Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 03:27 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

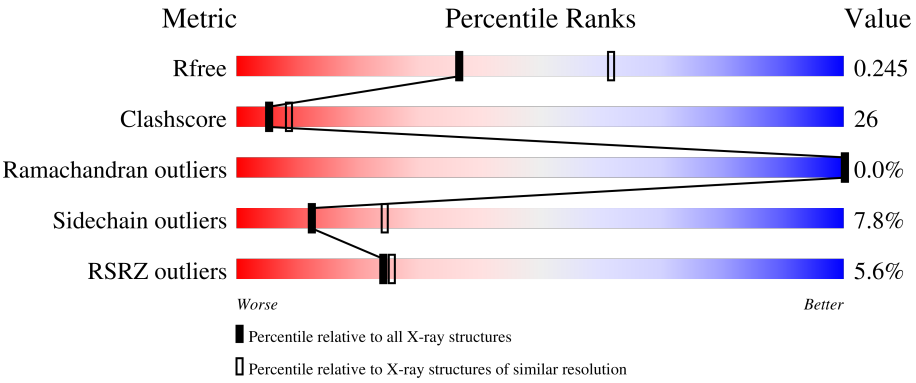
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	248	12% 54% 29% • 12%
1	A	248	5% 49% 38% • 10%
1	B	248	7% 53% 31% 5% 11%
1	D	248	7% 54% 31% 5% 10%
1	F	248	8% 54% 31% • 11%

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Mol	Chain	Length	Quality of chain
1	I	248	5% 55% 27% 5% 12%
1	K	248	13% 48% 36% 6% 11%
1	M	248	4% 56% 29% 5% 10%
1	O	248	10% 51% 33% 12%
1	Q	248	6% 48% 36% 6% 10%
1	S	248	6% 50% 35% 12%
1	U	248	7% 50% 33% 6% 11%
1	W	248	8% 54% 29% 5% 11%
1	Y	248	6% 53% 33% 5% 10%
2	2	291	3% 61% 21% 15%
2	C	291	4% 59% 24% 14%
2	E	291	4% 54% 28% 15%
2	G	291	% 64% 21% 14%
2	H	291	4% 60% 24% 14%
2	J	291	3% 62% 22% 13%
2	L	291	2% 57% 25% 14%
2	N	291	3% 64% 20% 13%
2	P	291	3% 61% 21% 14%
2	R	291	3% 60% 23% 15%
2	T	291	2% 62% 23% 14%
2	V	291	63% 21% 14%
2	X	291	3% 59% 23% 14%
2	Z	291	2% 57% 25% 16%

2 Entry composition (i)

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 mutation	UNP O33245
E	301	ALA	THR	engineered mutation	UNP O33245
G	301	ALA	THR	engineered mutation	UNP O33245
H	301	ALA	THR	engineered mutation	UNP O33245
J	301	ALA	THR	engineered mutation	UNP O33245
L	301	ALA	THR	engineered mutation	UNP O33245
N	301	ALA	THR	engineered mutation	UNP O33245
P	301	ALA	THR	engineered mutation	UNP O33245
R	301	ALA	THR	engineered mutation	UNP O33245
T	301	ALA	THR	engineered mutation	UNP O33245
V	301	ALA	THR	engineered mutation	UNP O33245
X	301	ALA	THR	engineered mutation	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	301	ALA	THR	engineered mutation	UNP O33245
2	301	ALA	THR	engineered mutation	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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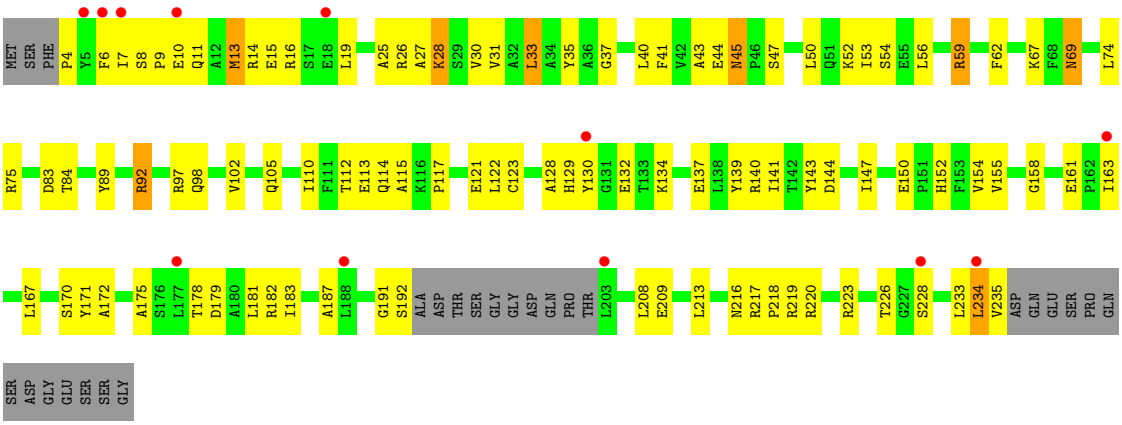
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	T	3	Total O 3 3	0	0
3	U	2	Total O 2 2	0	0
3	V	4	Total O 4 4	0	0
3	W	6	Total O 6 6	0	0
3	X	2	Total O 2 2	0	0
3	Y	6	Total O 6 6	0	0
3	Z	5	Total O 5 5	0	0
3	2	5	Total O 5 5	0	0
3	1	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

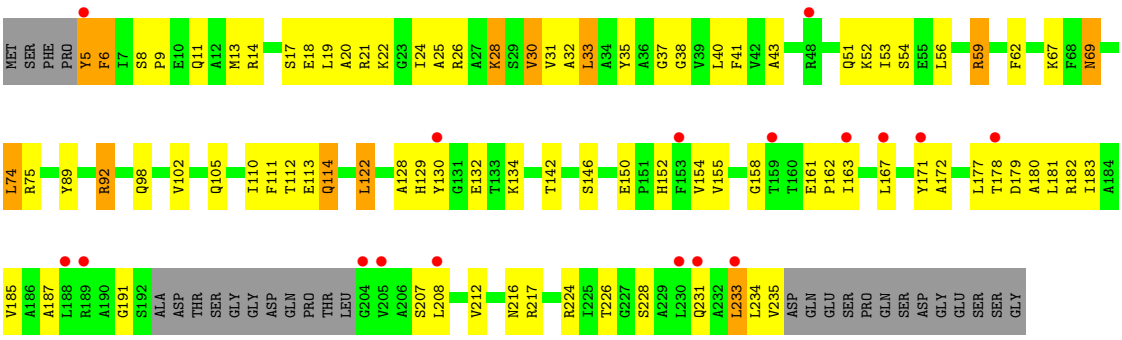
• Molecule 1: Proteasome subunit alpha

Chain A:



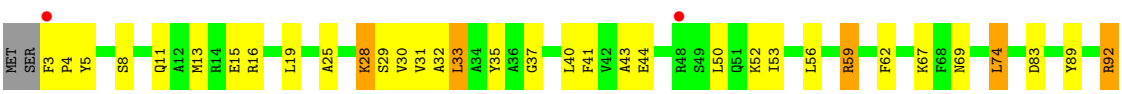
• Molecule 1: Proteasome subunit alpha

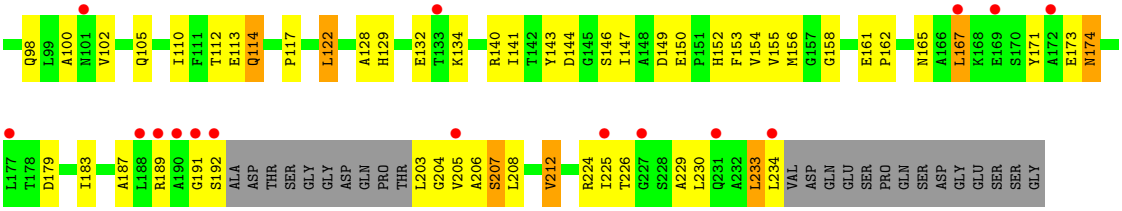
Chain B:



• Molecule 1: Proteasome subunit alpha

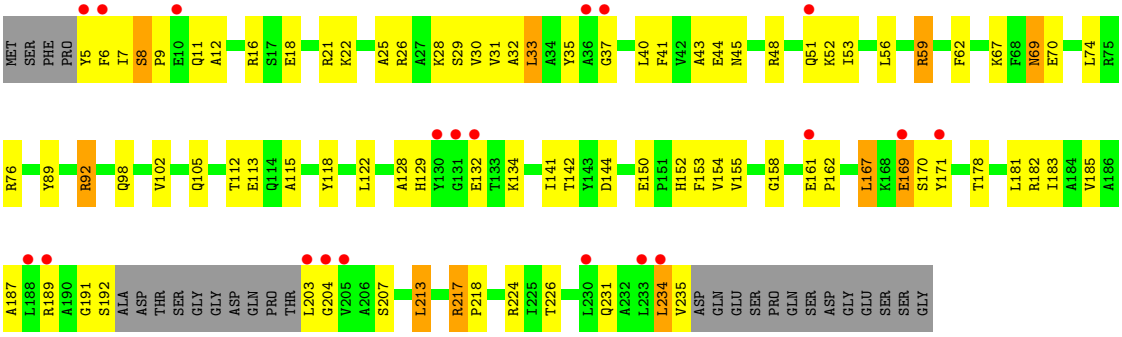
Chain D:





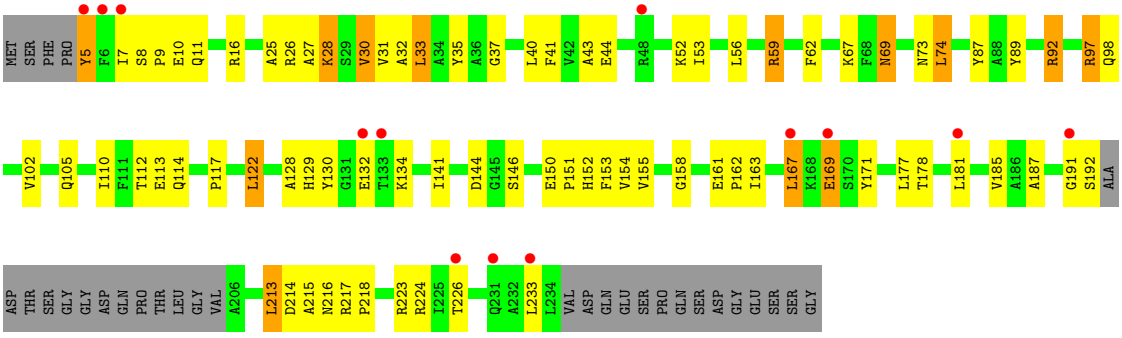
• Molecule 1: Proteasome subunit alpha

Chain F:



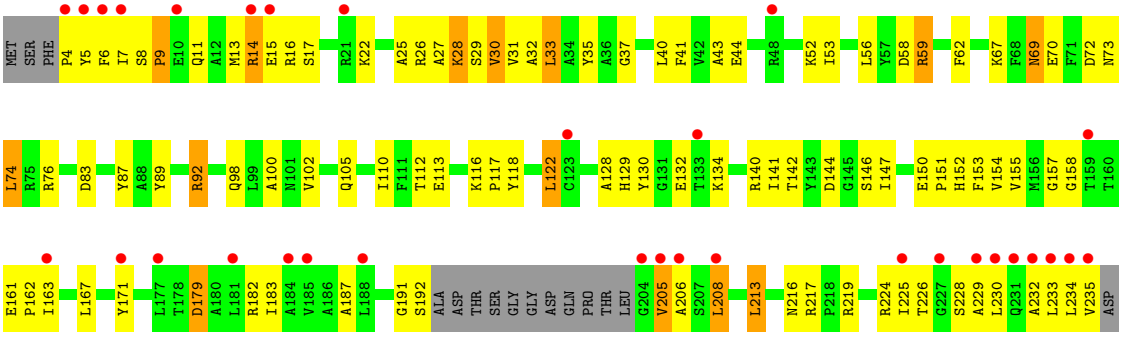
• Molecule 1: Proteasome subunit alpha

Chain I:



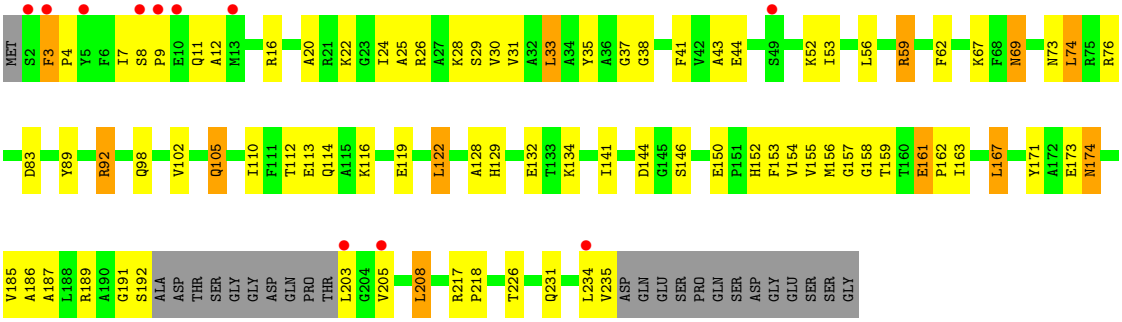
• Molecule 1: Proteasome subunit alpha

Chain K:



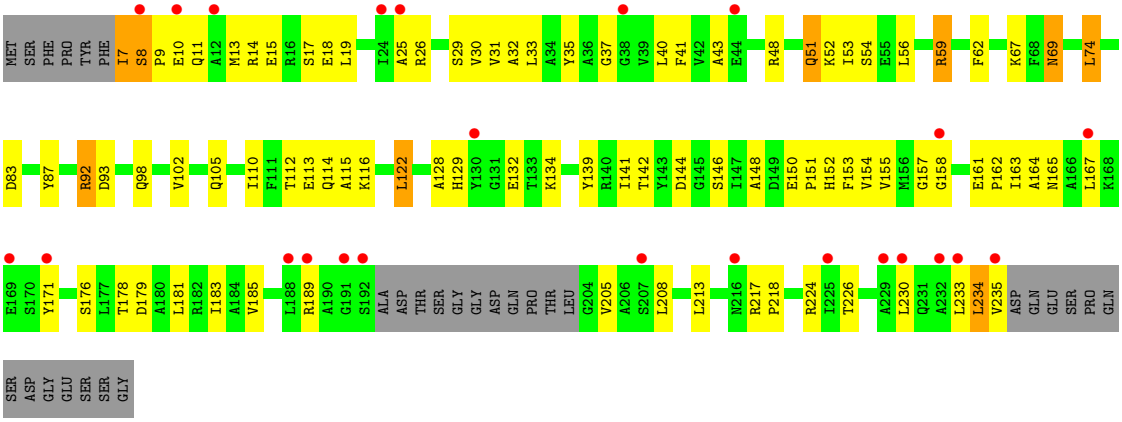
• Molecule 1: Proteasome subunit alpha

Chain M:



• Molecule 1: Proteasome subunit alpha

Chain O:

