



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:05 PM UTC

PDB ID : 3MKA / pdb_00003mka
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

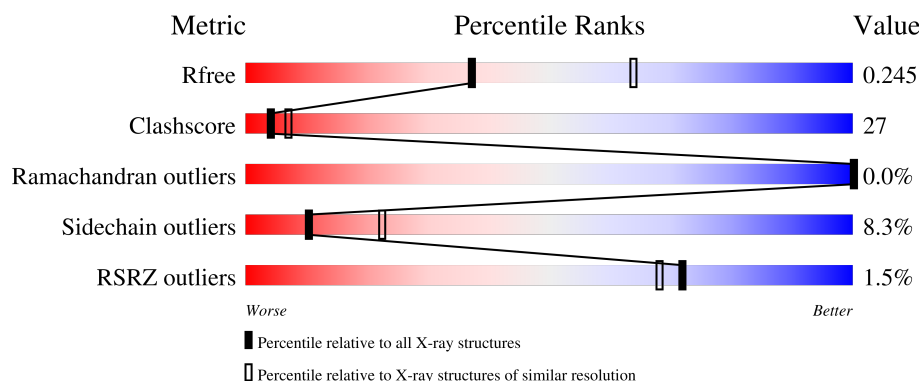
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



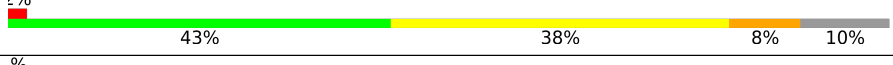
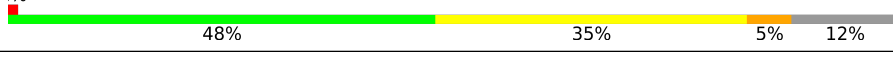
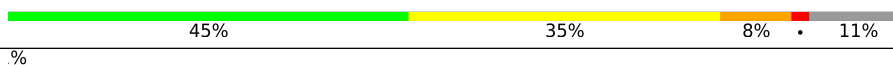
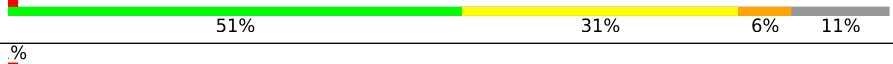
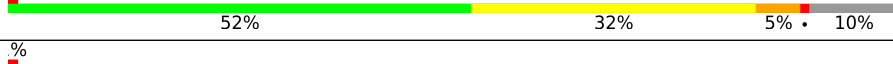
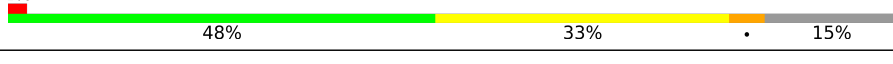
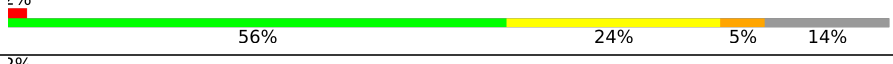
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	1	248	2% 51% 30% 7% 12%
1	A	248	% 47% 38% 5% 10%
1	B	248	48% 35% 6% 11%
1	D	248	2% 51% 30% 8% 10%
1	F	248	2% 51% 31% 6% 11%

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49801 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha.

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

- Molecule 2 is a protein called Proteasome subunit beta.

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

There are 14 discrepancies between the modelled and reference sequences:

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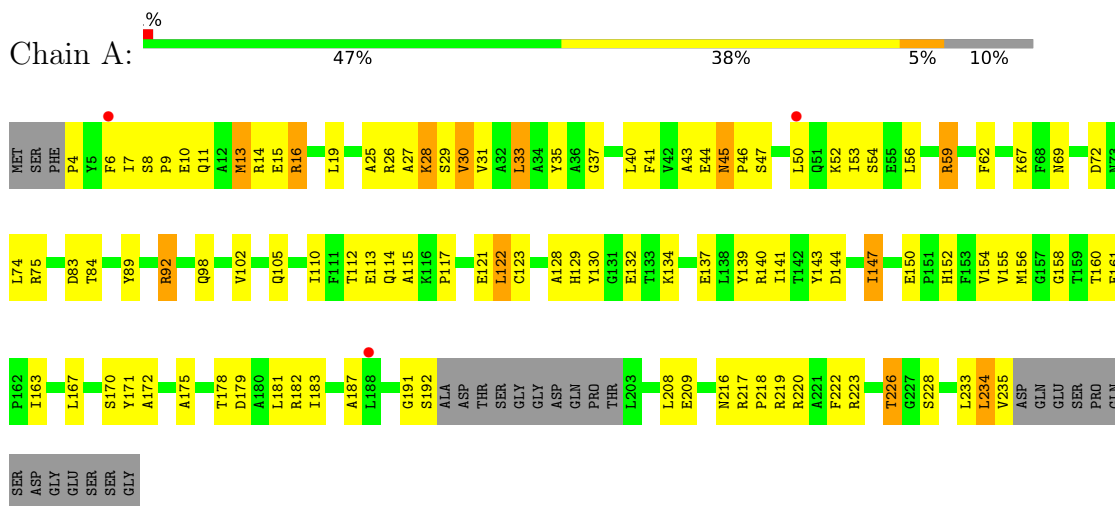
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	3	Total 3	O 3	0	0
3	U	2	Total 2	O 2	0	0
3	V	4	Total 4	O 4	0	0
3	W	6	Total 6	O 6	0	0
3	X	2	Total 2	O 2	0	0
3	Y	6	Total 6	O 6	0	0
3	Z	5	Total 5	O 5	0	0
3	2	5	Total 5	O 5	0	0
3	1	3	Total 3	O 3	0	0

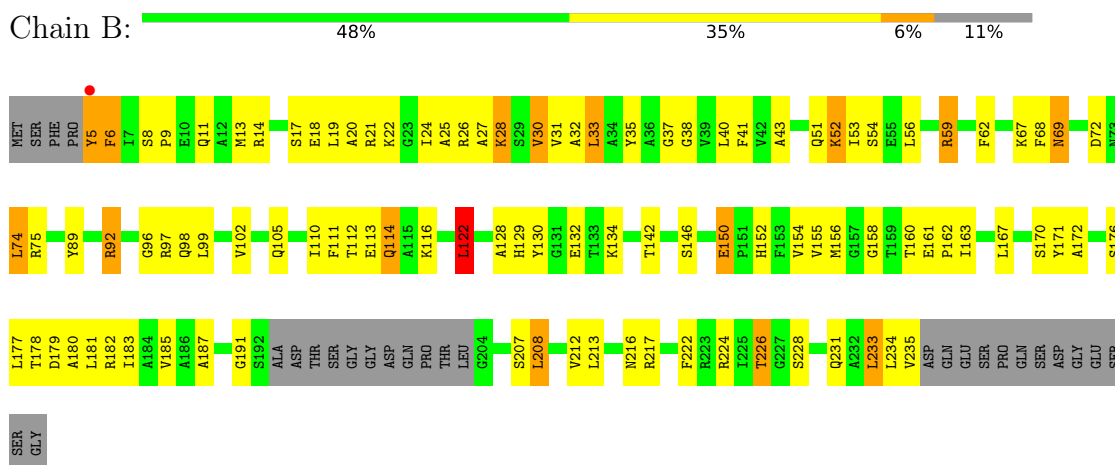
3 Residue-property plots [i](#)

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

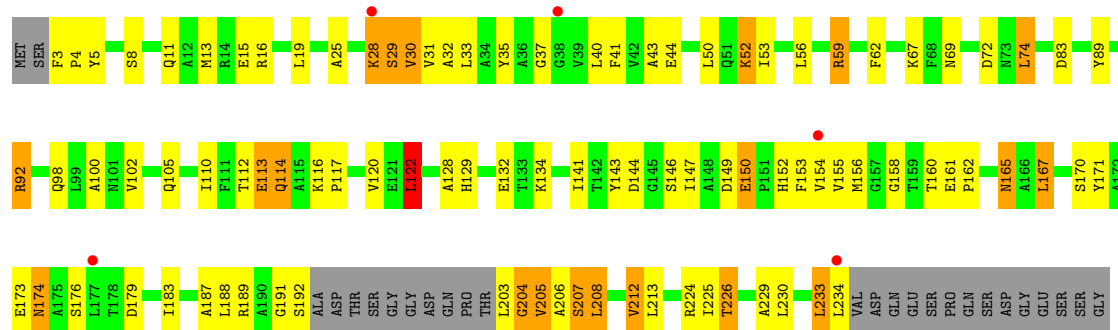


- Molecule 1: Proteasome subunit alpha

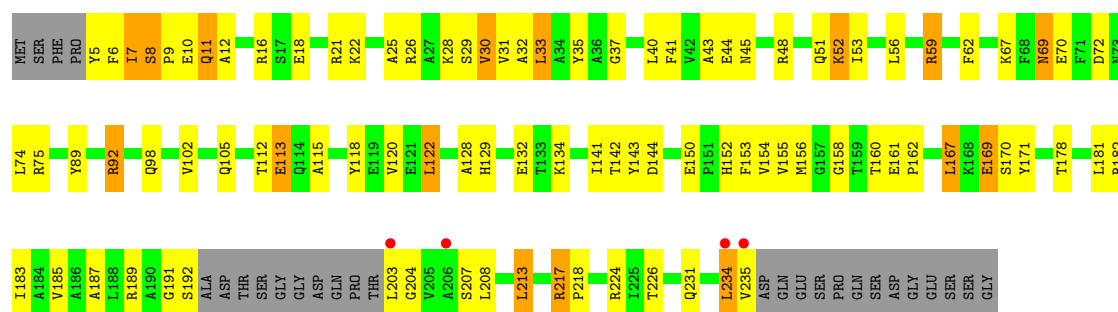


- Molecule 1: Proteasome subunit alpha

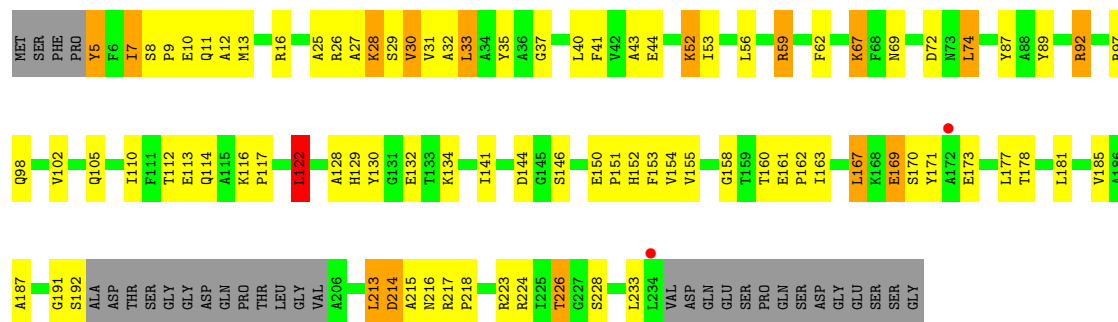




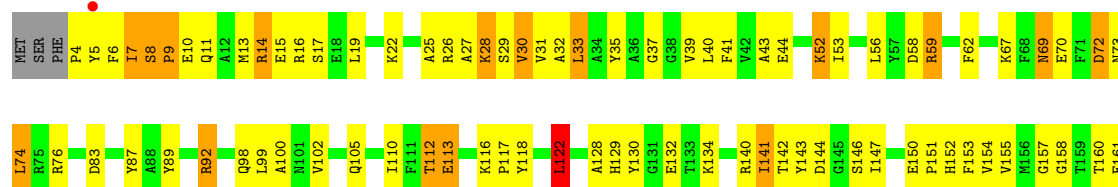
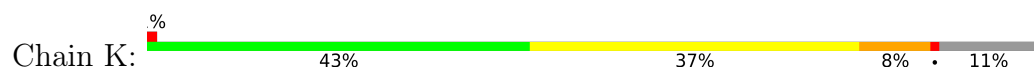
• Molecule 1: Proteasome subunit alpha

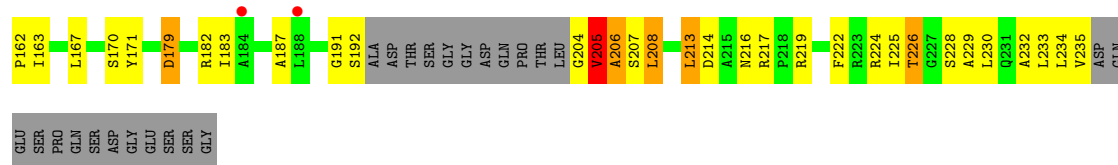


• Molecule 1: Proteasome subunit alpha



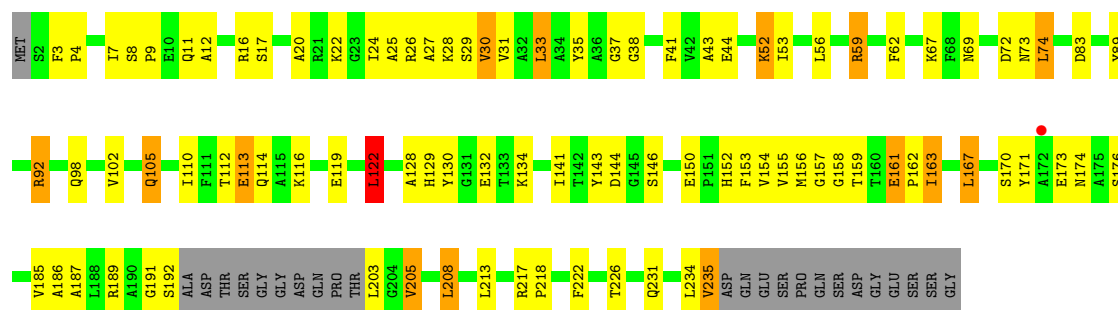
• Molecule 1: Proteasome subunit alpha





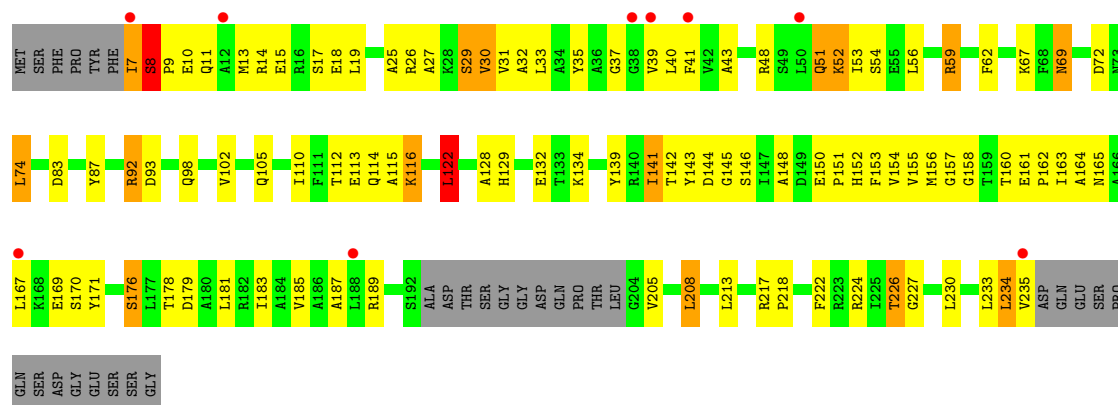
• Molecule 1: Proteasome subunit alpha

Chain M: 53% 31% 6% 10%



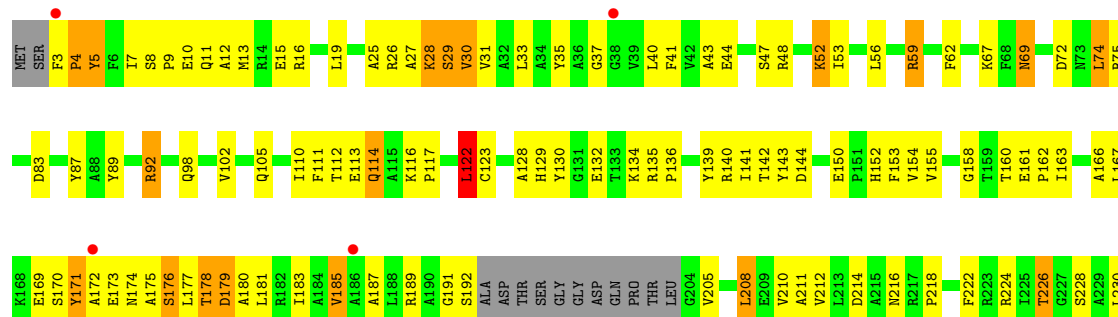
• Molecule 1: Proteasome subunit alpha

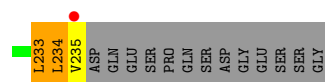
Chain O: 4% 46% 35% 6% 12%



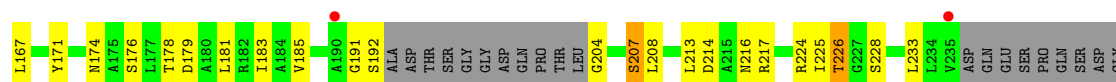
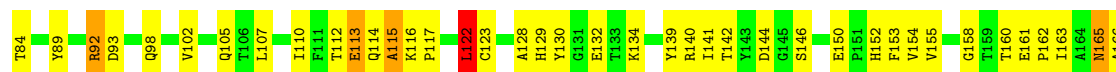
• Molecule 1: Proteasome subunit alpha

