Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:22 am BST

PDB ID	:	2TAA
Title	:	STRUCTURE AND POSSIBLE CATALYTIC RESIDUES OF TAKA-AMYLASE A
Authors	:	Kusunoki, M.; Matsuura, Y.; Tanaka, N.; Kakudo, M.
Deposited on	:	1982-10-18
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

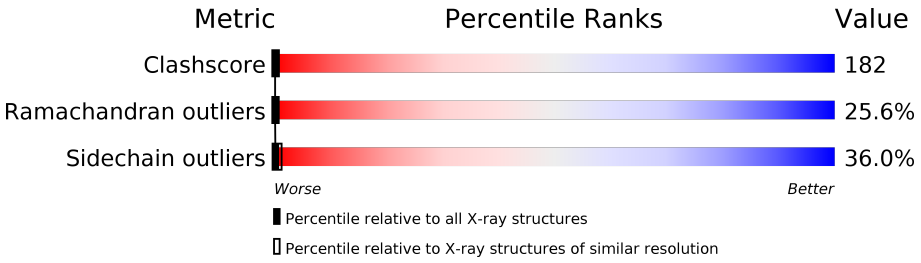
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	478	8% 29% 32% 30%
1	B	478	8% 29% 32% 31%
1	C	478	9% 28% 33% 30%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11073 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 TAKA-AMYLASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3690	2332	593	746	19			
1	B	478	Total	C	N	O	S	0	0	0
			3690	2332	593	746	19			
1	C	478	Total	C	N	O	S	0	0	0
			3690	2332	593	746	19			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

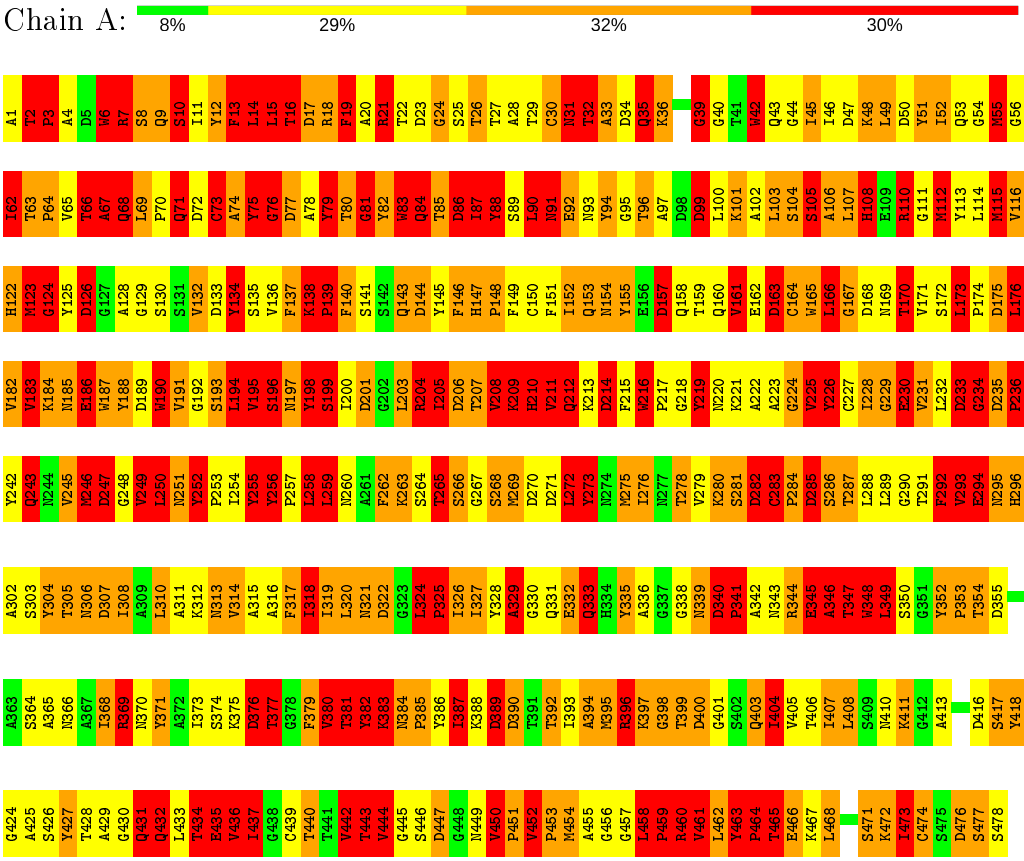
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

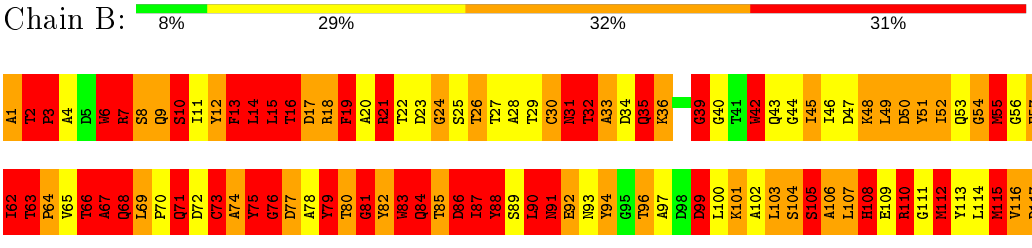
- Molecule 1: TAKA-AMYLASE A

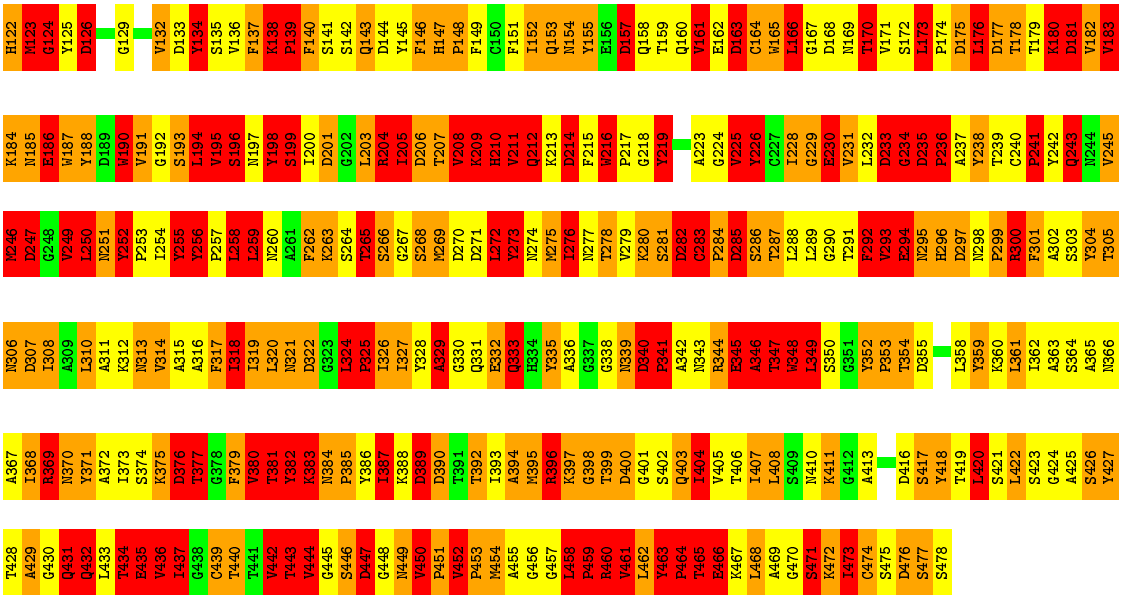
Chain A:



- Molecule 1: TAKA-AMYLASE A

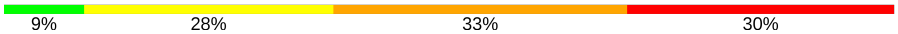
Chain B:

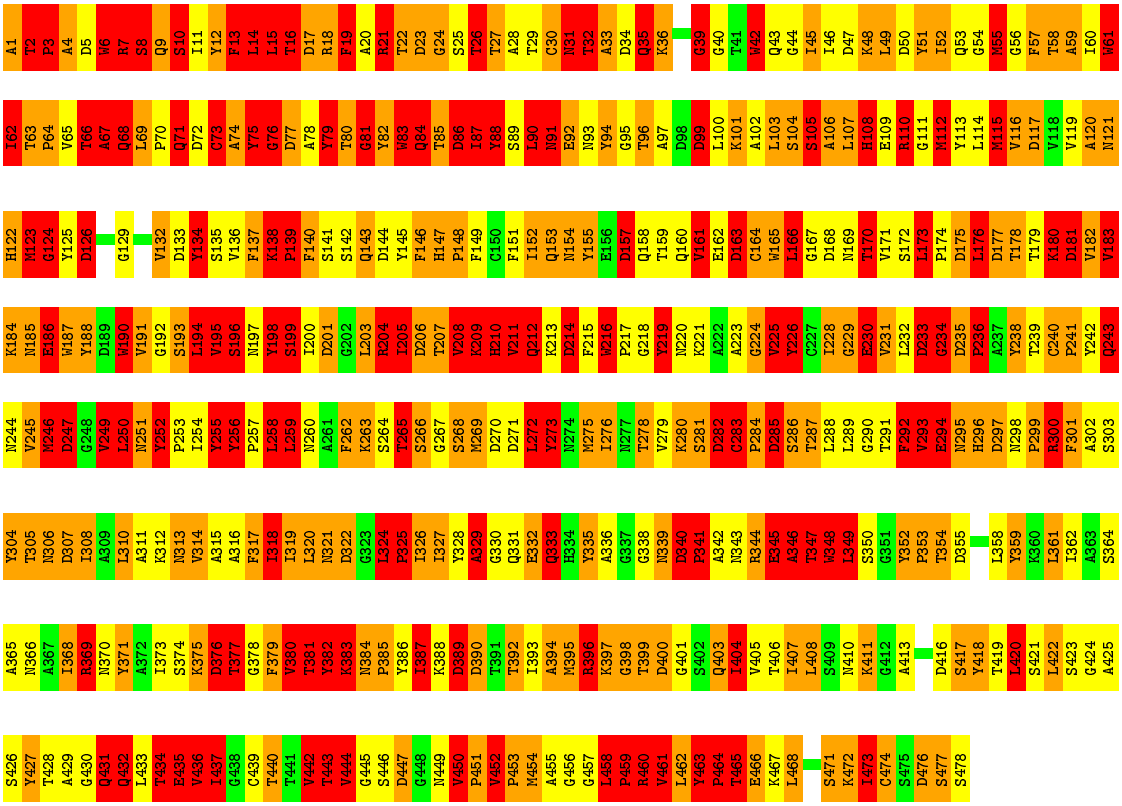




• Molecule 1: TAKA-AMYLASE A

Chain C:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.90Å 133.30Å 94.30Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11073	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.93	77/3782 (2.0%)	3.42	363/5163 (7.0%)
1	B	1.93	77/3782 (2.0%)	3.42	364/5163 (7.1%)
1	C	1.93	77/3782 (2.0%)	3.42	362/5163 (7.0%)
All	All	1.93	231/11346 (2.0%)	3.42	1089/15489 (7.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	87
1	B	2	87
1	C	2	87
All	All	6	261

All (231) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	463	TYR	CD1-CE1	-20.38	1.08	1.39
1	A	463	TYR	CD1-CE1	-20.38	1.08	1.39
1	C	463	TYR	CD1-CE1	-20.36	1.08	1.39
1	C	463	TYR	CZ-OH	19.61	1.71	1.37
1	A	463	TYR	CZ-OH	19.60	1.71	1.37
1	B	463	TYR	CZ-OH	19.59	1.71	1.37
1	C	404	ILE	N-CA	19.31	1.84	1.46
1	B	404	ILE	N-CA	19.30	1.84	1.46
1	A	404	ILE	N-CA	19.29	1.84	1.46
1	C	463	TYR	CD2-CE2	14.81	1.61	1.39
1	A	463	TYR	CD2-CE2	14.81	1.61	1.39
1	B	463	TYR	CD2-CE2	14.74	1.61	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	464	PRO	N-CD	-12.14	1.30	1.47
1	A	464	PRO	N-CD	-12.12	1.30	1.47
1	C	464	PRO	N-CD	-12.06	1.30	1.47
1	B	341	PRO	N-CD	-11.32	1.31	1.47
1	A	341	PRO	N-CD	-11.31	1.32	1.47
1	C	341	PRO	N-CD	-11.30	1.32	1.47
1	B	385	PRO	N-CD	-11.21	1.32	1.47
1	A	385	PRO	N-CD	-11.19	1.32	1.47
1	C	385	PRO	N-CD	-11.14	1.32	1.47
1	C	42	TRP	NE1-CE2	-10.97	1.23	1.37
1	B	42	TRP	NE1-CE2	-10.95	1.23	1.37
1	B	104	SER	CB-OG	-10.93	1.28	1.42
1	A	104	SER	CB-OG	-10.92	1.28	1.42
1	A	42	TRP	NE1-CE2	-10.90	1.23	1.37
1	C	104	SER	CB-OG	-10.86	1.28	1.42
1	C	139	PRO	N-CD	-10.41	1.33	1.47
1	B	139	PRO	N-CD	-10.37	1.33	1.47
1	A	139	PRO	N-CD	-10.35	1.33	1.47
1	A	404	ILE	C-O	10.22	1.42	1.23
1	B	404	ILE	C-O	10.21	1.42	1.23
1	C	404	ILE	C-O	10.19	1.42	1.23
1	A	83	TRP	NE1-CE2	-10.05	1.24	1.37
1	C	83	TRP	NE1-CE2	-10.04	1.24	1.37
1	B	83	TRP	NE1-CE2	-10.01	1.24	1.37
1	C	396	ARG	N-CA	9.69	1.65	1.46
1	B	396	ARG	N-CA	9.68	1.65	1.46
1	A	396	ARG	N-CA	9.66	1.65	1.46
1	B	460	ARG	CD-NE	9.58	1.62	1.46
1	A	460	ARG	CD-NE	9.57	1.62	1.46
1	C	460	ARG	CD-NE	9.51	1.62	1.46
1	C	463	TYR	CB-CG	9.18	1.65	1.51
1	A	463	TYR	CB-CG	9.18	1.65	1.51
1	B	463	TYR	CB-CG	9.16	1.65	1.51
1	B	212	GLN	N-CA	8.96	1.64	1.46
1	C	212	GLN	N-CA	8.95	1.64	1.46
1	A	212	GLN	N-CA	8.92	1.64	1.46
1	C	458	LEU	C-N	-8.82	1.17	1.34
1	A	458	LEU	C-N	-8.81	1.17	1.34
1	B	458	LEU	C-N	-8.80	1.17	1.34
1	B	464	PRO	CA-CB	8.29	1.70	1.53
1	A	464	PRO	CA-CB	8.28	1.70	1.53
1	C	464	PRO	CA-CB	8.26	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	459	PRO	N-CD	8.09	1.59	1.47
1	A	459	PRO	N-CD	8.08	1.59	1.47
1	A	341	PRO	N-CA	8.07	1.60	1.47
1	B	459	PRO	N-CD	8.05	1.59	1.47
1	B	341	PRO	N-CA	8.03	1.60	1.47
1	C	341	PRO	N-CA	8.02	1.60	1.47
1	C	300	ARG	NE-CZ	-7.92	1.22	1.33
1	A	300	ARG	NE-CZ	-7.85	1.22	1.33
1	B	211	VAL	CA-CB	-7.81	1.38	1.54
1	C	165	TRP	NE1-CE2	-7.79	1.27	1.37
1	B	300	ARG	NE-CZ	-7.79	1.23	1.33
1	A	211	VAL	CA-CB	-7.79	1.38	1.54
1	C	304	TYR	CZ-OH	-7.77	1.24	1.37
1	C	211	VAL	CA-CB	-7.75	1.38	1.54
1	B	165	TRP	NE1-CE2	-7.75	1.27	1.37
1	A	165	TRP	NE1-CE2	-7.75	1.27	1.37
1	B	304	TYR	CZ-OH	-7.72	1.24	1.37
1	C	348	TRP	NE1-CE2	-7.71	1.27	1.37
1	B	61	TRP	NE1-CE2	-7.70	1.27	1.37
1	C	61	TRP	NE1-CE2	-7.70	1.27	1.37
1	A	304	TYR	CZ-OH	-7.69	1.24	1.37
1	A	61	TRP	NE1-CE2	-7.69	1.27	1.37
1	A	348	TRP	NE1-CE2	-7.68	1.27	1.37
1	B	348	TRP	NE1-CE2	-7.66	1.27	1.37
1	B	404	ILE	CB-CG1	-7.58	1.32	1.54
1	A	404	ILE	CB-CG1	-7.57	1.32	1.54
1	C	404	ILE	CB-CG1	-7.57	1.32	1.54
1	C	82	TYR	CE2-CZ	-7.55	1.28	1.38
1	B	64	PRO	N-CD	-7.53	1.37	1.47
1	A	82	TYR	CE2-CZ	-7.52	1.28	1.38
1	C	64	PRO	N-CD	-7.51	1.37	1.47
1	A	64	PRO	N-CD	-7.50	1.37	1.47
1	B	82	TYR	CE2-CZ	-7.46	1.28	1.38
1	C	463	TYR	C-N	7.35	1.48	1.34
1	A	463	TYR	C-N	7.35	1.48	1.34
1	B	463	TYR	C-N	7.34	1.48	1.34
1	C	63	THR	CB-OG1	-7.25	1.28	1.43
1	B	63	THR	CB-OG1	-7.24	1.28	1.43
1	A	63	THR	CB-OG1	-7.23	1.28	1.43
1	C	64	PRO	N-CA	7.14	1.59	1.47
1	B	208	VAL	C-N	-7.14	1.17	1.34
1	B	404	ILE	CA-CB	7.13	1.71	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	ILE	CA-CB	7.12	1.71	1.54
1	A	208	VAL	C-N	-7.12	1.17	1.34
1	C	208	VAL	C-N	-7.11	1.17	1.34
1	C	404	ILE	CA-CB	7.11	1.71	1.54
1	A	64	PRO	N-CA	7.10	1.59	1.47
1	B	64	PRO	N-CA	7.08	1.59	1.47
1	C	166	LEU	C-N	6.97	1.45	1.33
1	A	166	LEU	C-N	6.94	1.45	1.33
1	B	166	LEU	C-N	6.89	1.45	1.33
1	C	397	LYS	N-CA	6.89	1.60	1.46
1	A	397	LYS	N-CA	6.87	1.60	1.46
1	B	397	LYS	N-CA	6.84	1.60	1.46
1	C	460	ARG	CZ-NH2	-6.78	1.24	1.33
1	B	6	TRP	NE1-CE2	-6.76	1.28	1.37
1	C	6	TRP	NE1-CE2	-6.75	1.28	1.37
1	A	6	TRP	NE1-CE2	-6.74	1.28	1.37
1	A	460	ARG	CZ-NH2	-6.73	1.24	1.33
1	A	139	PRO	N-CA	6.73	1.58	1.47
1	B	139	PRO	N-CA	6.72	1.58	1.47
1	B	460	ARG	CZ-NH2	-6.70	1.24	1.33
1	C	139	PRO	N-CA	6.67	1.58	1.47
1	A	187	TRP	NE1-CE2	-6.66	1.28	1.37
1	C	187	TRP	NE1-CE2	-6.66	1.28	1.37
1	B	187	TRP	NE1-CE2	-6.66	1.28	1.37
1	B	190	TRP	NE1-CE2	-6.64	1.28	1.37
1	C	190	TRP	NE1-CE2	-6.63	1.28	1.37
1	A	190	TRP	NE1-CE2	-6.62	1.28	1.37
1	B	216	TRP	CD2-CE2	-6.50	1.33	1.41
1	C	216	TRP	CD2-CE2	-6.48	1.33	1.41
1	A	216	TRP	CD2-CE2	-6.46	1.33	1.41
1	A	139	PRO	CA-C	6.36	1.65	1.52
1	B	139	PRO	CA-C	6.35	1.65	1.52
1	C	139	PRO	CA-C	6.35	1.65	1.52
1	A	83	TRP	CD1-NE1	-6.33	1.27	1.38
1	B	83	TRP	CD1-NE1	-6.33	1.27	1.38
1	A	398	GLY	N-CA	6.32	1.55	1.46
1	B	398	GLY	N-CA	6.31	1.55	1.46
1	C	83	TRP	CD1-NE1	-6.30	1.27	1.38
1	C	398	GLY	N-CA	6.29	1.55	1.46
1	B	463	TYR	CA-CB	6.25	1.67	1.53
1	C	435	GLU	N-CA	6.23	1.58	1.46
1	B	382	TYR	CZ-OH	-6.23	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	463	TYR	CA-CB	6.22	1.67	1.53
1	A	435	GLU	N-CA	6.22	1.58	1.46
1	B	435	GLU	N-CA	6.22	1.58	1.46
1	C	463	TYR	CA-CB	6.21	1.67	1.53
1	C	382	TYR	CZ-OH	-6.20	1.27	1.37
1	A	382	TYR	CZ-OH	-6.19	1.27	1.37
1	B	341	PRO	CA-C	6.09	1.65	1.52
1	A	341	PRO	CA-C	6.09	1.65	1.52
1	C	341	PRO	CA-C	6.09	1.65	1.52
1	B	447	ASP	N-CA	6.03	1.58	1.46
1	A	447	ASP	N-CA	6.00	1.58	1.46
1	C	463	TYR	CA-C	5.99	1.68	1.52
1	B	463	TYR	CA-C	5.98	1.68	1.52
1	A	463	TYR	CA-C	5.98	1.68	1.52
1	C	447	ASP	N-CA	5.97	1.58	1.46
1	B	348	TRP	CD1-NE1	-5.85	1.28	1.38
1	A	21	ARG	CZ-NH2	-5.85	1.25	1.33
1	B	21	ARG	CZ-NH2	-5.84	1.25	1.33
1	C	21	ARG	CZ-NH2	-5.84	1.25	1.33
1	A	348	TRP	CD1-NE1	-5.82	1.28	1.38
1	C	348	TRP	CD1-NE1	-5.80	1.28	1.38
1	C	167	GLY	N-CA	5.79	1.54	1.46