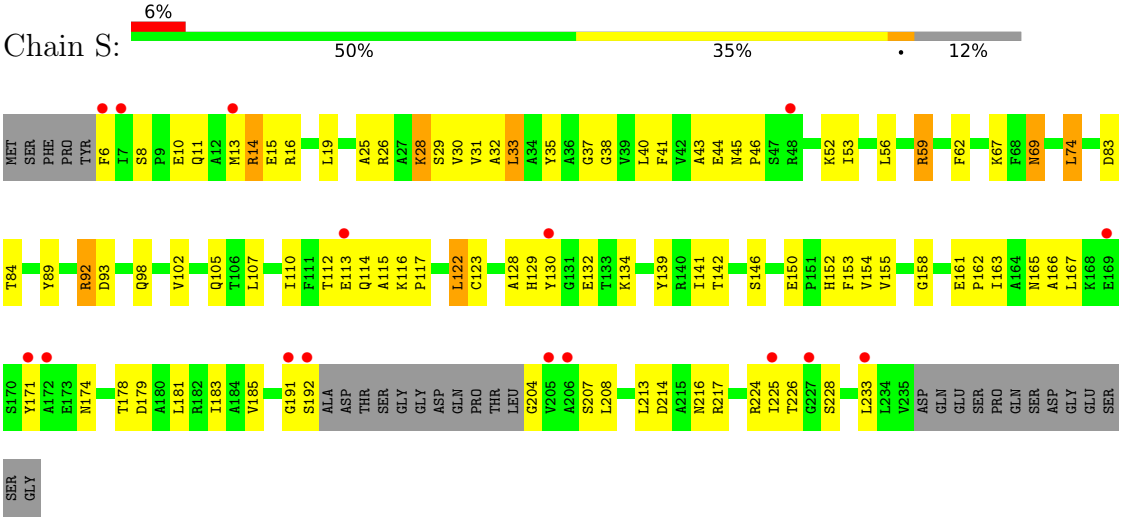


• Molecule 1: Proteasome subunit alpha

Chain Q:

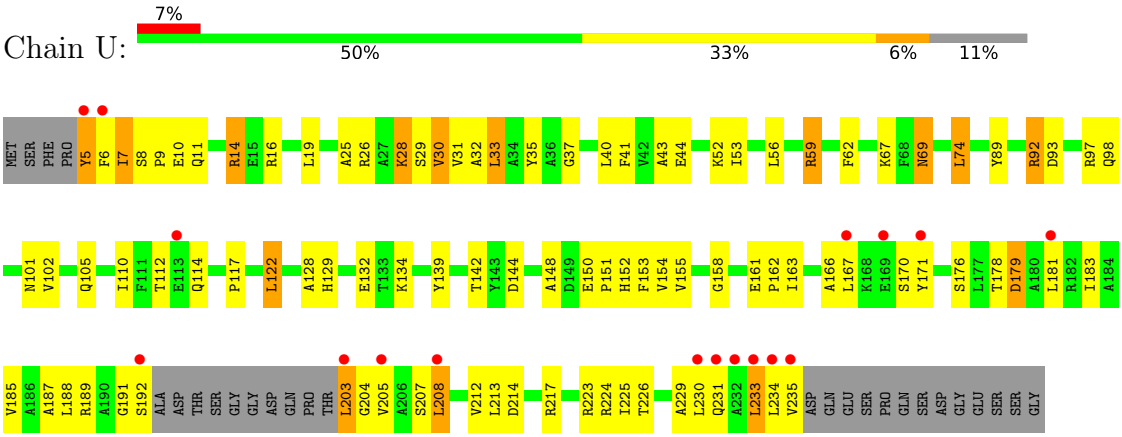
• Molecule 1: Proteasome subunit alpha

Chain S:



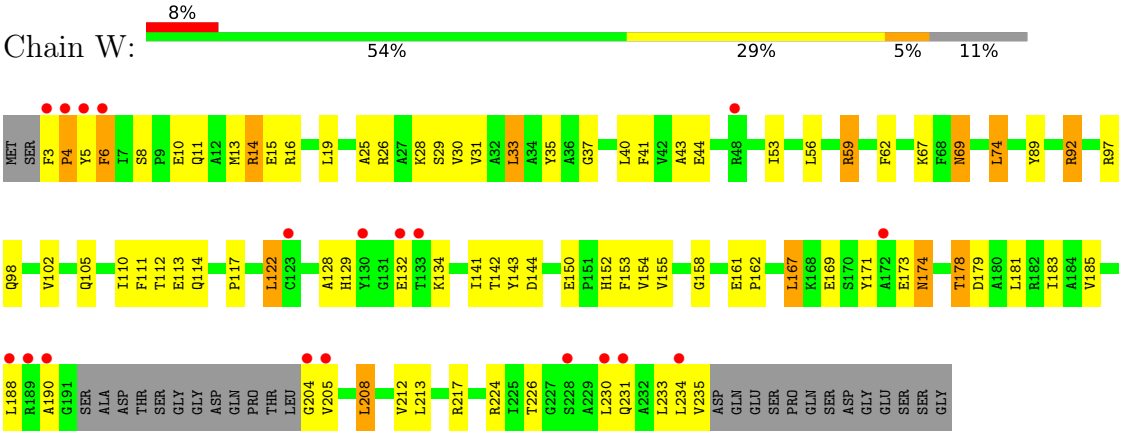
• Molecule 1: Proteasome subunit alpha

Chain U:



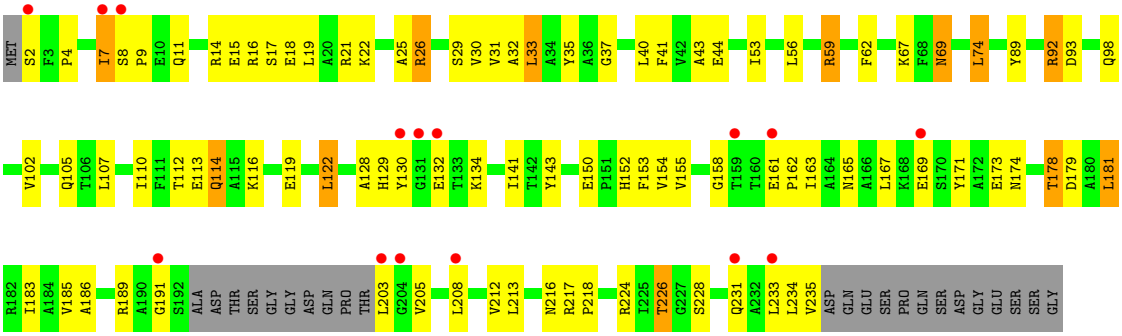
• Molecule 1: Proteasome subunit alpha

Chain W:



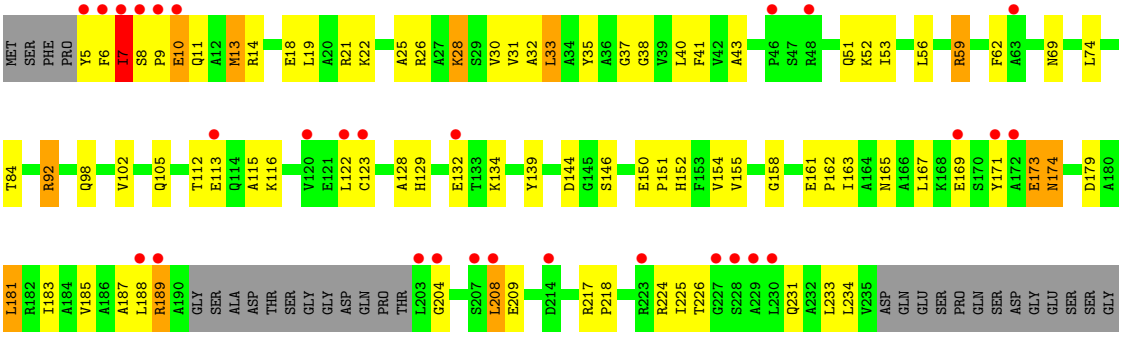
• Molecule 1: Proteasome subunit alpha

Chain Y:



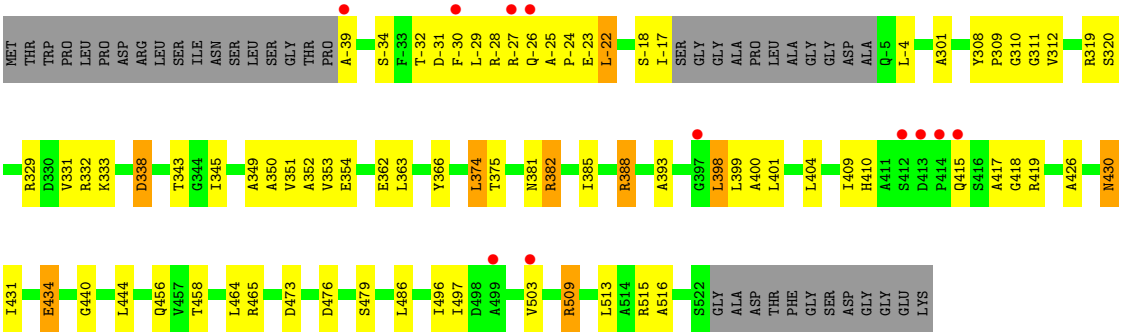
• Molecule 1: Proteasome subunit alpha

Chain 1:



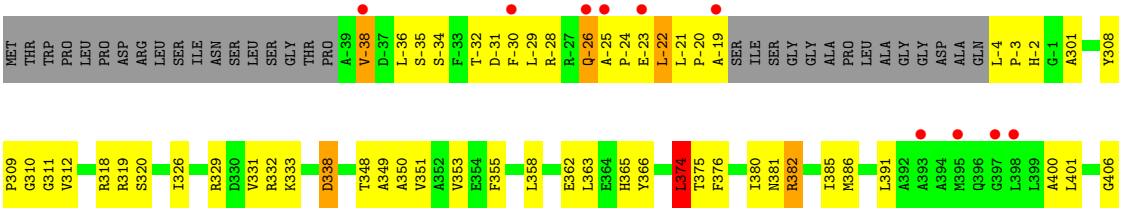
• Molecule 2: Proteasome subunit beta

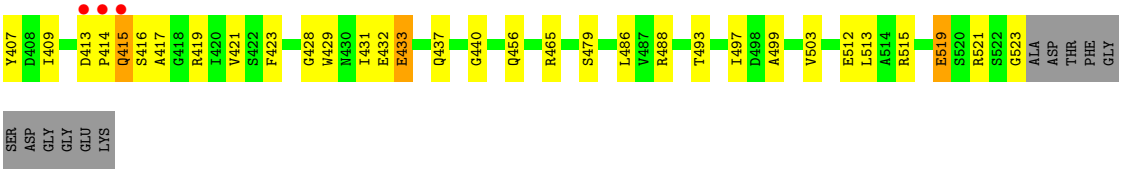
Chain C:



• Molecule 2: Proteasome subunit beta

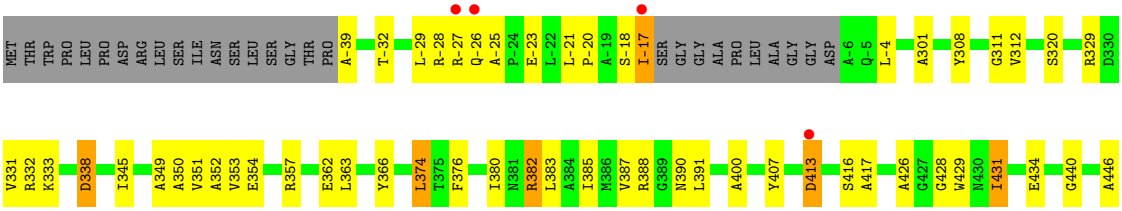
Chain E:

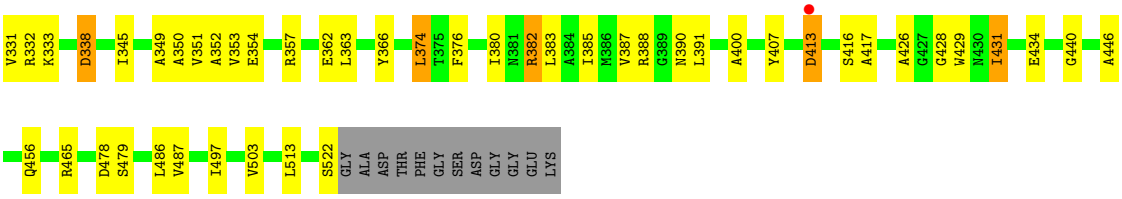




• Molecule 2: Proteasome subunit beta

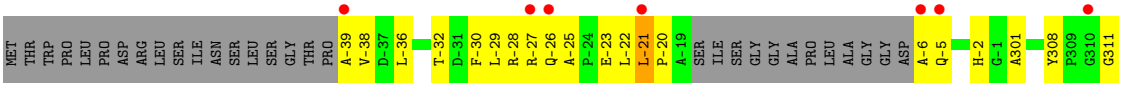
Chain G:





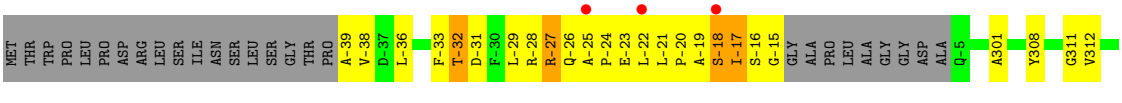
• Molecule 2: Proteasome subunit beta

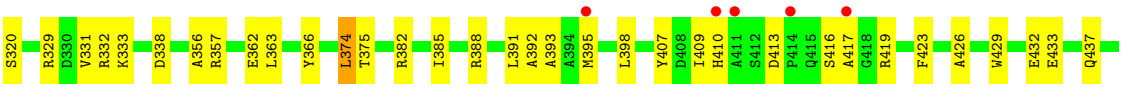
Chain H:

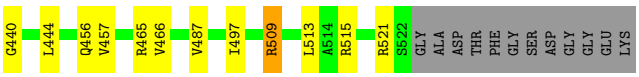


• Molecule 2: Proteasome subunit beta

Chain J:

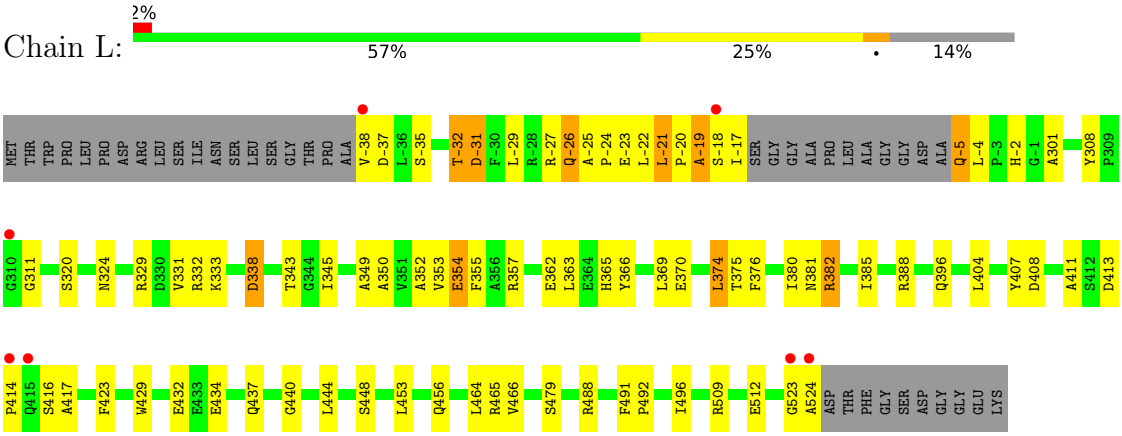






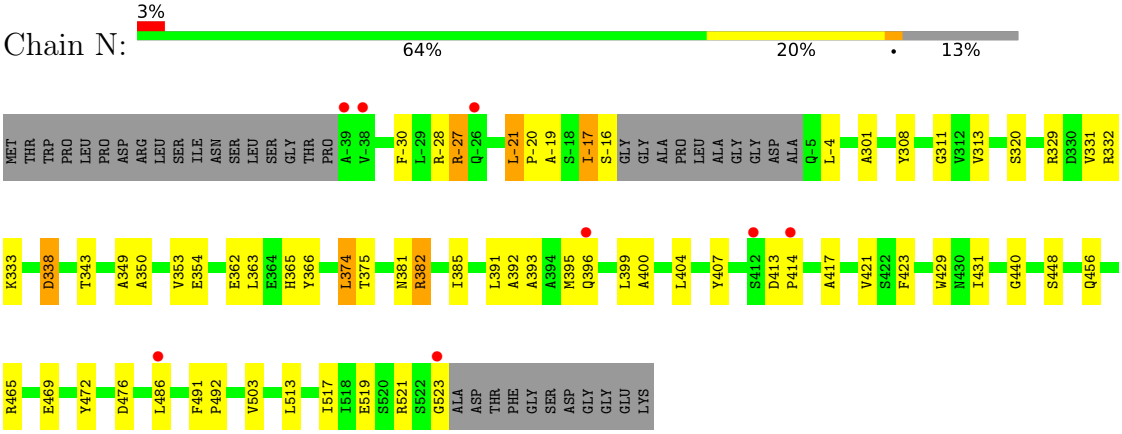
• Molecule 2: Proteasome subunit beta

Chain L:



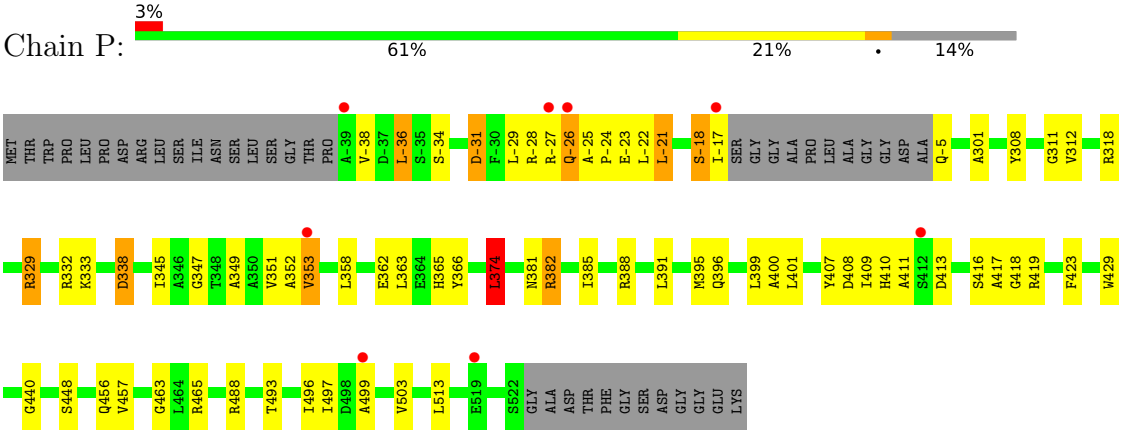
• Molecule 2: Proteasome subunit beta

Chain N:



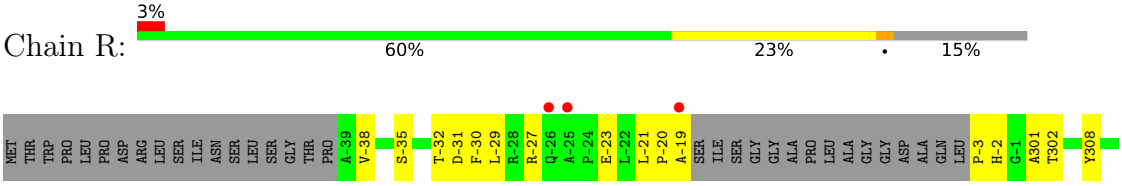
• Molecule 2: Proteasome subunit beta

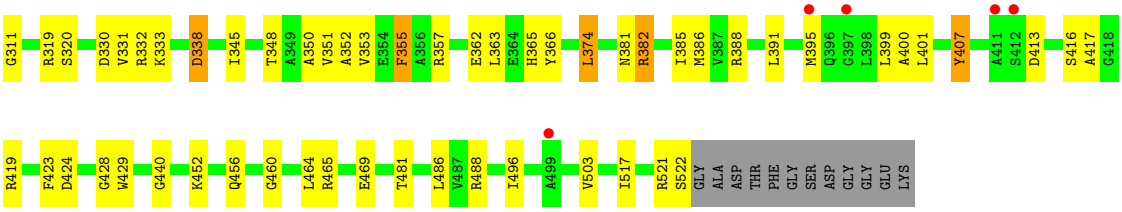
Chain P:



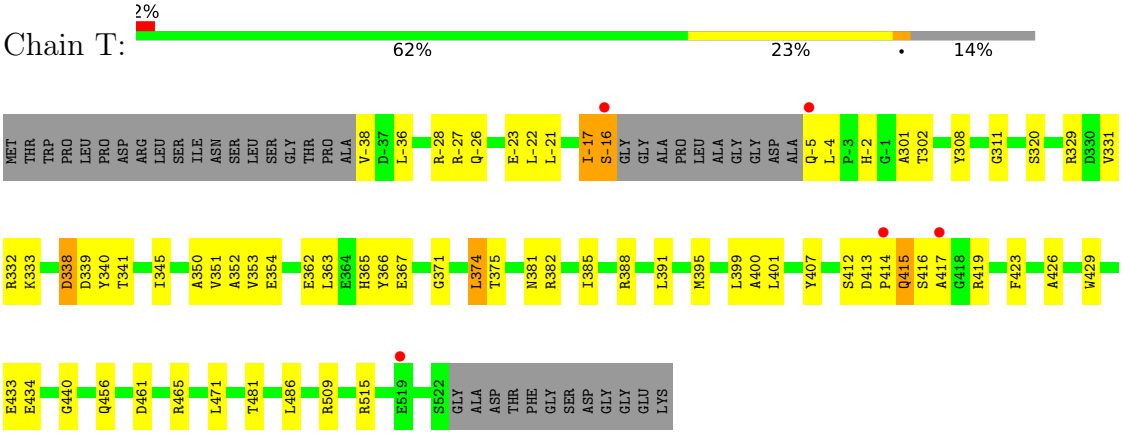
• Molecule 2: Proteasome subunit beta

Chain R:

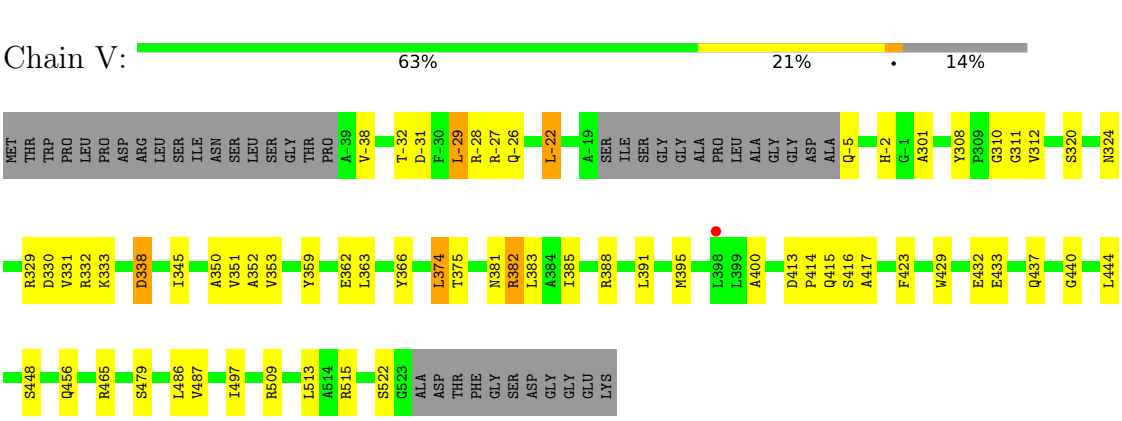




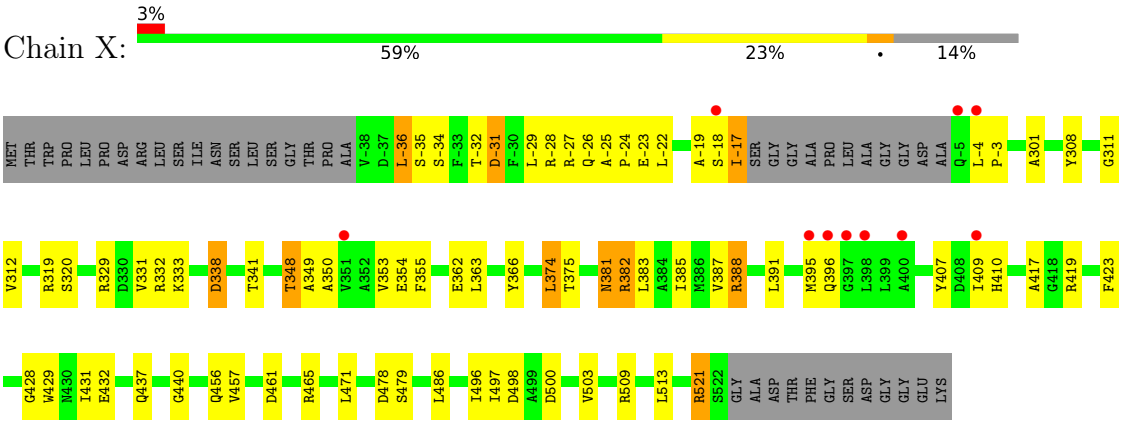
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

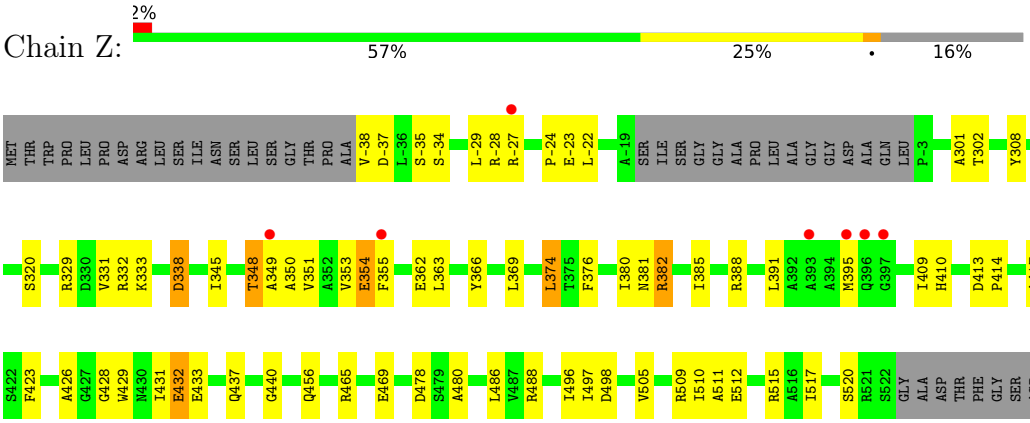


• Molecule 2: Proteasome subunit beta



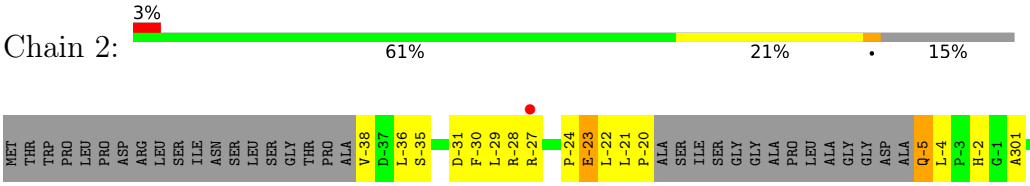
• Molecule 2: Proteasome subunit beta

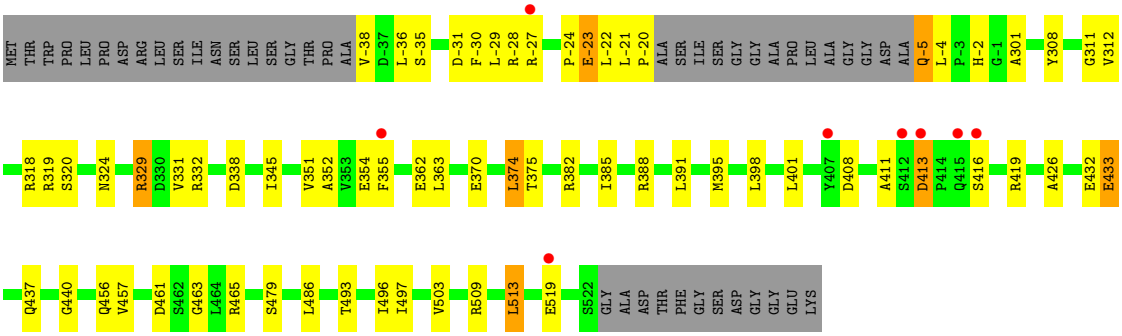
Chain Z:



• Molecule 2: Proteasome subunit beta

Chain 2:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.74 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.247 0.215 , 0.245	Depositor DCC
R_{free} test set	11802 reflections (5.05%)	wwPDB-VP
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]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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:HD12	1:Y:181:LEU:O	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:H:-27:ARG:HG2	2:H:-26:GLN:OE1	1.39	1.18
2:N:-17:ILE:CD1	2:N:392:ALA:HB3	1.74	1.18
1:A:7:ILE:O	1:B:5:TYR:HB3	1.42	1.18
2:N:413:ASP:OD1	2:N:414:PRO:HD2	1.40	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
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:T:426:ALA:HB2	2:2:-4:LEU:HD21	1.26	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
2:H:-6:ALA:N	2:H:-5:GLN:HB3	1.38	1.12
2:H:407:TYR:CE1	2:H:417:ALA:CB	2.31	1.12
1:S:35:TYR:CE1	1:S:37:GLY:CA	2.30	1.13
1:B:40:LEU:HD12	1:B:212:VAL:HG12	1.31	1.12
2:T:415:GLN:N	2:T:415:GLN:HE21	1.45	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
1:M:7:ILE:HG21	1:W:5:TYR:CE2	1.86	1.10
2:V:456:GLN:NE2	2:V:465:ARG:HH22	1.47	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:NE2	1:O:51:GLN:H	1.49	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:-17:ILE:O	2:T:-16:SER:HB2	1.47	1.09
1:1:8:SER:CB	1:1:11:GLN:HE21	1.64	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:D:3:PHE:CZ	1:F:6:PHE:HZ	1.70	1.08
1:W:181:LEU:O	1:W:185:VAL:HG23	1.53	1.08
1:U:35:TYR:CE1	1:U:37:GLY:CA	2.36	1.07
2:G:456:GLN:HE22	2:G:465:ARG:NH2	1.51	1.07
1:1:167:LEU:CD1	1:1:187:ALA:CB	2.33	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
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
1:1:8:SER:OG	1:1:11:GLN:HG2	1.56	1.05
2:C:456:GLN:NE2	2:C:465:ARG:HH22	1.53	1.04
1:I:181:LEU:O	1:I:185:VAL:HG23	1.56	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
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
2:R:456:GLN:HE22	2:R:465:ARG:NH2	1.55	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)
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:Z:348:THR:HB	2:Z:351:VAL:HG23	1.40	1.03
2:V:301:ALA:HB2	2:V:333:LYS:HZ3	1.20	1.02
1:M:7:ILE:HD13	1:W:5:TYR:HD2	1.12	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: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:H:-6:ALA:N	2:H:-5:GLN:CB	2.18	1.01
2:X:301:ALA:HB2	2:X:333:LYS:NZ	1.74	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
2:L:456:GLN:HE22	2:L:465:ARG:NH2	1.60	0.99
1:1:181:LEU:HD12	1:1:181:LEU:O	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:OE1	2:L:-26:GLN:HA	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	3:1:250:HOH:O	1.62	0.98
2:C:456:GLN:HE22	2:C:465:ARG:NH2	1.62	0.97
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.45	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:K:6:PHE:HB3	1:Q:4:PRO:HG3	1.45	0.97
1:Q:35:TYR:CZ	1:Q:37:GLY:HA3	1.98	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:M:7:ILE:CD1	1:W:5:TYR:HD2	1.78	0.96
1:1:179:ASP:O	1:1:183:ILE:HG13	1.65	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:N	1:O:51:GLN:HE21	1.67	0.93
2:J:-39:ALA:HA	2:T:-26:GLN:OE1	1.69	0.93
1:1:7:ILE:HB	1:1:11:GLN:HG3	1.46	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:HG2	2:X:521:ARG:HH11	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:H	1:O:51:GLN:HE21	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
2:C:-39:ALA:N	2:J:-26:GLN:CD	2.24	0.91
1:Y:179:ASP:O	1:Y:183:ILE:HG13	1.69	0.91
1:Y:181:LEU:HD12	1:Y:181:LEU:C	1.82	0.91
1:1:8:SER:N	1:1:11:GLN:HE21	1.67	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
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
1:1:8:SER:HB3	1:1:11:GLN:HE21	1.36	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
1:M:7:ILE:CG2	1:W:5:TYR:CE2	2.55	0.89
2:T:308:TYR:CZ	2:T:311:GLY:HA3	2.08	0.89
2:J:487:VAL:HG13	2:R:522:SER:O	1.71	0.89
2:R:456:GLN:HE22	2:R:465:ARG:HH22	0.91	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:HH11	2:X:521:ARG:CG	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:O	2:X:-17:ILE:HG12	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:HD23	1:O:19:LEU:C	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: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:HD22	1:W:174:ASN:N	1.73	0.86
1:1:8:SER:H	1:1:11:GLN:NE2	1.71	0.86
2:R:308:TYR:CZ	2:R:311:GLY:HA3	2.10	0.86
1:D:208:LEU:CD1	1:D:208:LEU:N	2.38	0.86
2:J:426:ALA:HB2	2:T:-4:LEU:HD21	1.55	0.86
1:B:22:LYS:O	1:B:26:ARG:HG3	1.75	0.86
1:B:178:THR:HA	1:B:233:LEU:CD2	2.05	0.86
1:1:8:SER:HB3	1:1:11:GLN:NE2	1.91	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:C	1:K:234:LEU:HD13	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: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
2:2:-28:ARG:HG2	2:2:-21:LEU:HD11	1.56	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:35:TYR:CD1	1:O:37:GLY:N	2.44	0.84
1:O:155:VAL:CG2	1:O:167:LEU:CD1	2.56	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
1:1:167:LEU:HD13	1:1:187:ALA:HB1	1.58	0.84
2:X:509:ARG:HH11	2:X:509:ARG:HG3	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:OE1	2:P:-26:GLN:HA	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:HE21	1:I:114:GLN:HA	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:8:SER:HG	1:O:11:GLN:HB3	1.42	0.82
1:O:155:VAL:HG21	1:O:167:LEU:CD1	2.09	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:K:4:PRO:HG3	1:W:5:TYR:CB	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:CG	2.15	0.81
1:A:6:PHE:HB3	1:B:5:TYR:HB2	1.62	0.81
1:F:25:ALA:O	1:F:158:GLY:HA2	1.80	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:T:426:ALA:CB	2:2:-4:LEU:HD21	2.09	0.81
2:2:456:GLN:HE22	2:2:465:ARG:HH22	1.28	0.81
2:C:-39:ALA:N	2:J:-26:GLN:NE2	2.29	0.81
1:I:129:HIS:HE1	3:I:250:HOH:O	1.63	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:OE1	2:G:-26:GLN:HA	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:OE1	2:L:354:GLU:CA	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:O	2:X:-17:ILE:CG1	2.30	0.80
1:M:7:ILE:HG21	1:W:5:TYR:HD2	1.27	0.80
1:U:59:ARG:HD2	1:U:129:HIS:HA	1.64	0.80
1:U:97:ARG:HH22	1:U:101:ASN:ND2	1.77	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: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
1:Q:230:LEU:O	1:Q:234:LEU:CD1	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:308:TYR:CZ	2:2:311:GLY:HA3	2.16	0.79
2:E:415:GLN:HE21	2:E:415:GLN:CA	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:HD23	1:U:233:LEU:H	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
2:C:434:GLU:OE1	2:C:434:GLU:CA	2.30	0.79
2:L:-18:SER:O	2:L:-17:ILE:CG2	2.30	0.79
1:1:8:SER:OG	1:1:11:GLN:CG	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:OE1	2:L:354:GLU:HA	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
2:C:-39:ALA:H2	2:J:-26:GLN:CD	1.85	0.78
2:G:456:GLN:HE22	2:G:465:ARG:HH22	0.81	0.78
1:Y:169:GLU:HA	1:Y:169:GLU:OE1	1.83	0.78
1:1:18:GLU:OE1	1:1:22:LYS:CE	2.30	0.78
1:F:169:GLU:HA	1:F:169:GLU:OE1	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:NE2	2:T:415:GLN:HA	1.97	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
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
1:K:4:PRO:CB	1:W:5:TYR:CG	2.67	0.78
2:L:308:TYR:CZ	2:L:311:GLY:HA3	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:153:PHE:CD2	1:Q:171:TYR:HD1	2.01	0.78
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: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: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
2:2:456:GLN:NE2	2:2:465:ARG:HH22	1.79	0.78
1:1:59:ARG:HD2	1:1:129:HIS:HA	1.65	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:HD13	1:O:234:LEU:C	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:N	1:W:174:ASN:ND2	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:-27:ARG:CG	2:H:-26:GLN:OE1	2.30	0.76
2:H:-23:GLU:HG2	2:P:-28:ARG:NH2	2.00	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:W:59:ARG:HD2	1:W:129:HIS:HA	1.68	0.75
1:1:173:GLU:CG	1:1:174:ASN:OD1	2.34	0.75
2:H:-32:THR:HG23	2:H:362:GLU:OE1	1.87	0.75
2:L:-26:GLN:OE1	2:L:-26:GLN:CA	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: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
2:Z:348:THR:CB	2:Z:351:VAL:CG2	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:25:ALA:O	1:1:158:GLY:HA2	1.86	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
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
1:1:167:LEU:HD11	1:1:187:ALA:CB	2.16	0.74
2:J:433:GLU:OE1	2:J:433:GLU:HA	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: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
1:1:150:GLU:HG3	1:1:154:VAL:HG22	1.69	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
2:G:-39:ALA:HB1	2:X:-26:GLN:OE1	1.88	0.73
1:Q:234:LEU:O	1:Q:235:VAL:HG23	1.88	0.73
1:O:35:TYR:HE1	1:O:37:GLY:HA3	1.45	0.73
1:1:33:LEU:CD1	1:1:40:LEU:HB3	2.18	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
1:1:152:HIS:CD2	1:1:171:TYR:HE2	2.07	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:F:5:TYR:HD1	1:W:11:GLN:HE22	1.37	0.72
2:J:465:ARG:HB3	2:J:465:ARG:NH1	2.04	0.72
1:M:154:VAL:HA	3:M:250:HOH:O	1.90	0.72
1:W:3:PHE:N	1:W:4:PRO:CA	2.51	0.72
2:2:413:ASP:OD1	2:2:416:SER:CB	2.30	0.72
1:1:35:TYR:CE1	1:1:37:GLY:HA3	2.24	0.72
1:S:115:ALA:HB1	1:U:6:PHE:CZ	2.25	0.72
2:X:509:ARG:HG3	2:X:509:ARG:NH1	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:33:LEU:H	1:K:33:LEU:HD12	1.54	0.72
1:K:152:HIS:CB	1:K:171:TYR:CE2	2.72	0.72
1:M:16:ARG:HB3	1:M:16:ARG:HH11	1.55	0.72
2:P:-26:GLN:OE1	2:P:-26:GLN:CA	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:CD1	1:Q:234:LEU:H	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
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
2:2:-28:ARG:CG	2:2:-21:LEU:HD11	2.21	0.71
1:D:35:TYR:CZ	1:D:37:GLY:HA3	2.21	0.71
1:F:11:GLN:OE1	1:F:11:GLN:HA	1.89	0.71
2:R:-30:PHE:HZ	2:Z:-38:VAL:CG2	2.04	0.71
2:X:350:ALA:O	2:X:353:VAL:HG12	1.91	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
1:1:167:LEU:HD12	1:1:187:ALA:HB2	1.70	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: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:41:PHE:HB3	1:U:53:ILE:HD13	1.71	0.70
1:U:176:SER:OG	1:U:179:ASP:CG	2.30	0.70
1:1:33:LEU:HD11	1:1:40:LEU:HB3	1.73	0.70
1:1:181:LEU:HD12	1:1:181:LEU:C	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:33:LEU:CD1	1:B:40:LEU:HB3	2.22	0.70
1:B:152:HIS:HB3	1:B:171:TYR:CE2	2.26	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
1:A:15:GLU:HB3	1:B:9:PRO:HG2	1.73	0.70
2:H:332:ARG:NH1	2:H:332:ARG:HB2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	2:N:332:ARG:HB2	2.07	0.70
2:T:338:ASP:C	2:T:338:ASP:OD1	2.29	0.70
2:T:415:GLN:N	2:T:415:GLN:NE2	2.30	0.70
2:2:362:GLU:OE2	2:2:382:ARG:HD3	1.92	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:C	1:O:234:LEU:CD1	2.60	0.70
2:P:465:ARG:HG3	2:P:513:LEU:HD11	1.74	0.70
1:U:7:ILE:HA	1:1:6:PHE:HA	1.73	0.70
1:M:35:TYR:CZ	1:M:37:GLY:HA3	2.27	0.70
2:G:332:ARG:HB2	2:G:332:ARG:HH11	1.56	0.69
1:1:173:GLU:C	1:1:174:ASN:OD1	2.30	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
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
2:2:-31:ASP:OD1	2:2:-27:ARG:NH2	2.26	0.69
1:U:7:ILE:HG13	1:U:8:SER:N	2.06	0.69
1:U:207:SER:O	1:U:208:LEU:CD1	2.40	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:O	2:P:-17:ILE:HG22	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
1:A:191:GLY:O	1:A:192:SER:HB2	1.93	0.69
2:G:-39:ALA:HB1	2:X:-26:GLN:HB3	1.73	0.69
2:G:301:ALA:CB	2:G:333:LYS:NZ	2.55	0.69
1:M:3:PHE:HD1	1:M:4:PRO:HD2	1.58	0.69
1:M:112:THR:HG22	1:M:113:GLU:OE2	1.93	0.69
2:P:332:ARG:NH1	2:P:332:ARG:HB2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:-37:ASP:OD1	2:Z:-35:SER:N	2.25	0.69
2:E:-30:PHE:CE1	2:E:-26:GLN:HG3	2.28	0.69
1:F:33:LEU:O	1:F:33:LEU:CD1	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:28:LYS:NZ	1:B:52:LYS:HE3	2.09	0.69
1:B:150:GLU:HG3	1:B:154:VAL:HG22	1.74	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:NH1	2:V:332:ARG:HB2	2.07	0.69
1:D:40:LEU:HA	1:D:212:VAL:HG12	1.74	0.68
1:D:167:LEU:HD13	1:D:187:ALA:HB2	1.74	0.68
1:M:59:ARG:HD2	1:M:129:HIS:HA	1.73	0.68
1:Q:89:TYR:CD1	2:Z:374:LEU:HD11	2.28	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
2:X:479:SER:HB2	2:2:479:SER:HB2	1.75	0.68
2:2:332:ARG:NH1	2:2:332:ARG:HB2	2.07	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:NE2	1:O:51:GLN:N	2.30	0.68
1:F:167:LEU:HD13	1:F:187:ALA:HB2	1.76	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
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
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:A:89:TYR:CD1	2:P:374:LEU:HD11	2.27	0.68
1:M:231:GLN:O	1:M:235:VAL:HG12	1.93	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:40:LEU:CD1	1:Q:212:VAL:CG1	2.72	0.68
1:Q:150:GLU:HG3	1:Q:154:VAL:HG22	1.75	0.68
1:Y:112:THR:HG22	1:Y:113:GLU:OE2	1.94	0.68
1:F:33:LEU:CD1	1:F:40:LEU:HB3	2.24	0.68
1:O:7:ILE:N	1:U:7:ILE:CD1	2.54	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:Y:163:ILE:HG12	1:Y:191:GLY:HA3	1.75	0.68
1:1:8:SER:H	1:1:11:GLN:CG	2.07	0.68
1:I:31:VAL:HG12	1:I:155:VAL:HG22	1.75	0.68
2:J:-38:VAL:HG11	1:S:84:THR:HG21	1.75	0.68
2:P:351:VAL:CG1	2:P:400:ALA:HB2	2.23	0.68
2:R:332:ARG:NH1	2:R:332:ARG:HB2	2.09	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
1:B:178:THR:CG2	1:B:233:LEU:HD23	2.12	0.67
1:Q:234:LEU:CD1	1:Q:234:LEU:N	2.57	0.67
1:Y:181:LEU:HD12	1:Y:185:VAL:HG23	1.76	0.67
2:2:-31:ASP:O	2:2:-27:ARG:HG3	1.95	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
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:C	1:U:188:LEU:HD23	2.15	0.67
2:Z:432:GLU:HG3	2:Z:437:GLN:HB2	1.77	0.67
2:2:-20:PRO:HB3	2:2:354:GLU:OE1	1.95	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:O	1:S:33:LEU:HD12	1.95	0.67
1:D:189:ARG:NH1	1:D:203:LEU:N	2.36	0.67
2:Z:-27:ARG:HG2	2:Z:-27:ARG:NH2	2.04	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:LYS:CE	1:I:28:LYS:H	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
2:2:456:GLN:HE22	2:2:465:ARG:NH2	1.93	0.66
1:D:11:GLN:HE22	1:Q:5:TYR:H	1.41	0.66
1:W:33:LEU:HD12	1:W:33:LEU:O	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:301:ALA:HB2	2:T:333:LYS:HE3	1.76	0.66
2:T:332:ARG:NH1	2:T:332:ARG:HB2	2.10	0.66
1:Y:173:GLU:HG3	1:Y:174:ASN:OD1	1.95	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:U:5:TYR:HB3	1:1:9:PRO:HD3	1.76	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:N	1:K:141:ILE:HD12	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
2:G:522:SER:HB3	2:V:487:VAL:HG13	1.77	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: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: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
2:J:426:ALA:HB2	2:T:-4:LEU:CD2	2.27	0.65
1:S:214:ASP:OD1	1:S:214:ASP:C	2.33	0.65
1:1:161:GLU:N	1:1:162:PRO:HD2	2.11	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
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
1:1:152:HIS:HB3	1:1:171:TYR:CE2	2.31	0.65
2:L:354:GLU:OE1	2:L:354:GLU:N	2.30	0.65
1:S:181:LEU:O	1:S:185:VAL:HG23	1.95	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