Chain Q: 2% 43% 38% 8% 10%

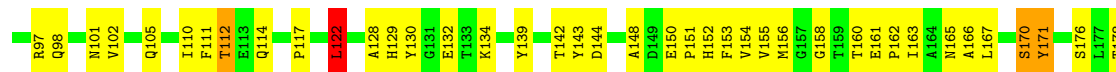




• Molecule 1: Proteasome subunit alpha



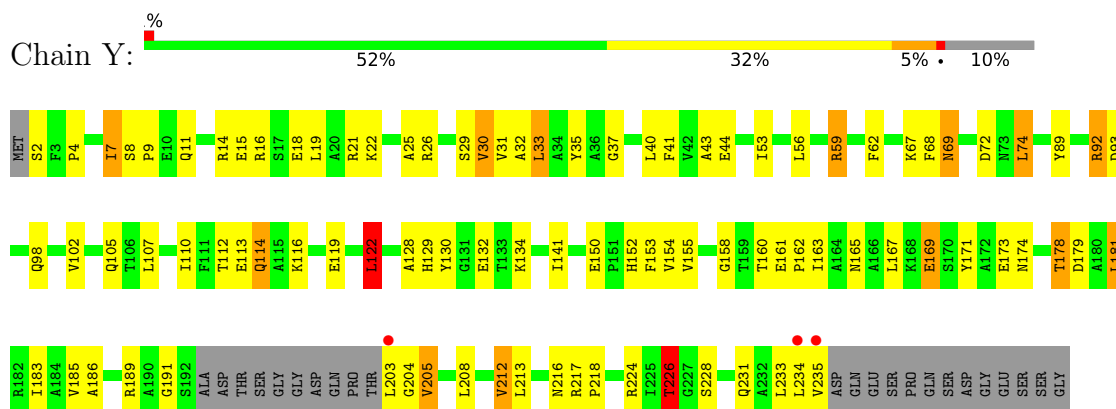
• Molecule 1: Proteasome subunit alpha



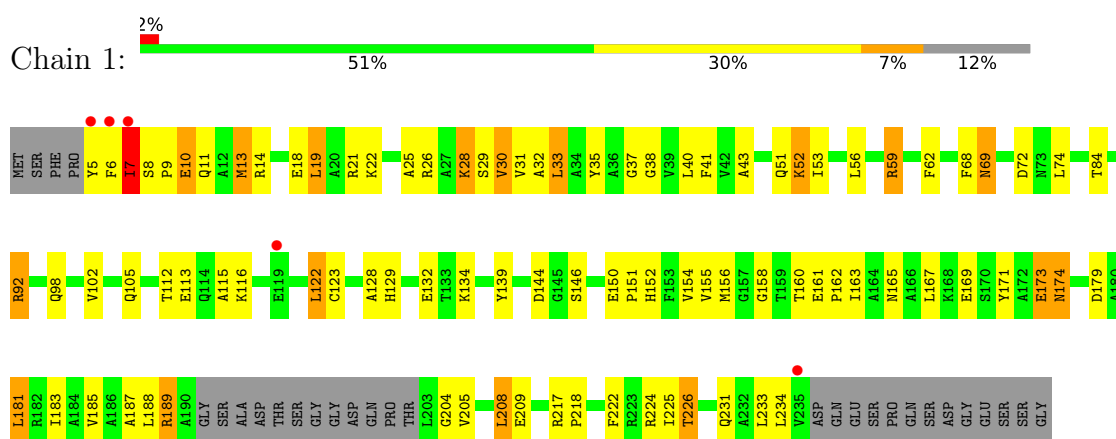
• Molecule 1: Proteasome subunit alpha



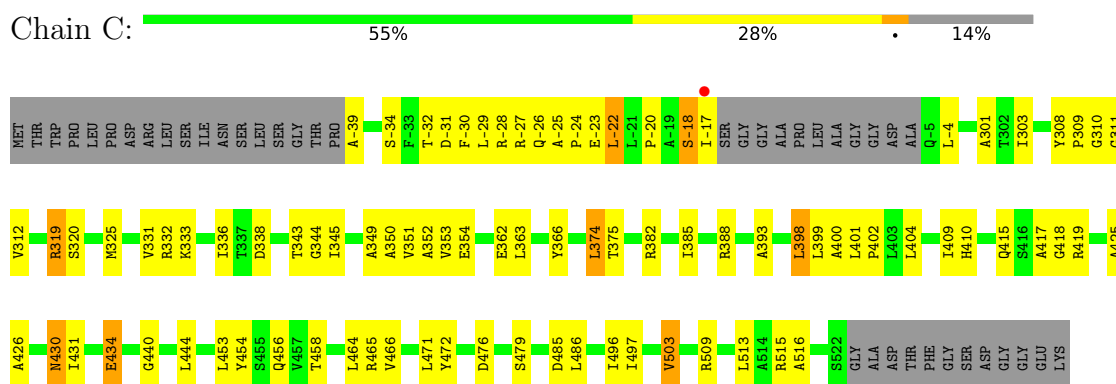
- Molecule 1: Proteasome subunit alpha



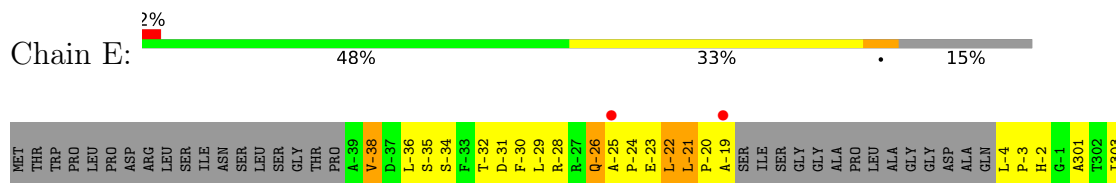
- Molecule 1: Proteasome subunit alpha

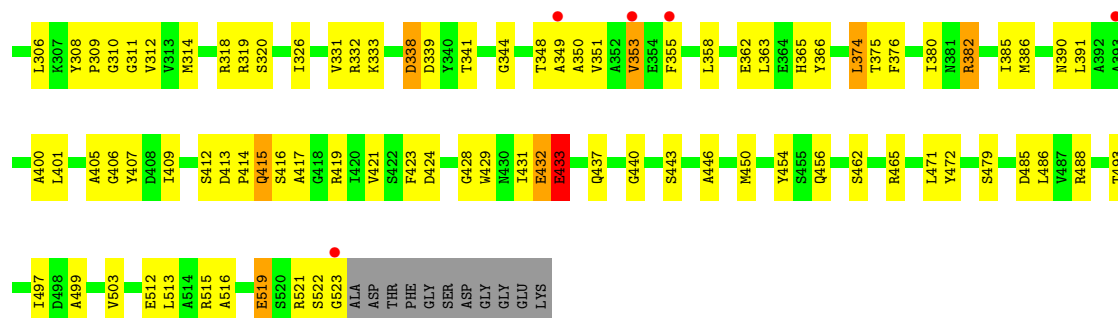


- Molecule 2: Proteasome subunit beta



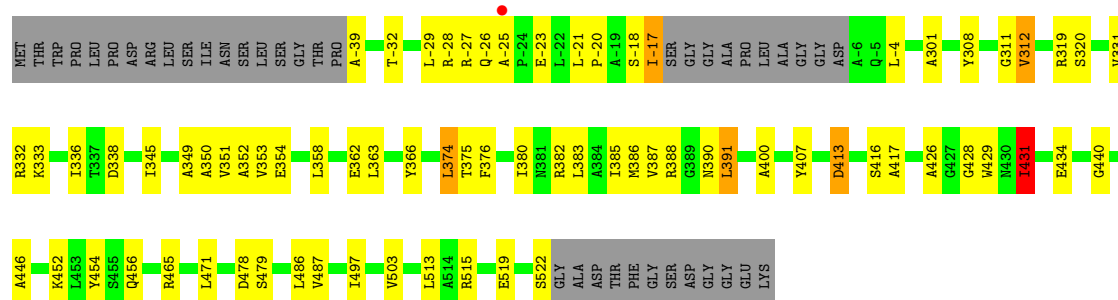
- Molecule 2: Proteasome subunit beta





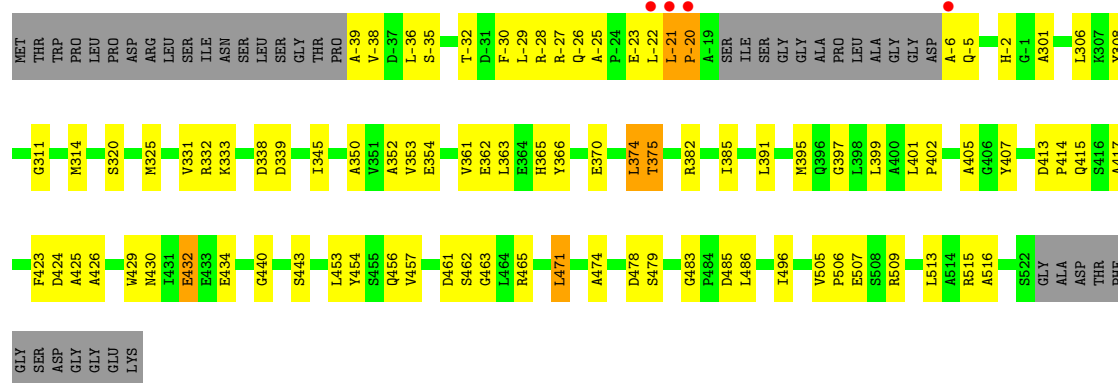
• Molecule 2: Proteasome subunit beta

Chain G: 61% 23% 14%



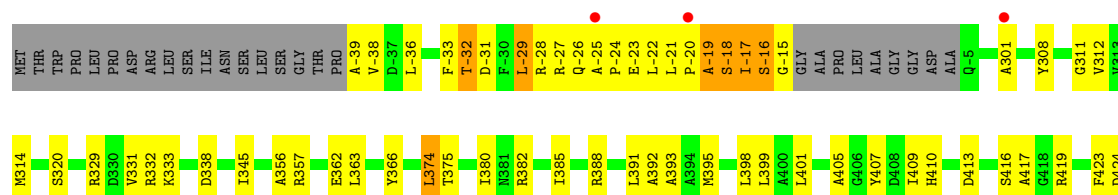
• Molecule 2: Proteasome subunit beta

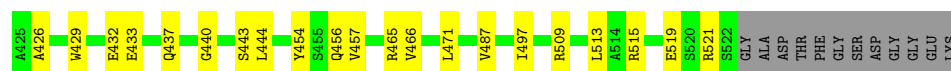
Chain H: 55% 29% 14%



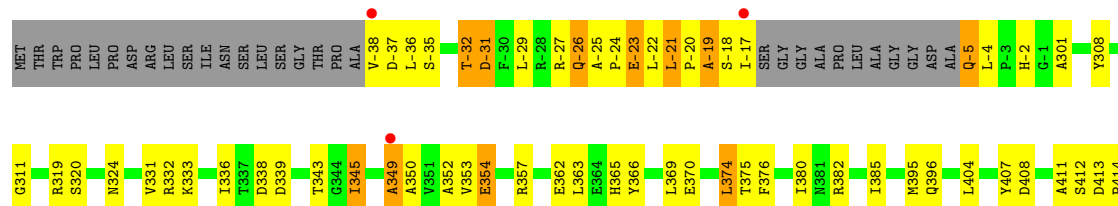
• Molecule 2: Proteasome subunit beta

Chain J: 58% 26% 13%

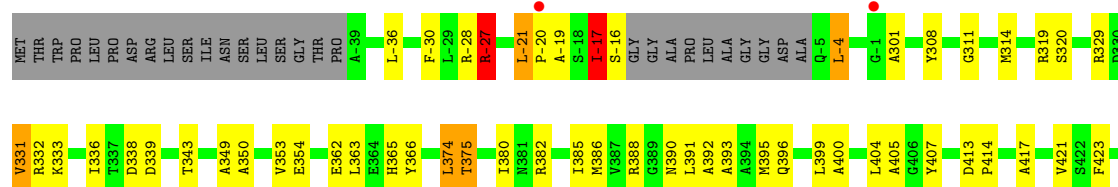




• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

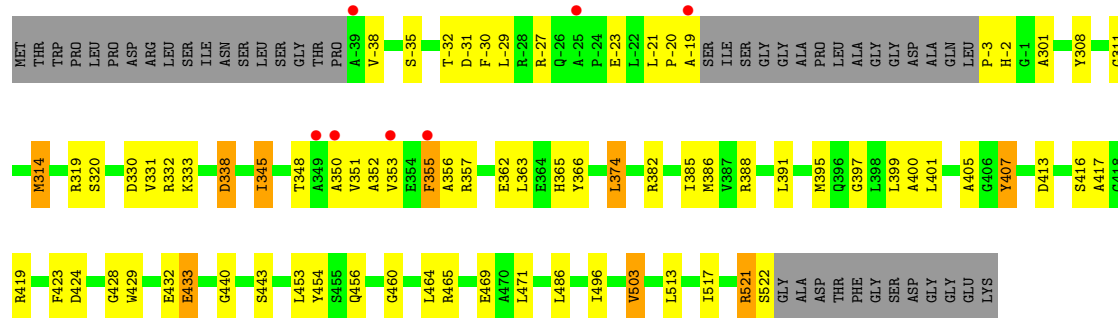


• Molecule 2: Proteasome subunit beta

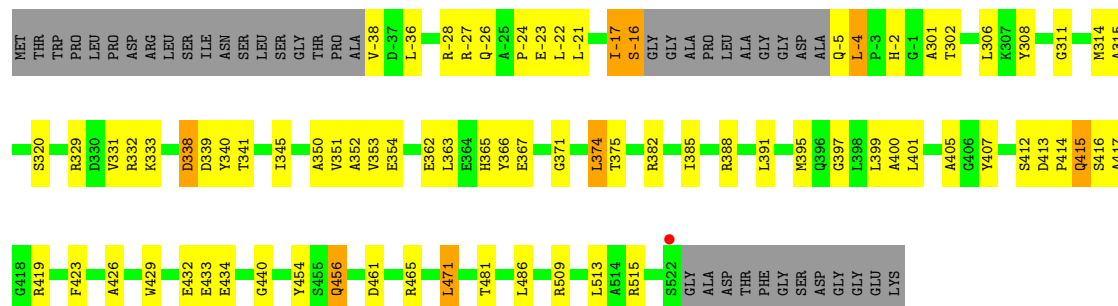


LYS

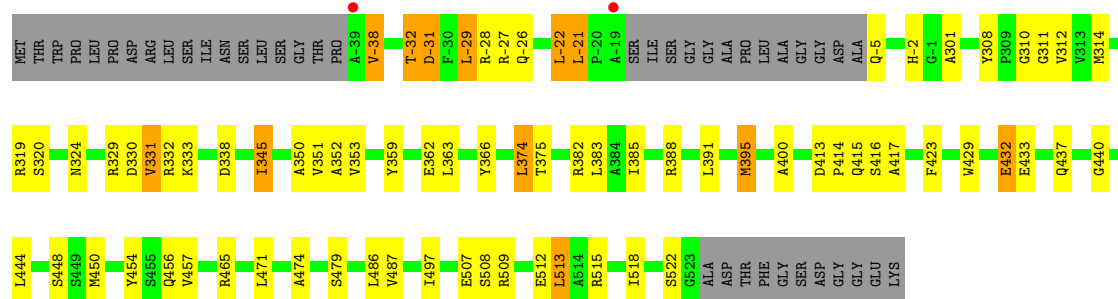
• Molecule 2: Proteasome subunit beta



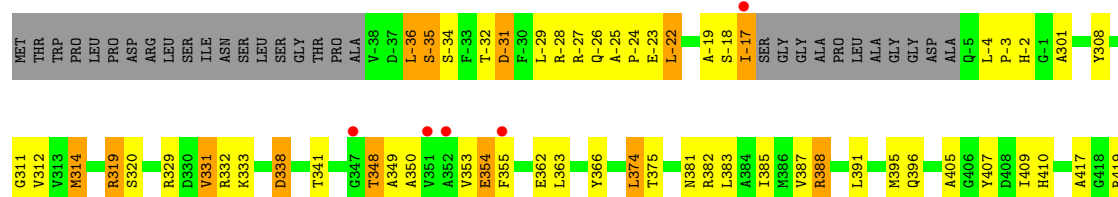
• Molecule 2: Proteasome subunit beta

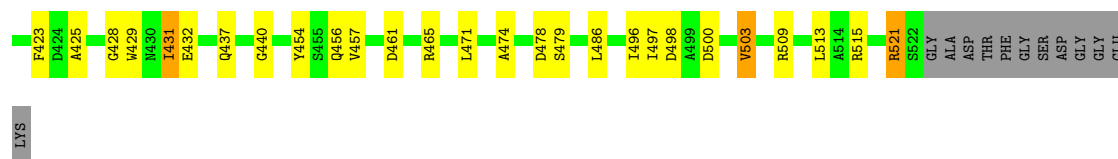


• Molecule 2: Proteasome subunit beta

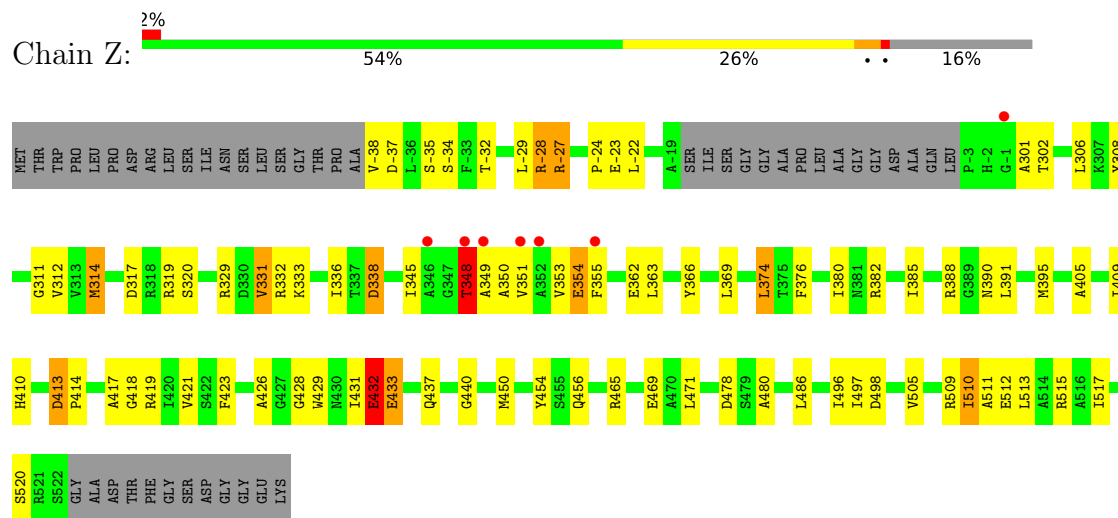


• Molecule 2: Proteasome subunit beta

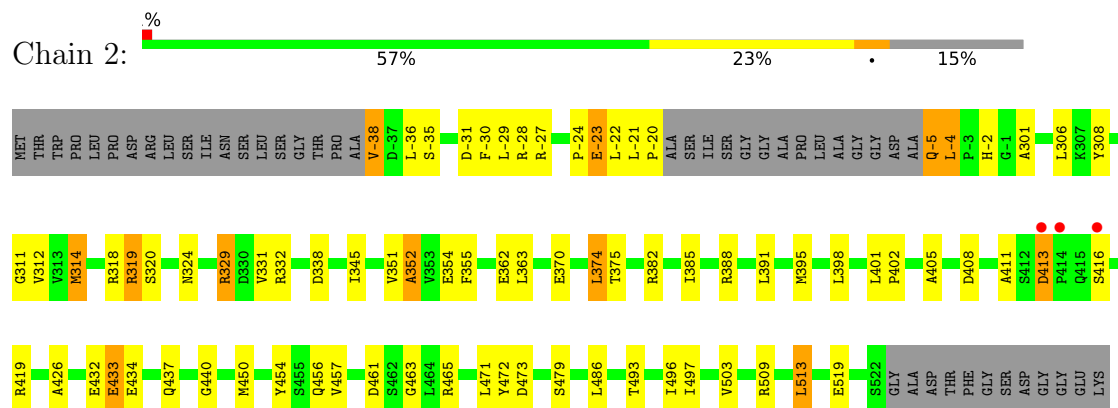




• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	173.93Å 115.42Å 199.58Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	29.77 – 2.51 29.77 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.77-2.51) 94.1 (29.77-2.51)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.247 0.215 , 0.245	Depositor DCC
R_{free} test set	11802 reflections (5.04%)	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 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49801	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.88	0/1720	1.12	7/2325 (0.3%)
1	A	0.92	0/1741	1.15	9/2353 (0.4%)
1	B	0.80	0/1722	1.14	15/2327 (0.6%)
1	D	0.87	2/1746 (0.1%)	1.21	17/2360 (0.7%)
1	F	0.90	1/1733 (0.1%)	1.19	11/2342 (0.5%)
1	I	0.91	2/1707 (0.1%)	1.21	11/2306 (0.5%)
1	K	0.85	0/1733	1.23	19/2342 (0.8%)
