	122	LEU
1	B	167	LEU
1	B	226	THR
1	B	228	SER
1	B	233	LEU
2	C	-22	LEU
2	C	329	ARG
2	C	338	ASP
2	C	353	VAL
2	C	363	LEU
2	C	374	LEU
2	C	381	ASN
2	C	382	ARG
2	C	398	LEU
2	C	430	ASN
2	C	434	GLU
2	C	509	ARG

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Mol	Chain	Res	Type
1	D	28	LYS
1	D	33	LEU
1	D	59	ARG
1	D	74	LEU
1	D	92	ARG
1	D	105	GLN
1	D	114	GLN
1	D	122	LEU
1	D	167	LEU
1	D	174	ASN
1	D	207	SER
1	D	212	VAL
1	D	226	THR
1	D	233	LEU
2	E	-34	SER
2	E	-26	GLN
2	E	-22	LEU
2	E	329	ARG
2	E	332	ARG
2	E	338	ASP
2	E	355	PHE
2	E	363	LEU
2	E	374	LEU
2	E	381	ASN
2	E	382	ARG
2	E	409	ILE
2	E	415	GLN
2	E	433	GLU
2	E	503	VAL
2	E	512	GLU
2	E	519	GLU
1	F	8	SER
1	F	26	ARG
1	F	33	LEU
1	F	48	ARG
1	F	59	ARG
1	F	69	ASN
1	F	74	LEU
1	F	92	ARG
1	F	105	GLN
1	F	122	LEU
1	F	167	LEU

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Mol	Chain	Res	Type
1	F	169	GLU
1	F	217	ARG
1	F	226	THR
1	F	234	LEU
2	G	-27	ARG
2	G	-17	ILE
2	G	329	ARG
2	G	363	LEU
2	G	374	LEU
2	G	382	ARG
2	G	413	ASP
2	G	431	ILE
2	G	434	GLU
2	G	503	VAL
2	G	513	LEU
2	H	-21	LEU
2	H	329	ARG
2	H	363	LEU
2	H	374	LEU
2	H	381	ASN
2	H	382	ARG
2	H	402	PRO
2	H	486	LEU
1	I	5	TYR
1	I	9	PRO
1	I	10	GLU
1	I	28	LYS
1	I	30	VAL
1	I	33	LEU
1	I	59	ARG
1	I	69	ASN
1	I	73	ASN
1	I	74	LEU
1	I	92	ARG
1	I	105	GLN
1	I	122	LEU
1	I	167	LEU
1	I	169	GLU
1	I	226	THR
2	J	-32	THR
2	J	-27	ARG
2	J	-18	SER

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Mol	Chain	Res	Type
2	J	-17	ILE
2	J	329	ARG
2	J	338	ASP
2	J	363	LEU
2	J	374	LEU
2	J	509	ARG
2	J	513	LEU
1	K	9	PRO
1	K	14	ARG
1	K	28	LYS
1	K	30	VAL
1	K	33	LEU
1	K	59	ARG
1	K	69	ASN
1	K	74	LEU
1	K	92	ARG
1	K	105	GLN
1	K	122	LEU
1	K	179	ASP
1	K	205	VAL
1	K	208	LEU
1	K	226	THR
1	K	228	SER
2	L	-32	THR
2	L	-31	ASP
2	L	-26	GLN
2	L	-21	LEU
2	L	-5	GLN
2	L	329	ARG
2	L	338	ASP
2	L	354	GLU
2	L	355	PHE
2	L	363	LEU
2	L	374	LEU
2	L	381	ASN
2	L	382	ARG
1	M	3	PHE
1	M	33	LEU
1	M	59	ARG
1	M	69	ASN
1	M	73	ASN
1	M	74	LEU

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Mol	Chain	Res	Type
1	M	92	ARG
1	M	105	GLN
1	M	122	LEU
1	M	159	THR
1	M	161	GLU
1	M	167	LEU
1	M	174	ASN
1	M	203	LEU
1	M	208	LEU
1	M	226	THR