1	C	434	THR	C-N	5.78	1.47	1.34
1	A	434	THR	C-N	5.77	1.47	1.34
1	B	167	GLY	N-CA	5.76	1.54	1.46
1	A	167	GLY	N-CA	5.75	1.54	1.46
1	B	434	THR	C-N	5.74	1.47	1.34
1	C	68	GLN	C-N	-5.70	1.21	1.34
1	A	397	LYS	CD-CE	5.70	1.65	1.51
1	A	68	GLN	C-N	-5.70	1.21	1.34
1	B	397	LYS	CD-CE	5.69	1.65	1.51
1	B	68	GLN	C-N	-5.68	1.21	1.34
1	C	397	LYS	CD-CE	5.68	1.65	1.51
1	B	42	TRP	CD1-NE1	-5.62	1.28	1.38
1	C	42	TRP	CD1-NE1	-5.62	1.28	1.38
1	A	42	TRP	CD1-NE1	-5.61	1.28	1.38
1	B	453	PRO	N-CD	-5.48	1.40	1.47
1	B	204	ARG	CZ-NH1	-5.45	1.25	1.33
1	A	453	PRO	N-CD	-5.42	1.40	1.47
1	C	103	LEU	CB-CG	5.41	1.68	1.52
1	A	103	LEU	CB-CG	5.41	1.68	1.52
1	B	459	PRO	N-CA	5.41	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	PRO	N-CA	5.41	1.56	1.47
1	C	204	ARG	CZ-NH1	-5.40	1.26	1.33
1	C	453	PRO	N-CD	-5.40	1.40	1.47
1	B	103	LEU	CB-CG	5.40	1.68	1.52
1	A	204	ARG	CZ-NH1	-5.37	1.26	1.33
1	C	459	PRO	N-CA	5.33	1.56	1.47
1	A	247	ASP	N-CA	5.33	1.57	1.46
1	B	247	ASP	N-CA	5.32	1.56	1.46
1	C	247	ASP	N-CA	5.31	1.56	1.46
1	C	132	VAL	CA-CB	-5.29	1.43	1.54
1	A	132	VAL	CA-CB	-5.29	1.43	1.54
1	B	132	VAL	CA-CB	-5.29	1.43	1.54
1	B	464	PRO	CA-C	5.28	1.63	1.52
1	A	427	TYR	CZ-OH	-5.27	1.28	1.37
1	C	168	ASP	N-CA	5.27	1.56	1.46
1	C	463	TYR	N-CA	5.27	1.56	1.46
1	A	463	TYR	N-CA	5.26	1.56	1.46
1	B	427	TYR	CZ-OH	-5.26	1.28	1.37
1	C	427	TYR	CZ-OH	-5.26	1.28	1.37
1	A	464	PRO	CA-C	5.24	1.63	1.52
1	A	166	LEU	N-CA	5.24	1.56	1.46
1	A	168	ASP	N-CA	5.23	1.56	1.46
1	B	463	TYR	N-CA	5.23	1.56	1.46
1	C	166	LEU	N-CA	5.22	1.56	1.46
1	B	168	ASP	N-CA	5.21	1.56	1.46
1	A	75	TYR	CE2-CZ	5.21	1.45	1.38
1	B	75	TYR	CE2-CZ	5.20	1.45	1.38
1	A	62	ILE	C-N	-5.20	1.22	1.34
1	C	216	TRP	NE1-CE2	-5.20	1.30	1.37
1	B	216	TRP	NE1-CE2	-5.19	1.30	1.37
1	C	464	PRO	CA-C	5.19	1.63	1.52
1	B	166	LEU	N-CA	5.19	1.56	1.46
1	B	62	ILE	C-N	-5.18	1.22	1.34
1	A	216	TRP	NE1-CE2	-5.17	1.30	1.37
1	C	62	ILE	C-N	-5.17	1.22	1.34
1	C	75	TYR	CE2-CZ	5.14	1.45	1.38
1	C	463	TYR	CE1-CZ	-5.13	1.31	1.38
1	A	341	PRO	C-N	5.10	1.45	1.34
1	C	293	VAL	N-CA	5.09	1.56	1.46
1	C	341	PRO	C-N	5.09	1.45	1.34
1	A	463	TYR	CE1-CZ	-5.08	1.31	1.38
1	B	341	PRO	C-N	5.07	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	VAL	N-CA	5.07	1.56	1.46
1	B	463	TYR	CE1-CZ	-5.07	1.31	1.38
1	C	139	PRO	C-N	5.05	1.45	1.34
1	A	81	GLY	C-N	5.05	1.45	1.34
1	A	139	PRO	C-N	5.04	1.45	1.34
1	C	81	GLY	C-N	5.04	1.45	1.34
1	B	81	GLY	C-N	5.04	1.45	1.34
1	B	293	VAL	N-CA	5.03	1.56	1.46
1	B	139	PRO	C-N	5.02	1.45	1.34

All (1089) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	300	ARG	NE-CZ-NH1	-56.15	92.22	120.30
1	A	300	ARG	NE-CZ-NH1	-56.10	92.25	120.30
1	C	300	ARG	NE-CZ-NH1	-56.05	92.27	120.30
1	C	19	PHE	CD1-CE1-CZ	-44.96	66.15	120.10
1	A	19	PHE	CD1-CE1-CZ	-44.94	66.17	120.10
1	B	19	PHE	CD1-CE1-CZ	-44.94	66.17	120.10
1	C	19	PHE	CZ-CE2-CD2	-44.54	66.65	120.10
1	A	19	PHE	CZ-CE2-CD2	-44.53	66.66	120.10
1	B	19	PHE	CZ-CE2-CD2	-44.53	66.66	120.10
1	B	464	PRO	CA-N-CD	-43.27	50.93	111.50
1	A	464	PRO	CA-N-CD	-43.26	50.94	111.50
1	C	464	PRO	CA-N-CD	-43.26	50.94	111.50
1	A	204	ARG	NE-CZ-NH1	-36.19	102.20	120.30
1	B	204	ARG	NE-CZ-NH1	-36.17	102.21	120.30
1	C	204	ARG	NE-CZ-NH1	-36.12	102.24	120.30
1	C	460	ARG	NE-CZ-NH2	-34.78	102.91	120.30
1	A	460	ARG	NE-CZ-NH2	-34.76	102.92	120.30
1	B	460	ARG	NE-CZ-NH2	-34.63	102.99	120.30
1	B	460	ARG	NE-CZ-NH1	34.40	137.50	120.30
1	C	460	ARG	NE-CZ-NH1	34.39	137.50	120.30
1	A	460	ARG	NE-CZ-NH1	34.38	137.49	120.30
1	C	138	LYS	C-N-CD	-29.46	55.78	120.60
1	A	138	LYS	C-N-CD	-29.46	55.80	120.60
1	B	138	LYS	C-N-CD	-29.43	55.85	120.60
1	B	139	PRO	CA-N-CD	-27.73	72.67	111.50
1	A	139	PRO	CA-N-CD	-27.70	72.72	111.50
1	C	139	PRO	CA-N-CD	-27.64	72.80	111.50
1	C	340	ASP	C-N-CD	-27.11	60.96	120.60
1	A	340	ASP	C-N-CD	-27.09	61.00	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	340	ASP	C-N-CD	-27.08	61.02	120.60
1	A	341	PRO	CA-N-CD	-24.62	77.03	111.50
1	C	341	PRO	CA-N-CD	-24.61	77.05	111.50
1	B	341	PRO	CA-N-CD	-24.60	77.06	111.50
1	C	459	PRO	N-CD-CG	-23.86	67.42	103.20
1	A	459	PRO	N-CD-CG	-23.84	67.44	103.20
1	B	459	PRO	N-CD-CG	-23.83	67.45	103.20
1	B	63	THR	CA-CB-CG2	-23.83	79.04	112.40
1	A	63	THR	CA-CB-CG2	-23.81	79.07	112.40
1	C	63	THR	CA-CB-CG2	-23.80	79.08	112.40
1	A	463	TYR	CZ-CE2-CD2	-23.26	98.86	119.80
1	B	463	TYR	CZ-CE2-CD2	-23.26	98.87	119.80
1	C	463	TYR	CZ-CE2-CD2	-23.21	98.92	119.80
1	B	21	ARG	NE-CZ-NH1	21.51	131.06	120.30
1	A	21	ARG	NE-CZ-NH1	21.41	131.01	120.30
1	C	21	ARG	NE-CZ-NH1	21.36	130.98	120.30
1	B	463	TYR	CG-CD1-CE1	-21.13	104.40	121.30
1	A	463	TYR	CG-CD1-CE1	-21.12	104.41	121.30
1	C	463	TYR	CG-CD1-CE1	-21.07	104.44	121.30
1	A	459	PRO	N-CA-CB	-20.49	78.71	103.30
1	B	459	PRO	N-CA-CB	-20.49	78.71	103.30
1	C	459	PRO	N-CA-CB	-20.46	78.75	103.30
1	B	300	ARG	NE-CZ-NH2	-20.12	110.24	120.30
1	A	300	ARG	NE-CZ-NH2	-20.11	110.25	120.30
1	C	300	ARG	NE-CZ-NH2	-20.08	110.26	120.30
1	C	396	ARG	NE-CZ-NH2	20.05	130.32	120.30
1	A	396	ARG	NE-CZ-NH2	20.03	130.31	120.30
1	B	396	ARG	NE-CZ-NH2	20.01	130.30	120.30
1	C	76	GLY	CA-C-O	-19.60	85.32	120.60
1	A	76	GLY	CA-C-O	-19.59	85.34	120.60
1	B	76	GLY	CA-C-O	-19.56	85.39	120.60
1	A	464	PRO	N-CA-CB	-19.46	79.94	103.30
1	A	204	ARG	NE-CZ-NH2	19.45	130.03	120.30
1	C	464	PRO	N-CA-CB	-19.45	79.96	103.30
1	B	464	PRO	N-CA-CB	-19.44	79.97	103.30
1	C	204	ARG	NE-CZ-NH2	19.42	130.01	120.30
1	B	204	ARG	NE-CZ-NH2	19.41	130.01	120.30
1	B	404	ILE	CA-CB-CG1	18.95	147.01	111.00
1	A	404	ILE	CA-CB-CG1	18.94	146.99	111.00
1	C	404	ILE	CA-CB-CG1	18.94	146.98	111.00
1	C	461	VAL	CA-C-O	-17.35	83.66	120.10
1	B	461	VAL	CA-C-O	-17.34	83.68	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	461	VAL	CA-C-O	-17.34	83.69	120.10
1	A	139	PRO	N-CA-CB	-16.90	83.02	103.30
1	C	139	PRO	N-CA-CB	-16.89	83.03	103.30
1	B	139	PRO	N-CA-CB	-16.89	83.04	103.30
1	A	396	ARG	O-C-N	-16.74	95.92	122.70
1	C	396	ARG	O-C-N	-16.73	95.93	122.70
1	B	396	ARG	O-C-N	-16.68	96.01	122.70
1	C	458	LEU	C-N-CD	-16.62	84.04	120.60
1	B	458	LEU	C-N-CD	-16.61	84.06	120.60
1	A	458	LEU	C-N-CD	-16.60	84.08	120.60
1	B	435	GLU	CA-C-O	-15.79	86.94	120.10
1	C	435	GLU	CA-C-O	-15.77	86.99	120.10
1	A	435	GLU	CA-C-O	-15.76	87.00	120.10
1	C	435	GLU	O-C-N	-15.66	97.64	122.70
1	A	435	GLU	O-C-N	-15.61	97.72	122.70
1	B	435	GLU	O-C-N	-15.57	97.79	122.70
1	B	81	GLY	CA-C-O	-15.45	92.79	120.60
1	A	81	GLY	CA-C-O	-15.44	92.81	120.60
1	C	81	GLY	CA-C-O	-15.43	92.83	120.60
1	C	464	PRO	CB-CG-CD	-15.16	47.38	106.50
1	A	464	PRO	CB-CG-CD	-15.15	47.40	106.50
1	B	464	PRO	CB-CG-CD	-15.15	47.40	106.50
1	A	341	PRO	N-CA-CB	-14.96	85.34	103.30
1	C	341	PRO	N-CA-CB	-14.96	85.34	103.30
1	B	341	PRO	N-CA-CB	-14.90	85.42	103.30
1	C	404	ILE	CB-CG1-CD1	-14.64	72.91	113.90
1	A	404	ILE	CB-CG1-CD1	-14.63	72.93	113.90
1	B	404	ILE	CB-CG1-CD1	-14.62	72.97	113.90
1	A	80	THR	C-N-CA	13.87	151.43	122.30
1	C	80	THR	C-N-CA	13.86	151.40	122.30
1	B	80	THR	C-N-CA	13.84	151.36	122.30
1	B	211	VAL	CA-CB-CG1	-13.81	90.19	110.90
1	C	211	VAL	CA-CB-CG1	-13.80	90.20	110.90
1	A	211	VAL	CA-CB-CG1	-13.80	90.20	110.90
1	C	195	VAL	CG1-CB-CG2	-13.76	88.89	110.90
1	B	134	TYR	CB-CG-CD1	-13.76	112.75	121.00
1	B	195	VAL	CG1-CB-CG2	-13.76	88.89	110.90
1	A	195	VAL	CG1-CB-CG2	-13.75	88.89	110.90
1	A	134	TYR	CB-CG-CD1	-13.73	112.76	121.00
1	C	134	TYR	CB-CG-CD1	-13.73	112.76	121.00
1	B	208	VAL	CG1-CB-CG2	-13.64	89.08	110.90
1	A	208	VAL	CG1-CB-CG2	-13.62	89.12	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	85	THR	CA-CB-CG2	-13.62	93.34	112.40
1	C	208	VAL	CG1-CB-CG2	-13.62	89.12	110.90