1:1:152:HIS:CD2	1:1:171:TYR:CE2	2.84	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
2:N:332:ARG:HB2	2:N:332:ARG:HH11	1.62	0.65
1:1:10:GLU:OE1	1:1:10:GLU:N	2.30	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
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
1:1:18:GLU:OE1	1:1:22:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:416:SER:O	2:2:419:ARG:NH1	2.30	0.64
1:F:169:GLU:OE1	1:F:169:GLU:N	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
1:1:8:SER:OG	1:1:11:GLN:NE2	2.30	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:HD23	1:U:188:LEU:O	1.98	0.64
2:2:301:ALA:O	2:2:440:GLY:HA3	1.98	0.64
1:1:18:GLU:OE2	1:1:21:ARG:NH2	2.30	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:C	1:O:19:LEU:CD2	2.66	0.64
1:U:92:ARG:HH11	1:U:92:ARG:CG	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:OD1	1:D:174:ASN:N	2.31	0.64
1:M:7:ILE:CD1	1:W:5:TYR:HB2	2.27	0.64
2:P:382:ARG:HH21	2:P:385:ILE:HD13	1.62	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:HH11	1:B:92:ARG:CG	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:OE1	1:I:169:GLU:N	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:B:18:GLU:OE2	1:B:21:ARG:NH1	2.30	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: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
1:1:174:ASN:OD1	1:1:174:ASN:N	2.32	0.63
1:D:16:ARG:HH21	1:M:4:PRO:CG	2.12	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: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:A:92:ARG:HH11	1:A:92:ARG:HG3	1.64	0.63
2:C:-39:ALA:H1	2:J:-26:GLN:NE2	1.96	0.63
1:F:181:LEU:O	1:F:185:VAL:HG23	1.98	0.63
1:Q:169:GLU:HA	1:Q:169:GLU:OE1	1.98	0.63
2:R:-29:LEU:HB3	2:R:-21:LEU:CD1	2.29	0.63
2:T:332:ARG:HB2	2:T:332:ARG:HH11	1.64	0.63
1:Y:205:VAL:HG21	1:Y:231:GLN:OE1	1.99	0.63
1:1:28:LYS:NZ	1:1:52:LYS:HE3	2.13	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:HB2	2:Z:332:ARG:HH11	1.64	0.63
1:O:141:ILE:HD12	1:O:141:ILE:N	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:NE2	2:L:-5:GLN:HA	2.14	0.62
1:M:92:ARG:HH11	1:M:92:ARG:CG	2.12	0.62
1:U:8:SER:N	1:1:5: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:HH11	1:M:16:ARG:CB	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
1:K:4:PRO:HB3	1:W:5:TYR:CD2	2.33	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
2:R:-30:PHE:CZ	2:Z:-38:VAL:CG2	2.82	0.62
2:X:350:ALA:O	2:X:353:VAL:CG1	2.47	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:HH11	1:K:92:ARG:CG	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
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
1:1:19:LEU:O	1:1:19:LEU:HD23	2.00	0.61
1:1:231:GLN:HA	1:1:234:LEU:HD12	1.80	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:HB2	2:V:332:ARG:HH11	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
1:S:141:ILE:N	1:S:141:ILE:HD12	2.14	0.61
1:W:173:GLU:HB3	1:W:174:ASN:ND2	2.15	0.61
2:X:332:ARG:NH1	2:X:332:ARG:HB2	2.15	0.61
2:2:416:SER:OG	2:2:419:ARG:NH2	2.30	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:U:93:ASP:OD1	2:2:375:THR:HG23	1.99	0.61
1:1:8:SER:H	1:1:11:GLN:CD	2.04	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: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
1:1:18:GLU:OE1	1:1:21:ARG:NH2	2.31	0.61
2:V:433:GLU:OE1	2:V:433:GLU:HA	2.00	0.61
2:2:391:LEU:O	2:2:395:MET:HG2	1.99	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:CG	1:Y:92:ARG:HH11	2.14	0.60
1:F:35:TYR:HE1	1:F:37:GLY:HA3	1.58	0.60
1:Q:7:ILE:HD11	1:Q:12:ALA:HA	1.83	0.60
1:Q:114:GLN:HE21	1:Q:114:GLN:HA	1.65	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:CG	1:F:92:ARG:HH11	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
1:D:19:LEU:HD12	1:K:9:PRO:HB3	1.81	0.60
2:H:485:ASP:C	2:H:485:ASP:OD1	2.39	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
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
2:2:332:ARG:HB2	2:2:332:ARG:HH11	1.67	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: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
1:1:225:ILE:HG21	1:1:233:LEU:HD12	1.82	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:HB2	2:J:332:ARG:HH11	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
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
1:1:167:LEU:HD11	1:1:187:ALA:HB3	1.84	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:HH11	1:D:92:ARG:CG	2.16	0.59
2:E:376:PHE:CE2	2:E:380:ILE:HD11	2.38	0.59
2:N:465:ARG:NH1	2:N:465:ARG:HB3	2.18	0.59
2:P:-17:ILE:O	2:P:-17:ILE:CG2	2.49	0.59
1:B:6:PHE:HD2	1:B:6:PHE:N	2.00	0.59
1:B:180:ALA:HA	1:B:183:ILE:HD12	1.85	0.59
1:I:92:ARG:CG	1:I:92:ARG:HH11	2.15	0.59
2:G:-17:ILE:C	2:G:-17:ILE:HD13	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
2:T:413:ASP:CG	2:T:414:PRO:HD2	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:217:ARG:HD2	1:1:218:PRO:HD2	1.85	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:HD22	2:L:-22:LEU:N	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: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:HB2	1:S:14:ARG:CZ	2.33	0.58
2:Z:496:ILE:HG13	2:Z:505:VAL:CG2	2.34	0.58
1:1:163:ILE:HD13	1:1:188:LEU:HD23	1.85	0.58
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
1:1:152:HIS:HB3	1:1:171:TYR:CZ	2.39	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:N	1:I:28:LYS:HE3	2.18	0.57
2:R:-30:PHE:HZ	2:Z:-38:VAL:HG23	1.68	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
1:D:19:LEU:HD12	1:K:9:PRO:CB	2.33	0.57
1:I:141:ILE:HD12	1:I:141:ILE:N	2.20	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
2:E:382:ARG:NH2	2:E:385:ILE:CD1	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:340:TYR:O	2:T:341:THR:HG22	2.03	0.57
1:1:31:VAL:HG12	1:1:155:VAL:HG22	1.87	0.57
1:1:92:ARG:CG	1:1:92:ARG:HH11	2.18	0.57
1:A:33:LEU:HD12	1:A:33:LEU:O	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:HH11	1:W:92:ARG:CG	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
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:OE1	1:U:231:GLN:HA	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
2:2:382:ARG:NH2	2:2:385:ILE:HD13	2.20	0.56
1:1:152:HIS:CG	1:1:171:TYR:CE2	2.93	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:B:161:GLU:CD	1:B:161:GLU:H	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
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:I:130:TYR:HE1	1:I:216:ASN:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:408:ASP:HB3	2:2:411:ALA:HB2	1.87	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
1:M:7:ILE:CG2	1:W:5:TYR:HD2	2.12	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:D:208:LEU:N	1:D:208:LEU:HD13	2.20	0.56
1:Q:92:ARG:CG	1:Q:92:ARG:HH11	2.19	0.56
1:Q:173:GLU:CG	1:Q:174:ASN:OD1	2.54	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
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
2:G:479:SER:HB2	2:V:479:SER:HB2	1.87	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
1:1:225:ILE:HG21	1:1:233:LEU:CD1	2.36	0.56
2:G:366:TYR:CE2	2:G:374:LEU:HD13	2.41	0.56
2:R:-27:ARG:HD2	2:R:-27:ARG:H	1.68	0.56
1:W:26:ARG:HB2	1:W:26:ARG:NH1	2.20	0.56
1:A:11:GLN:HE22	1:A:14:ARG:HH22	1.50	0.56
2:E:415:GLN:CA	2:E:415:GLN:NE2	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:H	1:A:161:GLU:CD	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:-30:PHE:HZ	2:R:-38:VAL:CG2	2.18	0.55
1:I:33:LEU:HD11	1:I:40:LEU:HB3	1.87	0.55
1:I:92:ARG:HH11	1:I:92:ARG:HG3	1.71	0.55
1:I:163:ILE:CD1	1:I:191:GLY:HA3	2.36	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: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:HH11	1:B:92:ARG:HG3	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:7:ILE:HD11	1:F:12:ALA:HA	1.87	0.55
1:F:189:ARG:HH21	1:F:203:LEU:HD21	1.69	0.55
1:O:161:GLU:CD	1:O:161:GLU:H	2.10	0.55
1:Q:142:THR:OG1	1:Q:144:ASP:HB3	2.06	0.55
1:U:231:GLN:OE1	1:U:231:GLN:CA	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:HE3	1:U:28:LYS:N	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:28:LYS:H	1:I:28:LYS:HE3	1.72	0.55
1:I:161:GLU:H	1:I:161:GLU:CD	2.10	0.55
2:J:515:ARG:HG2	2:J:515:ARG:HH11	1.72	0.55
1:U:7:ILE:HA	1:1:5:TYR:O	2.07	0.55
2:X:391:LEU:O	2:X:395:MET:HG2	2.06	0.55
2:E:-30:PHE:HZ	2:R:-38:VAL:HG23	1.71	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
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
2:2:-28:ARG:O	2:2:-24:PRO:HG3	2.07	0.55
2:R:456:GLN:NE2	2:R:465:ARG:NH2	2.25	0.54
1:U:224:ARG:HG2	1:U:224:ARG:HH11	1.72	0.54
2:X:332:ARG:HB2	2:X:332:ARG:HH11	1.71	0.54
1:D:16:ARG:NE	1:M:3:PHE:HE1	2.06	0.54
1:K:28:LYS:NZ	1:K:52:LYS:HE3	2.22	0.54
1:O:98:GLN:O	1:O:102:VAL:HG23	2.07	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:HD12	1:Y:141:ILE:N	2.23	0.54
1:Y:169:GLU:OE1	1:Y:169:GLU:CA	2.54	0.54
2:2:432:GLU:HG3	2:2:437:GLN:HB2	1.88	0.54
1:1:13:MET:HA	1:1:13:MET:CE	2.38	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:H	1:S:161:GLU:CD	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:83:ASP:OD2	2:P:365:HIS:ND1	2.29	0.54
1:O:152:HIS:CD2	1:O:171:TYR:CE2	2.95	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:N	1:I:5:TYR:HD1	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: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
1:1:8:SER:H	1:1:11:GLN:HG3	1.72	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:56:LEU:HG	1:I:62:PHE:HB2	1.90	0.54
1:I:129:HIS:HB2	1:I:132:GLU:CD	2.28	0.54
1:K:100:ALA:HB1	1:K:147:ILE:HD11	1.90	0.54
1:Q:26:ARG:NH1	1:Q:26:ARG:HB2	2.22	0.54
1:Q:161:GLU:H	1:Q:161:GLU:CD	2.11	0.54
2:T:413:ASP:OD1	2:T:413:ASP:C	2.46	0.54
1:Y:205:VAL:CG2	1:Y:231:GLN:OE1	2.56	0.54
1:D:13:MET:CE	1:Q:19:LEU:HD21	2.38	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:Y:181:LEU:CD1	1:Y:185:VAL:CG2	2.86	0.54
1:1:173:GLU:HG2	1:1:174:ASN:OD1	2.07	0.54
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: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
1:M:185:VAL:HG12	1:M:189:ARG:HH11	1.73	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
1:1:8:SER:OG	1:1:11:GLN:CD	2.46	0.53
1:1:19:LEU:HD23	1:1:19:LEU:C	2.28	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:C	2:E:338:ASP:OD1	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
2:H:-6:ALA:H1	2:H:-5:GLN:CB	2.02	0.53
1:Q:234:LEU:HD12	1:Q:234:LEU:H	1.68	0.53
1:U:11:GLN:CG	1:1:5:TYR:CE1	2.92	0.53
1:A:35:TYR:CD1	1:A:37:GLY:N	2.63	0.53
1:A:130:TYR:CD1	1:A:218:PRO:HA	2.43	0.53
2:E:391:LEU:HD12	2:E:391:LEU:O	2.08	0.53
2:G:-39:ALA:CB	2:X:-26:GLN:OE1	2.55	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:HH11	1:W:14:ARG:CG	2.21	0.53
1:W:28:LYS:HB3	1:W:44:GLU:HG3	1.89	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:OE1	2:G:-26:GLN:CA	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:HA	2:L:434:GLU:OE2	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:HD23	1:B:19:LEU:O	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:H	1:W:161:GLU:CD	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:O	1:O:234:LEU:CD1	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:28:LYS:NZ	1:I:52:LYS:HE3	2.24	0.52
1:I:163:ILE:CG1	1:I:191:GLY:HA3	2.38	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:28:LYS:H	1:B:28:LYS:HE2	1.73	0.52
1:B:129:HIS:HB2	1:B:132:GLU:CD	2.30	0.52
2:C:464:LEU:HG	2:C:464:LEU:O	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:9:PRO:HA	1:W:6:PHE:HE1	1.75	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: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:A:122:LEU:HD12	1:A:141:ILE:HB	1.90	0.52
1:A:130:TYR:CG	1:A:218:PRO:HA	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:35:TYR:CZ	1:1:37:GLY:CA	2.87	0.52
1:F:30:VAL:HG22	1:F:52:LYS:HZ3	1.75	0.52
1:F:170:SER:O	1:F:183:ILE:HD13	2.10	0.52
1:K:28:LYS:N	1:K:28:LYS:HE3	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:HD23	1:W:19:LEU:C	2.31	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
1:1:19: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
2:C:338:ASP:C	2:C:338:ASP:OD1	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
1:1:92:ARG:HH11	1:1:92:ARG:HG3	1.75	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:-30:PHE:CZ	2:P:-38:VAL:HG21	2.45	0.51
2:H:-28:ARG:CZ	2:H:-28:ARG:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:7:ILE:HB	1:1:11:GLN:CG	2.30	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:CZ	2:C:332:ARG:HB2	2.40	0.51
1:D:92:ARG:HH11	1:D:92:ARG:HG3	1.74	0.51
2:J:509:ARG:HH11	2:J:509:ARG:HG3	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:C	2:C:430:ASN:HD22	2.14	0.51
1:D:233:LEU:N	1:D:233:LEU:HD12	2.23	0.51
2:L:382:ARG:HD2	1:M:89:TYR:HE1	1.76	0.51
2:L:407:TYR:HE1	2:L:417:ALA:HB3	1.61	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
2:J:388:ARG:NH1	2:T:-21:LEU:O	2.44	0.51
1:S:114:GLN:HA	1:S:114:GLN:NE2	2.21	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:CE	1:Q:28:LYS:H	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:O	1:S:33:LEU:CD1	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: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:C:-26:GLN:CB	2:H:-39:ALA:CB	2.89	0.51
1:D:16:ARG:HH21	1:M:4:PRO:CD	2.24	0.51
2:H:350:ALA:O	2:H:353:VAL:HG12	2.11	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: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
1:1:112:THR:HG22	1:1:112:THR:O	2.11	0.51
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.93	0.50
1:B:171:TYR:CE1	1:B:172:ALA:O	2.64	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:HD12	1:F:141:ILE:N	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:A:15:GLU:OE1	1:B:8:SER:HA	2.11	0.50
1:D:144:ASP:OD2	1:D:146:SER:OG	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:173:GLU:HG3	1:1:174:ASN:OD1	2.09	0.50
1:A:67:LYS:HG2	1:A:69:ASN:HD21	1.77	0.50
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.94	0.50
1:F:178:THR:O	1:F:182:ARG:HG3	2.11	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:29:SER:OG	1:K:157:GLY:O	2.30	0.50
1:K:144:ASP:OD1	1:K:144:ASP: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
2:R:-30:PHE:CZ	2:Z:-38:VAL:HG23	2.45	0.50
1:Y:130:TYR:CE1	1:Y:216:ASN:O	2.64	0.50
1:D:129:HIS:HB2	1:D:132:GLU:CD	2.32	0.50
2:H:-23:GLU:HB3	2:P:-28:ARG:NH2	2.26	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
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.93	0.50
1:U:166:ALA:O	1:U:170:SER:OG	2.30	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
1:A:137:GLU:HG2	1:O:48:ARG:HH22	1.76	0.50
2:C:345:ILE:HB	2:C:352:ALA:HB1	1.92	0.50
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.94	0.50
1:D:144:ASP:OD1	1:D:144:ASP:O	2.30	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: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
2:2:-23:GLU:OE1	2:2:-23:GLU:O	2.30	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
1:Q:8:SER:HB2	1:Q:9:PRO:CD	2.42	0.50
1:Q:173:GLU:OE1	1:Q:174:ASN:OD1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:110:ILE:HG23	1:W:114:GLN:CG	2.24	0.50
1:1:33:LEU:HD12	1:1:33:LEU:O	2.12	0.50
1:1:56:LEU:HG	1:1:62:PHE:HB2	1.93	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:40:LEU:HD12	1:D:212:VAL:HG13	1.94	0.50
1:D:110:ILE:HG23	1:D:114:GLN:HG3	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