2	N	-27	ARG
2	N	-21	LEU
2	N	-17	ILE
2	N	-4	LEU
2	N	329	ARG
2	N	338	ASP
2	N	363	LEU
2	N	374	LEU
2	N	381	ASN
2	N	382	ARG
2	N	503	VAL
1	O	7	ILE
1	O	8	SER
1	O	17	SER
1	O	51	GLN
1	O	59	ARG
1	O	69	ASN
1	O	74	LEU
1	O	92	ARG
1	O	105	GLN
1	O	122	LEU
1	O	205	VAL
1	O	208	LEU
1	O	226	THR
1	O	234	LEU
2	P	-36	LEU
2	P	-31	ASP
2	P	-26	GLN
2	P	-21	LEU
2	P	-18	SER
2	P	-5	GLN
2	P	329	ARG

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Mol	Chain	Res	Type
2	P	338	ASP
2	P	353	VAL
2	P	363	LEU
2	P	374	LEU
2	P	381	ASN
2	P	382	ARG
2	P	503	VAL
1	Q	4	PRO
1	Q	5	TYR
1	Q	28	LYS
1	Q	59	ARG
1	Q	69	ASN
1	Q	74	LEU
1	Q	92	ARG
1	Q	105	GLN
1	Q	114	GLN
1	Q	122	LEU
1	Q	171	TYR
1	Q	174	ASN
1	Q	178	THR
1	Q	189	ARG
1	Q	208	LEU
1	Q	210	VAL
1	Q	226	THR
1	Q	228	SER
1	Q	234	LEU
2	R	-35	SER
2	R	-32	THR
2	R	338	ASP
2	R	355	PHE
2	R	363	LEU
2	R	374	LEU
2	R	381	ASN
2	R	382	ARG
2	R	407	TYR
1	S	10	GLU
1	S	13	MET
1	S	14	ARG
1	S	28	LYS
1	S	33	LEU
1	S	59	ARG
1	S	69	ASN

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Mol	Chain	Res	Type
1	S	74	LEU
1	S	92	ARG
1	S	105	GLN
1	S	122	LEU
1	S	208	LEU
1	S	226	THR
1	S	228	SER
2	T	-27	ARG
2	T	-22	LEU
2	T	-17	ILE
2	T	-16	SER
2	T	-5	GLN
2	T	329	ARG
2	T	338	ASP
2	T	363	LEU
2	T	374	LEU
2	T	381	ASN
2	T	412	SER
2	T	415	GLN
2	T	433	GLU
1	U	5	TYR
1	U	7	ILE
1	U	14	ARG
1	U	28	LYS
1	U	30	VAL
1	U	33	LEU
1	U	59	ARG
1	U	69	ASN
1	U	74	LEU
1	U	92	ARG
1	U	105	GLN
1	U	122	LEU
1	U	179	ASP
1	U	203	LEU
1	U	208	LEU
1	U	226	THR
1	U	233	LEU
2	V	-29	LEU
2	V	-22	LEU
2	V	329	ARG
2	V	338	ASP
2	V	363	LEU

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Mol	Chain	Res	Type
2	V	374	LEU
2	V	381	ASN
2	V	382	ARG
1	W	6	PHE
1	W	14	ARG
1	W	33	LEU
1	W	59	ARG
1	W	69	ASN
1	W	74	LEU
1	W	92	ARG
1	W	105	GLN
1	W	122	LEU
1	W	167	LEU
1	W	169	GLU
1	W	174	ASN
1	W	178	THR
1	W	188	LEU
1	W	208	LEU
1	W	217	ARG
1	W	226	THR
2	X	-36	LEU
2	X	-31	ASP
2	X	-17	ILE
2	X	329	ARG
2	X	338	ASP
2	X	348	THR
2	X	355	PHE
2	X	363	LEU
2	X	374	LEU
2	X	381	ASN
2	X	382	ARG
2	X	388	ARG
2	X	431	ILE
2	X	471	LEU
2	X	513	LEU
1	Y	7	ILE
1	Y	8	SER
1	Y	16	ARG
1	Y	26	ARG
1	Y	33	LEU
1	Y	59	ARG
1	Y	69	ASN