1	A	85	THR	CA-CB-CG2	-13.60	93.36	112.40
1	B	191	VAL	CA-CB-CG1	-13.59	90.52	110.90
1	A	191	VAL	CA-CB-CG1	-13.58	90.53	110.90
1	C	191	VAL	CA-CB-CG1	-13.57	90.55	110.90
1	B	85	THR	CA-CB-CG2	-13.55	93.42	112.40
1	C	76	GLY	O-C-N	12.93	143.38	122.70
1	A	76	GLY	O-C-N	12.92	143.38	122.70
1	B	76	GLY	O-C-N	12.90	143.35	122.70
1	B	418	TYR	CB-CG-CD2	12.87	128.72	121.00
1	C	463	TYR	CD1-CG-CD2	-12.83	103.79	117.90
1	A	418	TYR	CB-CG-CD2	12.81	128.69	121.00
1	A	463	TYR	CD1-CG-CD2	-12.81	103.81	117.90
1	B	463	TYR	CD1-CG-CD2	-12.78	103.84	117.90
1	C	418	TYR	CB-CG-CD2	12.71	128.62	121.00
1	A	55	MET	CA-CB-CG	12.68	134.86	113.30
1	B	55	MET	CA-CB-CG	12.67	134.84	113.30
1	C	55	MET	CA-CB-CG	12.66	134.83	113.30
1	A	404	ILE	O-C-N	-12.42	102.83	122.70
1	C	404	ILE	O-C-N	-12.42	102.83	122.70
1	B	404	ILE	O-C-N	-12.41	102.84	122.70
1	B	404	ILE	CA-CB-CG2	-12.25	86.39	110.90
1	A	404	ILE	CA-CB-CG2	-12.25	86.40	110.90
1	C	404	ILE	CA-CB-CG2	-12.25	86.41	110.90
1	B	123	MET	N-CA-CB	-12.03	88.94	110.60
1	C	463	TYR	CB-CG-CD1	12.03	128.22	121.00
1	C	123	MET	N-CA-CB	-12.01	88.98	110.60
1	A	123	MET	N-CA-CB	-12.01	88.98	110.60
1	A	463	TYR	CB-CG-CD1	11.94	128.16	121.00
1	B	463	TYR	CB-CG-CD1	11.90	128.14	121.00
1	B	418	TYR	CB-CG-CD1	-11.84	113.90	121.00
1	A	418	TYR	CB-CG-CD1	-11.83	113.90	121.00
1	B	341	PRO	N-CD-CG	-11.81	85.49	103.20
1	C	418	TYR	CB-CG-CD1	-11.81	113.92	121.00
1	C	341	PRO	N-CD-CG	-11.80	85.50	103.20
1	A	341	PRO	N-CD-CG	-11.79	85.52	103.20
1	B	163	ASP	CA-CB-CG	11.08	137.78	113.40
1	C	163	ASP	CA-CB-CG	11.07	137.76	113.40
1	A	163	ASP	CA-CB-CG	11.06	137.74	113.40
1	A	139	PRO	O-C-N	-10.94	105.20	122.70
1	B	139	PRO	O-C-N	-10.92	105.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	139	PRO	O-C-N	-10.91	105.24	122.70
1	C	19	PHE	CG-CD2-CE2	-10.84	108.88	120.80
1	A	19	PHE	CG-CD2-CE2	-10.82	108.89	120.80
1	B	19	PHE	CG-CD2-CE2	-10.79	108.93	120.80
1	A	91	ASN	CB-CA-C	-10.72	88.96	110.40
1	B	91	ASN	CB-CA-C	-10.72	88.97	110.40
1	C	91	ASN	CB-CA-C	-10.71	88.97	110.40
1	C	117	ASP	CB-CG-OD2	-10.69	108.68	118.30
1	C	96	THR	CA-CB-OG1	-10.67	86.60	109.00
1	A	96	THR	CA-CB-OG1	-10.66	86.60	109.00
1	B	96	THR	CA-CB-OG1	-10.65	86.64	109.00
1	C	463	TYR	CA-C-O	-10.64	97.75	120.10
1	A	463	TYR	CA-C-O	-10.62	97.79	120.10
1	B	463	TYR	CA-C-O	-10.62	97.80	120.10
1	A	117	ASP	CB-CG-OD2	-10.61	108.75	118.30
1	B	117	ASP	CB-CG-OD2	-10.61	108.75	118.30
1	B	404	ILE	CB-CA-C	10.50	132.61	111.60
1	C	404	ILE	CB-CA-C	10.50	132.60	111.60
1	A	404	ILE	CB-CA-C	10.49	132.58	111.60
1	A	250	LEU	CD1-CG-CD2	-10.46	79.13	110.50
1	B	250	LEU	CD1-CG-CD2	-10.46	79.14	110.50
1	C	250	LEU	CD1-CG-CD2	-10.45	79.16	110.50
1	A	396	ARG	NH1-CZ-NH2	-10.38	107.98	119.40
1	A	103	LEU	CB-CG-CD2	-10.38	93.35	111.00
1	C	396	ARG	NH1-CZ-NH2	-10.38	107.98	119.40
1	B	103	LEU	CB-CG-CD2	-10.38	93.36	111.00
1	B	396	ARG	NH1-CZ-NH2	-10.37	107.99	119.40
1	C	103	LEU	CB-CG-CD2	-10.36	93.39	111.00
1	C	82	TYR	CB-CG-CD2	10.31	127.18	121.00
1	A	82	TYR	CB-CG-CD2	10.28	127.17	121.00
1	B	82	TYR	CB-CG-CD2	10.24	127.15	121.00
1	A	461	VAL	O-C-N	-10.12	106.51	122.70
1	C	461	VAL	O-C-N	-10.10	106.54	122.70
1	A	452	VAL	CA-CB-CG2	-10.10	95.76	110.90
1	C	452	VAL	CA-CB-CG2	-10.09	95.77	110.90
1	B	461	VAL	O-C-N	-10.09	106.56	122.70
1	B	452	VAL	CA-CB-CG2	-10.06	95.81	110.90
1	C	110	ARG	NE-CZ-NH2	10.01	125.31	120.30
1	B	341	PRO	O-C-N	-10.00	106.69	122.70
1	B	110	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	A	341	PRO	O-C-N	-9.99	106.72	122.70
1	A	110	ARG	NE-CZ-NH2	9.98	125.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	341	PRO	O-C-N	-9.97	106.75	122.70
1	A	170	THR	CA-CB-CG2	-9.96	98.46	112.40
1	B	170	THR	CA-CB-CG2	-9.95	98.47	112.40
1	C	170	THR	CA-CB-CG2	-9.92	98.51	112.40
1	C	19	PHE	CB-CG-CD1	-9.79	113.94	120.80
1	C	19	PHE	CG-CD1-CE1	-9.77	110.05	120.80
1	A	19	PHE	CG-CD1-CE1	-9.77	110.06	120.80
1	B	76	GLY	CA-C-N	-9.74	95.76	117.20
1	B	19	PHE	CG-CD1-CE1	-9.74	110.09	120.80
1	A	76	GLY	CA-C-N	-9.74	95.78	117.20
1	A	19	PHE	CB-CG-CD1	-9.73	113.98	120.80
1	C	76	GLY	CA-C-N	-9.71	95.83	117.20
1	B	88	TYR	CB-CG-CD1	-9.70	115.18	121.00
1	B	19	PHE	CB-CG-CD1	-9.69	114.02	120.80
1	B	204	ARG	CD-NE-CZ	-9.68	110.05	123.60
1	A	88	TYR	CB-CG-CD1	-9.68	115.19	121.00
1	C	204	ARG	CD-NE-CZ	-9.68	110.05	123.60
1	A	204	ARG	CD-NE-CZ	-9.67	110.06	123.60
1	C	442	VAL	CA-CB-CG1	9.66	125.39	110.90
1	C	88	TYR	CB-CG-CD1	-9.65	115.21	121.00
1	A	442	VAL	CA-CB-CG1	9.64	125.36	110.90
1	B	442	VAL	CA-CB-CG1	9.62	125.33	110.90
1	B	340	ASP	O-C-N	9.47	139.09	121.10
1	A	340	ASP	O-C-N	9.46	139.06	121.10
1	C	340	ASP	O-C-N	9.44	139.03	121.10
1	B	346	ALA	N-CA-CB	-9.38	96.97	110.10
1	A	346	ALA	N-CA-CB	-9.38	96.97	110.10
1	C	346	ALA	N-CA-CB	-9.37	96.98	110.10
1	B	42	TRP	CD1-NE1-CE2	9.32	117.39	109.00
1	C	42	TRP	CD1-NE1-CE2	9.32	117.38	109.00
1	A	42	TRP	CD1-NE1-CE2	9.29	117.36	109.00
1	C	258	LEU	CB-CG-CD1	-9.27	95.24	111.00
1	A	258	LEU	CB-CG-CD1	-9.25	95.28	111.00
1	B	258	LEU	CB-CG-CD1	-9.24	95.29	111.00
1	A	82	TYR	CA-CB-CG	9.08	130.65	113.40
1	B	82	TYR	CA-CB-CG	9.08	130.65	113.40
1	A	225	VAL	CA-CB-CG2	9.06	124.50	110.90
1	B	225	VAL	CA-CB-CG2	9.06	124.50	110.90
1	C	82	TYR	CA-CB-CG	9.06	130.62	113.40
1	C	225	VAL	CA-CB-CG2	9.03	124.45	110.90
1	B	404	ILE	CA-C-O	9.03	139.06	120.10
1	C	404	ILE	CA-C-O	9.01	139.03	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	404	ILE	CA-C-O	9.01	139.02	120.10
1	B	233	ASP	CB-CG-OD1	-8.94	110.25	118.30
1	C	115	MET	CG-SD-CE	-8.93	85.92	100.20
1	A	115	MET	CG-SD-CE	-8.91	85.94	100.20
1	A	233	ASP	CB-CG-OD1	-8.90	110.29	118.30
1	B	115	MET	CG-SD-CE	-8.89	85.98	100.20
1	C	233	ASP	CB-CG-OD1	-8.84	110.35	118.30
1	B	371	TYR	CB-CG-CD1	-8.83	115.70	121.00
1	A	371	TYR	CB-CG-CD1	-8.82	115.71	121.00
1	B	346	ALA	CB-CA-C	-8.80	96.90	110.10
1	A	346	ALA	CB-CA-C	-8.79	96.91	110.10
1	C	371	TYR	CB-CG-CD1	-8.79	115.72	121.00
1	C	346	ALA	CB-CA-C	-8.79	96.92	110.10
1	A	188	TYR	CG-CD2-CE2	8.78	128.32	121.30
1	B	188	TYR	CG-CD2-CE2	8.76	128.31	121.30
1	A	420	LEU	CD1-CG-CD2	-8.75	84.25	110.50
1	C	420	LEU	CD1-CG-CD2	-8.75	84.25	110.50
1	B	420	LEU	CD1-CG-CD2	-8.74	84.27	110.50
1	B	188	TYR	CA-CB-CG	8.74	130.01	113.40
1	C	188	TYR	CG-CD2-CE2	8.73	128.29	121.30
1	C	463	TYR	C-N-CD	8.73	146.74	128.40
1	B	463	TYR	C-N-CD	8.73	146.73	128.40
1	A	188	TYR	CA-CB-CG	8.73	129.98	113.40
1	A	463	TYR	C-N-CD	8.71	146.70	128.40
1	C	188	TYR	CA-CB-CG	8.71	129.94	113.40
1	A	175	ASP	CB-CG-OD1	-8.62	110.55	118.30
1	B	65	VAL	CA-CB-CG1	8.61	123.82	110.90
1	A	65	VAL	CA-CB-CG1	8.61	123.81	110.90
1	C	65	VAL	CA-CB-CG1	8.60	123.80	110.90
1	C	435	GLU	N-CA-CB	8.59	126.06	110.60
1	A	459	PRO	N-CA-C	-8.59	89.78	112.10
1	B	175	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	B	459	PRO	N-CA-C	-8.58	89.79	112.10
1	C	459	PRO	N-CA-C	-8.58	89.79	112.10
1	B	318	ILE	CG1-CB-CG2	-8.58	92.53	111.40
1	A	435	GLU	N-CA-CB	8.57	126.03	110.60
1	B	435	GLU	N-CA-CB	8.57	126.03	110.60
1	C	175	ASP	CB-CG-OD1	-8.56	110.59	118.30
1	A	318	ILE	CG1-CB-CG2	-8.56	92.57	111.40
1	C	318	ILE	CG1-CB-CG2	-8.55	92.59	111.40
1	B	216	TRP	CH2-CZ2-CE2	8.51	125.91	117.40
1	A	225	VAL	N-CA-CB	-8.51	92.78	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	VAL	N-CA-CB	-8.51	92.79	111.50
1	C	225	VAL	N-CA-CB	-8.49	92.83	111.50
1	A	216	TRP	CH2-CZ2-CE2	8.46	125.86	117.40
1	A	396	ARG	CD-NE-CZ	-8.46	111.76	123.60
1	C	396	ARG	CD-NE-CZ	-8.45	111.77	123.60
1	B	396	ARG	CD-NE-CZ	-8.45	111.78	123.60
1	A	96	THR	OG1-CB-CG2	-8.44	90.58	110.00
1	C	216	TRP	CH2-CZ2-CE2	8.43	125.83	117.40