1:1:129:HIS:HB2	1:1:132:GLU:CD	2.32	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:HD12	2:Z:345:ILE:N	2.27	0.49
1:D:16:ARG:NH2	1:M:4:PRO:CG	2.75	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:29:SER:H	1:K:44:GLU:CG	2.25	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: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
1:1:204:GLY:O	1:1:208:LEU:HB2	2.13	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:O	2:C:-17:ILE:CG2	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:C	2:V:338:ASP:OD1	2.50	0.49
1:B:35:TYR:N	1:B:38:GLY:O	2.43	0.49
2:C:434:GLU:OE1	2:C:434:GLU:O	2.30	0.49
2:H:-27:ARG:O	2:H:-26:GLN:OE1	2.30	0.49
1:K:4:PRO:CG	1:W:5:TYR:CD2	2.95	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
2:T:388:ARG:NH1	2:2:-20:PRO:HA	2.28	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
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: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:C	2:P:338:ASP:OD1	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:C	2:Z:338:ASP:OD1	2.51	0.49
2:2:382:ARG:HH21	2:2:385:ILE:HD13	1.78	0.49
1:1:144:ASP:OD2	1:1:146:SER:OG	2.30	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:89:TYR:CD1	2:R:374:LEU:HD11	2.48	0.49
1:D:161:GLU:N	1:D:162:PRO:HD2	2.28	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:K:179:ASP:O	1:K:179:ASP:OD1	2.30	0.49
1:Q:171:TYR:CD2	1:Q:172:ALA:C	2.86	0.49
1:W:15:GLU:OE2	1:Y:9:PRO:CG	2.61	0.49
1:W:224:ARG:HG2	1:W:224:ARG:HH11	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:426:ALA:HB2	2:X:-4:LEU:HD21	1.95	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:C	2:L:338:ASP:OD1	2.51	0.49
1:S:191:GLY:O	1:S:192:SER:O	2.31	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:HD12	1:A:141:ILE:N	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:A:59:ARG:NH1	1:A:128:ALA:O	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:308:TYR:CZ	2:C:496:ILE:HD11	2.48	0.48
2:C:419:ARG:HG2	2:C:419:ARG:HH11	1.77	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
1:1:28:LYS:CE	1:1:28:LYS:H	2.26	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:92:ARG:HB3	2:V:375:THR:HG21	1.94	0.48
1:O:153:PHE:CD1	1:O:167:LEU:HD13	2.48	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
2:2:-20:PRO:CB	2:2:354:GLU:OE1	2.60	0.48
1:D:229:ALA:O	1:D:233:LEU:CD1	2.30	0.48
1:K:8:SER:HB2	1:K:9:PRO:HD2	1.95	0.48
1:K:224:ARG:HG2	1:K:224:ARG:HH11	1.78	0.48
2:N:448:SER:HB3	2:V:448:SER:HB3	1.96	0.48
1:O:67:LYS:HG2	1:O:69:ASN:HD21	1.78	0.48
2:R:464:LEU:HG	2:R:464:LEU:O	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:X:366:TYR:CE2	2:X:374:LEU:HD13	2.49	0.48
1:F:22:LYS:HE3	1:F:22:LYS:HB2	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
2:2:461:ASP:OD1	2:2:509:ARG:NH2	2.41	0.48
1:D:16:ARG:NE	1:M:3:PHE:CE1	2.82	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: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
1:1:98:GLN:O	1:1:102:VAL:HG23	2.14	0.48
1:B:8:SER:HA	1:B:9:PRO:HD2	1.74	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
2:C:409:ILE:CD1	2:C:410:HIS:CE1	2.95	0.48
1:D:19:LEU:CD1	1:K:9:PRO:HB3	2.44	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:Q:214:ASP:OD1	1:Q:214:ASP:C	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:HD23	1:W:19:LEU:O	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:HG3	2:J:509:ARG:NH1	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:27:ALA:HB1	1:Q:28:LYS:CE	2.45	0.47
1:Q:179:ASP:O	1:Q:183:ILE:HG13	2.14	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:HH11	1:K:14:ARG:HG3	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: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:HG2	1:U:224:ARG:NH1	2.30	0.47
1:W:173:GLU:HB3	1:W:174:ASN:HD21	1.76	0.47
1:1:224:ARG:HH11	1:1:224:ARG:HG2	1.80	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:-20:PRO:HA	2:R:388:ARG:NH1	2.29	0.47
2:E:421:VAL:HG22	2:E:431:ILE:HG12	1.96	0.47
2:G:388:ARG:HG3	2:X:-19:ALA:HB2	1.97	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: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: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:D:141:ILE:HD12	1:D:141:ILE:N	2.30	0.47
1:F:7:ILE:HD12	1:F:11:GLN:HB3	1.96	0.47
1:F:67:LYS:HG2	1:F:69:ASN:HD21	1.80	0.47
2:G:478:ASP:OD1	2:V:324:ASN:HB3	2.15	0.47
2:H:515:ARG:O	2:H:516:ALA:C	2.53	0.47
1:I:5:TYR:N	1:U:5:TYR:HH	2.12	0.47
1:I:26:ARG:NH1	1:I:26:ARG:HB2	2.29	0.47
2:J:-18:SER:O	2:J:398:LEU:CD1	2.63	0.47
2:J:407:TYR:CE1	2:J:417:ALA:HB3	2.49	0.47
1:K:142:THR:HG1	1:K:144:ASP:HB3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:-38:VAL:HG23	2:N:-30:PHE:CZ	2.49	0.47
1:M:154:VAL:CA	3:M:250:HOH:O	2.57	0.47
2:P:-27:ARG:C	2:P:-26:GLN:OE1	2.53	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:HD12	2:T:-4:LEU:N	2.30	0.47
1:U:179:ASP:OD1	1:U:179:ASP:N	2.48	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: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
2:V:-26:GLN:NE2	2:2:-38:VAL:N	2.63	0.47
1:B:5:TYR:HE2	1:O:11:GLN:NE2	2.01	0.47
1:D:167:LEU:HD12	1:D:167:LEU:HA	1.61	0.47
1:F:92:ARG:HB3	2:N:375:THR:HG21	1.96	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
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
1:1:181:LEU:O	1:1:185:VAL:HG23	2.14	0.47
2:H:513:LEU:HD12	2:H:513:LEU:HA	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:HH11	1:W:92:ARG:HG3	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:HG2	1:I:224:ARG:NH1	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:HG2	1:B:224:ARG:HH11	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:N	2:X:486:LEU:HD12	2.31	0.46
1:Y:17:SER:HG	1:Y:143:TYR:HH	1.63	0.46
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.97	0.46
1:A:181:LEU:HD23	1:A:233:LEU:HB3	1.96	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:D:13:MET:HE1	1:Q:116:LYS:HD2	1.97	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: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:HD12	1:U:208:LEU:HA	1.35	0.46
2:V:-26:GLN:HE22	2:2:-38:VAL:N	2.11	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:10:GLU:OE1	1:1:10:GLU:CA	2.63	0.46
1:1:161:GLU:N	1:1:162:PRO:CD	2.79	0.46
1:A:45:ASN:OD1	1:A:209:GLU:OE1	2.34	0.46
1:F:7:ILE:CG2	1:W:8:SER:HB3	2.46	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
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: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
1:1:28:LYS:N	1:1:28:LYS:HE3	2.30	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
2:2:320:SER:HB2	2:2:331:VAL:HG21	1.97	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:HH11	2:L:332:ARG:CB	2.29	0.46
1:M:29:SER:OG	1:M:157:GLY:O	2.33	0.46
1:O:54:SER:HB3	3:O:249:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:308:TYR:CE2	2:2:496:ILE:HD11	2.51	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
2:2:-29:LEU:CD2	2:2:-22:LEU:HD12	2.45	0.46
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:33:LEU:HD11	1:S:40:LEU:HB3	1.97	0.45
1:S:142:THR:OG1	1:S:146:SER:HB2	2.16	0.45
2:V:330:ASP:OD2	2:2:433:GLU:HG3	2.16	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
2:C:479:SER:HB2	2:E:479:SER:HB2	1.98	0.45
1:F:9:PRO:HA	1:W:6:PHE:CE1	2.50	0.45
1:F:11:GLN:OE1	1:F:11:GLN:CA	2.59	0.45
1:F:92:ARG:CG	1:F:92:ARG:NH1	2.76	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:HA	1:W:114:GLN:HE21	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
1:1:8:SER:O	1:1:11:GLN:CG	2.64	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
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:7:ILE:HB	1:Q:11:GLN:OE1	2.15	0.45
1:Q:152:HIS:CB	1:Q:171:TYR:HE1	2.08	0.45
1:Q:208:LEU:HA	1:Q:208:LEU:HD12	1.77	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
2:2:312:VAL:HG12	2:2:497:ILE:HB	1.98	0.45
1:B:98:GLN:HG2	2:H:370:GLU:OE1	2.16	0.45
1:D:5:TYR:OH	1:Y:7:ILE:O	2.22	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:K:4:PRO:CB	1:W:5:TYR:CZ	3.00	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
1:1:13: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
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:HH11	2:V:332:ARG:CB	2.29	0.45
1:A:6:PHE:CB	1:B:5:TYR:HB2	2.40	0.45
1:B:207:SER:O	1:B:208:LEU:HD12	2.16	0.45
2:C:419:ARG:NH1	2:C:419:ARG:HG2	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:HD12	2:P:401:LEU:HA	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
1:U:208:LEU:HD13	1:U:208:LEU:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:509:ARG:CZ	2:V:513:LEU:HD21	2.47	0.45
2:2:-36:LEU:O	2:2:-35:SER:HB2	2.16	0.45
1:B:187:ALA:O	1:B:191:GLY:N	2.47	0.45
2:G:-4:LEU:HD22	2:G:-4:LEU:N	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
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
2:2:388:ARG:HG3	2:2:426:ALA:O	2.17	0.45
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:O	1:I:144:ASP:OD2	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
2:2:332:ARG:HH11	2:2:332:ARG:CB	2.30	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:E:-30:PHE:CZ	2:R:-38:VAL:CG2	2.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:388:ARG:NH2	2:T:354:GLU:OE2	2.50	0.44
2:N:472:TYR:HD2	2:N:521:ARG:NH1	2.14	0.44
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
1:S:30:VAL:HG22	1:S:52:LYS:HZ3	1.83	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:HD12	2:C:513:LEU:HA	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:B:11:GLN:HG3	1:B:14:ARG:NH1	2.32	0.44
2:C:398:LEU:HA	2:C:398:LEU:HD12	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:30:VAL:HG22	1:Q:52:LYS:NZ	2.31	0.44
1:Q:205:VAL:O	1:Q:205:VAL:CG1	2.66	0.44
2:Z:418:GLY:O	2:Z:419:ARG:NH1	2.50	0.44
1:1:150:GLU:CG	1:1:154:VAL:HG22	2.45	0.44
1:A:19:LEU:O	1:A:19:LEU:HD23	2.18	0.44
2:G:390:ASN:CG	2:G:390:ASN:O	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:67:LYS:HG2	1:U:69:ASN:ND2	2.32	0.44
1:U:231:GLN:NE2	1:U:235:VAL:HG21	2.19	0.44
2:V:310:GLY:H	2:V:415:GLN:HA	1.83	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:W:161:GLU:N	1:W:162:PRO:HD2	2.32	0.44
1:Y:22:LYS:HB3	1:Y:26:ARG:HH21	1.82	0.44
1:Y:35:TYR:OH	1:Y:37:GLY:HA3	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:28:LYS:HZ2	1:1:52:LYS:HE3	1.80	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:29:SER:H	1:M:44:GLU:CG	2.31	0.44
1:M:59:ARG:NH2	1:M:217:ARG:O	2.46	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:HZ2	1:S:116:LYS:HG2	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:HD12	1:Y:167:LEU:HA	1.86	0.44
1:A:67:LYS:HG2	1:A:69:ASN:ND2	2.33	0.44
1:A:217:ARG:NH2	1:A:223:ARG:NE	2.65	0.44
2:E:-30:PHE:CD2	2:E:-30:PHE:C	2.91	0.44
2:E:350:ALA:HB2	2:R:428:GLY:HA3	2.00	0.44
2:G:487:VAL:HG13	2:V:522:SER:HB3	1.99	0.44
2:H:308:TYR:CD1	2:H:308:TYR:C	2.91	0.44
1:I:163:ILE:HG23	1:I:187:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:ARG:NH1	1:I:223:ARG:HG2	2.33	0.44
1:M:7:ILE:HD13	1:W:5:TYR:HB2	1.97	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:X:312:VAL:HG12	2:X:497:ILE:HB	1.99	0.44
2:2:486:LEU:CD1	2:2:486:LEU:N	2.81	0.44
1:1:33:LEU:HD12	1:1:33:LEU:H	1.83	0.44
2:C:388:ARG:O	2:C:388:ARG:HG2	2.18	0.43
2:C:486:LEU:N	2:C:486:LEU:CD1	2.81	0.43
1:D:92:ARG:CG	1:D:92:ARG:NH1	2.78	0.43
1:D:161:GLU:CD	1:D:161:GLU:N	2.70	0.43
1:D:161:GLU:O	1:D:165:ASN:ND2	2.51	0.43
2:H:456:GLN:NE2	2:H:465:ARG:NH2	2.32	0.43
1:K:217:ARG:HA	1:K:217:ARG:HD3	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: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:HH11	2:P:332:ARG:CB	2.27	0.43
1:Q:29:SER:N	1:Q:44:GLU:OE1	2.49	0.43
1:Q:171:TYR:HE2	1:Q:173:GLU:CA	2.31	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
1:1:92:ARG:CG	1:1:92:ARG:NH1	2.79	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:E:375:THR:HG21	1:K:92:ARG:HB3	1.99	0.43
2:G:426:ALA:HB2	2:X:-4:LEU:CD2	2.47	0.43
2:H:401:LEU:HD12	2:H:401:LEU:HA	1.83	0.43
2:J:-22:LEU:HD12	2:J:-22:LEU:N	2.33	0.43
2:N:472:TYR:HD2	2:N:521:ARG:HH12	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:-4:LEU:O	2:2:-2:HIS:HD2	2.01	0.43
1:1:33:LEU:CD1	1:1:33:LEU:O	2.66	0.43
2:C:401:LEU:HD12	2:C:401:LEU:HA	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:T:-38:VAL:CG2	2:2:-30:PHE:HZ	2.31	0.43
2:V:301:ALA:HB1	2:V:333:LYS:HD3	1.98	0.43
2:Z:-35:SER:HB3	2:Z:369:LEU:CD1	2.48	0.43
2:Z:-23:GLU:O	2:Z:-23:GLU:HG3	2.17	0.43
2:Z:432:GLU:OE1	2:Z:432:GLU:HA	2.17	0.43
2:E:401:LEU:HD12	2:E:401:LEU:HA	1.76	0.43
2:H:-21:LEU:HA	2:H:-21:LEU:HD12	1.71	0.43
1:M:30:VAL:HG22	1:M:52:LYS:NZ	2.34	0.43
1:M:129:HIS:HB2	1:M:132:GLU:CD	2.39	0.43
1:Q:19:LEU:HD23	1:Q:19:LEU:O	2.17	0.43
1:Q:172:ALA:CB	1:Q:175:ALA:HB2	2.48	0.43
1:S:8:SER:HB3	1:S:11:GLN:CG	2.48	0.43
1:S:116:LYS:HG2	1:S:117:PRO:O	2.19	0.43
2:2:318:ARG:HD3	2:2:493:THR:HG23	2.00	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
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:I:7:ILE:HG12	1:S:6:PHE:O	2.19	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
2:T:-4:LEU:N	2:T:-4:LEU:CD1	2.82	0.43
1:W:98:GLN:O	1:W:102:VAL:HG23	2.19	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
2:C:473:ASP:OD2	2:R:452:LYS:NZ	2.35	0.43
1:D:11:GLN:NE2	1:Q:5:TYR:H	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LEU:CD1	1:D:234:LEU:N	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
2:T:-17:ILE:HG12	2:T:-16:SER:H	1.83	0.43
2:X:388:ARG:HE	2:X:388:ARG:HB2	1.41	0.43
2:2:-5:GLN:HE21	2:2:-5:GLN:HB2	1.66	0.43
2:2:338:ASP:C	2:2:338:ASP:OD1	2.57	0.43
1:A:170:SER:OG	1:A:183:ILE:CG2	2.67	0.43
1:A:182:ARG:HH12	1:A:235:VAL:HA	1.84	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:J:374:LEU:HD11	1:S:89:TYR:CD1	2.54	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:R:-30:PHE:CE2	2:Z:-38:VAL:HG21	2.53	0.43
1:U:29:SER:H	1:U:44:GLU:CG	2.31	0.43
1:U:150:GLU:CG	1:U:154:VAL:HG22	2.43	0.43
2:X:-23:GLU:HG2	2:X:-22:LEU:N	2.34	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:HH11	2:T:332:ARG:CB	2.30	0.43
2:Z:348:THR:OG1	2:Z:351:VAL:CG2	2.66	0.43
1:A:28:LYS:HB2	1:A:52:LYS:HZ2	1.83	0.43
2:C:-26:GLN:CG	2:H:-39:ALA:HB1	2.49	0.43
2:C:430:ASN:ND2	2:C:431:ILE:O	2.51	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
1:1:173:GLU:CB	1:1:174:ASN:OD1	2.66	0.43
1:D:19:LEU:HD23	1:D:19:LEU:C	2.40	0.42
1:D:59:ARG:CD	1:D:129:HIS:HA	2.44	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:30:VAL:HG22	1:I:52:LYS:HZ3	1.84	0.42
1:I:33:LEU:O	1:I:33:LEU:CD1	2.65	0.42
2:J:382:ARG:HH21	2:J:385:ILE:HD13	1.83	0.42
1:K:32:ALA:O	1:K:153:PHE:HA	2.19	0.42
1:K:140:ARG:C	1:K:141:ILE:HD12	2.39	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
1:D:3:PHE:HZ	1:F:6:PHE:HZ	1.49	0.42
2:E:-28:ARG:NH2	2:E:-21:LEU:HD23	2.33	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:32:ALA:O	1:S:153:PHE:HA	2.19	0.42
1:S:167:LEU:O	1:S:171:TYR:N	2.51	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: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:30:VAL:HG22	1:D:52:LYS:NZ	2.34	0.42
1:D:207:SER:O	1:D:208:LEU:CD1	2.38	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
1:1:26:ARG:O	1:1:26:ARG:CG	2.66	0.42
1:A:115:ALA:HB3	1:B:112:THR:HG22	2.01	0.42
2:C:-4:LEU:HD22	2:H:426:ALA:HB2	2.02	0.42
1:D:224:ARG:HG2	1:D:224:ARG:HH11	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