1	M	0.94	0/1759	1.17	9/2378 (0.4%)
1	O	0.84	0/1700	1.19	20/2297 (0.9%)
1	Q	0.86	0/1745	1.18	14/2359 (0.6%)
1	S	0.87	1/1712 (0.1%)	1.20	14/2313 (0.6%)
1	U	0.90	2/1733 (0.1%)	1.19	17/2342 (0.7%)
1	W	0.94	0/1739	1.17	13/2351 (0.6%)
1	Y	0.87	1/1759 (0.1%)	1.15	8/2378 (0.3%)
2	2	1.02	2/1858 (0.1%)	1.17	6/2520 (0.2%)
2	C	1.08	2/1882 (0.1%)	1.16	10/2553 (0.4%)
2	E	0.98	3/1863 (0.2%)	1.20	10/2527 (0.4%)
2	G	1.10	3/1887 (0.2%)	1.18	6/2560 (0.2%)
2	H	1.09	3/1872 (0.2%)	1.19	15/2538 (0.6%)
2	J	1.03	3/1892 (0.2%)	1.17	8/2566 (0.3%)
2	L	1.00	2/1886 (0.1%)	1.16	9/2558 (0.4%)
2	N	1.07	2/1892 (0.1%)	1.20	19/2566 (0.7%)
2	P	0.94	0/1882	1.17	13/2553 (0.5%)
2	R	0.94	3/1851 (0.2%)	1.14	6/2510 (0.2%)
2	T	1.05	1/1883 (0.1%)	1.16	6/2554 (0.2%)
2	V	1.10	5/1872 (0.3%)	1.19	9/2539 (0.4%)
2	X	1.01	2/1877 (0.1%)	1.19	7/2546 (0.3%)
2	Z	1.08	2/1846 (0.1%)	1.19	12/2503 (0.5%)
All	All	0.97	42/50492 (0.1%)	1.18	320/68366 (0.5%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	446	ALA	CA-CB	-8.40	1.40	1.53
1	Y	165	ASN	C-N	8.24	1.44	1.33
2	Z	450	MET	SD-CE	7.88	1.99	1.79
2	J	345	ILE	C-N	-7.84	1.22	1.33
1	U	165	ASN	C-N	7.25	1.43	1.33
2	V	457	VAL	CA-CB	7.23	1.62	1.54
2	L	345	ILE	C-N	-7.07	1.23	1.33
2	V	450	MET	SD-CE	6.58	1.96	1.79
2	R	345	ILE	C-N	6.39	1.42	1.33
2	J	356	ALA	C-N	-6.37	1.25	1.33
1	S	165	ASN	C-N	-6.32	1.25	1.33
2	G	431	ILE	CA-CB	-6.27	1.46	1.54
2	L	421	VAL	CA-CB	6.24	1.62	1.54
1	F	120	VAL	CA-CB	6.14	1.64	1.55
2	C	325	MET	SD-CE	6.10	1.94	1.79
2	H	325	MET	SD-CE	6.03	1.94	1.79
2	H	474	ALA	C-O	-6.01	1.17	1.24
2	2	450	MET	SD-CE	5.92	1.94	1.79
2	E	450	MET	SD-CE	5.89	1.94	1.79
1	D	165	ASN	C-N	5.87	1.41	1.33
2	V	518	ILE	CA-CB	-5.79	1.47	1.54
2	C	466	VAL	CA-CB	-5.79	1.47	1.54
2	G	515	ARG	C-O	-5.78	1.17	1.24
2	X	474	ALA	C-O	-5.73	1.17	1.24
2	2	314	MET	SD-CE	-5.71	1.65	1.79
2	V	474	ALA	C-O	-5.70	1.17	1.24
2	N	446	ALA	CA-CB	-5.67	1.44	1.53
2	E	341	THR	CA-CB	5.65	1.63	1.53
2	J	401	LEU	C-O	-5.65	1.19	1.25
1	D	120	VAL	CA-CB	5.64	1.63	1.55
2	Z	314	MET	SD-CE	-5.59	1.65	1.79
2	T	315	ALA	CA-CB	-5.46	1.43	1.54
1	I	67	LYS	CA-C	5.31	1.60	1.52
2	N	386	MET	SD-CE	5.29	1.92	1.79
2	R	356	ALA	C-N	5.21	1.40	1.33
2	V	314	MET	SD-CE	-5.15	1.66	1.79
1	I	13	MET	SD-CE	5.15	1.92	1.79
2	E	446	ALA	CA-CB	-5.14	1.45	1.53
1	U	7	ILE	CA-CB	5.10	1.61	1.54
2	R	314	MET	SD-CE	-5.08	1.66	1.79
2	X	314	MET	SD-CE	-5.05	1.67	1.79
2	H	361	VAL	CA-CB	-5.03	1.48	1.54