1	C	96	THR	OG1-CB-CG2	-8.43	90.61	110.00
1	B	96	THR	OG1-CB-CG2	-8.43	90.61	110.00
1	C	225	VAL	CA-CB-CG1	8.40	123.51	110.90
1	B	225	VAL	CA-CB-CG1	8.39	123.49	110.90
1	A	225	VAL	CA-CB-CG1	8.38	123.48	110.90
1	C	208	VAL	CB-CA-C	8.36	127.28	111.40
1	A	208	VAL	CB-CA-C	8.35	127.27	111.40
1	B	208	VAL	CB-CA-C	8.35	127.27	111.40
1	B	235	ASP	CB-CG-OD1	8.32	125.79	118.30
1	C	163	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	B	99	ASP	CB-CG-OD1	-8.31	110.82	118.30
1	A	99	ASP	CB-CG-OD1	-8.30	110.83	118.30
1	A	235	ASP	CB-CG-OD1	8.30	125.77	118.30
1	B	84	GLN	CA-CB-CG	8.30	131.66	113.40
1	C	84	GLN	CA-CB-CG	8.29	131.65	113.40
1	A	163	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	A	84	GLN	CA-CB-CG	8.29	131.63	113.40
1	C	235	ASP	CB-CG-OD1	8.29	125.76	118.30
1	C	99	ASP	CB-CG-OD1	-8.29	110.84	118.30
1	B	341	PRO	CA-CB-CG	-8.27	88.28	104.00
1	A	341	PRO	CA-CB-CG	-8.27	88.29	104.00
1	C	341	PRO	CA-CB-CG	-8.26	88.31	104.00
1	A	188	TYR	CB-CG-CD1	8.25	125.95	121.00
1	C	188	TYR	CB-CG-CD1	8.25	125.95	121.00
1	B	188	TYR	CB-CG-CD1	8.24	125.94	121.00
1	C	396	ARG	CA-C-N	8.24	135.33	117.20
1	A	396	ARG	CA-C-N	8.23	135.30	117.20
1	B	396	ARG	CA-C-N	8.21	135.27	117.20
1	B	64	PRO	CA-N-CD	-8.21	100.00	111.50
1	C	64	PRO	CA-N-CD	-8.21	100.01	111.50
1	B	163	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	64	PRO	CA-N-CD	-8.21	100.01	111.50
1	A	163	ASP	CB-CG-OD1	8.20	125.68	118.30
1	B	163	ASP	CB-CG-OD1	8.18	125.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	163	ASP	CB-CG-OD1	8.16	125.64	118.30
1	B	198	TYR	CB-CG-CD1	-8.16	116.11	121.00
1	A	198	TYR	CB-CG-CD1	-8.13	116.12	121.00
1	C	112	MET	CA-CB-CG	8.12	127.11	113.30
1	B	112	MET	CA-CB-CG	8.12	127.10	113.30
1	A	112	MET	CA-CB-CG	8.11	127.09	113.30
1	C	198	TYR	CB-CG-CD1	-8.09	116.15	121.00
1	B	468	LEU	CD1-CG-CD2	-8.07	86.28	110.50
1	C	468	LEU	CD1-CG-CD2	-8.06	86.31	110.50
1	A	468	LEU	CD1-CG-CD2	-8.06	86.33	110.50
1	A	452	VAL	CA-CB-CG1	-8.03	98.85	110.90
1	B	452	VAL	CA-CB-CG1	-8.03	98.85	110.90
1	C	452	VAL	CA-CB-CG1	-8.01	98.89	110.90
1	B	283	CYS	CB-CA-C	-8.00	94.39	110.40
1	A	283	CYS	CB-CA-C	-8.00	94.41	110.40
1	C	283	CYS	CB-CA-C	-7.97	94.45	110.40
1	B	191	VAL	CG1-CB-CG2	-7.96	98.16	110.90
1	A	191	VAL	CG1-CB-CG2	-7.96	98.17	110.90
1	C	191	VAL	CG1-CB-CG2	-7.95	98.19	110.90
1	C	19	PHE	CD1-CG-CD2	7.83	128.47	118.30
1	B	340	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	A	340	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	19	PHE	CD1-CG-CD2	7.81	128.45	118.30
1	C	230	GLU	CA-CB-CG	7.81	130.57	113.40
1	C	340	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	230	GLU	CA-CB-CG	7.79	130.53	113.40
1	B	19	PHE	CD1-CG-CD2	7.79	128.42	118.30
1	B	452	VAL	CG1-CB-CG2	7.78	123.35	110.90
1	C	452	VAL	CG1-CB-CG2	7.77	123.34	110.90
1	A	452	VAL	CG1-CB-CG2	7.77	123.33	110.90
1	B	230	GLU	CA-CB-CG	7.76	130.48	113.40
1	B	67	ALA	CA-C-O	-7.71	103.91	120.10
1	C	63	THR	CA-CB-OG1	-7.70	92.83	109.00
1	A	67	ALA	CA-C-O	-7.68	103.96	120.10
1	C	67	ALA	CA-C-O	-7.68	103.96	120.10
1	A	10	SER	N-CA-CB	-7.68	98.98	110.50
1	C	10	SER	N-CA-CB	-7.68	98.98	110.50
1	A	63	THR	CA-CB-OG1	-7.67	92.89	109.00
1	B	10	SER	N-CA-CB	-7.66	99.00	110.50
1	B	63	THR	CA-CB-OG1	-7.66	92.92	109.00
1	B	88	TYR	CB-CG-CD2	7.65	125.59	121.00
1	C	147	HIS	CA-CB-CG	7.61	126.53	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	147	HIS	CA-CB-CG	7.60	126.52	113.60
1	A	147	HIS	CA-CB-CG	7.60	126.52	113.60
1	A	47	ASP	CA-CB-CG	7.58	130.07	113.40
1	C	47	ASP	CA-CB-CG	7.57	130.06	113.40
1	A	88	TYR	CB-CG-CD2	7.57	125.54	121.00
1	B	47	ASP	CA-CB-CG	7.57	130.05	113.40
1	B	325	PRO	N-CA-CB	-7.57	94.22	103.30
1	A	325	PRO	N-CA-CB	-7.51	94.28	103.30
1	C	325	PRO	N-CA-CB	-7.51	94.29	103.30
1	B	64	PRO	CA-CB-CG	-7.50	89.75	104.00
1	A	64	PRO	CA-CB-CG	-7.50	89.75	104.00
1	B	211	VAL	CA-C-O	-7.50	104.35	120.10
1	C	88	TYR	CB-CG-CD2	7.50	125.50	121.00
1	A	211	VAL	CA-C-O	-7.48	104.39	120.10
1	B	463	TYR	N-CA-CB	-7.47	97.14	110.60
1	C	211	VAL	CA-C-O	-7.47	104.42	120.10
1	A	463	TYR	N-CA-CB	-7.45	97.19	110.60
1	C	64	PRO	CA-CB-CG	-7.45	89.84	104.00
1	C	463	TYR	N-CA-CB	-7.44	97.20	110.60
1	B	265	THR	CA-CB-CG2	7.41	122.77	112.40
1	A	265	THR	CA-CB-CG2	7.40	122.76	112.40
1	C	265	THR	CA-CB-CG2	7.38	122.74	112.40
1	A	155	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	B	155	TYR	CB-CG-CD2	-7.37	116.58	121.00
1	B	14	LEU	CD1-CG-CD2	-7.37	88.40	110.50
1	A	14	LEU	CD1-CG-CD2	-7.36	88.43	110.50
1	B	465	THR	CA-CB-OG1	7.35	124.43	109.00
1	A	465	THR	CA-CB-OG1	7.35	124.43	109.00
1	C	47	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	14	LEU	CD1-CG-CD2	-7.34	88.47	110.50
1	C	465	THR	CA-CB-OG1	7.34	124.41	109.00
1	A	47	ASP	CB-CG-OD2	7.33	124.90	118.30
1	B	427	TYR	CA-CB-CG	7.33	127.33	113.40
1	C	155	TYR	CB-CG-CD2	-7.33	116.61	121.00
1	B	47	ASP	CB-CG-OD2	7.30	124.87	118.30
1	C	137	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	A	427	TYR	CA-CB-CG	7.29	127.26	113.40
1	B	137	PHE	CB-CG-CD1	-7.29	115.70	120.80
1	B	63	THR	N-CA-C	7.29	130.68	111.00
1	C	427	TYR	CA-CB-CG	7.28	127.23	113.40
1	C	434	THR	O-C-N	7.28	134.35	122.70
1	A	434	THR	O-C-N	7.28	134.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	THR	N-CA-C	7.27	130.63	111.00
1	B	434	THR	O-C-N	7.27	134.34	122.70
1	C	63	THR	N-CA-C	7.27	130.64	111.00
1	A	137	PHE	CB-CG-CD1	-7.27	115.71	120.80
1	C	67	ALA	CB-CA-C	-7.25	99.22	110.10
1	B	247	ASP	N-CA-CB	7.24	123.64	110.60
1	A	67	ALA	CB-CA-C	-7.24	99.24	110.10
1	A	247	ASP	N-CA-CB	7.24	123.62	110.60
1	A	139	PRO	CA-C-N	7.22	133.09	117.20
1	B	67	ALA	CB-CA-C	-7.22	99.26	110.10
1	C	247	ASP	N-CA-CB	7.22	123.60	110.60
1	C	139	PRO	CA-C-N	7.22	133.08	117.20
1	C	376	ASP	O-C-N	-7.22	111.15	122.70
1	A	376	ASP	O-C-N	-7.21	111.16	122.70
1	B	376	ASP	O-C-N	-7.21	111.17	122.70
1	B	138	LYS	CA-C-O	-7.20	104.97	120.10
1	B	139	PRO	CA-C-N	7.20	133.05	117.20
1	C	2	THR	CA-CB-CG2	7.19	122.47	112.40
1	A	138	LYS	CA-C-O	-7.19	105.01	120.10
1	A	2	THR	CA-CB-CG2	7.18	122.46	112.40
1	C	138	LYS	CA-C-O	-7.18	105.03	120.10
1	B	2	THR	CA-CB-CG2	7.15	122.42	112.40
1	A	173	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	C	173	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	B	173	LEU	CB-CG-CD2	-7.13	98.87	111.00
1	B	245	VAL	CA-CB-CG2	7.11	121.56	110.90
1	B	209	LYS	N-CA-CB	-7.09	97.83	110.60
1	B	341	PRO	C-N-CA	7.09	139.42	121.70
1	C	341	PRO	C-N-CA	7.08	139.40	121.70
1	A	341	PRO	C-N-CA	7.08	139.40	121.70
1	B	318	ILE	CA-CB-CG2	7.07	125.05	110.90
1	A	245	VAL	CA-CB-CG2	7.07	121.50	110.90
1	C	245	VAL	CA-CB-CG2	7.07	121.50	110.90
1	C	318	ILE	CA-CB-CG2	7.07	125.03	110.90
1	A	209	LYS	N-CA-CB	-7.06	97.89	110.60
1	C	209	LYS	N-CA-CB	-7.05	97.90	110.60
1	A	318	ILE	CA-CB-CG2	7.05	125.01	110.90
1	B	341	PRO	CA-C-N	7.05	132.72	117.20
1	C	341	PRO	CA-C-N	7.05	132.71	117.20
1	A	341	PRO	CA-C-N	7.05	132.70	117.20
1	B	63	THR	N-CA-CB	-7.04	96.93	110.30
1	A	63	THR	N-CA-CB	-7.03	96.94	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	THR	N-CA-CB	-7.02	96.95	110.30
1	B	439	CYS	CA-CB-SG	-7.01	101.38	114.00
1	A	439	CYS	CA-CB-SG	-7.00	101.40	114.00
1	C	198	TYR	O-C-N	7.00	133.90	122.70
1	C	439	CYS	CA-CB-SG	-7.00	101.40	114.00
1	A	198	TYR	O-C-N	6.99	133.89	122.70
1	B	198	TYR	O-C-N	6.99	133.89	122.70
1	C	283	CYS	N-CA-CB	-6.99	98.02	110.60
1	C	85	THR	OG1-CB-CG2	-6.97	93.97	110.00
1	B	85	THR	OG1-CB-CG2	-6.97	93.98	110.00
1	A	283	CYS	N-CA-CB	-6.96	98.08	110.60
1	B	283	CYS	N-CA-CB	-6.96	98.08	110.60
1	A	85	THR	OG1-CB-CG2	-6.95	94.01	110.00