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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:HD3	2:J:521:ARG:HA	1.87	0.42
1:K:16:ARG:HG3	1:M:9:PRO:CG	2.49	0.42
2:N:476:ASP:O	2:P:329:ARG:NH2	2.52	0.42
1:O:26:ARG:CG	1:O:26:ARG:O	2.67	0.42
1:Q:48:ARG:O	1:Q:48:ARG:HG2	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:A:28:LYS:CE	1:A:28:LYS:H	2.32	0.42
1:A:234:LEU:O	1:A:235:VAL:CG2	2.68	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:NH1	1:U:26:ARG:HB2	2.34	0.42
2:V:-29:LEU:HA	2:V:-29:LEU:HD12	1.72	0.42
2:X:-28:ARG:O	2:X:-24:PRO:HG3	2.19	0.42
2:2:308:TYR:CE2	2:2:311:GLY:HA3	2.51	0.42
1:1:8:SER:O	1:1:11:GLN:HG2	2.19	0.42
1:D:3:PHE:HE1	1:F:6:PHE:HE2	1.52	0.42
1:D:233:LEU:CD1	1:D:233:LEU:H	2.32	0.42
2:E:433:GLU:H	2:E:433:GLU:HG2	1.67	0.42
2:G:-17:ILE:C	2:G:-17:ILE:CD1	2.88	0.42
2:G:486:LEU:N	2:G:486:LEU:CD1	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
2:P:-21:LEU:O	2:V:388:ARG:NH1	2.53	0.42
1:U:30:VAL:HG22	1:U:52:LYS:NZ	2.35	0.42
2:V:415:GLN:OE1	2:V:415:GLN:CA	2.67	0.42
1:1:10:GLU:O	1:1:14:ARG:HB2	2.20	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:-30:PHE:HZ	2:P:-38:VAL:CG2	2.32	0.42
2:H:-23:GLU:HB3	2:P:-28:ARG:HH22	1.83	0.42
2:L:376:PHE:CE2	2:L:380:ILE:HD11	2.55	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:401:LEU:HD12	2:2:401:LEU:HA	1.87	0.42
1:1:18:GLU:OE2	1:1:21:ARG:NE	2.52	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:HG2	1:F:224:ARG:HH11	1.85	0.42
2:G:366:TYR:CD2	2:G:374:LEU:HD13	2.55	0.42
1:I:8:SER:O	1:I:11:GLN:N	2.53	0.42
1:I:130:TYR:CG	1:I:218:PRO:HA	2.55	0.42
2:L:-38:VAL:HG12	2:L:-37:ASP:N	2.33	0.42
2:L:308:TYR:CE2	2:L:311:GLY:HA3	2.55	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:U:89:TYR:CE1	2:2:382:ARG:HD2	2.54	0.42
1:W:33:LEU:HB3	1:W:153:PHE:HB3	2.01	0.42
2:Z:433:GLU:OE1	2:Z:433:GLU:CA	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:CD2	2:L:-22:LEU:H	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: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:26:ARG:O	1:S:26:ARG:CG	2.68	0.42
1:S:224:ARG:HG2	1:S:224:ARG:NH1	2.34	0.42
2:2:416:SER:O	2:2:419:ARG:CZ	2.68	0.42
1:A:27:ALA:HB1	1:A:28:LYS:HE2	2.02	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:332:ARG:HH11	2:J:332:ARG:CB	2.32	0.41
1:K:26:ARG:HB2	1:K:26:ARG:CZ	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
1:1:35:TYR:CE1	1:1:37:GLY:CA	2.98	0.41
1:1:188:LEU:O	1:1:189:ARG:C	2.59	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:HE21	2:E:415:GLN:N	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:O	2:V:-38:VAL:HG13	2.20	0.41
1:W:14:ARG:NH1	1:W:14:ARG:CG	2.80	0.41
2:X:419:ARG:HG2	2:X:419:ARG:HH11	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
2:2:345:ILE:HB	2:2:352:ALA:HB1	2.01	0.41
1:A:9:PRO:CD	1:A:10:GLU:H	2.32	0.41
1:A:161:GLU:CD	1:A:161:GLU:N	2.73	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:O	2:J:-38:VAL:CG1	2.67	0.41
2:J:419:ARG:NH1	2:J:419:ARG:HG2	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:HA	2:R:521:ARG:HD3	1.82	0.41
1:S:28:LYS:H	1:S:28:LYS:HE3	1.85	0.41
1:S:107:LEU:HD23	1:S:107:LEU:HA	1.94	0.41
1:U:26:ARG:O	1:U:26:ARG:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:40:LEU:CD1	1:U:212:VAL:CG1	2.98	0.41
2:X:301:ALA:HB1	2:X:333:LYS:NZ	2.24	0.41
2:C:310:GLY:HA2	2:C:415:GLN:HA	2.01	0.41
1:D:234:LEU:N	1:D:234:LEU:HD12	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:N	2:Z:486:LEU:CD1	2.84	0.41
1:1:150:GLU:HA	1:1:151:PRO:HD3	1.89	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:33:LEU:O	1:K:33:LEU:HD13	2.20	0.41
1:K:56:LEU:HD23	1:K:56:LEU:HA	1.88	0.41
1:K:150:GLU:CG	1:K:154:VAL:HG22	2.47	0.41
1:M:7:ILE:HD11	1:W:5:TYR:HB2	2.02	0.41
1:M:129:HIS:HE1	3:M:253:HOH:O	2.04	0.41
1:U:5:TYR:CD1	1:U:5:TYR:N	2.87	0.41
2:V:388:ARG:O	2:V:388:ARG:HG2	2.20	0.41
1:Y:26:ARG:HE	1:Y:26:ARG:HB2	1.75	0.41
1:1:8:SER:N	1:1:11:GLN:HG3	2.34	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:-28:ARG:HG3	2:P:-21:LEU:HD21	2.00	0.41
2:P:-21:LEU:HD12	2:P:-21:LEU:HA	1.81	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:54:SER:CB	1:A:75:ARG:HD2	2.51	0.41
1:A:59:ARG:NH2	1:A:217:ARG:O	2.47	0.41
1:A:163:ILE:O	1:A:167:LEU:HB2	2.19	0.41
1:F:213:LEU:HD23	1:F:213:LEU:HA	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:HD23	1:Y:107:LEU:HA	1.94	0.41
1:A:235:VAL:O	1:A:235:VAL:HG12	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:N	2:N:486:LEU:HD12	2.35	0.41
1:O:161:GLU:CD	1:O:161:GLU:N	2.74	0.41
2:P:-26:GLN:HB3	2:V:-38:VAL:HG12	2.03	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: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
1:1:8:SER:N	1:1:11:GLN:CG	2.79	0.41
1:B:35:TYR:HE1	1:B:37:GLY:HA3	1.58	0.41
2:C:-4:LEU:HD13	2:C:398:LEU:HD11	2.03	0.41
2:C:388:ARG:HG3	2:C:426:ALA:O	2.21	0.41
1:D:11:GLN:CD	1:Q:5:TYR:HD1	2.24	0.41
1:D:28:LYS:H	1:D:28:LYS:HE3	1.86	0.41
1:D:32:ALA:O	1:D:153:PHE:HA	2.21	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
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
2:P:-23:GLU:HG2	2:P:-22:LEU:HG	2.02	0.41
1:Q:233:LEU:HA	1:Q:233:LEU:HD23	1.73	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
1:S:45:ASN:HA	1:S:46:PRO:HD2	1.89	0.41
2:T:367:GLU:O	2:T:371:GLY:N	2.53	0.41
2:Z:498:ASP:C	2:Z:498:ASP:OD1	2.59	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:CD1	1:U:234:LEU:N	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: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:O	2:X:496:ILE:HG23	2.21	0.40
1:Y:59:ARG:CD	1:Y:129:HIS:HA	2.44	0.40
1:1:33:LEU:HD12	1:1:40:LEU:HB3	2.00	0.40
1:1:112:THR:O	1:1:112:THR:CG2	2.69	0.40
1:B:54:SER:CB	1:B:75:ARG:HD2	2.51	0.40
1:B:130:TYR:HE1	1:B:216:ASN:O	2.04	0.40
2:H:471:LEU:HD12	2:H:471:LEU:HA	1.93	0.40
1:I:161:GLU:CD	1:I:161:GLU:N	2.73	0.40
1:K:167:LEU:HD23	1:K:167:LEU:HA	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:-32:THR:CG2	2:X:-31:ASP:N	2.84	0.40
2:X:-25:ALA:N	2:X:-24:PRO:HD3	2.36	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: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:87:TYR:O	2:R:357:ARG:NH1	2.54	0.40
1:Q:167:LEU:HA	1:Q:167:LEU:HD23	1.85	0.40
1:S:35:TYR:HD1	1:S:37:GLY:H	1.50	0.40
1:U:98:GLN:HG2	2:2:370:GLU:OE1	2.22	0.40
2:V:-22:LEU:HA	2:V:-22:LEU:HD12	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
1:1:32:ALA:HA	1:1:40:LEU:O	2.21	0.40
1:1:123:CYS:HA	1:1:139:TYR:O	2.22	0.40
1:A:4:PRO:HB3	1:B:11:GLN:CD	2.41	0.40
1:A:44:GLU:C	1:A:45:ASN:HD22	2.24	0.40
1:A:84:THR:HG22	2:P:-36:LEU:HD11	2.02	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
2:J:375:THR:HG23	1:S:93:ASP:OD1	2.21	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:Q:40:LEU:HD13	1:Q:212:VAL:HG11	2.03	0.40
1:Q:173:GLU:O	1:Q:174:ASN:OD1	2.40	0.40
2:R:486:LEU:N	2:R:486:LEU:CD1	2.84	0.40
2:T:471:LEU:HD12	2:T:471:LEU:HA	1.95	0.40
1:U:112:THR:HG23	1:1:115:ALA:HB3	2.03	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: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
1:Y:56:LEU:HD23	1:Y:56:LEU:HA	1.91	0.40
1:Y:186:ALA:O	1:Y:189:ARG:CG	2.70	0.40
2:2:319:ARG:CG	2:2:320:SER:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:513:LEU:HA	2:2:513:LEU:HD12	1.78	0.40
1:A:33:LEU:CD1	1:A:33:LEU:O	2.69	0.40
1:B:33:LEU:HD12	1:B:40:LEU:HB3	2.01	0.40
1:D:29:SER:N	1:D:44:GLU:OE1	2.50	0.40
1:D:30:VAL:HG22	1:D:52:LYS:HZ3	1.86	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:O	2:L:509:ARG:HD2	2.22	0.40
1:M:56:LEU:HD23	1:M:56:LEU:HA	1.91	0.40
1:M:67:LYS:HG2	1:M:69:ASN:ND2	2.36	0.40
1:M:205:VAL:HG23	1:M:234:LEU:CD1	2.51	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:O	2:X:457:VAL:HG12	2.20	0.40
1:1:35:TYR:CE2	1:1:38:GLY:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	215/248 (87%)	204 (95%)	10 (5%)	1 (0%)	29 48
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%)	29	48
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%)	34	54
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 (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	168/192 (88%)	150 (89%)	18 (11%)	6	13
1	A	171/192 (89%)	157 (92%)	14 (8%)	11	22
1	B	168/192 (88%)	152 (90%)	16 (10%)	8	17
1	D	171/192 (89%)	157 (92%)	14 (8%)	11	22
1	F	170/192 (88%)	155 (91%)	15 (9%)	10	19
1	I	167/192 (87%)	151 (90%)	16 (10%)	8	16
1	K	170/192 (88%)	154 (91%)	16 (9%)	8	17
1	M	173/192 (90%)	157 (91%)	16 (9%)	9	18
1	O	167/192 (87%)	153 (92%)	14 (8%)	11	21
1	Q	171/192 (89%)	152 (89%)	19 (11%)	6	11
1	S	168/192 (88%)	154 (92%)	14 (8%)	11	22
1	U	170/192 (88%)	153 (90%)	17 (10%)	7	15
1	W	170/192 (88%)	153 (90%)	17 (10%)	7	15
1	Y	173/192 (90%)	155 (90%)	18 (10%)	7	13
2	2	186/216 (86%)	175 (94%)	11 (6%)	19	37
2	C	188/216 (87%)	176 (94%)	12 (6%)	17	33
2	E	185/216 (86%)	168 (91%)	17 (9%)	9	18
2	G	188/216 (87%)	177 (94%)	11 (6%)	19	37
2	H	186/216 (86%)	178 (96%)	8 (4%)	29	53
2	J	189/216 (88%)	179 (95%)	10 (5%)	22	43
2	L	188/216 (87%)	175 (93%)	13 (7%)	15	30
2	N	189/216 (88%)	178 (94%)	11 (6%)	20	38
2	P	188/216 (87%)	174 (93%)	14 (7%)	13	27
2	R	184/216 (85%)	175 (95%)	9 (5%)	25	47
2	T	189/216 (88%)	176 (93%)	13 (7%)	15	30
2	V	186/216 (86%)	178 (96%)	8 (4%)	29	53
2	X	188/216 (87%)	173 (92%)	15 (8%)	12	23
2	Z	184/216 (85%)	169 (92%)	15 (8%)	11	22
All	All	4995/5712 (87%)	4604 (92%)	391 (8%)	12	24