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Mol	Chain	Res	Type
1	Y	74	LEU
1	Y	92	ARG
1	Y	105	GLN
1	Y	114	GLN
1	Y	122	LEU
1	Y	178	THR
1	Y	181	LEU
1	Y	203	LEU
1	Y	208	LEU
1	Y	226	THR
1	Y	228	SER
2	Z	-34	SER
2	Z	-22	LEU
2	Z	329	ARG
2	Z	338	ASP
2	Z	348	THR
2	Z	354	GLU
2	Z	355	PHE
2	Z	363	LEU
2	Z	374	LEU
2	Z	381	ASN
2	Z	382	ARG
2	Z	432	GLU
2	Z	509	ARG
2	Z	510	ILE
2	Z	520	SER
2	2	-23	GLU
2	2	-5	GLN
2	2	329	ARG
2	2	355	PHE
2	2	363	LEU
2	2	374	LEU
2	2	413	ASP
2	2	433	GLU
2	2	503	VAL
2	2	513	LEU
2	2	519	GLU
1	1	7	ILE
1	1	10	GLU
1	1	13	MET
1	1	28	LYS
1	1	33	LEU

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Mol	Chain	Res	Type
1	1	59	ARG
1	1	69	ASN
1	1	74	LEU
1	1	92	ARG
1	1	105	GLN
1	1	116	LYS
1	1	122	LEU
1	1	173	GLU
1	1	174	ASN
1	1	181	LEU
1	1	189	ARG
1	1	208	LEU
1	1	226	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	69	ASN
1	A	73	ASN
1	A	105	GLN
1	A	165	ASN
1	B	51	GLN
1	B	69	ASN
1	B	101	ASN
1	B	105	GLN
1	B	114	GLN
1	B	152	HIS
1	B	165	ASN
2	C	430	ASN
2	C	456	GLN
1	D	11	GLN
1	D	51	GLN
1	D	69	ASN
1	D	105	GLN
1	D	165	ASN
2	E	-2	HIS
2	E	415	GLN
2	E	456	GLN
1	F	51	GLN
1	F	69	ASN
1	F	73	ASN

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Mol	Chain	Res	Type
1	F	101	ASN
1	F	105	GLN
1	F	165	ASN
2	G	456	GLN
2	H	-5	GLN
2	H	456	GLN
1	I	51	GLN
1	I	69	ASN
1	I	73	ASN
1	I	114	GLN
1	I	152	HIS
1	I	165	ASN
2	J	-2	HIS
2	J	456	GLN
1	K	51	GLN
1	K	69	ASN
1	K	73	ASN
1	K	101	ASN
1	K	129	HIS
2	L	-5	GLN
2	L	456	GLN
1	M	51	GLN
1	M	69	ASN
1	M	73	ASN
1	M	101	ASN
1	M	105	GLN
2	N	396	GLN
2	N	456	GLN
1	O	51	GLN
1	O	69	ASN
1	O	73	ASN
1	O	101	ASN
1	O	105	GLN
1	O	114	GLN
1	O	152	HIS
1	Q	51	GLN
1	Q	69	ASN
1	Q	73	ASN
1	Q	105	GLN
1	Q	114	GLN
2	R	-2	HIS
2	R	456	GLN

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Mol	Chain	Res	Type
1	S	69	ASN
1	S	73	ASN
1	S	101	ASN
1	S	105	GLN
1	S	114	GLN
1	S	174	ASN
2	T	-5	GLN
2	T	410	HIS
2	T	415	GLN
2	T	456	GLN
1	U	51	GLN
1	U	69	ASN
1	U	73	ASN
1	U	101	ASN
1	U	105	GLN
1	U	129	HIS
1	U	165	ASN
2	V	-26	GLN
2	V	-2	HIS
2	V	456	GLN
1	W	69	ASN
1	W	105	GLN
1	W	114	GLN
1	W	174	ASN
2	X	-5	GLN
2	X	456	GLN
1	Y	51	GLN
1	Y	69	ASN
1	Y	73	ASN
1	Y	165	ASN