1	C	126	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	B	436	VAL	CG1-CB-CG2	-6.93	99.82	110.90
1	B	21	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	436	VAL	CG1-CB-CG2	-6.92	99.83	110.90
1	C	436	VAL	CG1-CB-CG2	-6.92	99.83	110.90
1	A	126	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	C	196	SER	N-CA-CB	-6.90	100.15	110.50
1	A	196	SER	N-CA-CB	-6.90	100.15	110.50
1	B	196	SER	N-CA-CB	-6.89	100.17	110.50
1	C	466	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	C	211	VAL	N-CA-C	6.88	129.57	111.00
1	B	143	GLN	CA-CB-CG	6.87	128.51	113.40
1	B	466	GLU	OE1-CD-OE2	-6.87	115.06	123.30
1	B	126	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	A	21	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	211	VAL	N-CA-C	6.87	129.54	111.00
1	C	18	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	7	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	143	GLN	CA-CB-CG	6.86	128.49	113.40
1	C	329	ALA	CB-CA-C	-6.86	99.81	110.10
1	A	329	ALA	CB-CA-C	-6.86	99.82	110.10
1	B	444	VAL	N-CA-CB	-6.86	96.42	111.50
1	C	143	GLN	CA-CB-CG	6.85	128.48	113.40
1	A	466	GLU	OE1-CD-OE2	-6.85	115.08	123.30
1	B	329	ALA	CB-CA-C	-6.85	99.82	110.10
1	B	211	VAL	N-CA-C	6.85	129.50	111.00
1	A	444	VAL	N-CA-CB	-6.84	96.45	111.50
1	C	444	VAL	N-CA-CB	-6.84	96.46	111.50
1	C	21	ARG	NE-CZ-NH2	-6.83	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	18	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	42	TRP	CA-CB-CG	6.83	126.67	113.70
1	B	443	THR	O-C-N	-6.82	111.78	122.70
1	C	443	THR	O-C-N	-6.82	111.78	122.70
1	A	42	TRP	CA-CB-CG	6.81	126.64	113.70
1	C	471	SER	N-CA-CB	-6.81	100.28	110.50
1	A	443	THR	O-C-N	-6.80	111.82	122.70
1	A	18	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	471	SER	N-CA-CB	-6.80	100.31	110.50
1	C	82	TYR	CG-CD2-CE2	6.79	126.74	121.30
1	A	471	SER	N-CA-CB	-6.79	100.31	110.50
1	C	42	TRP	CA-CB-CG	6.79	126.61	113.70
1	C	262	PHE	CB-CG-CD2	6.78	125.55	120.80
1	A	82	TYR	CG-CD2-CE2	6.78	126.72	121.30
1	B	82	TYR	CG-CD2-CE2	6.75	126.70	121.30
1	C	463	TYR	N-CA-C	6.74	129.18	111.00
1	A	7	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	458	LEU	C-N-CA	6.73	150.26	122.00
1	C	7	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	463	TYR	N-CA-C	6.72	129.16	111.00
1	B	63	THR	OG1-CB-CG2	6.72	125.47	110.00
1	B	463	TYR	N-CA-C	6.72	129.16	111.00
1	B	211	VAL	CA-CB-CG2	6.72	120.97	110.90
1	A	458	LEU	C-N-CA	6.71	150.20	122.00
1	C	458	LEU	C-N-CA	6.71	150.19	122.00
1	A	63	THR	OG1-CB-CG2	6.70	125.41	110.00
1	B	124	GLY	N-CA-C	6.69	129.84	113.10
1	A	124	GLY	N-CA-C	6.69	129.83	113.10
1	C	124	GLY	N-CA-C	6.69	129.83	113.10
1	C	63	THR	OG1-CB-CG2	6.68	125.37	110.00
1	C	211	VAL	CA-CB-CG2	6.68	120.92	110.90
1	A	211	VAL	CA-CB-CG2	6.68	120.92	110.90
1	C	101	LYS	CD-CE-NZ	6.67	127.04	111.70
1	A	262	PHE	CB-CG-CD2	6.67	125.47	120.80
1	B	101	LYS	CD-CE-NZ	6.66	127.03	111.70
1	A	101	LYS	CD-CE-NZ	6.66	127.02	111.70
1	B	21	ARG	NH1-CZ-NH2	-6.66	112.08	119.40
1	C	140	PHE	CB-CG-CD1	6.65	125.45	120.80
1	B	62	ILE	CB-CG1-CD1	-6.65	95.29	113.90
1	B	434	THR	C-N-CA	6.65	138.32	121.70
1	C	62	ILE	CB-CG1-CD1	-6.64	95.30	113.90
1	A	21	ARG	NH1-CZ-NH2	-6.64	112.10	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	PHE	CB-CG-CD1	6.63	125.44	120.80
1	C	21	ARG	NH1-CZ-NH2	-6.63	112.10	119.40
1	C	434	THR	C-N-CA	6.63	138.28	121.70
1	A	62	ILE	CB-CG1-CD1	-6.63	95.33	113.90
1	A	434	THR	C-N-CA	6.63	138.28	121.70
1	B	157	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	A	201	ASP	CB-CA-C	-6.62	97.16	110.40
1	B	201	ASP	CB-CA-C	-6.62	97.16	110.40
1	C	201	ASP	CB-CA-C	-6.62	97.16	110.40
1	B	262	PHE	CB-CG-CD2	6.62	125.43	120.80
1	C	282	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	A	157	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	A	282	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	C	157	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	B	140	PHE	CB-CG-CD1	6.58	125.40	120.80
1	B	335	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	C	219	TYR	CG-CD2-CE2	-6.56	116.05	121.30
1	B	282	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	B	80	THR	CA-C-N	-6.54	103.12	116.20
1	C	138	LYS	O-C-N	6.54	133.52	121.10
1	A	335	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	B	138	LYS	O-C-N	6.53	133.50	121.10
1	A	219	TYR	CG-CD2-CE2	-6.52	116.08	121.30
1	B	219	TYR	CG-CD2-CE2	-6.52	116.09	121.30
1	A	80	THR	CA-C-N	-6.51	103.18	116.20
1	A	138	LYS	O-C-N	6.51	133.46	121.10
1	C	80	THR	CA-C-N	-6.51	103.19	116.20
1	C	229	GLY	C-N-CA	6.49	137.93	121.70
1	A	229	GLY	C-N-CA	6.49	137.93	121.70
1	B	229	GLY	C-N-CA	6.48	137.91	121.70
1	C	335	TYR	CB-CG-CD1	-6.47	117.11	121.00
1	B	458	LEU	N-CA-C	6.47	128.46	111.00
1	A	458	LEU	N-CA-C	6.46	128.45	111.00
1	B	64	PRO	N-CA-CB	6.46	111.05	103.30
1	C	458	LEU	N-CA-C	6.45	128.43	111.00
1	A	64	PRO	N-CA-CB	6.45	111.04	103.30
1	B	463	TYR	CB-CG-CD2	6.45	124.87	121.00
1	A	463	TYR	CB-CG-CD2	6.43	124.86	121.00
1	A	459	PRO	CA-N-CD	-6.43	102.50	111.50
1	C	64	PRO	N-CA-CB	6.42	111.01	103.30
1	C	459	PRO	CA-N-CD	-6.42	102.51	111.50
1	B	306	ASN	N-CA-CB	6.41	122.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	306	ASN	N-CA-CB	6.41	122.13	110.60
1	B	459	PRO	CA-N-CD	-6.40	102.54	111.50
1	C	55	MET	CB-CG-SD	6.40	131.60	112.40
1	B	75	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	B	55	MET	CB-CG-SD	6.39	131.58	112.40
1	C	61	TRP	C-N-CA	-6.39	105.72	121.70
1	C	463	TYR	CB-CG-CD2	6.39	124.83	121.00
1	A	55	MET	CB-CG-SD	6.39	131.56	112.40
1	B	61	TRP	C-N-CA	-6.39	105.73	121.70
1	C	256	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	61	TRP	C-N-CA	-6.37	105.77	121.70
1	A	256	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	B	403	GLN	C-N-CA	6.37	137.62	121.70
1	A	75	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	C	306	ASN	N-CA-CB	6.37	122.06	110.60
1	C	403	GLN	C-N-CA	6.37	137.62	121.70
1	A	403	GLN	C-N-CA	6.36	137.60	121.70
1	C	390	ASP	CA-CB-CG	6.36	127.39	113.40
1	A	390	ASP	CA-CB-CG	6.34	127.35	113.40
1	B	190	TRP	CE2-CD2-CG	6.33	112.37	107.30
1	C	75	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	B	390	ASP	CA-CB-CG	6.32	127.30	113.40
1	B	256	TYR	CB-CG-CD2	-6.31	117.21	121.00
1	C	262	PHE	CB-CG-CD1	-6.30	116.39	120.80
1	A	333	GLN	CA-CB-CG	6.29	127.25	113.40
1	B	233	ASP	OD1-CG-OD2	6.29	135.25	123.30
1	C	190	TRP	CE2-CD2-CG	6.29	112.33	107.30
1	B	191	VAL	CA-CB-CG2	6.29	120.33	110.90
1	A	191	VAL	CA-CB-CG2	6.29	120.33	110.90
1	B	333	GLN	CA-CB-CG	6.28	127.22	113.40
1	B	42	TRP	CD1-CG-CD2	-6.28	101.28	106.30
1	C	333	GLN	CA-CB-CG	6.27	127.20	113.40
1	A	190	TRP	CE2-CD2-CG	6.27	112.32	107.30
1	A	233	ASP	OD1-CG-OD2	6.27	135.22	123.30
1	C	233	ASP	OD1-CG-OD2	6.27	135.21	123.30
1	B	262	PHE	CB-CG-CD1	-6.27	116.41	120.80
1	C	191	VAL	CA-CB-CG2	6.26	120.30	110.90
1	C	42	TRP	CD1-CG-CD2	-6.24	101.31	106.30
1	C	345	GLU	N-CA-CB	6.23	121.82	110.60
1	B	345	GLU	N-CA-CB	6.23	121.81	110.60
1	B	369	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	42	TRP	CD1-CG-CD2	-6.22	101.32	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	PHE	CB-CG-CD1	-6.22	116.45	120.80
1	A	345	GLU	N-CA-CB	6.22	121.79	110.60
1	A	369	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	66	THR	CA-CB-OG1	6.21	122.04	109.00
1	C	49	LEU	O-C-N	-6.20	112.78	122.70
1	A	49	LEU	O-C-N	-6.20	112.78	122.70
1	A	66	THR	CA-CB-OG1	6.20	122.01	109.00
1	C	104	SER	CB-CA-C	-6.20	98.33	110.10
1	C	369	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	C	187	TRP	CE2-CD2-CG	6.18	112.25	107.30
1	A	104	SER	CB-CA-C	-6.18	98.36	110.10