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	-38	VAL	N-CA-C	-8.78	96.24	108.27
1	U	112	THR	N-CA-C	8.57	120.70	111.36
1	S	213	LEU	N-CA-C	-8.47	94.93	108.73
1	K	10	GLU	N-CA-C	8.40	120.43	111.28
1	Y	165	ASN	O-C-N	-8.40	113.42	122.07
1	K	213	LEU	N-CA-C	-8.38	94.87	108.52
2	N	454	TYR	N-CA-C	8.37	120.41	111.28
2	R	432	GLU	N-CA-C	8.33	121.59	108.67
1	D	116	LYS	CA-C-N	-8.31	112.23	120.21
1	D	116	LYS	C-N-CA	-8.31	112.23	120.21
1	Y	213	LEU	N-CA-C	-8.29	95.00	108.52
2	Z	413	ASP	CA-C-N	8.18	127.83	119.82
2	Z	413	ASP	C-N-CA	8.18	127.83	119.82
1	I	213	LEU	N-CA-C	-8.18	95.19	108.52
2	N	-17	ILE	N-CA-C	8.16	118.94	110.62
1	K	72	ASP	N-CA-C	-8.13	102.50	111.36
1	M	72	ASP	N-CA-C	-8.13	102.50	111.36
2	X	-35	SER	N-CA-C	-8.10	101.07	111.92
2	Z	454	TYR	N-CA-C	8.08	120.09	111.28
2	G	391	LEU	N-CA-C	7.97	119.60	111.07
2	J	356	ALA	CA-C-N	7.86	131.45	120.29
2	J	356	ALA	C-N-CA	7.86	131.45	120.29
1	I	173	GLU	N-CA-C	7.84	119.82	111.28
1	1	160	THR	N-CA-C	7.83	123.01	113.38
2	J	454	TYR	N-CA-C	7.77	119.75	111.28
1	Q	176	SER	N-CA-C	-7.76	100.27	110.43
1	F	7	ILE	N-CA-C	7.74	120.11	108.80
1	1	122	LEU	N-CA-C	7.69	120.85	109.24
2	V	454	TYR	N-CA-C	7.69	119.66	111.28
1	Q	72	ASP	N-CA-C	-7.64	103.03	111.36
1	S	7	ILE	N-CA-C	-7.60	101.62	110.21
1	Y	72	ASP	N-CA-C	-7.60	103.08	111.36
1	F	72	ASP	N-CA-C	-7.52	103.16	111.36
1	O	72	ASP	N-CA-C	-7.50	103.19	111.36
1	Y	122	LEU	N-CA-C	7.48	120.53	109.24
2	E	433	GLU	N-CA-C	-7.44	103.80	113.17
1	U	205	VAL	N-CA-C	-7.44	101.75	111.05
1	F	122	LEU	N-CA-C	7.40	120.41	109.24
1	S	72	ASP	N-CA-C	-7.39	103.31	111.36
1	S	122	LEU	N-CA-C	7.37	120.37	109.24
1	K	205	VAL	CB-CA-C	-7.36	102.55	111.97
2	L	454	TYR	N-CA-C	7.36	119.30	111.28
1	S	160	THR	N-CA-C	7.25	122.48	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	52	LYS	N-CA-C	-7.25	103.88	114.39
2	J	356	ALA	O-C-N	-7.23	114.46	122.12
1	U	122	LEU	N-CA-C	7.22	120.15	109.24
2	R	454	TYR	N-CA-C	7.22	119.15	111.28
2	V	512	GLU	N-CA-C	-7.17	102.88	111.69
1	K	205	VAL	N-CA-C	7.15	117.28	110.42
1	W	213	LEU	N-CA-C	-7.13	96.90	108.52
2	V	432	GLU	N-CA-C	7.13	119.41	109.15
1	I	72	ASP	N-CA-C	-7.10	103.62	111.36
2	C	454	TYR	N-CA-C	7.09	119.01	111.28
1	U	72	ASP	N-CA-C	-7.06	103.66	111.36
1	B	176	SER	N-CA-C	-7.04	101.23	110.53
1	S	115	ALA	N-CA-C	-7.04	103.53	111.14
1	S	12	ALA	N-CA-C	7.03	118.64	110.97
1	D	208	LEU	N-CA-C	7.02	120.08	109.41
1	K	122	LEU	N-CA-C	7.02	119.84	109.24
1	A	72	ASP	N-CA-C	-7.00	103.73	111.36
1	M	122	LEU	N-CA-C	7.00	119.81	109.24
2	X	454	TYR	N-CA-C	6.98	118.89	111.28
2	P	454	TYR	N-CA-C	6.98	118.89	111.28
1	I	160	THR	N-CA-C	6.98	122.09	112.04
1	W	116	LYS	CA-C-N	-6.96	113.53	120.21
1	W	116	LYS	C-N-CA	-6.96	113.53	120.21
1	F	10	GLU	N-CA-C	-6.96	103.70	111.28
1	I	122	LEU	N-CA-C	6.96	119.74	109.24
2	P	-38	VAL	N-CA-C	6.95	117.44	106.88
1	Q	122	LEU	N-CA-C	6.94	119.72	109.24
1	Q	160	THR	N-CA-C	6.94	122.04	112.04
2	N	434	GLU	CA-C-N	-6.90	115.35	123.08
2	N	434	GLU	C-N-CA	-6.90	115.35	123.08
2	H	354	GLU	N-CA-C	-6.88	103.86	111.36
2	H	-36	LEU	O-C-N	-6.88	114.08	122.20
1	D	122	LEU	N-CA-C	6.87	119.61	109.24
2	L	433	GLU	N-CA-C	-6.84	104.61	114.12
1	M	52	LYS	N-CA-C	-6.82	104.51	114.39
1	B	160	THR	N-CA-C	6.73	121.73	112.04
2	Z	-28	ARG	N-CA-C	-6.71	103.89	111.07
2	2	454	TYR	N-CA-C	6.70	119.44	111.33
1	A	46	PRO	N-CA-C	-6.68	104.82	113.57
1	D	176	SER	N-CA-C	-6.67	101.69	110.43
1	Q	52	LYS	N-CA-C	-6.67	104.73	114.39
1	W	160	THR	N-CA-C	6.65	121.62	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	432	GLU	N-CA-C	6.64	119.35	109.59
1	A	160	THR	N-CA-C	6.64	121.59	112.04
2	H	454	TYR	N-CA-C	6.62	118.50	111.28
1	K	226	THR	N-CA-C	6.62	119.78	109.52
1	I	52	LYS	N-CA-C	-6.62	104.79	114.39
1	K	143	TYR	N-CA-C	-6.62	104.10	111.71
1	U	213	LEU	N-CA-C	-6.62	96.89	108.20
2	T	432	GLU	N-CA-C	6.58	118.63	109.15
1	O	160	THR	N-CA-C	6.56	121.49	112.04
1	D	213	LEU	N-CA-C	-6.56	98.04	108.73
2	E	432	GLU	N-CA-C	6.54	119.20	109.59
1	K	206	ALA	N-CA-C	-6.54	105.17	113.01
1	B	170	SER	N-CA-C	6.52	120.94	112.92
1	F	160	THR	N-CA-C	6.52	121.43	112.04
1	U	165	ASN	O-C-N	-6.51	115.37	122.07
1	D	160	THR	N-CA-C	6.51	121.41	112.04
1	Q	143	TYR	N-CA-C	-6.49	104.21	111.28
1	O	122	LEU	N-CA-C	6.48	119.03	109.24
2	C	336	ILE	N-CA-C	-6.47	100.35	108.89
1	W	226	THR	N-CA-C	6.46	119.53	109.52
2	L	522	SER	N-CA-C	6.45	119.27	111.40
1	A	122	LEU	N-CA-C	6.43	118.95	109.24
1	W	222	PHE	N-CA-C	6.40	119.50	109.96
2	H	432	GLU	N-CA-C	6.38	119.02	109.25
1	M	170	SER	N-CA-C	6.38	121.85	113.30
1	B	122	LEU	N-CA-C	6.38	118.87	109.24
2	J	443	SER	N-CA-C	6.37	119.04	111.71
1	1	52	LYS	N-CA-C	-6.35	105.18	114.39
1	U	170	SER	N-CA-C	6.34	118.27	111.36
2	L	395	MET	N-CA-C	-6.32	105.05	112.89
1	D	72	ASP	N-CA-C	-6.32	104.48	111.36
2	2	472	TYR	N-CA-C	-6.31	104.48	111.36
1	O	143	TYR	N-CA-C	-6.31	104.45	111.71
1	K	7	ILE	N-CA-C	6.29	117.98	108.80
2	G	454	TYR	N-CA-C	6.27	118.12	111.28
1	B	52	LYS	N-CA-C	-6.25	105.33	114.39
2	N	-27	ARG	N-CA-C	6.25	118.17	111.36
1	Y	160	THR	N-CA-C	6.21	120.98	112.04
2	G	375	THR	N-CA-C	-6.19	102.36	110.53
1	O	52	LYS	N-CA-C	-6.19	105.41	114.39
2	V	395	MET	N-CA-C	-6.19	104.64	111.82
1	F	75	ARG	N-CA-C	-6.18	104.62	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	431	ILE	N-CA-C	-6.18	99.68	108.58
1	B	27	ALA	N-CA-C	6.17	119.65	110.52
2	V	-21	LEU	N-CA-C	6.15	117.40	109.65
2	Z	331	VAL	N-CA-C	6.15	117.35	109.30
2	T	454	TYR	N-CA-C	6.14	118.76	111.33
1	S	207	SER	N-CA-C	6.13	120.38	112.41
2	L	-36	LEU	N-CA-C	-6.13	99.21	109.07
1	K	113	GLU	N-CA-C	6.12	120.89	113.17
1	Y	204	GLY	N-CA-C	6.10	122.26	110.66
2	P	-38	VAL	CB-CA-C	-6.10	103.45	111.81
1	D	205	VAL	CB-CA-C	-6.09	103.92	112.14
1	Q	3	PHE	CA-C-N	6.09	127.45	119.84
1	Q	3	PHE	C-N-CA	6.09	127.45	119.84
1	U	160	THR	N-CA-C	6.07	120.89	112.45
1	M	176	SER	N-CA-C	-6.07	102.52	110.53
2	E	454	TYR	N-CA-C	6.06	117.89	111.28
2	Z	336	ILE	N-CA-C	-6.05	101.73	109.30
1	K	160	THR	N-CA-C	6.05	120.75	112.04
1	F	213	LEU	N-CA-C	-6.05	96.50	107.75
1	O	227	GLY	N-CA-C	6.04	122.34	111.34
1	O	226	THR	N-CA-C	6.03	118.86	109.52
2	P	434	GLU	N-CA-C	6.01	118.79	111.82
2	R	443	SER	N-CA-C	5.99	118.60	111.71
2	R	521	ARG	N-CA-C	-5.97	104.77	111.28
2	N	319	ARG	N-CA-C	5.97	119.32	110.48
2	N	336	ILE	N-CA-C	-5.96	101.02	108.89
1	B	226	THR	N-CA-C	5.94	119.24	109.85
2	C	503	VAL	N-CA-C	5.92	117.28	108.46
1	S	226	THR	N-CA-C	5.92	119.20	109.85
1	B	72	ASP	N-CA-C	-5.90	104.79	112.23
2	P	339	ASP	N-CA-C	5.90	119.58	112.38
2	P	432	GLU	N-CA-C	5.90	117.81	108.67
1	D	52	LYS	N-CA-C	-5.88	105.87	114.39
2	2	352	ALA	N-CA-C	5.88	118.92	111.69
1	Q	226	THR	N-CA-C	5.87	118.62	109.52
1	U	222	PHE	N-CA-C	5.87	118.77	109.96
2	E	522	SER	N-CA-C	-5.87	106.20	113.19
1	K	112	THR	N-CA-C	5.85	117.74	111.36
1	U	8	SER	CA-C-N	5.85	127.15	119.84
1	U	8	SER	C-N-CA	5.85	127.15	119.84
1	O	222	PHE	N-CA-C	5.84	118.73	109.96
1	U	52	LYS	N-CA-C	-5.84	105.92	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	331	VAL	N-CA-C	5.83	116.93	109.30
1	D	113	GLU	N-CA-C	5.82	121.26	114.04
1	W	72	ASP	N-CA-C	-5.81	105.03	111.36
1	W	122	LEU	N-CA-C	5.79	117.98	109.24
1	1	72	ASP	N-CA-C	-5.77	105.07	111.36
1	O	208	LEU	N-CA-C	5.76	118.45	109.52
2	G	431	ILE	CB-CA-C	-5.74	103.79	110.91
2	H	453	LEU	N-CA-C	5.73	119.89	113.01
1	I	29	SER	N-CA-C	5.73	119.03	110.14
1	W	113	GLU	N-CA-C	5.73	121.15	114.04
1	O	170	SER	N-CA-C	5.73	120.26	113.16
1	Q	166	ALA	N-CA-C	-5.70	105.07	111.28
1	1	29	SER	N-CA-C	5.69	118.96	110.14
1	S	52	LYS	N-CA-C	-5.69	106.14	114.39
2	J	399	LEU	N-CA-C	5.69	118.51	109.24
2	J	-19	ALA	N-CA-C	-5.68	103.17	111.30
1	K	170	SER	N-CA-C	5.68	120.94	112.94
2	X	431	ILE	N-CA-C	-5.64	99.60	108.23
2	H	375	THR	N-CA-C	-5.63	103.09	110.53
1	I	226	THR	N-CA-C	5.63	118.25	109.52
1	W	143	TYR	N-CA-C	-5.62	105.24	111.71
2	Z	-27	ARG	N-CA-C	5.62	117.48	111.36
1	1	226	THR	N-CA-C	5.61	118.22	109.52
1	U	171	TYR	N-CA-C	5.61	118.36	110.23
1	K	52	LYS	N-CA-C	-5.60	106.28	114.39
1	K	222	PHE	N-CA-C	5.60	118.35	110.23
2	N	375	THR	N-CA-C	-5.60	103.52	110.41
2	R	397	GLY	N-CA-C	5.60	121.52	114.25
1	F	208	LEU	N-CA-C	5.59	119.09	110.42
1	Q	222	PHE	N-CA-C	5.59	118.34	109.96
1	O	27	ALA	N-CA-C	5.57	118.78	110.14
1	S	176	SER	N-CA-C	-5.57	103.13	110.43
2	H	425	ALA	N-CA-C	5.56	119.16	112.38
2	C	472	TYR	N-CA-C	-5.55	105.14	111.14
2	H	-20	PRO	N-CA-C	5.55	121.25	113.53
1	D	204	GLY	N-CA-C	5.54	119.63	112.54
1	W	176	SER	N-CA-C	-5.54	103.22	110.53
1	D	205	VAL	N-CA-C	-5.53	104.98	110.62
1	1	222	PHE	N-CA-C	5.53	118.26	109.96
1	I	214	ASP	N-CA-C	5.53	117.98	109.07
1	W	52	LYS	N-CA-C	-5.53	106.37	114.39
2	V	-31	ASP	N-CA-C	-5.52	105.26	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	434	GLU	N-CA-C	5.51	118.22	111.82
2	H	462	SER	N-CA-C	-5.51	104.92	111.69
2	P	425	ALA	N-CA-C	5.50	119.09	112.38
1	I	170	SER	N-CA-C	5.50	120.10	113.17
2	V	345	ILE	N-CA-C	5.48	115.78	108.11
2	E	412	SER	N-CA-C	5.47	117.24	111.28
1	U	226	THR	N-CA-C	5.47	118.00	109.52
2	E	339	ASP	N-CA-C	5.46	119.04	112.38
1	O	176	SER	N-CA-C	-5.46	103.32	110.53
1	B	222	PHE	N-CA-C	5.45	118.23	110.10
2	C	-18	SER	N-CA-C	5.44	117.95	108.76
2	T	397	GLY	N-CA-C	5.43	121.15	114.69
2	L	336	ILE	N-CA-C	-5.43	101.67	108.84
1	A	16	ARG	N-CA-C	-5.42	105.27	111.07
2	H	505	VAL	CA-C-N	-5.42	114.21	119.90
2	H	505	VAL	C-N-CA	-5.42	114.21	119.90
2	L	339	ASP	N-CA-C	5.42	118.99	112.38
2	E	472	TYR	N-CA-C	-5.42	105.29	111.14
1	Q	29	SER	N-CA-C	5.41	118.53	110.14
2	T	-4	LEU	N-CA-C	5.41	117.54	110.08
1	A	29	SER	N-CA-C	5.39	118.50	110.14
2	X	515	ARG	N-CA-C	-5.39	105.40	111.28
2	N	380	ILE	CB-CA-C	-5.39	105.07	111.97
2	T	456	GLN	CA-C-N	-5.37	115.65	122.37
2	T	456	GLN	C-N-CA	-5.37	115.65	122.37
1	I	7	ILE	N-CA-C	5.37	116.63	108.80
2	H	-35	SER	N-CA-C	-5.36	106.04	112.58
2	X	425	ALA	N-CA-C	5.36	118.92	112.38
2	P	-35	SER	N-CA-C	-5.35	106.05	112.58
1	B	213	LEU	N-CA-C	-5.35	99.05	108.20
1	D	226	THR	N-CA-C	5.35	117.81	109.52
1	Y	226	THR	N-CA-C	5.33	117.78	109.52
2	G	336	ILE	N-CA-C	-5.33	100.65	108.54
2	L	349	ALA	N-CA-C	5.33	116.77	111.07
2	N	432	GLU	N-CA-C	5.33	116.93	108.67
1	A	147	ILE	N-CA-C	5.32	115.55	108.11
1	F	113	GLU	N-CA-C	5.32	120.78	113.97
2	Z	433	GLU	N-CA-C	5.32	118.23	111.69
2	G	319	ARG	N-CA-C	5.31	118.33	110.48
1	S	113	GLU	N-CA-C	5.30	121.15	114.31
1	K	214	ASP	N-CA-C	5.29	117.14	108.52
2	C	453	LEU	N-CA-C	5.29	119.36	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	443	SER	N-CA-C	5.29	117.79	111.71
2	N	433	GLU	N-CA-C	-5.29	106.33	112.89
1	U	143	TYR	N-CA-C	-5.29	105.63	111.71
2	X	319	ARG	N-CA-C	5.26	118.69	110.32
1	D	170	SER	N-CA-C	5.26	119.79	113.17
2	2	402	PRO	N-CA-C	5.25	120.44	111.68
1	O	8	SER	N-CA-C	5.24	117.00	109.04
2	V	319	ARG	N-CA-C	5.24	118.23	110.48
1	M	27	ALA	N-CA-C	5.22	118.24	110.52
1	B	150	GLU	N-CA-C	5.20	116.47	109.24
1	D	150	GLU	N-CA-C	5.20	116.47	109.24
1	U	208	LEU	N-CA-C	5.20	117.58	109.52
2	V	331	VAL	N-CA-C	5.20	116.11	109.30
1	O	169	GLU	N-CA-C	5.19	117.02	111.36
2	Z	319	ARG	N-CA-C	5.19	118.57	110.32
1	B	68	PHE	N-CA-C	5.18	117.34	111.02
1	Q	233	LEU	N-CA-C	5.17	116.92	111.28
2	Z	510	ILE	N-CA-C	-5.17	106.10	111.58
2	C	319	ARG	N-CA-C	5.17	118.13	110.48
1	B	208	LEU	N-CA-C	5.17	117.82	109.40
1	O	29	SER	N-CA-C	5.17	118.16	109.95
1	O	145	GLY	N-CA-C	-5.17	107.98	115.27
2	H	443	SER	N-CA-C	5.16	117.65	111.71
2	N	465	ARG	N-CA-C	-5.16	105.31	111.03
2	N	-4	LEU	CA-C-N	5.15	125.39	119.83
2	N	-4	LEU	C-N-CA	5.15	125.39	119.83
2	N	518	ILE	CB-CA-C	-5.14	105.20	112.14
2	C	-20	PRO	N-CA-C	-5.12	105.57	112.48
1	Y	205	VAL	N-CA-C	5.12	119.98	109.34
1	O	39	VAL	N-CA-C	5.11	115.26	108.11
1	A	222	PHE	N-CA-C	5.11	117.71	110.10
2	P	331	VAL	N-CA-C	5.10	115.98	109.30
1	Q	75	ARG	N-CA-C	-5.10	105.63	111.14
2	C	425	ALA	N-CA-C	5.10	118.60	112.38
1	F	143	TYR	N-CA-C	-5.10	105.85	111.71
2	C	402	PRO	N-CA-C	5.09	120.27	111.77
2	Z	348	THR	N-CA-C	5.09	117.61	110.23
1	U	56	LEU	N-CA-C	-5.09	106.17	112.93
1	D	29	SER	N-CA-C	5.08	118.02	110.14
2	N	462	SER	N-CA-C	-5.08	105.82	111.36
2	P	397	GLY	N-CA-C	5.08	121.13	115.08
2	P	399	LEU	N-CA-C	5.08	117.84	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	8	SER	N-CA-C	5.08	117.06	110.40
2	P	472	TYR	N-CA-C	-5.08	105.65	111.14
1	K	39	VAL	N-CA-C	5.08	115.21	108.11
2	L	319	ARG	N-CA-C	5.07	117.99	110.48
2	N	-36	LEU	N-CA-C	-5.07	106.78	113.17
1	B	116	LYS	CA-C-N	-5.07	115.56	120.98
1	B	116	LYS	C-N-CA	-5.07	115.56	120.98
1	O	213	LEU	N-CA-C	-5.06	97.19	107.41
2	E	462	SER	N-CA-C	-5.05	105.86	111.36
2	H	397	GLY	N-CA-C	5.05	121.77	115.21
2	J	380	ILE	CB-CA-C	-5.04	105.51	111.97
1	O	116	LYS	CA-C-N	-5.04	115.37	120.21
1	O	116	LYS	C-N-CA	-5.04	115.37	120.21
2	N	331	VAL	N-CA-C	5.03	115.89	109.30
2	R	453	LEU	N-CA-C	5.03	119.27	113.18
1	W	29	SER	N-CA-C	5.03	117.94	110.14
2	H	339	ASP	N-CA-C	5.03	118.51	112.38
1	M	222	PHE	N-CA-C	5.02	117.57	110.10
1	S	165	ASN	CA-C-N	-5.01	113.56	120.28
1	S	165	ASN	C-N-CA	-5.01	113.56	120.28
1	M	213	LEU	N-CA-C	-5.01	97.85	107.57
1	M	113	GLU	N-CA-C	5.01	120.38	113.97
2	N	339	ASP	N-CA-C	5.01	118.49	112.38
2	2	319	ARG	N-CA-C	5.00	117.89	110.48
1	A	226	THR	N-CA-C	5.00	117.27	109.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1693	0	1688	138	0
1	A	1713	0	1713	131	0
1	B	1695	0	1685	129	0
1	D	1717	0	1712	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1706	0	1705	93	0
1	I	1680	0	1673	102	0
1	K	1705	0	1702	154	0
1	M	1730	0	1726	115	0
1	O	1675	0	1676	107	0
1	Q	1716	0	1710	151	0
1	S	1686	0	1685	107	0
1	U	1706	0	1705	161	0
1	W	1710	0	1705	128	0
1	Y	1730	0	1726	92	0
2	2	1829	0	1824	69	0
2	C	1853	0	1850	106	0
2	E	1834	0	1829	101	0
2	G	1858	0	1855	78	0
2	H	1844	0	1841	111	0
2	J	1863	0	1858	88	0
2	L	1857	0	1853	102	0
2	N	1863	0	1858	78	0
2	P	1853	0	1850	103	0
2	R	1822	0	1815	84	0
2	T	1854	0	1850	76	0
2	V	1843	0	1837	75	0
2	X	1848	0	1845	96	0
2	Z	1817	0	1810	86	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2715	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 27.