2	Z	410	HIS
2	Z	456	GLN
2	2	-5	GLN
2	2	-2	HIS
2	2	415	GLN
2	2	456	GLN
1	1	11	GLN
1	1	69	ASN
1	1	73	ASN
1	1	105	GLN
1	1	152	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	1	219/248 (88%)	0.69	29 (13%) 4 3	48, 86, 121, 152	0
1	A	222/248 (89%)	0.24	13 (5%) 23 24	43, 81, 117, 145	0
1	B	220/248 (88%)	0.41	17 (7%) 14 14	48, 88, 127, 145	0
1	D	222/248 (89%)	0.41	19 (8%) 11 11	52, 92, 126, 144	0
1	F	221/248 (89%)	0.49	20 (9%) 10 10	45, 86, 126, 147	0
1	I	217/248 (87%)	0.29	13 (5%) 23 23	45, 80, 123, 149	0
1	K	221/248 (89%)	0.82	33 (14%) 3 2	48, 98, 135, 148	0
1	M	224/248 (90%)	0.28	12 (5%) 26 27	45, 78, 127, 147	0
1	O	218/248 (87%)	0.60	25 (11%) 5 5	50, 97, 137, 150	0
1	Q	222/248 (89%)	0.50	16 (7%) 16 16	48, 96, 131, 140	0
1	S	219/248 (88%)	0.51	17 (7%) 14 14	46, 85, 129, 140	0
1	U	221/248 (89%)	0.38	17 (7%) 14 14	49, 88, 130, 144	0
1	W	221/248 (89%)	0.51	19 (8%) 11 11	48, 81, 125, 149	0
1	Y	224/248 (90%)	0.41	17 (7%) 15 14	53, 93, 132, 142	0
2	2	246/291 (84%)	0.09	8 (3%) 47 50	48, 68, 97, 107	0
2	C	250/291 (85%)	0.13	10 (4%) 39 41	51, 73, 111, 143	0
2	E	248/291 (85%)	0.22	14 (5%) 25 26	30, 77, 115, 132	0
2	G	251/291 (86%)	0.02	5 (1%) 65 67	45, 67, 115, 141	0
2	H	249/291 (85%)	0.20	13 (5%) 28 29	45, 71, 113, 136	0
2	J	252/291 (86%)	0.09	8 (3%) 48 51	47, 70, 109, 135	0
2	L	251/291 (86%)	0.13	8 (3%) 48 51	51, 75, 116, 140	0
2	N	252/291 (86%)	0.12	8 (3%) 48 51	44, 70, 115, 144	0
2	P	250/291 (85%)	0.18	8 (3%) 48 51	47, 75, 114, 144	0
2	R	246/291 (84%)	0.16	9 (3%) 42 44	30, 82, 118, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	250/291 (85%)	-0.02	5 (2%) 65 67	40, 68, 110, 137	0
2	V	249/291 (85%)	-0.12	1 (0%) 92 92	47, 68, 112, 136	0
2	X	249/291 (85%)	0.11	11 (4%) 35 37	44, 65, 115, 144	0
2	Z	245/291 (84%)	0.05	7 (2%) 52 55	49, 73, 115, 131	0
All	All	6579/7546 (87%)	0.27	382 (5%) 24 24	30, 78, 124, 152	0

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	5	TYR	11.7
1	U	5	TYR	10.0
1	1	6	PHE	9.4
1	W	4	PRO	7.7
1	K	7	ILE	7.6
1	A	6	PHE	7.5
1	K	231	GLN	6.9
2	X	397	GLY	6.3
1	1	5	TYR	6.2
1	K	6	PHE	6.1
1	1	7	ILE	6.1
1	M	2	SER	5.8
1	Q	233	LEU	5.7