1	B	104	SER	CB-CA-C	-6.18	98.36	110.10
1	B	49	LEU	O-C-N	-6.18	112.82	122.70
1	C	66	THR	CA-CB-OG1	6.16	121.94	109.00
1	A	103	LEU	CB-CG-CD1	6.16	121.47	111.00
1	C	103	LEU	CB-CG-CD1	6.16	121.47	111.00
1	B	411	LYS	CB-CG-CD	-6.16	95.59	111.60
1	B	103	LEU	CB-CG-CD1	6.15	121.46	111.00
1	A	411	LYS	CB-CG-CD	-6.15	95.61	111.60
1	B	464	PRO	CB-CA-C	6.15	127.37	112.00
1	A	300	ARG	CB-CG-CD	6.14	127.57	111.60
1	C	411	LYS	CB-CG-CD	-6.14	95.63	111.60
1	C	300	ARG	CB-CG-CD	6.14	127.56	111.60
1	A	464	PRO	CB-CA-C	6.13	127.34	112.00
1	B	75	TYR	CD1-CE1-CZ	6.13	125.32	119.80
1	C	464	PRO	CB-CA-C	6.13	127.34	112.00
1	B	458	LEU	CB-CA-C	-6.13	98.55	110.20
1	B	300	ARG	CB-CG-CD	6.13	127.53	111.60
1	C	75	TYR	CD1-CE1-CZ	6.13	125.31	119.80
1	B	187	TRP	CE2-CD2-CG	6.12	112.20	107.30
1	A	187	TRP	CE2-CD2-CG	6.12	112.20	107.30
1	A	398	GLY	N-CA-C	6.12	128.40	113.10
1	B	398	GLY	N-CA-C	6.12	128.41	113.10
1	A	458	LEU	CB-CA-C	-6.12	98.57	110.20
1	B	265	THR	O-C-N	-6.12	112.91	122.70
1	B	273	TYR	CB-CA-C	-6.12	98.17	110.40
1	C	285	ASP	O-C-N	6.11	132.48	122.70
1	C	398	GLY	N-CA-C	6.11	128.38	113.10
1	A	335	TYR	CA-CB-CG	6.11	125.01	113.40
1	B	285	ASP	O-C-N	6.11	132.47	122.70
1	B	473	ILE	CA-CB-CG1	6.11	122.61	111.00
1	C	335	TYR	CA-CB-CG	6.11	125.00	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	265	THR	O-C-N	-6.10	112.93	122.70
1	A	75	TYR	CD1-CE1-CZ	6.10	125.29	119.80
1	A	273	TYR	CB-CA-C	-6.10	98.20	110.40
1	B	15	LEU	C-N-CA	6.10	136.95	121.70
1	B	335	TYR	CA-CB-CG	6.10	124.99	113.40
1	C	458	LEU	CB-CA-C	-6.10	98.61	110.20
1	C	473	ILE	CA-CB-CG1	6.09	122.58	111.00
1	A	285	ASP	O-C-N	6.09	132.45	122.70
1	A	15	LEU	C-N-CA	6.09	136.93	121.70
1	A	473	ILE	CA-CB-CG1	6.09	122.57	111.00
1	C	273	TYR	CB-CA-C	-6.09	98.22	110.40
1	C	265	THR	O-C-N	-6.08	112.98	122.70
1	C	15	LEU	C-N-CA	6.07	136.88	121.70
1	A	404	ILE	CG1-CB-CG2	6.04	124.69	111.40
1	C	404	ILE	CG1-CB-CG2	6.04	124.69	111.40
1	B	404	ILE	CG1-CB-CG2	6.03	124.67	111.40
1	B	132	VAL	CG1-CB-CG2	6.01	120.52	110.90
1	A	225	VAL	O-C-N	-6.00	113.10	122.70
1	B	229	GLY	CA-C-N	-6.00	104.00	117.20
1	C	132	VAL	CG1-CB-CG2	6.00	120.50	110.90
1	C	225	VAL	O-C-N	-6.00	113.11	122.70
1	A	132	VAL	CG1-CB-CG2	5.99	120.48	110.90
1	A	229	GLY	N-CA-C	-5.99	98.14	113.10
1	B	225	VAL	O-C-N	-5.99	113.12	122.70
1	A	432	GLN	CB-CA-C	5.98	122.37	110.40
1	B	229	GLY	N-CA-C	-5.98	98.14	113.10
1	C	432	GLN	CB-CA-C	5.98	122.37	110.40
1	A	154	ASN	N-CA-C	-5.98	94.85	111.00
1	C	45	ILE	CA-CB-CG2	5.98	122.85	110.90
1	A	229	GLY	CA-C-N	-5.97	104.06	117.20
1	B	154	ASN	N-CA-C	-5.97	94.89	111.00
1	B	432	GLN	CB-CA-C	5.97	122.33	110.40
1	B	51	TYR	CG-CD2-CE2	-5.96	116.53	121.30
1	C	154	ASN	N-CA-C	-5.96	94.89	111.00
1	C	229	GLY	N-CA-C	-5.96	98.19	113.10
1	B	45	ILE	CA-CB-CG2	5.96	122.82	110.90
1	B	210	HIS	CA-CB-CG	5.96	123.73	113.60
1	C	210	HIS	CA-CB-CG	5.96	123.73	113.60
1	A	45	ILE	CA-CB-CG2	5.96	122.82	110.90
1	A	210	HIS	CA-CB-CG	5.96	123.73	113.60
1	C	434	THR	CA-C-O	-5.96	107.59	120.10
1	B	434	THR	CA-C-O	-5.96	107.59	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	229	GLY	CA-C-N	-5.95	104.10	117.20
1	C	392	THR	CA-CB-CG2	5.95	120.73	112.40
1	A	434	THR	CA-C-O	-5.95	107.61	120.10
1	C	51	TYR	CG-CD2-CE2	-5.95	116.54	121.30
1	A	51	TYR	CG-CD2-CE2	-5.93	116.55	121.30
1	A	392	THR	CA-CB-CG2	5.93	120.70	112.40
1	B	16	THR	CA-CB-CG2	-5.91	104.13	112.40
1	B	392	THR	CA-CB-CG2	5.91	120.67	112.40
1	C	432	GLN	N-CA-CB	-5.90	99.98	110.60
1	C	226	TYR	O-C-N	-5.89	113.27	122.70
1	A	16	THR	CA-CB-CG2	-5.88	104.17	112.40
1	A	432	GLN	N-CA-CB	-5.88	100.02	110.60
1	B	387	ILE	CB-CG1-CD1	-5.87	97.46	113.90
1	B	208	VAL	CA-C-N	-5.87	104.29	117.20
1	A	226	TYR	O-C-N	-5.86	113.32	122.70
1	B	432	GLN	N-CA-CB	-5.86	100.05	110.60
1	A	387	ILE	CB-CG1-CD1	-5.86	97.49	113.90
1	B	252	TYR	CG-CD2-CE2	-5.86	116.61	121.30
1	C	208	VAL	CA-C-N	-5.86	104.32	117.20
1	C	387	ILE	CB-CG1-CD1	-5.85	97.51	113.90
1	A	208	VAL	CA-C-N	-5.85	104.33	117.20
1	B	219	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	252	TYR	CG-CD2-CE2	-5.85	116.62	121.30
1	C	270	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	16	THR	CA-CB-CG2	-5.84	104.22	112.40
1	B	226	TYR	O-C-N	-5.84	113.36	122.70
1	C	252	TYR	CG-CD2-CE2	-5.83	116.63	121.30
1	A	226	TYR	N-CA-C	5.82	126.72	111.00
1	A	341	PRO	N-CA-C	5.82	127.24	112.10
1	B	341	PRO	N-CA-C	5.82	127.23	112.10
1	C	397	LYS	CA-C-N	5.82	127.84	116.20
1	C	341	PRO	N-CA-C	5.82	127.22	112.10
1	A	270	ASP	CB-CG-OD2	5.82	123.53	118.30
1	C	226	TYR	N-CA-C	5.82	126.70	111.00
1	B	226	TYR	N-CA-C	5.81	126.70	111.00
1	A	219	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	B	397	LYS	CA-C-N	5.80	127.81	116.20
1	A	397	LYS	CA-C-N	5.80	127.81	116.20
1	B	270	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	65	VAL	CB-CA-C	-5.80	100.39	111.40
1	B	347	THR	O-C-N	-5.79	113.43	122.70
1	A	205	ILE	CB-CG1-CD1	-5.79	97.69	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	ALA	CA-C-O	-5.79	107.95	120.10
1	C	219	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	B	205	ILE	CB-CG1-CD1	-5.78	97.70	113.90
1	C	205	ILE	CB-CG1-CD1	-5.78	97.71	113.90
1	A	1	ALA	CA-C-O	-5.78	107.97	120.10
1	A	347	THR	O-C-N	-5.78	113.46	122.70
1	B	473	ILE	CA-CB-CG2	5.78	122.45	110.90
1	A	65	VAL	CB-CA-C	-5.77	100.44	111.40
1	B	1	ALA	CA-C-O	-5.77	107.98	120.10
1	A	473	ILE	CA-CB-CG2	5.77	122.43	110.90
1	B	73	CYS	CA-CB-SG	5.77	124.38	114.00
1	C	473	ILE	CA-CB-CG2	5.76	122.43	110.90
1	A	73	CYS	CA-CB-SG	5.76	124.37	114.00
1	C	59	ALA	N-CA-CB	-5.76	102.03	110.10
1	C	73	CYS	CA-CB-SG	5.76	124.37	114.00
1	B	65	VAL	CB-CA-C	-5.76	100.46	111.40
1	C	137	PHE	CB-CG-CD2	5.76	124.83	120.80
1	A	134	TYR	CB-CG-CD2	5.75	124.45	121.00
1	A	59	ALA	N-CA-CB	-5.75	102.05	110.10
1	B	21	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	380	VAL	CA-CB-CG1	5.75	119.52	110.90
1	A	19	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	B	59	ALA	N-CA-CB	-5.74	102.06	110.10
1	A	21	ARG	CD-NE-CZ	5.74	131.64	123.60
1	B	137	PHE	CB-CG-CD2	5.74	124.82	120.80
1	C	347	THR	O-C-N	-5.74	113.52	122.70
1	C	380	VAL	CA-CB-CG1	5.74	119.51	110.90
1	A	137	PHE	CB-CG-CD2	5.74	124.82	120.80
1	A	380	VAL	CA-CB-CG1	5.74	119.50	110.90
1	C	21	ARG	CD-NE-CZ	5.74	131.63	123.60
1	B	146	PHE	CB-CG-CD1	-5.73	116.79	120.80
1	B	19	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	C	19	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	C	134	TYR	CB-CG-CD2	5.72	124.43	121.00
1	C	230	GLU	CB-CA-C	-5.72	98.96	110.40
1	C	343	ASN	CA-CB-CG	-5.72	100.82	113.40
1	A	381	THR	O-C-N	5.72	131.85	122.70
1	C	55	MET	O-C-N	-5.72	113.48	123.20
1	B	207	THR	C-N-CA	5.71	135.99	121.70
1	A	55	MET	O-C-N	-5.71	113.49	123.20
1	B	96	THR	O-C-N	-5.71	113.56	122.70
1	B	134	TYR	CB-CG-CD2	5.71	124.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	55	MET	O-C-N	-5.71	113.49	123.20
1	A	343	ASN	CA-CB-CG	-5.71	100.85	113.40
1	C	207	THR	C-N-CA	5.71	135.97	121.70
1	A	146	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	C	185	ASN	CA-C-N	-5.70	104.67	117.20
1	C	381	THR	O-C-N	5.70	131.81	122.70
1	A	230	GLU	CB-CA-C	-5.69	99.01	110.40
1	A	185	ASN	CA-C-N	-5.69	104.68	117.20
1	A	207	THR	C-N-CA	5.69	135.93	121.70
1	B	185	ASN	CA-C-N	-5.69	104.67	117.20
1	A	96	THR	O-C-N	-5.69	113.60	122.70
1	B	343	ASN	CA-CB-CG	-5.69	100.88	113.40
1	C	146	PHE	CB-CG-CD1	-5.69	116.82	120.80
1	B	234	GLY	N-CA-C	5.68	127.31	113.10
1	C	234	GLY	N-CA-C	5.68	127.31	113.10
1	B	381	THR	O-C-N	5.68	131.79	122.70
1	A	234	GLY	N-CA-C	5.67	127.28	113.10