All (2715) 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:207:SER:C	1:D:208:LEU:HD12	1.56	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
2:L:413:ASP:OD1	2:L:414:PRO:HD2	1.36	1.24
1:W:173:GLU:C	1:W:174:ASN:HD22	1.45	1.23
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:301:ALA:HB2	2:R:333:LYS:HZ3	1.05	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
1:Y:35:TYR:CE1	1:Y:37:GLY:CA	2.30	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
2:X:301:ALA:HB2	2:X:333:LYS:HZ3	1.08	1.12
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
2:T:-17:ILE:O	2:T:-16:SER:HB2	1.47	1.09
1:I:8:SER:CB	1:I: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:207:SER:C	1:D:208:LEU:CD1	2.30	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
2:V:301:ALA:HB2	2:V:333:LYS:HZ3	1.18	1.03
1:D:3:PHE:CE1	1:F:6:PHE:HZ	1.68	1.03
1:D:13:MET:HE1	1:Q:116:LYS:HD2	1.40	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
1:M:7:ILE:HD13	1:W:5:TYR:HD2	1.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:181:LEU:HD12	1:I: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: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:I:250:HOH:O	1.62	0.98
2:C:456:GLN:HE22	2:C:465:ARG:NH2	1.62	0.97
1:I:30:VAL:HG13	1:I: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
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
2:R:301:ALA:CB	2:R:333:LYS:HZ3	1.78	0.96
1:U:167:LEU:HA	1:U:170:SER:OG	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:-39:ALA:N	2:J:-26:GLN:CD	2.24	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:Y:181:LEU:HD12	1:Y:181:LEU:C	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:18:GLU:CD	1:1:21:ARG:HH21	1.76	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:O:19:LEU:HD23	1:O:19:LEU:C	1.94	0.92
1:A:19:LEU:HD12	1:B:9:PRO:HB2	1.51	0.92
2:C:409:ILE:HG13	2:C:410:HIS:ND1	1.85	0.92
1:S:15:GLU:OE2	1:1:9:PRO:HD2	1.69	0.92
1:U:214:ASP:HB3	1:U:217:ARG:HG3	1.50	0.91
2:P:407:TYR:CE1	2:P:417:ALA:HB3	2.05	0.91
2:2:-28:ARG:HG2	2:2:-21:LEU:CD1	2.00	0.91
2:E:456:GLN:HE22	2:E:465:ARG:NH2	1.68	0.91
2:N:-21:LEU:HD12	2:N:-20:PRO:HD3	1.49	0.91
1:D:15:GLU:OE2	1:K:8:SER:HB2	1.70	0.91
1:D:35:TYR:HE1	1:D:37:GLY:HA3	1.22	0.91
2:G:362:GLU:OE2	2:G:382:ARG:HD3	1.69	0.91
1:Y:179:ASP:O	1:Y:183:ILE:HG13	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:234:LEU:C	1:K:234:LEU:HD13	1.96	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
1:W:173:GLU:C	1:W:174:ASN:ND2	2.30	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:HD21	1:A:52:LYS:CD	1.86	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:382:ARG:NH2	2:X:385:ILE:HD13	1.92	0.84
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
2:C:-39:ALA:H2	2:J:-26:GLN:CD	1.85	0.83
2:P:301:ALA:HB2	2:P:333:LYS:HZ3	1.44	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
2:H:-27:ARG:HG2	2:H:-26:GLN:CD	2.04	0.82
1:Q:40:LEU:HD12	1:Q:212:VAL:CG1	2.09	0.82
1:A:7:ILE:HD12	1:A:11:GLN:CG	2.10	0.82
1:S:25:ALA:O	1:S:158:GLY:HA2	1.79	0.82
1:F:203:LEU:N	1:F:234:LEU:HD11	1.94	0.82
1:B:5:TYR:HE2	1:O:11:GLN:HE22	1.27	0.82
2:E:-36:LEU:HD12	2:E:-31:ASP:OD2	1.80	0.82
2:N:301:ALA:HB2	2:N:333:LYS:NZ	1.93	0.82
1:O:155:VAL:HG21	1:O:167:LEU:CD1	2.09	0.82
2:H:407:TYR:CZ	2:H:417:ALA:CB	2.62	0.82
1:O:234:LEU:HD13	1:O:234:LEU:C	2.03	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:H:-27:ARG:NE	2:H:-26:GLN:CD	2.39	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
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
1:Q:171:TYR:CD2	1:Q:171:TYR:C	2.56	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:-39:ALA:N	2:J:-26:GLN:NE2	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:358:LEU:HD23	2:E:386:MET:HE3	1.64	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:171:TYR:CE2	1:Q:172:ALA:C	2.61	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:G:456:GLN:HE22	2:G:465:ARG:HH22	0.81	0.78
1:1:18:GLU:OE1	1:1:22:LYS:CE	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:-26:GLN:CD	2:H:-39:ALA:HB1	2.09	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:F:169:GLU:OE1	1:F:169:GLU:HA	1.84	0.78
1:Y:169:GLU:HA	1:Y:169:GLU:OE1	1.83	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
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:B:234:LEU:O	1:B:235:VAL:CG2	2.30	0.77
1:M:163:ILE:HD11	1:M:191:GLY:HA3	1.65	0.77
1:M:186:ALA:HA	1:M:189:ARG:CZ	2.13	0.77
1:U:11:GLN:HG2	1:1:5:TYR:CE1	2.20	0.77
1:B:59:ARG:HD2	1:B:129:HIS:HA	1.67	0.77
1:I:25:ALA:O	1:I:158:GLY:HA2	1.84	0.77
2:J:301:ALA:CB	2:J:333:LYS:NZ	2.48	0.77
1:M:16:ARG:HB3	1:M:16:ARG:NH1	2.00	0.77
1:B:25:ALA:O	1:B:158:GLY:HA2	1.84	0.77
1:K:5:TYR:CD1	1:M:11:GLN:CG	2.63	0.77
1:W:174:ASN:ND2	1:W:174:ASN:N	2.30	0.77
1:Q:181:LEU:O	1:Q:185:VAL:CG2	2.32	0.77
1:D:59:ARG:HD2	1:D:129:HIS:HA	1.66	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:13:MET:HE3	1:O:116:LYS:HD2	1.65	0.76
2:H:-27:ARG:HE	2:H:-26:GLN:CD	1.94	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:Q:171:TYR:C	1:Q:171:TYR:HD2	1.94	0.75
1:W:59:ARG:HD2	1:W:129:HIS:HA	1.68	0.75
1:I:173:GLU:CG	1:I: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:I:191:GLY:O	1:I:192:SER:C	2.30	0.75
1:U:176:SER:OG	1:U:179:ASP:CG	2.30	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:I:181:LEU:HD12	1:I:181:LEU:C	2.11	0.75
1:D:173:GLU:C	1:D:174:ASN:OD1	2.30	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:Q:173:GLU:C	1:Q:174:ASN:OD1	2.30	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
2:T:338:ASP:C	2:T:338:ASP:OD1	2.29	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:CD1	1:A:40:LEU:HB3	2.17	0.74
1:O:234:LEU:C	1:O:234:LEU:CD1	2.60	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
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
1:1:173:GLU:C	1:1:174:ASN:OD1	2.30	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
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:A:7:ILE:C	1:B:5:TYR:HB3	2.13	0.73
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:K:179:ASP:OD1	1:K:179:ASP:C	2.31	0.73
1:O:8:SER:HG	1:O:11:GLN:HB3	1.52	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:U:188:LEU:C	1:U:188:LEU:HD23	2.15	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:U:167:LEU:HA	1:U:170:SER:HG	1.55	0.72
1:O:41:PHE:HB3	1:O:53:ILE:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:41:PHE:HB3	1:I: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
1:Q:153:PHE:HD2	1:Q:171:TYR:HD1	1.38	0.71
1:I:167:LEU:HD12	1:I: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:A:178:THR:O	1:A:182:ARG:HG3	1.91	0.70
1:U:41:PHE:HB3	1:U:53:ILE:HD13	1.71	0.70
1:I:33:LEU:HD11	1:I:40:LEU:HB3	1.73	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:K:150:GLU:HG3	1:K:154:VAL:HG22	1.73	0.70
1:A:13:MET:HE3	1:O:116:LYS:CD	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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
1:U:13:MET:HE2	1:U:111:PHE:HE2	1.56	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
1:U:207:SER:C	1:U:208:LEU:HD13	2.16	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
2:T:414:PRO:C	2:T:415:GLN:HE21	2.01	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
1:O:19:LEU:C	1:O:19:LEU:CD2	2.66	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: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)
1:S:214:ASP:OD1	1:S:214:ASP:C	2.33	0.69
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
2:L:-18:SER:C	2:L:-17:ILE:HG22	2.18	0.68
1:O:51:GLN:NE2	1:O:51:GLN:N	2.30	0.68
2:V:301:ALA:CB	2:V:333:LYS:HZ3	1.95	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
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
2:H:413:ASP:OD1	2:H:413:ASP:C	2.36	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
1:Y:181:LEU:C	1:Y:181:LEU:CD1	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:8:SER:H	1:I: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:I:9:PRO:CD	2.41	0.67
1:U:5:TYR:HB2	1:I: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
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:Q:234:LEU:C	1:Q:235:VAL:HG23	2.20	0.67
1:U:181:LEU:CD2	1:U:234:LEU:HD12	2.24	0.67
2:C:-39:ALA:H1	2:J:-26:GLN:CD	1.99	0.67
1:K:4:PRO:CG	1:W:5:TYR:CG	2.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:301:ALA:CB	2:X:333:LYS:HZ2	2.06	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
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
1:A:11:GLN:CD	1:A:14:ARG:HH21	2.02	0.66
2:C:308:TYR:OH	2:C:496:ILE:HD11	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
1:D:191:GLY:O	1:D:192:SER:HB2	1.94	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
2:V:-26:GLN:HE22	2:2:-38:VAL:H1	1.43	0.66
1:Y:2:SER:O	1:Y:4:PRO:HD3	1.95	0.66
1:1:8:SER:H	1:1:11:GLN:CD	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:19:LEU:HD23	1:B:19:LEU:C	2.21	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:-18:SER:O	2:X:-17:ILE:C	2.39	0.65
1:A:9:PRO:CG	1:O:15:GLU:HB3	2.26	0.65
2:H:-29:LEU:O	2:H:-25:ALA:C	2.39	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
2:R:301:ALA:HB1	2:R:333:LYS:HZ2	1.62	0.65
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:I:161:GLU:N	1:I: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: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:I:152:HIS:HB3	1:I: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:H:485:ASP:C	2:H:485:ASP:OD1	2.39	0.65
2:T:338:ASP:OD1	2:T:339:ASP:N	2.30	0.65
1:I:152:HIS:CD2	1:I: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:U:207:SER:C	1:U:208:LEU:CD1	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:351:VAL:CG1	2:E:400:ALA:HB2	2.27	0.64
1:K:234:LEU:C	1:K:234:LEU:CD1	2.69	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
2:C:430:ASN:ND2	2:C:431:ILE:C	2.55	0.64
1:M:7:ILE:CD1	1:W:5:TYR:CD2	2.65	0.64
1:O:35:TYR:CZ	1:O:37:GLY:CA	2.72	0.64
1:Y:18:GLU:OE1	1:Y:21:ARG:NH2	2.30	0.64
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:167:LEU:CA	1:U:170:SER:HG	2.09	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:-17:ILE:C	2:G:-17:ILE:HD13	2.23	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:G:391:LEU:HD12	2:G:391:LEU:C	2.22	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
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
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
1:Y:234:LEU:C	1:Y:235:VAL:HG23	2.23	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
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
2:T:413:ASP:CG	2:T:414:PRO:HD2	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:430:ASN:ND2	2:C:430:ASN:C	2.57	0.62
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
1:I:169:GLU:OE1	1:I:169:GLU:HA	1.99	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:Q:169:GLU:HA	1:Q:169:GLU:OE1	1.98	0.62
1:U:8:SER:N	1:I:5:TYR:O	2.32	0.62
2:Z:312:VAL:HG12	2:Z:497:ILE:HB	1.81	0.62
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
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:S:19:LEU:C	1:S:19:LEU:HD23	2.25	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:D:161:GLU:H	1:D:161:GLU:CD	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:LYS:HB2	1:A:52:LYS:HZ2	1.65	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
1:U:13:MET:HA	1:U:13:MET:HE3	1.82	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:129:HIS:HB2	1:S:132:GLU:CD	2.26	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:B:161:GLU:CD	1:B:161:GLU:H	2.08	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
1:I:214:ASP:OD1	1:I:214:ASP:C	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:465:ARG:HB3	2:J:465:ARG:HH11	1.66	0.61
2:L:-23:GLU:CD	2:L:-23:GLU:H	2.09	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:308:TYR:CE1	2:X:311:GLY:HA3	2.35	0.61
1:F:129:HIS:HB2	1:F:132:GLU:CD	2.26	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
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:A:161:GLU:H	1:A:161:GLU:CD	2.09	0.60
1:D:19:LEU:HD12	1:K:9:PRO:HB3	1.81	0.60
2:Z:348:THR:CG2	2:Z:351:VAL:HG23	2.30	0.60
1:B:112:THR:HG22	1:B:113:GLU:OE2	2.01	0.60
1:O:161:GLU:CD	1:O:161:GLU:H	2.10	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
2:P:301:ALA:CB	2:P:333:LYS:HZ3	2.13	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:Q:163:ILE:HG23	1:Q:187:ALA:C	2.26	0.60
1:Y:128:ALA:HB2	1:Y:134:LYS:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:GLY:O	1:D:208:LEU:HD13	2.01	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
1:F:189:ARG:HH21	1:F:203:LEU:HD23	1.65	0.59
1:W:129:HIS:HB2	1:W:132:GLU:CD	2.27	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
2:C:-4:LEU:CD1	2:C:398:LEU:HD11	2.33	0.59
1:I:161:GLU:H	1:I:161:GLU:CD	2.10	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
2:X:301:ALA:HB1	2:X:333:LYS:HZ2	1.67	0.59
1:Y:31:VAL:HG12	1:Y:155:VAL:HG22	1.84	0.59
1:B:13:MET:HE3	1:B:111:PHE:HE2	1.67	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
2:R:355:PHE:CE2	2:R:386:MET:HE2	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
1:K:234:LEU:O	1:K:235:VAL:C	2.45	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:S:161:GLU:H	1:S:161:GLU:CD	2.11	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
2:H:-27:ARG:C	2:H:-26:GLN:OE1	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:92:ARG:CG	1:I:92:ARG:HH11	2.15	0.59
2:J:-38:VAL:O	2:J:-36:LEU:HD22	2.03	0.59
1:Y:161:GLU:H	1:Y:161:GLU:CD	2.11	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: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
2:J:-16:SER:O	2:J:-15:GLY:C	2.46	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:T:413:ASP:OD1	2:T:413:ASP:C	2.46	0.58
1:I:19:LEU:HD23	1:I:19:LEU:C	2.28	0.58
1:I:129:HIS:HB2	1:I:132:GLU:CD	2.28	0.58
1:Q:161:GLU:H	1:Q:161:GLU:CD	2.11	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:Q:171:TYR:HE2	1:Q:172:ALA:C	2.11	0.58
2:C:-29:LEU:CD2	2:C:-25:ALA:HB3	2.34	0.58
2:L:-18:SER:C	2:L:-17:ILE:CG2	2.77	0.58
1:M:98:GLN:O	1:M:102:VAL:HG23	2.03	0.58