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

Sometimes 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	-6:ALA	C	-5:GLN	N	4.40

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	219/248 (88%)	0.69	29 (13%) 3 3	48, 86, 121, 152	0
1	A	222/248 (89%)	0.24	12 (5%) 25 27	43, 81, 117, 145	0
1	B	220/248 (88%)	0.40	17 (7%) 13 13	48, 88, 127, 145	0
1	D	222/248 (89%)	0.40	18 (8%) 12 12	52, 92, 126, 144	0
1	F	221/248 (89%)	0.49	20 (9%) 9 9	45, 86, 126, 147	0
1	I	217/248 (87%)	0.29	13 (5%) 21 22	45, 80, 123, 149	0
1	K	221/248 (89%)	0.81	32 (14%) 2 2	48, 98, 135, 148	0
1	M	224/248 (90%)	0.28	11 (4%) 29 31	45, 78, 127, 147	0
1	O	218/248 (87%)	0.60	24 (11%) 5 5	50, 97, 137, 150	0
1	Q	222/248 (89%)	0.50	16 (7%) 15 16	48, 96, 131, 140	0
1	S	219/248 (88%)	0.50	16 (7%) 15 15	46, 85, 129, 140	0
1	U	221/248 (89%)	0.38	17 (7%) 13 13	49, 88, 130, 144	0
1	W	221/248 (89%)	0.51	19 (8%) 10 10	48, 81, 125, 149	0
1	Y	224/248 (90%)	0.41	15 (6%) 17 18	53, 93, 132, 142	0
2	2	246/291 (84%)	0.09	8 (3%) 46 50	48, 68, 97, 107	0
2	C	250/291 (85%)	0.13	11 (4%) 34 37	51, 73, 111, 143	0
2	E	248/291 (85%)	0.22	13 (5%) 27 29	30, 77, 115, 132	0
2	G	251/291 (86%)	0.02	4 (1%) 72 74	44, 67, 115, 141	0
2	H	249/291 (85%)	0.20	13 (5%) 27 29	45, 71, 113, 136	0
2	J	252/291 (86%)	0.09	8 (3%) 47 51	47, 70, 109, 135	0
2	L	251/291 (86%)	0.13	7 (2%) 53 56	51, 75, 116, 140	0
2	N	252/291 (86%)	0.12	8 (3%) 47 51	44, 70, 115, 144	0
2	P	250/291 (85%)	0.19	8 (3%) 47 51	47, 75, 114, 144	0
2	R	246/291 (84%)	0.16	8 (3%) 46 50	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 68	40, 68, 110, 137	0
2	V	249/291 (85%)	-0.13	1 (0%) 92 93	47, 68, 112, 136	0
2	X	249/291 (85%)	0.11	10 (4%) 38 41	44, 65, 115, 144	0
2	Z	245/291 (84%)	0.06	7 (2%) 51 55	49, 73, 115, 131	0
All	All	6579/7546 (87%)	0.27	370 (5%) 24 25	30, 78, 124, 152	0

All (370) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	5	TYR	11.4
1	U	5	TYR	10.1
1	1	6	PHE	9.2
1	W	4	PRO	7.7
1	A	6	PHE	7.5
1	K	7	ILE	7.3
1	K	231	GLN	7.0
2	X	397	GLY	6.2
1	1	7	ILE	6.1
1	1	5	TYR	6.1
1	K	6	PHE	6.0
1	M	2	SER	5.8
1	Q	233	LEU	5.6
1	K	188	LEU	5.2
1	S	205	VAL	5.1
1	U	234	LEU	5.1
1	B	205	VAL	5.1
1	1	230	LEU	5.1
1	1	10	GLU	5.1
2	G	-17	ILE	5.0
1	O	188	LEU	4.9
2	H	-26	GLN	4.9
1	I	7	ILE	4.7
1	Y	191	GLY	4.7
1	F	234	LEU	4.7
1	U	203	LEU	4.7
2	H	417	ALA	4.6
1	K	233	LEU	4.6
1	W	188	LEU	4.6
2	H	310	GLY	4.6
1	F	6	PHE	4.6
1	O	167	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	H	-39	ALA	4.5
1	M	205	VAL	4.5
1	O	233	LEU	4.5
1	I	6	PHE	4.5
1	Q	130	TYR	4.5
1	D	172	ALA	4.4
2	H	-6	ALA	4.4
1	U	205	VAL	4.3
1	W	205	VAL	4.3
1	S	191	GLY	4.2
1	I	5	TYR	4.2
2	P	-17	ILE	4.1
1	K	205	VAL	4.1
1	K	21	ARG	4.1
1	1	203	LEU	4.0
1	O	225	ILE	4.0
1	O	235	VAL	4.0
1	K	225	ILE	4.0
1	S	172	ALA	4.0
1	F	130	TYR	4.0
1	B	188	LEU	3.9
1	S	169	GLU	3.9
1	U	232	ALA	3.9
2	H	414	PRO	3.9
1	W	3	PHE	3.9
1	B	5	TYR	3.9
1	A	5	TYR	3.9
1	O	192	SER	3.8
2	C	414	PRO	3.8
1	W	204	GLY	3.7
2	2	412	SER	3.7
1	D	188	LEU	3.7
1	W	6	PHE	3.7
1	U	208	LEU	3.7
2	C	415	GLN	3.7
1	Y	169	GLU	3.7
1	K	235	VAL	3.7
2	E	397	GLY	3.6
1	Q	192	SER	3.6
1	S	192	SER	3.6
1	U	167	LEU	3.6
2	T	-5	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	Q	169	GLU	3.6
1	W	133	THR	3.6
1	F	188	LEU	3.6
2	R	499	ALA	3.6
1	U	6	PHE	3.5
1	D	177	LEU	3.5
1	B	231	GLN	3.5
1	F	203	LEU	3.5
2	C	-27	ARG	3.5
1	A	234	LEU	3.5
1	F	230	LEU	3.5
1	Y	132	GLU	3.4
1	B	167	LEU	3.4
2	2	413	ASP	3.4
2	H	-27	ARG	3.4
1	D	133	THR	3.4
1	1	8	SER	3.4
1	D	3	PHE	3.4
1	F	5	TYR	3.4
1	Y	233	LEU	3.4
1	Q	230	LEU	3.4
1	K	229	ALA	3.4
1	M	8	SER	3.4
1	U	233	LEU	3.4
1	K	206	ALA	3.4
1	A	188	LEU	3.3
1	S	6	PHE	3.3
1	O	130	TYR	3.3
1	O	10	GLU	3.3
1	D	192	SER	3.3
1	I	226	THR	3.3
2	L	414	PRO	3.3
1	Q	232	ALA	3.3
1	O	44	GLU	3.3
1	1	229	ALA	3.3
2	E	-25	ALA	3.3
2	X	351	VAL	3.3
1	O	169	GLU	3.3
1	Q	234	LEU	3.3
1	I	231	GLN	3.3
1	O	8	SER	3.3
1	Q	188	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	204	GLY	3.3
2	E	-19	ALA	3.2
2	H	415	GLN	3.2
1	K	171	TYR	3.2
2	H	-21	LEU	3.2
1	U	171	TYR	3.2
2	C	413	ASP	3.2
2	J	414	PRO	3.2
2	G	413	ASP	3.2
1	S	233	LEU	3.2
1	M	5	TYR	3.1
2	L	415	GLN	3.1
2	X	-5	GLN	3.1
1	Q	3	PHE	3.1
2	L	524	ALA	3.1
2	N	-38	VAL	3.1
2	P	412	SER	3.1
1	Y	130	TYR	3.1
1	D	205	VAL	3.1
2	J	-18	SER	3.1
2	R	412	SER	3.1
1	B	163	ILE	3.1
1	U	235	VAL	3.1
1	S	7	ILE	3.1
1	K	14	ARG	3.0
1	W	189	ARG	3.0
2	X	398	LEU	3.0
1	F	205	VAL	3.0
1	U	231	GLN	3.0
1	K	133	THR	3.0
1	S	13	MET	3.0
2	X	395	MET	3.0
1	O	24	ILE	3.0
1	K	230	LEU	3.0
1	F	233	LEU	3.0
1	K	123	CYS	2.9
1	B	171	TYR	2.9
1	M	234	LEU	2.9
1	K	181	LEU	2.9
2	N	-39	ALA	2.9
1	S	48	ARG	2.9
1	Y	8	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	1	9	PRO	2.9
1	W	130	TYR	2.9
1	Q	135	ARG	2.9
1	D	167	LEU	2.9
1	S	171	TYR	2.9
2	R	395	MET	2.8
2	L	310	GLY	2.8
1	I	169	GLU	2.8
1	S	113	GLU	2.8
1	F	36	ALA	2.8
2	P	-26	GLN	2.8
2	E	-26	GLN	2.8
2	Z	349	ALA	2.8
1	F	161	GLU	2.8
1	F	204	GLY	2.8
2	C	397	GLY	2.8
1	B	230	LEU	2.8
1	1	48	ARG	2.8
1	F	169	GLU	2.7
1	W	231	GLN	2.7
2	2	407	TYR	2.7
1	K	234	LEU	2.7
2	L	-18	SER	2.7
2	T	414	PRO	2.7
1	B	189	ARG	2.7
1	Y	2	SER	2.7
1	S	227	GLY	2.7
2	P	519	GLU	2.7
2	P	499	ALA	2.7
1	O	189	ARG	2.7
2	E	413	ASP	2.7
1	U	192	SER	2.6
2	C	499	ALA	2.6
2	H	411	ALA	2.6
1	D	191	GLY	2.6
1	F	131	GLY	2.6
1	K	177	LEU	2.6
1	K	4	PRO	2.6
1	O	12	ALA	2.6
2	P	353	VAL	2.6
1	K	48	ARG	2.6
2	J	417	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	204	GLY	2.6
1	Q	216	ASN	2.6
2	2	415	GLN	2.6
2	L	-38	VAL	2.6
1	B	208	LEU	2.6
1	K	10	GLU	2.6
2	2	416	SER	2.6
1	K	5	TYR	2.6
2	C	-39	ALA	2.5
1	Y	231	GLN	2.5
2	J	395	MET	2.5
2	Z	397	GLY	2.5
1	1	113	GLU	2.5
2	2	519	GLU	2.5
1	I	233	LEU	2.5
1	1	169	GLU	2.5
1	K	232	ALA	2.5
1	1	228	SER	2.5
2	G	-26	GLN	2.5
2	N	396	GLN	2.5
1	A	177	LEU	2.5
1	O	38	GLY	2.5
1	1	204	GLY	2.5
2	C	-26	GLN	2.5
2	R	-25	ALA	2.5
1	A	7	ILE	2.5
2	N	412	SER	2.5
1	W	190	ALA	2.5
1	A	10	GLU	2.5
1	K	185	VAL	2.5
2	T	-16	SER	2.5
2	X	409	ILE	2.5
1	M	203	LEU	2.4
2	N	-26	GLN	2.4
1	A	130	TYR	2.4
1	F	10	GLU	2.4
2	N	414	PRO	2.4
2	H	407	TYR	2.4
1	F	132	GLU	2.4
2	C	-30	PHE	2.4
1	Q	191	GLY	2.4
1	I	133	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	171	TYR	2.4
1	B	159	THR	2.4
2	E	393	ALA	2.4
2	T	417	ALA	2.4
1	F	189	ARG	2.4
1	K	227	GLY	2.4
1	Y	204	GLY	2.4
1	B	178	THR	2.4
1	K	208	LEU	2.4
1	O	230	LEU	2.4
2	X	-4	LEU	2.4
2	2	-27	ARG	2.4
2	E	415	GLN	2.4
1	M	9	PRO	2.4
1	D	234	LEU	2.4
1	Y	208	LEU	2.4
2	R	-19	ALA	2.4
1	D	189	ARG	2.3
1	D	231	GLN	2.3
1	1	207	SER	2.3
2	N	486	LEU	2.3
1	1	223	ARG	2.3
2	P	-27	ARG	2.3
2	2	355	PHE	2.3
1	O	216	ASN	2.3
2	Z	393	ALA	2.3
1	U	181	LEU	2.3
2	G	-27	ARG	2.3
1	1	46	PRO	2.3
2	E	395	MET	2.3
1	A	163	ILE	2.3
1	W	230	LEU	2.3
2	X	396	GLN	2.3
1	I	132	GLU	2.3
1	M	10	GLU	2.3
1	B	48	ARG	2.3
1	Y	131	GLY	2.3
2	E	-30	PHE	2.3
1	U	230	LEU	2.3
1	Y	161	GLU	2.3
1	1	132	GLU	2.3
1	I	48	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	228	SER	2.3
1	O	171	TYR	2.3
1	Y	203	LEU	2.3
1	1	123	CYS	2.3
1	1	189	ARG	2.2
1	M	13	MET	2.2
2	N	523	GLY	2.2
1	M	3	PHE	2.2
1	U	113	GLU	2.2
2	T	519	GLU	2.2
1	I	167	LEU	2.2
2	J	-22	LEU	2.2
1	S	130	TYR	2.2
1	O	191	GLY	2.2
1	Q	205	VAL	2.2
1	W	228	SER	2.2
1	S	225	ILE	2.2
2	P	-39	ALA	2.2
2	L	523	GLY	2.2
1	W	132	GLU	2.2
1	D	190	ALA	2.2
1	1	208	LEU	2.2
1	1	214	ASP	2.2
1	S	206	ALA	2.2
1	1	63	ALA	2.2
2	X	-18	SER	2.2
2	E	-23	GLU	2.2
1	K	159	THR	2.2
1	A	18	GLU	2.2
1	B	130	TYR	2.2
2	C	412	SER	2.2
1	O	232	ALA	2.2
1	W	172	ALA	2.2
2	Z	355	PHE	2.2
1	W	123	CYS	2.2
2	X	400	ALA	2.1
1	D	225	ILE	2.1
1	F	51	GLN	2.1
1	1	172	ALA	2.1
2	H	418	GLY	2.1
2	J	-25	ALA	2.1
1	Q	231	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	410	HIS	2.1
1	D	101	ASN	2.1
2	Z	395	MET	2.1
1	D	227	GLY	2.1
1	F	37	GLY	2.1
2	R	411	ALA	2.1
2	H	-5	GLN	2.1
2	Z	396	GLN	2.1
1	Q	153	PHE	2.1
2	V	398	LEU	2.1
1	K	15	GLU	2.1
1	M	49	SER	2.1
2	R	397	GLY	2.1
1	K	184	ALA	2.1
1	O	229	ALA	2.1
1	U	169	GLU	2.1
2	R	-26	GLN	2.1
1	D	48	ARG	2.1
1	Y	159	THR	2.1
1	1	171	TYR	2.1
2	Z	-27	ARG	2.1
1	A	203	LEU	2.1
1	B	233	LEU	2.1
2	E	398	LEU	2.1
1	1	227	GLY	2.1
1	D	169	GLU	2.1
1	1	120	VAL	2.1
2	E	-38	VAL	2.1
1	Y	7	ILE	2.1
1	I	181	LEU	2.1
1	O	207	SER	2.1
1	W	234	LEU	2.1
1	1	188	LEU	2.1
1	W	48	ARG	2.1
1	O	25	ALA	2.0
2	E	414	PRO	2.0
2	J	411	ALA	2.0
1	B	153	PHE	2.0
1	1	122	LEU	2.0
1	Q	158	GLY	2.0
1	I	191	GLY	2.0
1	O	158	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	503	VAL	2.0
1	K	163	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.