1	B	230	GLU	CB-CA-C	-5.66	99.07	110.40
1	C	96	THR	O-C-N	-5.66	113.64	122.70
1	C	140	PHE	CB-CG-CD2	-5.66	116.83	120.80
1	B	383	LYS	N-CA-CB	-5.65	100.43	110.60
1	B	297	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	229	GLY	O-C-N	5.64	131.73	122.70
1	A	383	LYS	N-CA-CB	-5.64	100.45	110.60
1	B	18	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	181	ASP	N-CA-C	5.64	126.23	111.00
1	A	297	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	297	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	181	ASP	N-CA-C	5.63	126.21	111.00
1	C	383	LYS	N-CA-CB	-5.63	100.46	110.60
1	B	181	ASP	N-CA-C	5.63	126.19	111.00
1	C	167	GLY	N-CA-C	5.62	127.16	113.10
1	B	465	THR	N-CA-CB	-5.62	99.62	110.30
1	A	229	GLY	O-C-N	5.62	131.68	122.70
1	B	167	GLY	N-CA-C	5.61	127.14	113.10
1	B	463	TYR	O-C-N	5.61	131.76	121.10
1	A	465	THR	N-CA-CB	-5.61	99.64	110.30
1	C	465	THR	N-CA-CB	-5.61	99.65	110.30
1	A	167	GLY	N-CA-C	5.61	127.12	113.10
1	C	198	TYR	N-CA-CB	5.60	120.69	110.60
1	A	52	ILE	CA-CB-CG2	5.60	122.10	110.90
1	A	140	PHE	CB-CG-CD2	-5.60	116.88	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	463	TYR	O-C-N	5.60	131.74	121.10
1	B	52	ILE	CA-CB-CG2	5.60	122.10	110.90
1	C	198	TYR	CA-C-O	-5.60	108.34	120.10
1	B	368	ILE	CG1-CB-CG2	-5.60	99.08	111.40
1	A	82	TYR	C-N-CA	5.60	135.69	121.70
1	A	198	TYR	N-CA-CB	5.59	120.67	110.60
1	C	247	ASP	CA-CB-CG	5.59	125.70	113.40
1	C	463	TYR	O-C-N	5.59	131.73	121.10
1	A	368	ILE	CG1-CB-CG2	-5.59	99.10	111.40
1	C	229	GLY	O-C-N	5.59	131.64	122.70
1	B	198	TYR	CA-C-O	-5.59	108.36	120.10
1	B	198	TYR	N-CA-CB	5.59	120.66	110.60
1	A	49	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	C	82	TYR	C-N-CA	5.58	135.66	121.70
1	C	49	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	C	52	ILE	CA-CB-CG2	5.58	122.06	110.90
1	A	198	TYR	CA-C-O	-5.58	108.39	120.10
1	C	99	ASP	CB-CA-C	-5.58	99.25	110.40
1	A	99	ASP	CB-CA-C	-5.58	99.25	110.40
1	A	247	ASP	CA-CB-CG	5.58	125.67	113.40
1	B	82	TYR	C-N-CA	5.58	135.64	121.70
1	B	99	ASP	CB-CA-C	-5.58	99.25	110.40
1	B	396	ARG	CG-CD-NE	5.57	123.50	111.80
1	C	368	ILE	CG1-CB-CG2	-5.57	99.14	111.40
1	C	376	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	247	ASP	CA-CB-CG	5.57	125.65	113.40
1	B	49	LEU	CB-CG-CD1	-5.57	101.54	111.00
1	C	396	ARG	CG-CD-NE	5.57	123.49	111.80
1	C	199	SER	CB-CA-C	-5.56	99.53	110.10
1	A	396	ARG	CG-CD-NE	5.56	123.48	111.80
1	C	83	TRP	CE2-CD2-CG	-5.56	102.85	107.30
1	A	83	TRP	CE2-CD2-CG	-5.56	102.86	107.30
1	A	199	SER	CB-CA-C	-5.55	99.56	110.10
1	B	140	PHE	CB-CG-CD2	-5.55	116.92	120.80
1	A	376	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	199	SER	CB-CA-C	-5.54	99.57	110.10
1	B	376	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	82	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	B	83	TRP	CE2-CD2-CG	-5.52	102.88	107.30
1	C	82	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	300	ARG	NH1-CZ-NH2	5.52	125.47	119.40
1	C	300	ARG	NH1-CZ-NH2	5.52	125.47	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	300	ARG	NH1-CZ-NH2	5.51	125.47	119.40
1	C	18	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	154	ASN	CA-CB-CG	5.50	125.51	113.40
1	C	166	LEU	CB-CA-C	5.50	120.65	110.20
1	A	82	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	166	LEU	CB-CA-C	5.49	120.64	110.20
1	A	154	ASN	CA-CB-CG	5.49	125.48	113.40
1	B	255	TYR	CA-CB-CG	5.48	123.82	113.40
1	B	166	LEU	CB-CA-C	5.48	120.61	110.20
1	B	326	ILE	CB-CG1-CD1	5.48	129.24	113.90
1	A	18	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	181	ASP	N-CA-CB	-5.47	100.76	110.60
1	A	326	ILE	CB-CG1-CD1	5.47	129.21	113.90
1	B	154	ASN	CA-CB-CG	5.47	125.43	113.40
1	C	326	ILE	CB-CG1-CD1	5.46	129.20	113.90
1	B	181	ASP	N-CA-CB	-5.46	100.77	110.60
1	A	255	TYR	CA-CB-CG	5.45	123.76	113.40
1	C	255	TYR	CA-CB-CG	5.45	123.76	113.40
1	C	377	THR	CA-CB-CG2	5.45	120.03	112.40
1	B	411	LYS	N-CA-CB	-5.45	100.79	110.60
1	B	8	SER	C-N-CA	5.44	135.30	121.70
1	C	181	ASP	N-CA-CB	-5.44	100.81	110.60
1	C	186	GLU	CA-CB-CG	5.44	125.37	113.40
1	A	377	THR	CA-CB-CG2	5.44	120.01	112.40
1	B	377	THR	CA-CB-CG2	5.44	120.01	112.40
1	B	404	ILE	C-N-CA	-5.43	108.12	121.70
1	C	8	SER	C-N-CA	5.43	135.28	121.70
1	A	8	SER	C-N-CA	5.43	135.28	121.70
1	A	411	LYS	N-CA-CB	-5.43	100.83	110.60
1	C	292	PHE	C-N-CA	5.43	135.27	121.70
1	C	252	TYR	N-CA-C	5.43	125.66	111.00
1	B	186	GLU	CA-CB-CG	5.43	125.34	113.40
1	A	252	TYR	N-CA-C	5.42	125.64	111.00
1	A	186	GLU	CA-CB-CG	5.42	125.33	113.40
1	B	389	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	404	ILE	C-N-CA	-5.41	108.17	121.70
1	C	411	LYS	N-CA-CB	-5.41	100.86	110.60
1	B	252	TYR	N-CA-C	5.41	125.61	111.00
1	A	292	PHE	C-N-CA	5.41	135.22	121.70
1	C	404	ILE	C-N-CA	-5.41	108.18	121.70
1	A	246	MET	N-CA-C	5.40	125.59	111.00
1	B	292	PHE	C-N-CA	5.40	135.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3	PRO	N-CA-C	5.40	126.15	112.10
1	A	3	PRO	N-CA-C	5.40	126.14	112.10
1	B	246	MET	N-CA-C	5.40	125.58	111.00
1	A	389	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	435	GLU	CA-C-N	5.39	129.07	117.20
1	B	3	PRO	N-CA-C	5.39	126.12	112.10
1	C	198	TYR	C-N-CA	5.39	135.18	121.70
1	C	369	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
1	B	435	GLU	CA-C-N	5.39	129.06	117.20
1	C	435	GLU	CA-C-N	5.39	129.06	117.20
1	B	198	TYR	C-N-CA	5.38	135.16	121.70
1	A	198	TYR	C-N-CA	5.38	135.16	121.70
1	C	246	MET	N-CA-C	5.38	125.53	111.00
1	B	245	VAL	CG1-CB-CG2	-5.37	102.30	110.90
1	C	135	SER	N-CA-CB	-5.37	102.44	110.50
1	A	369	ARG	NH1-CZ-NH2	-5.37	113.50	119.40
1	C	245	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	C	327	ILE	CA-CB-CG2	-5.37	100.17	110.90
1	A	245	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	B	327	ILE	CA-CB-CG2	-5.35	100.19	110.90
1	A	327	ILE	CA-CB-CG2	-5.35	100.20	110.90
1	B	116	VAL	CA-CB-CG2	5.35	118.92	110.90
1	A	135	SER	N-CA-CB	-5.34	102.48	110.50
1	A	178	THR	CA-CB-CG2	5.34	119.88	112.40
1	A	161	VAL	C-N-CA	5.34	135.05	121.70
1	C	161	VAL	C-N-CA	5.34	135.05	121.70
1	C	178	THR	CA-CB-CG2	5.33	119.87	112.40
1	C	209	LYS	CA-CB-CG	5.33	125.14	113.40
1	B	369	ARG	NH1-CZ-NH2	-5.33	113.53	119.40
1	B	135	SER	N-CA-CB	-5.33	102.51	110.50
1	B	161	VAL	C-N-CA	5.33	135.01	121.70
1	B	83	TRP	CA-C-O	-5.32	108.92	120.10
1	B	450	VAL	N-CA-C	5.32	125.37	111.00
1	C	116	VAL	CA-CB-CG2	5.32	118.88	110.90
1	B	209	LYS	CA-CB-CG	5.32	125.10	113.40
1	A	450	VAL	N-CA-C	5.32	125.35	111.00
1	B	178	THR	CA-CB-CG2	5.32	119.84	112.40
1	C	83	TRP	CA-C-O	-5.32	108.94	120.10
1	A	209	LYS	CA-CB-CG	5.31	125.09	113.40
1	A	83	TRP	CA-C-O	-5.31	108.94	120.10
1	A	116	VAL	CA-CB-CG2	5.31	118.87	110.90
1	C	389	ASP	CB-CG-OD2	5.31	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	243	GLN	OE1-CD-NE2	-5.31	109.69	121.90
1	C	15	LEU	CA-CB-CG	-5.31	103.09	115.30
1	C	450	VAL	N-CA-C	5.30	125.31	111.00
1	A	243	GLN	OE1-CD-NE2	-5.30	109.71	121.90
1	B	15	LEU	CA-CB-CG	-5.30	103.11	115.30
1	C	411	LYS	CA-C-N	5.30	126.79	116.20
1	A	15	LEU	CA-CB-CG	-5.29	103.12	115.30
1	A	13	PHE	CA-C-O	-5.28	109.00	120.10
1	B	148	PRO	CA-N-CD	-5.28	104.11	111.50
1	B	319	ILE	CA-CB-CG2	5.28	121.46	110.90
1	A	411	LYS	CA-C-N	5.28	126.76	116.20
1	B	243	GLN	OE1-CD-NE2	-5.28	109.76	121.90
1	C	13	PHE	CA-C-O	-5.28	109.02	120.10
1	A	319	ILE	CA-CB-CG2	5.27	121.44	110.90
1	B	411	LYS	CA-C-N	5.27	126.74	116.20
1	C	319	ILE	CA-CB-CG2	5.26	121.42	110.90
1	B	13	PHE	CA-C-O	-5.26	109.06	120.10
1	C	466	GLU	CG-CD-OE2	5.25	128.81	118.30
1	A	148	PRO	CA-N-CD	-5.25	104.15	111.50
1	C	266	SER	CB-CA-C	-5.25	100.13	110.10