2:P:-27:ARG:NE	2:P:-26:GLN:CD	2.61	0.58
2:P:407:TYR:CE1	2:P:417:ALA:CB	2.82	0.58
1:W:33:LEU:O	1:W:33:LEU:CD1	2.51	0.58
1:I:8:SER:OG	1:I:11:GLN:CD	2.46	0.58
1:U:205:VAL:HG21	1:U:231:GLN:HB2	1.84	0.58
1:I:217:ARG:HD2	1:I:218:PRO:HD2	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:319:ARG:HG3	2:C:320:SER:N	2.19	0.57
2:E:338:ASP:C	2:E:338:ASP:OD1	2.46	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
1:1:13:MET:HA	1:1:13:MET:HE3	1.85	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
2:T:340:TYR:O	2:T:341:THR:HG22	2.03	0.57
2:T:340:TYR:C	2:T:341:THR:CG2	2.78	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
2:Z:511:ALA:HB1	2:Z:515:ARG:HH21	1.69	0.57
1:F:161:GLU:H	1:F:161:GLU:CD	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:129:HIS:HB2	1:Q:132:GLU:CD	2.30	0.57
1:S:28:LYS:NZ	1:S:52:LYS:HE3	2.20	0.57
2:T:486:LEU:HG	2:T:515:ARG:NH1	2.19	0.57
1:B:129:HIS:HB2	1:B:132:GLU:CD	2.30	0.57
1:U:191:GLY:O	1:U:192:SER:C	2.47	0.57
2:V:301:ALA:CB	2:V:333:LYS:HZ2	2.15	0.57
1:W:15:GLU:CD	1:Y:9:PRO:HG2	2.29	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
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
1:1:19:LEU:C	1:1:19:LEU:CD2	2.78	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
1:D:25:ALA:O	1:D:158:GLY:HA2	2.05	0.56
2:G:-29:LEU:O	2:G:-25:ALA:C	2.49	0.56
1:K:58:ASP:OD1	1:K:219:ARG:NH1	2.39	0.56
1:K:161:GLU:H	1:K:161:GLU:CD	2.12	0.56
2:N:382:ARG:NH2	2:N:385:ILE:HD13	2.21	0.56
2:R:407:TYR:C	2:R:407:TYR:CD2	2.84	0.56
2:T:382:ARG:NH2	2:T:385:ILE:HD13	2.20	0.56
1:W:19:LEU:HD23	1:W:19:LEU:C	2.31	0.56
1:W:161:GLU:H	1:W:161:GLU:CD	2.12	0.56
1:I:130:TYR:HE1	1:I:216:ASN:O	1.88	0.56
1:I:152:HIS:CD2	1:I:171:TYR:CE2	2.92	0.56
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:176:SER:HG	1:U:179:ASP:CG	2.11	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
1:A:129:HIS:HB2	1:A:132:GLU:CD	2.31	0.56
1:K:129:HIS:HB2	1:K:132:GLU:CD	2.30	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
2:C:338:ASP:C	2:C:338:ASP:OD1	2.49	0.56
2:C:430:ASN:C	2:C:430:ASN:HD22	2.14	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:I:225:ILE:HG21	1:I: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
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
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:I:5:TYR:CZ	2.40	0.55
1:B:92:ARG:HH11	1:B:92:ARG:HG3	1.70	0.55
2:E:-26:GLN:OE1	2:E:-26:GLN:HA	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:-29:LEU:O	2:J:-25:ALA:C	2.49	0.55
1:Q:13:MET:HE1	1:Q:111:PHE:HE2	1.72	0.55
1:Q:142:THR:OG1	1:Q:144:ASP:HB3	2.06	0.55
1:Q:234:LEU:C	1:Q:235:VAL:CG2	2.79	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:R:338:ASP:C	2:R:338:ASP:OD1	2.50	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: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
2:P:407:TYR:HE1	2:P:417:ALA:HB3	1.67	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
1:D:129:HIS:HB2	1:D:132:GLU:CD	2.32	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
2:J:515:ARG:HG2	2:J:515:ARG:HH11	1.72	0.55
1:U:7:ILE:HA	1:I:5:TYR:O	2.07	0.55
2:X:391:LEU:O	2:X:395:MET:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:U:161:GLU:CD	1:U:161:GLU:H	2.16	0.54
1:1:129:HIS:HB2	1:1:132:GLU:CD	2.32	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
1:D:67:LYS:NZ	1:K:144:ASP:OD1	2.39	0.54
1:F:129:HIS:HE1	3:F:251:HOH:O	1.90	0.54
1:I:27:ALA:HB1	1:I:28:LYS:CE	2.37	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
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:X:350:ALA:C	2:X:353:VAL:HG12	2.33	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
2:V:338:ASP:C	2:V:338:ASP:OD1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:LEU:CD1	1:F:33:LEU:C	2.80	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
1:1:8:SER:H	1:1:11:GLN:HG3	1.72	0.54
1:A:13:MET:CE	1:O:116:LYS:CD	2.86	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: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:171:TYR:CD2	1:Q:172:ALA:C	2.86	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:O:129:HIS:HB2	1:O:132:GLU:CD	2.33	0.54
2:P:338:ASP:C	2:P:338:ASP:OD1	2.51	0.54
1:Y:129:HIS:HB2	1:Y:132:GLU:CD	2.33	0.54
1:Y:181:LEU:CD1	1:Y:185:VAL:CG2	2.86	0.54
2:Z:338:ASP:C	2:Z:338:ASP:OD1	2.51	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:B:234:LEU:C	1:B:235:VAL:HG23	2.29	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: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
2:C:-29:LEU:HD23	2:C:-25:ALA:HB3	1.90	0.53
1:F:98:GLN:O	1:F:102:VAL:HG23	2.08	0.53
2:L:338:ASP:C	2:L:338:ASP:OD1	2.51	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
1:U:129:HIS:HB2	1:U:132:GLU:CD	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:338:ASP:C	2:H:338:ASP:OD1	2.51	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:P:314:MET:HE3	2:P:405:ALA:HB2	1.91	0.53
2:R:382:ARG:NH2	2:R:385:ILE:HD13	2.24	0.53
2:E:-28:ARG:HB2	2:E:-21:LEU:HD21	1.91	0.53
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
2:T:-2:HIS:C	2:T:-2:HIS:ND1	2.66	0.53
1:Q:214:ASP:OD1	1:Q:214:ASP:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:ILE:CG1	1:I:191:GLY:HA3	2.38	0.52
2:J:-28:ARG:NH2	2:T:-23:GLU:CD	2.67	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: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
2:C:464:LEU:O	2:C:464:LEU:HG	2.10	0.52
2:C:515:ARG:O	2:C:516:ALA:C	2.52	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:340:TYR:C	2:T:341:THR:HG23	2.33	0.52
2:C:366:TYR:CE2	2:C:374:LEU:HD13	2.44	0.52
1:D:13:MET:HE2	1:Q:19:LEU:HD11	1.92	0.52
2:R:407:TYR:C	2:R:407:TYR:HD2	2.18	0.52
1:B:33:LEU:CD1	1:B:33:LEU:O	2.58	0.52
2:H:515:ARG:O	2:H:516:ALA:C	2.53	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: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
1:I:224:ARG:HH11	1:I:224:ARG:HG2	1.75	0.52
2:P:-27:ARG:C	2:P:-26:GLN:OE1	2.53	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:I:51:GLN:HA	1:I:209:GLU:OE2	2.10	0.52
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
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:I:92:ARG:HH11	1:I: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
2:L:432:GLU:CD	2:L:437:GLN:HE21	2.18	0.51
1:I:7:ILE:HB	1:I: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:E:358:LEU:HD23	2:E:386:MET:CE	2.39	0.51
2:J:509:ARG:HH11	2:J:509:ARG:HG3	1.74	0.51
2:L:382:ARG:HH21	2:L:385:ILE:HD13	1.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:7:ILE:HD13	1:A:15:GLU:CD	2.35	0.51
1:B:182:ARG:CG	1:B:183:ILE:N	2.72	0.51
2:E:413:ASP:HB2	2:E:416:SER:HG	1.72	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
1:U:166:ALA:C	1:U:170:SER:HG	2.16	0.51
2:X:-36:LEU:O	2:X:-35:SER:HB2	2.11	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
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:19:LEU:HD23	1:Q:19:LEU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:R:382:ARG:HH21	2:R:385:ILE:HD13	1.75	0.51
1:I:112:THR:HG22	1:I: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: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
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
2:Z:-29:LEU:O	2:Z:-28:ARG:C	2.54	0.50
1:I:173:GLU:HG3	1:I: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:2:314:MET:HE3	2:2:405:ALA:HB2	1.94	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
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
1:Q:176:SER:OG	1:Q:179:ASP:CG	2.54	0.50
2:V:-5:GLN:NE2	2:V:-2:HIS:CE1	2.80	0.50
1:W:33:LEU:CD1	1:W:33:LEU:C	2.84	0.50
1:W:152:HIS:HB3	1:W:171:TYR:CE2	2.47	0.50
1:W:204:GLY:O	1:W:208:LEU:HB2	2.12	0.50
2:C:382:ARG:HD2	1:I:89:TYR:CE1	2.47	0.49
1:F:16:ARG:NH2	1:F:115:ALA:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:ASN:O	1:I:216:ASN:OD1	2.30	0.49
1:I:216:ASN:C	1:I:216:ASN:OD1	2.55	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
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
2:C:349:ALA:O	2:C:350:ALA:C	2.54	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:R:-2:HIS:C	2:R:-2:HIS:CD2	2.91	0.49
2:V:301:ALA:HB2	2:V:333:LYS:CE	2.42	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
1:1:28:LYS:HZ2	1:1:52:LYS:HE3	1.75	0.49
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:I:116:LYS:NZ	1:I:117:PRO:O	2.43	0.49
2:J:301:ALA:O	2:J:440:GLY:HA3	2.13	0.49
2:N:338:ASP:C	2:N:338:ASP:OD1	2.56	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
1:U:188:LEU:C	1:U:188:LEU:CD2	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:165:ASN:O	1:S:166:ALA:C	2.53	0.49
2:T:314:MET:HE3	2:T:405:ALA:HB2	1.94	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
2:X:314:MET:HE3	2:X:405:ALA:HB2	1.93	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:I:30:VAL:HG22	1:I:52:LYS:HZ3	1.77	0.49
1:O:144:ASP:OD1	1:O:146:SER:OG	2.30	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
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
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: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
1:S:30:VAL:HG22	1:S:52:LYS:HZ3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:191:GLY:O	1:S:192:SER:O	2.31	0.49
1:Y:116:LYS:NZ	1:Y:119:GLU:OE2	2.42	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:C:-29:LEU:O	2:C:-25:ALA:C	2.56	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:G:390:ASN:CG	2:G:390:ASN:O	2.56	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:203:LEU:C	1:U:207:SER:OG	2.56	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:E:-30:PHE:C	2:E:-30:PHE:CD2	2.91	0.48
2:H:308:TYR:CD1	2:H:308:TYR:C	2.91	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:U:19:LEU:HD23	1:U:19:LEU:C	2.38	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
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:D:161:GLU:CD	1:D:161:GLU:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:U:8:SER:HA	1:U:9:PRO:HD2	1.61	0.48
2:V:-26:GLN:NE2	2:2:-38:VAL:H1	2.10	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: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
2:G:-23:GLU:HG3	2:N:-28:ARG:HD2	1.95	0.48
2:H:314:MET:HE3	2:H:405:ALA:HB2	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
2:P:302:THR:OG1	2:P:481:THR:OG1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:K:30:VAL:HG13	1:K:43:ALA:CB	2.27	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
1:A:234:LEU:C	1:A:235:VAL:CG2	2.86	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
2:2:338:ASP:C	2:2:338:ASP:OD1	2.57	0.48
1:A:123:CYS:HA	1:A:139:TYR:O	2.14	0.47
1:A:234:LEU:C	1:A:235:VAL:HG23	2.38	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:-26:GLN:C	2:P:-24:PRO:HD3	2.39	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:Z:469:GLU:HG3	2:Z:517:ILE:HD13	1.95	0.47
1:K:144:ASP:OD2	1:K:146:SER:OG	2.30	0.47
1:O:13:MET:HE3	1:O:13:MET:HB3	1.85	0.47
2:P:-17:ILE:HG21	2:P:396:GLN:CD	2.39	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
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
1:B:161:GLU:CD	1:B:161:GLU:N	2.72	0.47
2:J:308:TYR:CD1	2:J:308:TYR:C	2.91	0.47
2:N:399:LEU:HG	2:N:400:ALA:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:140:ARG:C	1:K:141:ILE:HD12	2.39	0.47
1:S:35:TYR:N	1:S:38:GLY:O	2.46	0.47
2:T:375:THR:HG21	1:I:92:ARG:HB3	1.96	0.47
1:U:13:MET:HE2	1:U:111:PHE:CE2	2.45	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:I:224:ARG:HH11	1:I: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:M:155:VAL:C	1:M:156:MET:HG3	2.39	0.47
1:Q:7:ILE:CD1	1:Q:12:ALA:HA	2.45	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:Y:19:LEU:C	1:Y:19:LEU:HD23	2.40	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:D:207:SER:C	1:D:208:LEU:HD13	2.31	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
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
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:R:351:VAL:HG12	2:R:400:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:Y:19:LEU:O	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:G:-17:ILE:C	2:G:-17:ILE:CD1	2.88	0.47
2:G:358:LEU:HD23	2:G:386:MET:HE3	1.95	0.47
2:H:-27:ARG:CG	2:H:-26:GLN:CD	2.84	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
1:M:129:HIS:HB2	1:M:132:GLU:CD	2.39	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:19:LEU:HD23	1:D:19:LEU:C	2.40	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: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:X:338:ASP:OD2	2:X:341:THR:OG1	2.30	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: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:I:188:LEU:O	1:I:189:ARG:C	2.59	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:301:ALA:HB1	2:V:333:LYS:HZ2	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:A:161:GLU:CD	1:A:161:GLU:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:179:ASP:O	1:W:183:ILE:HG13	2.15	0.46
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
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
2:E:314:MET:HE3	2:E:405:ALA:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:SER:HB3	3:O:249:HOH:O	2.16	0.46
2:R:-3:PRO:O	2:R:348:THR:HA	2.16	0.46
2:R:314:MET:HE3	2:R:405:ALA:HB2	1.96	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:E:521:ARG:C	2:E:523:GLY:H	2.23	0.46
1:O:114:GLN:O	1:O:115:ALA:C	2.58	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
1:U:8:SER:H	1:1:5:TYR:C	2.23	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
1:O:161:GLU:CD	1:O:161:GLU:N	2.74	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:496:ILE:HG13	2:Z:505:VAL:HG22	1.97	0.45
2:Z:498:ASP:C	2:Z:498:ASP:OD1	2.59	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
1:K:142:THR:HG1	1:K:144:ASP:HB3	1.79	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
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
2:Z:314:MET:HE3	2:Z:405:ALA:HB2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:301:ALA:HB2	2:L:333:LYS:CE	2.46	0.45