1	K	188	LEU	5.2
1	1	230	LEU	5.2
1	S	205	VAL	5.1
1	1	10	GLU	5.1
1	U	234	LEU	5.1
1	B	205	VAL	5.0
2	G	-17	ILE	4.9
1	O	188	LEU	4.8
2	H	-26	GLN	4.8
1	I	7	ILE	4.8
1	Y	191	GLY	4.7
1	I	6	PHE	4.6
1	U	203	LEU	4.6
1	F	6	PHE	4.6
1	F	234	LEU	4.6
1	Q	130	TYR	4.6
2	H	417	ALA	4.6
1	M	205	VAL	4.6
1	K	233	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	172	ALA	4.5
1	O	167	LEU	4.5
1	W	188	LEU	4.5
2	H	310	GLY	4.5
1	O	233	LEU	4.4
2	H	-39	ALA	4.4
1	S	191	GLY	4.4
2	H	-6	ALA	4.4
1	U	205	VAL	4.3
1	W	205	VAL	4.2
1	K	21	ARG	4.2
1	I	5	TYR	4.1
2	P	-17	ILE	4.1
1	K	205	VAL	4.1
1	U	232	ALA	4.0
1	S	172	ALA	4.0
1	S	169	GLU	4.0
1	K	225	ILE	3.9
1	B	5	TYR	3.9
1	O	235	VAL	3.9
1	1	203	LEU	3.9
1	W	3	PHE	3.9
1	O	225	ILE	3.9
1	O	192	SER	3.9
1	F	130	TYR	3.9
1	B	188	LEU	3.9
2	H	414	PRO	3.9
1	A	5	TYR	3.9
2	C	414	PRO	3.8
2	2	412	SER	3.8
1	W	204	GLY	3.7
2	C	415	GLN	3.7
1	K	235	VAL	3.7
1	W	6	PHE	3.7
2	E	397	GLY	3.7
1	S	192	SER	3.7
1	Y	169	GLU	3.6
1	U	167	LEU	3.6
1	Q	192	SER	3.6
1	D	188	LEU	3.6
2	R	499	ALA	3.6
2	T	-5	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	Q	169	GLU	3.6
1	B	231	GLN	3.6
1	W	133	THR	3.5
1	U	208	LEU	3.5
2	2	413	ASP	3.5
1	D	133	THR	3.5
1	B	167	LEU	3.5
1	D	177	LEU	3.5
1	F	188	LEU	3.5
1	F	203	LEU	3.5
1	U	6	PHE	3.5
1	Q	230	LEU	3.5
1	M	8	SER	3.5
1	D	3	PHE	3.4
1	Y	132	GLU	3.4
2	C	-27	ARG	3.4
1	D	192	SER	3.4
1	A	234	LEU	3.4
1	U	233	LEU	3.4
1	Q	232	ALA	3.4
1	O	169	GLU	3.4
2	H	-27	ARG	3.4
1	O	8	SER	3.4
1	F	5	TYR	3.4
1	F	230	LEU	3.4
1	Y	233	LEU	3.4
1	1	8	SER	3.4
1	1	229	ALA	3.4
1	O	10	GLU	3.4
1	K	206	ALA	3.4
1	K	229	ALA	3.3
2	L	414	PRO	3.3
2	X	351	VAL	3.3
1	A	188	LEU	3.3
1	S	6	PHE	3.3
1	I	226	THR	3.3
2	E	-25	ALA	3.3
2	H	-21	LEU	3.3
1	O	44	GLU	3.3
1	Q	188	LEU	3.3
1	Q	234	LEU	3.3
1	I	231	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	130	TYR	3.3
1	S	233	LEU	3.2
2	E	-19	ALA	3.2
1	M	5	TYR	3.2
2	C	413	ASP	3.2
2	G	413	ASP	3.2
1	K	171	TYR	3.2
1	U	171	TYR	3.2
1	B	204	GLY	3.2
2	H	415	GLN	3.2
2	L	415	GLN	3.2
2	X	-5	GLN	3.2
1	S	7	ILE	3.2
2	J	414	PRO	3.2
2	L	524	ALA	3.1
2	N	-38	VAL	3.1
1	Y	130	TYR	3.1
2	J	-18	SER	3.1
1	F	205	VAL	3.1
1	B	163	ILE	3.1
1	O	24	ILE	3.0
1	S	48	ARG	3.0
1	U	235	VAL	3.0
1	Q	3	PHE	3.0
1	B	171	TYR	3.0
1	U	231	GLN	3.0
1	D	205	VAL	3.0
2	X	395	MET	3.0
2	P	412	SER	3.0
2	R	412	SER	3.0
1	S	13	MET	3.0
1	W	189	ARG	3.0
1	M	234	LEU	3.0
1	Q	135	ARG	3.0
1	K	123	CYS	2.9
1	Y	8	SER	2.9
1	K	230	LEU	2.9
1	K	14	ARG	2.9
1	K	133	THR	2.9
2	X	398	LEU	2.9
1	F	233	LEU	2.9
1	F	161	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	1	9	PRO	2.9
2	L	310	GLY	2.9
1	D	167	LEU	2.9
1	W	130	TYR	2.9
1	K	181	LEU	2.9
2	N	-39	ALA	2.9
1	F	36	ALA	2.8
1	S	171	TYR	2.8
2	T	414	PRO	2.8
1	O	189	ARG	2.8
2	Z	349	ALA	2.8
2	E	-26	GLN	2.8
2	P	-26	GLN	2.8
2	R	395	MET	2.8
1	I	169	GLU	2.8
1	U	192	SER	2.8
1	1	48	ARG	2.8
2	2	407	TYR	2.8
1	S	113	GLU	2.8
1	F	204	GLY	2.8
1	B	230	LEU	2.7
2	P	499	ALA	2.7
1	F	169	GLU	2.7
2	L	-18	SER	2.7
1	W	231	GLN	2.7
1	D	191	GLY	2.7
2	C	397	GLY	2.7
1	B	189	ARG	2.7
2	2	415	GLN	2.7
1	K	234	LEU	2.7
1	S	227	GLY	2.7
1	Y	2	SER	2.7
2	P	519	GLU	2.7
2	E	413	ASP	2.7
1	K	48	ARG	2.7
2	H	411	ALA	2.6
1	K	177	LEU	2.6
1	F	131	GLY	2.6
2	2	416	SER	2.6
2	P	353	VAL	2.6
1	1	169	GLU	2.6
1	Q	216	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	4	PRO	2.6
2	C	499	ALA	2.6
2	J	417	ALA	2.6
1	1	228	SER	2.6
1	Y	231	GLN	2.6
1	K	10	GLU	2.6
1	B	159	THR	2.5
1	K	232	ALA	2.5
1	O	12	ALA	2.5
2	2	519	GLU	2.6
1	K	204	GLY	2.5
2	Z	397	GLY	2.5
2	J	395	MET	2.5
1	K	5	TYR	2.5
1	I	233	LEU	2.5
1	K	185	VAL	2.5
1	M	203	LEU	2.5
1	A	177	LEU	2.5
1	B	208	LEU	2.5
1	A	7	ILE	2.5
2	C	-26	GLN	2.5
1	D	234	LEU	2.5
1	O	38	GLY	2.5
2	X	-4	LEU	2.5
1	1	113	GLU	2.5
1	M	9	PRO	2.5
2	C	-39	ALA	2.5
1	W	190	ALA	2.5
1	Y	204	GLY	2.5
2	R	-25	ALA	2.5
1	F	10	GLU	2.5
1	F	171	TYR	2.4
1	1	204	GLY	2.4
2	X	409	ILE	2.4
1	Q	191	GLY	2.4
2	N	-26	GLN	2.4
2	N	414	PRO	2.4
1	A	10	GLU	2.4
2	T	-16	SER	2.4
1	I	48	ARG	2.4
2	C	-30	PHE	2.4
2	N	396	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	393	ALA	2.4
2	T	417	ALA	2.4
2	N	412	SER	2.4
2	L	-38	VAL	2.4
1	A	130	TYR	2.4
1	D	231	GLN	2.4
1	F	189	ARG	2.4
2	E	415	GLN	2.4
2	H	407	TYR	2.4
1	F	132	GLU	2.4
1	K	227	GLY	2.4
2	2	-27	ARG	2.4
2	E	395	MET	2.4
1	B	178	THR	2.4
2	G	-26	GLN	2.4
1	K	208	LEU	2.4
1	M	10	GLU	2.3
1	A	228	SER	2.3
1	I	133	THR	2.3
1	O	230	LEU	2.3