2:R:308:TYR:CE2	2:R:311:GLY:C	2.94	0.45
2:R:407:TYR:CE2	2:R:417:ALA:HB1	2.51	0.45
2:R:424:ASP:C	2:R:424:ASP:OD1	2.59	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:I:13:MET:HE3	1:I:13:MET:CA	2.46	0.45
1:A:7:ILE:CD1	1:A:15:GLU:CD	2.89	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:O:30:VAL:HG22	1:O:52:LYS:NZ	2.31	0.45
1:Q:7:ILE:HB	1:Q:11:GLN:OE1	2.15	0.45
1:Q:140:ARG:C	1:Q:141:ILE:HD12	2.42	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
1:D:11:GLN:CD	1:Q:5:TYR:HD1	2.24	0.45
2:E:351:VAL:HG11	2:E:400:ALA:HB2	1.98	0.45
1:I:161:GLU:CD	1:I:161:GLU:N	2.73	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:I:152:HIS:CB	1:I:171:TYR:CE2	2.98	0.45
1:A:4:PRO:HB3	1:B:11:GLN:CD	2.41	0.45
1:F:33:LEU:HD12	1:F:33:LEU:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:205:VAL:O	1:W:205:VAL:HG12	2.15	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
2:G:338:ASP:C	2:G:338:ASP:OD1	2.59	0.45
1:K:22:LYS:O	1:K:25:ALA:HB3	2.16	0.45
1:K:191:GLY:O	1:K:192:SER:C	2.58	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
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:A:44:GLU:C	1:A:45:ASN:HD22	2.24	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
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
1:B:33:LEU:CD1	1:B:33:LEU:C	2.90	0.45
1:I:129:HIS:O	1:I:130:TYR:C	2.60	0.45
1:Q:211:ALA:C	1:Q:212:VAL:HG13	2.41	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
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: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
1:K:144:ASP:OD1	1:K:144:ASP:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:303:ILE:HD13	2:C:344:GLY:C	2.42	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:T:351:VAL:CG1	2:T:400:ALA:HB2	2.47	0.44
1:U:167:LEU:CA	1:U:170:SER:OG	2.46	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
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
2:X:-2:HIS:ND1	2:X:-2:HIS:C	2.75	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
2:E:-29:LEU:O	2:E:-25:ALA:C	2.60	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:28:LYS:HZ2	1:K:52:LYS:HE3	1.81	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: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
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:8:SER:O	1:K:9:PRO:C	2.60	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: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
2:X:-32:THR:HG23	2:X:-31:ASP:N	2.33	0.44
1:A:156:MET:HE3	1:A:156:MET:HB2	1.87	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:28:LYS:HZ2	1:S:52:LYS:HE3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:161:GLU:CD	1:Y:161:GLU:N	2.75	0.44
1:Y:167:LEU:HD12	1:Y:167:LEU:HA	1.86	0.44
2:2:306:LEU:C	2:2:306:LEU:HD12	2.42	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: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
1:I:163:ILE:HG23	1:I:187:ALA:O	2.18	0.44
1:I:217:ARG:NH1	1:I:223:ARG:HG2	2.33	0.44
1:M:7:ILE:HD13	1:W:5:TYR:HB2	1.97	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:V:413:ASP:OD1	2:V:413:ASP:C	2.60	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: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:35:TYR:CZ	1:Q:37:GLY:C	2.96	0.43
1:Q:130:TYR:CE1	1:Q:216:ASN:O	2.71	0.43
1:U:204:GLY:O	1:U:205:VAL:C	2.61	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
2:E:521:ARG:C	2:E:523:GLY:N	2.75	0.43
1:F:32:ALA:O	1:F:153:PHE:HA	2.17	0.43
1:F:156:MET:HE3	1:F:156:MET:HB2	1.93	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:306:LEU:HD12	2:P:306:LEU:C	2.43	0.43
2:P:332:ARG:HH11	2:P:332:ARG:CB	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:338:ASP:OD1	2:J:338:ASP:C	2.60	0.43
2:N:472:TYR:HD2	2:N:521:ARG:HH12	1.66	0.43
1:Q:8:SER:HB2	1:Q:9:PRO:HD2	2.00	0.43
1:U:205:VAL:HG22	1:U:230:LEU:HG	2.01	0.43
2:V:345:ILE:HB	2:V:352:ALA:HB1	1.99	0.43
2:V:486:LEU:N	2:V:486:LEU:HD12	2.33	0.43
2:2:-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
2:2:-31:ASP:CG	2:2:-27:ARG:HH21	2.26	0.43
1:1:156:MET:HE3	1:1:156:MET:HB2	1.89	0.43
1:B:19:LEU:C	1:B:19:LEU:CD2	2.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:116:LYS:HG2	1:S:117:PRO:O	2.19	0.43
1:U:11:GLN:O	1:U:12:ALA:C	2.61	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
1:S:142:THR:OG1	1:S:144:ASP:OD1	2.30	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
2:C:366:TYR:CD2	2:C:374:LEU:HD13	2.54	0.43
1:D:11:GLN:NE2	1:Q:5:TYR:H	2.13	0.43
1:D:234:LEU:CD1	1:D:234:LEU:N	2.81	0.43
2:E:303:ILE:HD13	2:E:344:GLY:C	2.44	0.43
2:E:320:SER:HB2	2:E:331:VAL:HG21	2.00	0.43
2:E:515:ARG:O	2:E:516:ALA:C	2.61	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:T:-17:ILE:HG12	2:T:-16:SER:H	1.83	0.43
1:U:231:GLN:O	1:U:231:GLN:CD	2.62	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
1:1:35:TYR:CD2	1:1:38:GLY:C	2.97	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:314:MET:HE3	2:J:405:ALA:HB2	2.01	0.43
2:J:374:LEU:HD11	1:S:89:TYR:CD1	2.54	0.43
2:L:424:ASP:C	2:L:424:ASP:OD1	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:306:LEU:C	2:E:306:LEU:HD12	2.44	0.43
1:F:161:GLU:CD	1:F:161:GLU:N	2.76	0.43
2:H:457:VAL:HG13	2:H:463:GLY:CA	2.48	0.43
1:I:11:GLN:O	1:I:12:ALA:C	2.62	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:B:156:MET:HE3	1:B:156:MET:HB2	1.92	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:I:173:GLU:CB	1:I:174:ASN:OD1	2.66	0.43
1:D:59:ARG:CD	1:D:129:HIS:HA	2.44	0.42
1:D:225:ILE:HG21	1:D:233:LEU:CD2	2.49	0.42
2:E:406:GLY:O	2:E:419:ARG:N	2.46	0.42
1:F:56:LEU:HD23	1:F:56:LEU:HA	1.89	0.42
2:H:345:ILE:HB	2:H:352:ALA:HB1	2.00	0.42
1:I:33:LEU: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
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:140:ARG:C	1:S:141:ILE:HD12	2.43	0.42
1:S:174:ASN:HD22	1:S:174:ASN:N	2.16	0.42
2:T:302:THR:OG1	2:T:481:THR:OG1	2.29	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
1:I:150:GLU:HA	1:I:151:PRO:HD3	1.88	0.42
2:J:424:ASP:C	2:J:424:ASP:OD1	2.62	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:33:LEU:CD1	1:S:33:LEU:C	2.92	0.42
1:S:167:LEU:O	1:S:171:TYR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:129:HIS:O	1:M:130:TYR:C	2.62	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:I:26:ARG:O	1:I: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
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
1:K:19:LEU:C	1:K:19:LEU:HD23	2.44	0.42
2:N:476:ASP:O	2:P:329:ARG:NH2	2.52	0.42
1:Q:48:ARG:O	1:Q:48:ARG:HG2	2.19	0.42
1:Q:161:GLU:CD	1:Q:161:GLU:N	2.74	0.42
2:R:399:LEU:HD11	2:R:401:LEU:HD13	2.01	0.42
2:T:306:LEU:C	2:T:306:LEU:HD12	2.44	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:G:452:LYS:HZ1	2:2:473:ASP:CG	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:142:THR:HG1	1:Q:144:ASP:HB3	1.84	0.42
1:Q:176:SER:HG	1:Q:179:ASP:CG	2.23	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: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:26:ARG:O	1:O:26:ARG:CG	2.67	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
2:P:358:LEU:HD23	2:P:386:MET:HE3	2.01	0.42
2:R:433:GLU:CD	2:R:433:GLU:N	2.76	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:H:413:ASP:CG	2:H:414:PRO:HD2	2.43	0.42
2:L:376:PHE:CE2	2:L:380:ILE:HD11	2.55	0.42
1:Q:135:ARG:O	1:Q:136:PRO:C	2.61	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:156:MET:HE3	1:O:156:MET:HB2	1.90	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
1:1:68:PHE:O	1:1:69:ASN:C	2.61	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:H:424:ASP:C	2:H:424:ASP:OD1	2.63	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: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:I:33:LEU:CD1	1:I:33:LEU:C	2.93	0.42
1:K:163:ILE:HG23	1:K:187:ALA:O	2.20	0.42
1:O:163:ILE:HG23	1:O:187:ALA:C	2.45	0.42
1:Q:205:VAL:O	1:Q:205:VAL:CG1	2.66	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
1:U:204:GLY:C	1:U:206:ALA:N	2.73	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
1:F:16:ARG:HH22	1:F:115:ALA:C	2.28	0.41
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:M:116:LYS:NZ	1:M:119:GLU:OE2	2.49	0.41
2:N:314:MET:HE3	2:N:405:ALA:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:172:ALA:HB3	1:A:175:ALA:HB2	2.03	0.41
1:B:96:GLY:O	1:B:97:ARG:C	2.62	0.41
2:C:-4:LEU:CD1	2:C:398:LEU:CD1	2.97	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
1:S:15:GLU:CD	1:1:9:PRO:HD2	2.43	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
1:U:156:MET:HE3	1:U:156:MET:HB2	1.94	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:B:178:THR:CA	1:B:233:LEU:CD2	2.82	0.41
2:E:485:ASP:C	2:E:485:ASP:OD1	2.63	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
1:U:40:LEU:CD1	1:U:212:VAL:CG1	2.98	0.41
1:W:161:GLU:CD	1:W:161:GLU:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LEU:N	1:D:234:LEU:HD12	2.35	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:M:17:SER:OG	1:M:143:TYR:OH	2.38	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
1:U:216:ASN:O	1:U:216:ASN:CG	2.63	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:O:30:VAL:HG22	1:O:52:LYS:HZ3	1.85	0.41
1:U:5:TYR:CD1	1:U:5:TYR:N	2.87	0.41
1:U:129:HIS:O	1:U:130:TYR:C	2.64	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:E:390:ASN:CG	2:E:390:ASN:O	2.62	0.41
2:E:424:ASP:OD1	2:E:424:ASP:C	2.64	0.41
2:N:308:TYR:CD1	2:N:308:TYR:C	2.99	0.41
1:O:155:VAL:C	1:O:156:MET:HG3	2.45	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
1:W:33:LEU:HD12	1:W:33:LEU:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:VAL:HG22	1:D:52:LYS:HZ3	1.85	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
2:N:491:PHE:HB3	2:N:492:PRO:HD2	2.02	0.41
1:O:33:LEU:HD12	1:O:33:LEU:C	2.45	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
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
2:P:424:ASP:C	2:P:424:ASP:OD1	2.63	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
2:C:434:GLU:OE1	2:C:434:GLU:C	2.63	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:156:MET:HE3	1:M:156:MET:HB2	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:367:GLU:O	2:T:371:GLY:N	2.53	0.41
1:W:129:HIS:O	1:W:130:TYR:C	2.64	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
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
2:Z:478:ASP:OD1	2:Z:478:ASP:C	2.63	0.41
1:B:13:MET:HE3	1:B:111:PHE:CE2	2.52	0.40
2:H:506:PRO:O	2:H:507:GLU:C	2.65	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: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:C:485:ASP:C	2:C:485:ASP:OD1	2.64	0.40
2:H:306:LEU:C	2:H:306:LEU:HD12	2.46	0.40
2:H:471:LEU:HD12	2:H:471:LEU:HA	1.93	0.40
1:K:167:LEU:HD23	1:K:167:LEU:HA	1.58	0.40
1:K:204:GLY:O	1:K:207:SER:OG	2.30	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:S:67:LYS:HG2	1:S:69:ASN:ND2	2.36	0.40
1:S:161:GLU:CD	1:S:161:GLU:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:350:ALA:HA	2:X:353:VAL:HG12	2.03	0.40
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:N:465:ARG:O	2:N:466:VAL:C	2.64	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: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:33:LEU:HD12	1:D:33:LEU:C	2.40	0.40
1:D:189:ARG:O	1:D:192:SER:N	2.55	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: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
2:N:388:ARG:C	2:N:390:ASN:H	2.30	0.40
1:O:9:PRO:O	1:O:13:MET:HG2	2.21	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:30:VAL:HG22	1:U:52:LYS:HZ3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:PHE:O	1:Y:69:ASN:C	2.64	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
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: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
2:N:459:ASP:O	2:N:460:GLY:C	2.60	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:V:507:GLU:O	2:V:508:SER:C	2.64	0.40
2:X:457:VAL:O	2:X:457:VAL:HG12	2.20	0.40
2:Z:306:LEU:C	2:Z:306:LEU:HD12	2.46	0.40
2:Z:388:ARG:C	2:Z:390:ASN:H	2.29	0.40
2:2:-31:ASP:CG	2:2:-27:ARG:NH2	2.79	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%)	24	43
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
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%)	24	43
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%)	30	49
2	N	248/291 (85%)	244 (98%)	4 (2%)	0	100	100
2	P	246/291 (84%)	244 (99%)	2 (1%)	0	100	100
2	R	242/291 (83%)	240 (99%)	2 (1%)	0	100	100
2	T	246/291 (84%)	243 (99%)	3 (1%)	0	100	100
2	V	245/291 (84%)	244 (100%)	1 (0%)	0	100	100
2	X	245/291 (84%)	244 (100%)	1 (0%)	0	100	100
2	Z	241/291 (83%)	240 (100%)	1 (0%)	0	100	100
All	All	6466/7546 (86%)	6271 (97%)	192 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	168/192 (88%)	147 (88%)	21 (12%)	4	9
1	A	171/192 (89%)	157 (92%)	14 (8%)	10	23
1	B	168/192 (88%)	151 (90%)	17 (10%)	7	15
1	D	171/192 (89%)	156 (91%)	15 (9%)	9	20
1	F	170/192 (88%)	153 (90%)	17 (10%)	7	15
1	I	167/192 (87%)	152 (91%)	15 (9%)	9	19
1	K	170/192 (88%)	152 (89%)	18 (11%)	6	14
1	M	173/192 (90%)	156 (90%)	17 (10%)	7	16
1	O	167/192 (87%)	151 (90%)	16 (10%)	8	17
1	Q	171/192 (89%)	150 (88%)	21 (12%)	4	10
1	S	168/192 (88%)	154 (92%)	14 (8%)	10	22
1	U	170/192 (88%)	152 (89%)	18 (11%)	6	14
1	W	170/192 (88%)	152 (89%)	18 (11%)	6	14
1	Y	173/192 (90%)	153 (88%)	20 (12%)	5	11
2	2	186/216 (86%)	172 (92%)	14 (8%)	12	26
2	C	188/216 (87%)	180 (96%)	8 (4%)	26	51
2	E	185/216 (86%)	167 (90%)	18 (10%)	8	17
2	G	188/216 (87%)	176 (94%)	12 (6%)	16	33
2	H	186/216 (86%)	179 (96%)	7 (4%)	29	56
2	J	189/216 (88%)	178 (94%)	11 (6%)	18	38
2	L	188/216 (87%)	175 (93%)	13 (7%)	14	30
2	N	189/216 (88%)	179 (95%)	10 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	188/216 (87%)	176 (94%)	12 (6%)	16	33
2	R	184/216 (85%)	173 (94%)	11 (6%)	17	36
2	T	189/216 (88%)	174 (92%)	15 (8%)	11	24
2	V	186/216 (86%)	176 (95%)	10 (5%)	20	41
2	X	188/216 (87%)	171 (91%)	17 (9%)	9	19
2	Z	184/216 (85%)	168 (91%)	16 (9%)	9	21
All	All	4995/5712 (87%)	4580 (92%)	415 (8%)	10	22

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	28	LYS
1	A	30	VAL
1	A	33	LEU
1	A	45	ASN
1	A	59	ARG
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	99	LEU
1	B	105	GLN
1	B	114	GLN
1	B	122	LEU
1	B	167	LEU
1	B	226	THR

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Mol	Chain	Res	Type
1	B	228	SER
1	B	233	LEU
2	C	-22	LEU
2	C	353	VAL
2	C	363	LEU
2	C	374	LEU
2	C	398	LEU
2	C	430	ASN
2	C	434	GLU
2	C	471	LEU
1	D	28	LYS
1	D	30	VAL
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	188	LEU
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	-21	LEU
2	E	332	ARG
2	E	338	ASP
2	E	353	VAL
2	E	355	PHE
2	E	363	LEU
2	E	374	LEU
2	E	382	ARG
2	E	409	ILE
2	E	415	GLN
2	E	433	GLU
2	E	471	LEU
2	E	503	VAL
2	E	512	GLU

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Mol	Chain	Res	Type
2	E	519	GLU
1	F	8	SER
1	F	11	GLN
1	F	26	ARG
1	F	30	VAL
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
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	312	VAL
2	G	363	LEU
2	G	374	LEU
2	G	413	ASP
2	G	431	ILE
2	G	434	GLU
2	G	471	LEU
2	G	503	VAL
2	G	513	LEU
2	G	519	GLU
2	H	-21	LEU
2	H	363	LEU
2	H	374	LEU
2	H	402	PRO
2	H	434	GLU
2	H	471	LEU
2	H	486	LEU
1	I	5	TYR
1	I	9	PRO
1	I	10	GLU
1	I	28	LYS
1	I	30	VAL

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Mol	Chain	Res	Type
1	I	33	LEU
1	I	59	ARG
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
1	I	228	SER
2	J	-32	THR
2	J	-29	LEU
2	J	-18	SER
2	J	-17	ILE
2	J	-16	SER
2	J	329	ARG
2	J	363	LEU
2	J	374	LEU
2	J	471	LEU
2	J	513	LEU
2	J	519	GLU
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	99	LEU
1	K	105	GLN
1	K	122	LEU
1	K	141	ILE
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

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Mol	Chain	Res	Type
2	L	-23	GLU
2	L	-21	LEU
2	L	-5	GLN
2	L	354	GLU
2	L	363	LEU
2	L	374	LEU
2	L	412	SER
2	L	416	SER
2	L	471	LEU
2	L	513	LEU
1	M	30	VAL
1	M	33	LEU
1	M	59	ARG
1	M	73	ASN
1	M	74	LEU
1	M	92	ARG
1	M	105	GLN
1	M	122	LEU
1	M	159	THR
1	M	161	GLU
1	M	163	ILE
1	M	167	LEU
1	M	203	LEU
1	M	205	VAL
1	M	208	LEU
1	M	226	THR
1	M	235	VAL
2	N	-27	ARG
2	N	-21	LEU
2	N	-17	ILE
2	N	-4	LEU
2	N	329	ARG
2	N	363	LEU
2	N	374	LEU
2	N	471	LEU
2	N	503	VAL
2	N	513	LEU
1	O	7	ILE
1	O	8	SER
1	O	17	SER
1	O	30	VAL
1	O	51	GLN

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Mol	Chain	Res	Type
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	141	ILE
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	-23	GLU
2	P	-21	LEU
2	P	-18	SER
2	P	-5	GLN
2	P	353	VAL
2	P	363	LEU
2	P	374	LEU
2	P	471	LEU
2	P	503	VAL
1	Q	4	PRO
1	Q	5	TYR
1	Q	28	LYS
1	Q	30	VAL
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	178	THR
1	Q	179	ASP
1	Q	185	VAL
1	Q	189	ARG
1	Q	208	LEU
1	Q	210	VAL
1	Q	226	THR

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Mol	Chain	Res	Type
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	407	TYR
2	R	433	GLU
2	R	471	LEU
2	R	503	VAL
2	R	513	LEU
1	S	10	GLU
1	S	13	MET
1	S	28	LYS
1	S	30	VAL
1	S	33	LEU
1	S	59	ARG
1	S	69	ASN
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	-24	PRO
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	412	SER
2	T	415	GLN
2	T	433	GLU
2	T	471	LEU
2	T	513	LEU

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Mol	Chain	Res	Type
1	U	5	TYR
1	U	7	ILE
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	183	ILE
1	U	203	LEU
1	U	205	VAL
1	U	208	LEU
1	U	226	THR
1	U	233	LEU
2	V	-38	VAL
2	V	-32	THR
2	V	-29	LEU
2	V	-22	LEU
2	V	-21	LEU
2	V	329	ARG
2	V	363	LEU
2	V	374	LEU
2	V	471	LEU
2	V	513	LEU
1	W	6	PHE
1	W	30	VAL
1	W	33	LEU
1	W	59	ARG
1	W	74	LEU
1	W	92	ARG
1	W	99	LEU
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	185	VAL

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Mol	Chain	Res	Type
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	-22	LEU
2	X	-17	ILE
2	X	329	ARG
2	X	338	ASP
2	X	348	THR
2	X	354	GLU
2	X	355	PHE
2	X	363	LEU
2	X	374	LEU
2	X	388	ARG
2	X	431	ILE
2	X	471	LEU
2	X	503	VAL
2	X	513	LEU
2	X	521	ARG
1	Y	7	ILE
1	Y	8	SER
1	Y	16	ARG
1	Y	30	VAL
1	Y	33	LEU
1	Y	59	ARG
1	Y	69	ASN
1	Y	74	LEU
1	Y	92	ARG
1	Y	105	GLN
1	Y	114	GLN
1	Y	122	LEU
1	Y	169	GLU
1	Y	178	THR
1	Y	181	LEU
1	Y	203	LEU
1	Y	208	LEU
1	Y	212	VAL
1	Y	226	THR
1	Y	228	SER
2	Z	-34	SER

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Mol	Chain	Res	Type
2	Z	-32	THR
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	432	GLU
2	Z	471	LEU
2	Z	509	ARG
2	Z	510	ILE
2	Z	513	LEU
2	Z	520	SER
2	2	-38	VAL
2	2	-23	GLU
2	2	-5	GLN
2	2	-4	LEU
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	471	LEU
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	19	LEU
1	1	28	LYS
1	1	30	VAL
1	1	33	LEU
1	1	59	ARG
1	1	69	ASN
1	1	74	LEU
1	1	92	ARG
1	1	105	GLN
1	1	116	LYS

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Mol	Chain	Res	Type
1	1	122	LEU
1	1	173	GLU
1	1	174	ASN
1	1	181	LEU
1	1	189	ARG
1	1	205	VAL
1	1	208	LEU
1	1	226	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) 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	129	HIS
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	129	HIS
1	B	165	ASN
2	C	381	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
1	F	101	ASN
1	F	105	GLN
1	F	114	GLN

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Mol	Chain	Res	Type
1	F	165	ASN
2	G	410	HIS
2	G	456	GLN
2	H	-5	GLN
2	H	381	ASN
2	H	456	GLN
1	I	51	GLN
1	I	69	ASN
1	I	114	GLN
1	I	129	HIS
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	381	ASN
2	L	456	GLN
1	M	51	GLN
1	M	69	ASN
1	M	105	GLN
2	N	381	ASN
2	N	396	GLN
2	N	430	ASN
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	129	HIS
1	O	152	HIS
2	P	410	HIS
1	Q	51	GLN
1	Q	69	ASN
1	Q	73	ASN
1	Q	105	GLN
1	Q	114	GLN
1	Q	129	HIS

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Mol	Chain	Res	Type
2	R	-2	HIS
2	R	381	ASN
2	R	456	GLN
1	S	69	ASN
1	S	73	ASN
1	S	101	ASN
1	S	105	GLN
1	S	114	GLN
1	S	129	HIS
1	S	174	ASN
2	T	-5	GLN
2	T	381	ASN
2	T	410	HIS
2	T	415	GLN
2	T	456	GLN
1	U	51	GLN
1	U	69	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	381	ASN
2	V	456	GLN
1	W	11	GLN
1	W	51	GLN
1	W	69	ASN
1	W	105	GLN
1	W	114	GLN
1	W	129	HIS
1	W	152	HIS
1	W	174	ASN
2	X	-5	GLN
2	X	381	ASN
2	X	456	GLN
1	Y	51	GLN
1	Y	69	ASN
1	Y	73	ASN
1	Y	165	ASN
2	Z	381	ASN
2	Z	410	HIS

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Mol	Chain	Res	Type
2	Z	415	GLN
2	Z	456	GLN
2	2	-5	GLN
2	2	-2	HIS
2	2	381	ASN
2	2	415	GLN
2	2	430	ASN
2	2	456	GLN
1	1	11	GLN
1	1	51	GLN
1	1	69	ASN
1	1	73	ASN
1	1	101	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	219/248 (88%)	0.16	5 (2%) 61 57	48, 86, 121, 152	0
1	A	222/248 (89%)	0.15	3 (1%) 73 70	43, 81, 117, 145	0
1	B	220/248 (88%)	0.12	1 (0%) 87 85	48, 88, 127, 145	0
1	D	222/248 (89%)	0.36	5 (2%) 61 57	52, 92, 126, 144	0
1	F	221/248 (89%)	0.09	4 (1%) 67 64	45, 86, 126, 147	0
1	I	217/248 (87%)	0.05	2 (0%) 81 78	45, 80, 123, 149	0
1	K	221/248 (89%)	0.49	3 (1%) 73 70	48, 98, 135, 148	0
1	M	224/248 (90%)	0.09	1 (0%) 88 86	45, 78, 127, 147	0
1	O	218/248 (87%)	0.37	9 (4%) 41 37	50, 97, 137, 150	0
1	Q	222/248 (89%)	0.35	5 (2%) 61 57	48, 96, 131, 140	0
1	S	219/248 (88%)	0.09	3 (1%) 73 70	46, 85, 129, 140	0
1	U	221/248 (89%)	0.09	1 (0%) 87 85	49, 88, 130, 144	0
1	W	221/248 (89%)	-0.04	2 (0%) 81 78	48, 81, 125, 149	0
1	Y	224/248 (90%)	0.11	3 (1%) 75 71	53, 93, 132, 142	0
2	2	246/291 (84%)	-0.16	3 (1%) 76 73	48, 68, 97, 107	0
2	C	250/291 (85%)	-0.09	1 (0%) 88 86	51, 73, 111, 143	0
2	E	248/291 (85%)	0.08	7 (2%) 55 50	30, 77, 115, 132	0
2	G	251/291 (86%)	-0.13	1 (0%) 88 86	44, 67, 115, 141	0
2	H	249/291 (85%)	-0.08	4 (1%) 70 67	45, 71, 113, 136	0
2	J	252/291 (86%)	-0.21	3 (1%) 76 73	47, 70, 109, 135	0
2	L	251/291 (86%)	-0.07	4 (1%) 70 67	51, 75, 116, 140	0
2	N	252/291 (86%)	-0.20	3 (1%) 76 73	44, 70, 115, 144	0
2	P	250/291 (85%)	-0.07	3 (1%) 76 73	47, 75, 114, 144	0
2	R	246/291 (84%)	0.08	7 (2%) 55 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%)	-0.28	1 (0%) 88 86	40, 68, 110, 137	0
2	V	249/291 (85%)	-0.18	2 (0%) 82 80	47, 68, 112, 136	0
2	X	249/291 (85%)	-0.08	5 (2%) 65 61	44, 65, 115, 144	0
2	Z	245/291 (84%)	-0.02	7 (2%) 53 49	49, 73, 115, 131	0
All	All	6579/7546 (87%)	0.03	98 (1%) 72 68	30, 78, 124, 152	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	PHE	5.2
2	E	-19	ALA	4.4
2	X	351	VAL	4.2
1	F	235	VAL	4.0
2	V	-19	ALA	3.8
2	Z	352	ALA	3.4
2	L	-17	ILE	3.4
1	F	203	LEU	3.4
1	1	6	PHE	3.4
1	Y	234	LEU	3.4
2	Z	-1	GLY	3.4
2	C	-17	ILE	3.4
1	1	5	TYR	3.3
2	R	-19	ALA	3.3
1	U	6	PHE	3.1
2	Z	349	ALA	3.1
1	Q	235	VAL	3.1
1	Y	235	VAL	3.1
1	K	188	LEU	3.0
2	Z	355	PHE	3.0
1	O	188	LEU	2.9
2	R	349	ALA	2.9
1	D	234	LEU	2.9
1	O	38	GLY	2.9
2	H	-20	PRO	2.8
1	O	167	LEU	2.8
1	I	234	LEU	2.8
1	O	7	ILE	2.8
2	H	-6	ALA	2.8
1	A	188	LEU	2.7
2	X	347	GLY	2.7
2	H	-21	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	V	-39	ALA	2.6
2	X	355	PHE	2.6
1	W	235	VAL	2.6
1	W	5	TYR	2.6
1	O	235	VAL	2.6
2	R	353	VAL	2.6
1	K	5	TYR	2.6
1	D	38	GLY	2.5
2	2	413	ASP	2.5
2	E	-25	ALA	2.5
2	R	-25	ALA	2.5
2	P	-19	ALA	2.5
1	D	28	LYS	2.5
1	Y	203	LEU	2.5
1	F	206	ALA	2.5
2	X	-17	ILE	2.4
2	E	393	ALA	2.4
1	F	234	LEU	2.4
1	K	184	ALA	2.4
2	L	349	ALA	2.4
2	2	416	SER	2.4
1	Q	38	GLY	2.4
2	Z	351	VAL	2.4
2	N	523	GLY	2.3
1	Q	3	PHE	2.3
2	P	347	GLY	2.3
1	O	41	PHE	2.3
2	E	353	VAL	2.3
1	1	235	VAL	2.3
2	X	352	ALA	2.3
1	O	50	LEU	2.3
2	R	355	PHE	2.3
2	R	350	ALA	2.2
2	H	-22	LEU	2.2
1	O	12	ALA	2.2
2	N	-1	GLY	2.2
2	L	-38	VAL	2.2
1	M	172	ALA	2.2
1	B	5	TYR	2.2
2	Z	348	THR	2.2
1	D	177	LEU	2.2
1	1	7	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	6	PHE	2.2
2	Z	346	ALA	2.2
2	P	-18	SER	2.2
1	D	154	VAL	2.1
1	O	39	VAL	2.1
1	Q	172	ALA	2.1
2	G	-25	ALA	2.1
2	E	355	PHE	2.1
2	J	-25	ALA	2.1
1	A	50	LEU	2.1
2	E	523	GLY	2.1
2	N	-20	PRO	2.1
2	2	414	PRO	2.1
1	S	235	VAL	2.1
2	J	301	ALA	2.1
2	L	524	ALA	2.1
1	1	119	GLU	2.1
1	S	190	ALA	2.1
1	Q	186	ALA	2.0
2	E	349	ALA	2.0
2	R	-39	ALA	2.0
2	J	-20	PRO	2.0
1	I	172	ALA	2.0
2	T	522	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.