1	B	48	ARG	2.3
1	1	189	ARG	2.3
1	A	163	ILE	2.3
1	O	171	TYR	2.3
2	R	-19	ALA	2.3
1	Y	208	LEU	2.3
1	1	223	ARG	2.3
2	X	396	GLN	2.3
1	O	216	ASN	2.3
1	W	228	SER	2.3
1	D	189	ARG	2.3
1	U	230	LEU	2.3
1	Y	203	LEU	2.3
1	1	46	PRO	2.3
1	K	159	THR	2.3
1	O	191	GLY	2.3
1	U	181	LEU	2.3
2	J	-22	LEU	2.3
2	2	355	PHE	2.3
1	W	230	LEU	2.3
2	N	486	LEU	2.3
1	U	113	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	-27	ARG	2.3
2	N	523	GLY	2.3
2	E	-30	PHE	2.3
1	I	167	LEU	2.3
1	Y	161	GLU	2.3
1	1	123	CYS	2.3
1	M	13	MET	2.2
1	Y	131	GLY	2.2
1	D	190	ALA	2.2
1	1	132	GLU	2.2
1	1	207	SER	2.2
2	T	519	GLU	2.2
2	X	400	ALA	2.2
2	Z	393	ALA	2.2
1	S	130	TYR	2.2
1	1	214	ASP	2.2
2	L	523	GLY	2.2
2	E	-23	GLU	2.2
1	O	7	ILE	2.2
1	O	229	ALA	2.2
1	I	132	GLU	2.2
1	Q	205	VAL	2.2
1	O	232	ALA	2.2
1	S	206	ALA	2.2
1	W	172	ALA	2.2
2	P	-39	ALA	2.2
1	D	227	GLY	2.2
2	R	397	GLY	2.2
1	B	130	TYR	2.2
2	C	412	SER	2.2
1	A	18	GLU	2.2
1	Q	231	GLN	2.2
1	W	132	GLU	2.2
1	1	63	ALA	2.2
1	D	169	GLU	2.2
2	X	-18	SER	2.2
1	S	225	ILE	2.2
1	M	3	PHE	2.2
2	G	-27	ARG	2.2
2	Z	355	PHE	2.2
1	F	51	GLN	2.1
2	J	410	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	184	ALA	2.1
1	D	48	ARG	2.1
1	D	101	ASN	2.1
1	D	225	ILE	2.1
1	U	169	GLU	2.1
1	W	123	CYS	2.1
1	K	15	GLU	2.1
1	1	172	ALA	2.1
1	1	227	GLY	2.1
1	Q	153	PHE	2.1
2	Z	395	MET	2.1
1	F	37	GLY	2.1
2	H	418	GLY	2.1
2	J	-25	ALA	2.1
2	H	-5	GLN	2.1
2	J	411	ALA	2.1
2	X	487	VAL	2.1
1	Y	159	THR	2.1
2	E	414	PRO	2.1
1	B	153	PHE	2.1
1	1	208	LEU	2.1
1	1	120	VAL	2.1
1	W	48	ARG	2.1
1	Y	171	TYR	2.1
1	B	233	LEU	2.1
1	M	49	SER	2.1
1	O	207	SER	2.1
2	V	398	LEU	2.1
2	R	-26	GLN	2.1
2	Z	396	GLN	2.1
2	R	411	ALA	2.0
1	1	171	TYR	2.0
1	A	203	LEU	2.0
1	D	230	LEU	2.0
1	I	181	LEU	2.0
1	S	231	GLN	2.0
1	1	122	LEU	2.0
1	1	188	LEU	2.0
2	E	398	LEU	2.0
2	G	396	GLN	2.0
1	I	191	GLY	2.0
1	O	158	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	L	-25	ALA	2.0
2	Z	352	ALA	2.0
1	W	234	LEU	2.0
1	Y	7	ILE	2.0
1	M	6	PHE	2.0
1	A	229	ALA	2.0
1	O	25	ALA	2.0
1	Y	11	GLN	2.0
1	K	192	SER	2.0
2	E	-38	VAL	2.0
1	Q	158	GLY	2.0
1	K	163	ILE	2.0
2	E	355	PHE	2.0
2	R	-3	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.