1	B	81	GLY	N-CA-C	-5.24	100.00	113.10
1	A	71	GLN	CB-CG-CD	5.24	125.22	111.60
1	A	81	GLY	N-CA-C	-5.24	100.00	113.10
1	A	266	SER	CB-CA-C	-5.24	100.14	110.10
1	C	71	GLN	CB-CG-CD	5.24	125.22	111.60
1	A	259	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	B	96	THR	CA-CB-CG2	5.24	119.73	112.40
1	B	259	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	466	GLU	CG-CD-OE2	5.23	128.77	118.30
1	C	81	GLY	N-CA-C	-5.23	100.02	113.10
1	B	71	GLN	CB-CG-CD	5.23	125.20	111.60
1	A	266	SER	CA-CB-OG	-5.23	97.09	111.20
1	B	266	SER	CB-CA-C	-5.23	100.17	110.10
1	B	466	GLU	CG-CD-OE2	5.22	128.75	118.30
1	B	266	SER	CA-CB-OG	-5.22	97.11	111.20
1	B	347	THR	CA-CB-OG1	5.22	119.96	109.00
1	C	153	GLN	CB-CG-CD	5.22	125.17	111.60
1	B	87	ILE	CA-CB-CG2	5.22	121.33	110.90
1	C	110	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	C	266	SER	CA-CB-OG	-5.21	97.13	111.20
1	B	236	PRO	CB-CA-C	-5.21	98.97	112.00
1	C	148	PRO	CA-N-CD	-5.21	104.21	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	347	THR	CA-CB-OG1	5.21	119.94	109.00
1	A	347	THR	CA-CB-OG1	5.21	119.94	109.00
1	A	87	ILE	CA-CB-CG2	5.20	121.31	110.90
1	A	96	THR	CA-CB-CG2	5.20	119.68	112.40
1	A	153	GLN	CB-CG-CD	5.20	125.12	111.60
1	C	87	ILE	CA-CB-CG2	5.20	121.30	110.90
1	C	259	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	C	211	VAL	CB-CA-C	-5.20	101.53	111.40
1	C	236	PRO	CB-CA-C	-5.20	99.01	112.00
1	B	153	GLN	CB-CG-CD	5.19	125.10	111.60
1	B	216	TRP	CE3-CZ3-CH2	-5.19	115.49	121.20
1	B	203	LEU	CB-CA-C	-5.19	100.34	110.20
1	A	203	LEU	CB-CA-C	-5.19	100.34	110.20
1	A	110	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	A	236	PRO	CB-CA-C	-5.18	99.04	112.00
1	B	7	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	203	LEU	CB-CA-C	-5.18	100.35	110.20
1	C	435	GLU	C-N-CA	5.18	134.66	121.70
1	C	442	VAL	N-CA-CB	-5.18	100.09	111.50
1	A	211	VAL	CB-CA-C	-5.18	101.55	111.40
1	B	211	VAL	CB-CA-C	-5.18	101.55	111.40
1	C	96	THR	CA-CB-CG2	5.18	119.66	112.40
1	B	442	VAL	N-CA-CB	-5.18	100.10	111.50
1	A	216	TRP	CE3-CZ3-CH2	-5.18	115.50	121.20
1	A	442	VAL	N-CA-CB	-5.18	100.11	111.50
1	A	4	ALA	N-CA-CB	-5.17	102.86	110.10
1	A	435	GLU	C-N-CA	5.17	134.63	121.70
1	B	58	THR	O-C-N	-5.17	114.43	122.70
1	B	4	ALA	N-CA-CB	-5.17	102.86	110.10
1	B	110	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	B	435	GLU	C-N-CA	5.17	134.61	121.70
1	A	58	THR	O-C-N	-5.16	114.44	122.70
1	B	134	TYR	CG-CD2-CE2	-5.15	117.18	121.30
1	B	7	ARG	C-N-CA	5.15	134.58	121.70
1	C	58	THR	O-C-N	-5.15	114.46	122.70
1	A	243	GLN	CG-CD-NE2	5.14	129.05	116.70
1	C	4	ALA	N-CA-CB	-5.14	102.90	110.10
1	C	216	TRP	CE3-CZ3-CH2	-5.14	115.54	121.20
1	B	75	TYR	CG-CD1-CE1	-5.14	117.19	121.30
1	A	7	ARG	C-N-CA	5.14	134.55	121.70
1	B	139	PRO	CA-CB-CG	-5.14	94.24	104.00
1	C	126	ASP	CB-CG-OD2	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	243	GLN	CG-CD-NE2	5.14	129.03	116.70
1	C	139	PRO	CA-CB-CG	-5.13	94.25	104.00
1	B	243	GLN	CG-CD-NE2	5.13	129.02	116.70
1	C	134	TYR	CG-CD2-CE2	-5.13	117.20	121.30
1	B	126	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	294	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	A	139	PRO	CA-CB-CG	-5.12	94.28	104.00
1	A	18	ARG	CA-CB-CG	5.12	124.66	113.40
1	C	176	LEU	CB-CA-C	-5.12	100.48	110.20
1	C	18	ARG	CA-CB-CG	5.11	124.64	113.40
1	A	126	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	7	ARG	C-N-CA	5.11	134.47	121.70
1	C	294	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	A	176	LEU	CB-CA-C	-5.11	100.50	110.20
1	B	18	ARG	CA-CB-CG	5.10	124.62	113.40
1	A	75	TYR	CG-CD1-CE1	-5.10	117.22	121.30
1	C	252	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	134	TYR	CG-CD2-CE2	-5.09	117.22	121.30
1	B	176	LEU	CB-CA-C	-5.09	100.52	110.20
1	A	294	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	B	80	THR	O-C-N	5.09	131.85	123.20
1	C	75	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	A	7	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	32	THR	N-CA-C	5.07	124.70	111.00
1	B	32	THR	N-CA-C	5.07	124.69	111.00
1	C	32	THR	N-CA-C	5.06	124.67	111.00
1	C	66	THR	CB-CA-C	-5.06	97.94	111.60
1	C	96	THR	N-CA-C	5.06	124.65	111.00
1	B	66	THR	CB-CA-C	-5.06	97.95	111.60
1	C	7	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	66	THR	CB-CA-C	-5.05	97.95	111.60
1	C	382	TYR	CG-CD2-CE2	-5.05	117.26	121.30
1	A	80	THR	O-C-N	5.05	131.79	123.20
1	A	96	THR	N-CA-C	5.04	124.62	111.00
1	A	252	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	B	252	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	B	96	THR	N-CA-C	5.04	124.60	111.00
1	C	80	THR	O-C-N	5.03	131.76	123.20
1	A	249	VAL	N-CA-C	5.02	124.56	111.00
1	B	241	PRO	CA-N-CD	-5.02	104.47	111.50
1	C	249	VAL	N-CA-C	5.02	124.55	111.00
1	A	382	TYR	CG-CD2-CE2	-5.02	117.28	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	19	PHE	CA-CB-CG	5.02	125.94	113.90
1	B	249	VAL	N-CA-C	5.02	124.54	111.00
1	C	95	GLY	C-N-CA	5.01	134.24	121.70
1	A	19	PHE	CA-CB-CG	5.01	125.92	113.90
1	B	73	CYS	CA-C-O	-5.01	109.58	120.10
1	B	85	THR	CA-C-O	5.00	130.61	120.10
1	A	73	CYS	CA-C-O	-5.00	109.59	120.10
1	A	95	GLY	C-N-CA	5.00	134.21	121.70
1	B	19	PHE	CA-CB-CG	5.00	125.91	113.90
1	B	382	TYR	CG-CD2-CE2	-5.00	117.30	121.30

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	208	VAL	CA
1	A	404	ILE	CB
1	B	208	VAL	CA
1	B	404	ILE	CB
1	C	208	VAL	CA
1	C	404	ILE	CB

All (261) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	SER	Mainchain
1	A	108	HIS	Mainchain
1	A	123	MET	Mainchain
1	A	13	PHE	Mainchain
1	A	134	TYR	Sidechain
1	A	138	LYS	Mainchain,Peptide
1	A	15	LEU	Mainchain
1	A	157	ASP	Sidechain
1	A	17	ASP	Mainchain
1	A	194	LEU	Mainchain
1	A	195	VAL	Mainchain
1	A	2	THR	Mainchain
1	A	204	ARG	Sidechain
1	A	205	ILE	Mainchain
1	A	208	VAL	Mainchain
1	A	209	LYS	Mainchain
1	A	211	VAL	Mainchain
1	A	212	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	219	TYR	Sidechain
1	A	24	GLY	Mainchain
1	A	243	GLN	Sidechain
1	A	246	MET	Mainchain
1	A	249	VAL	Mainchain
1	A	250	LEU	Mainchain
1	A	252	TYR	Mainchain
1	A	255	TYR	Sidechain
1	A	256	TYR	Mainchain
1	A	258	LEU	Mainchain
1	A	259	LEU	Mainchain
1	A	26	THR	Mainchain
1	A	265	THR	Mainchain
1	A	272	LEU	Mainchain
1	A	273	TYR	Mainchain
1	A	278	THR	Mainchain
1	A	282	ASP	Mainchain
1	A	284	PRO	Mainchain
1	A	292	PHE	Mainchain
1	A	294	GLU	Sidechain
1	A	300	ARG	Sidechain,Mainchain
1	A	31	ASN	Mainchain
1	A	310	LEU	Mainchain
1	A	313	ASN	Sidechain
1	A	324	LEU	Mainchain
1	A	325	PRO	Mainchain
1	A	329	ALA	Mainchain
1	A	340	ASP	Mainchain,Peptide
1	A	346	ALA	Mainchain
1	A	347	THR	Mainchain
1	A	35	GLN	Mainchain
1	A	353	PRO	Mainchain
1	A	376	ASP	Mainchain
1	A	39	GLY	Mainchain
1	A	394	ALA	Mainchain
1	A	396	ARG	Sidechain,Mainchain
1	A	404	ILE	Mainchain
1	A	431	GLN	Sidechain
1	A	432	GLN	Sidechain
1	A	435	GLU	Sidechain,Mainchain
1	A	452	VAL	Mainchain
1	A	458	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	460	ARG	Sidechain
1	A	461	VAL	Mainchain
1	A	463	TYR	Sidechain
1	A	54	GLY	Mainchain
1	A	61	TRP	Mainchain
1	A	66	THR	Mainchain
1	A	68	GLN	Sidechain
1	A	7	ARG	Sidechain
1	A	73	CYS	Mainchain
1	A	74	ALA	Mainchain
1	A	75	TYR	Sidechain
1	A	76	GLY	Mainchain
1	A	79	TYR	Sidechain
1	A	81	GLY	Mainchain
1	A	86	ASP	Mainchain
1	A	87	ILE	Mainchain
1	A	91	ASN	Sidechain,Mainchain
1	A	93	ASN	Mainchain
1	A	94	TYR	Sidechain,Mainchain
1	A	99	ASP	Sidechain
1	B	105	SER	Mainchain
1	B	108	HIS	Mainchain
1	B	123	MET	Mainchain
1	B	13	PHE	Mainchain
1	B	134	TYR	Sidechain
1	B	138	LYS	Mainchain,Peptide
1	B	15	LEU	Mainchain
1	B	157	ASP	Sidechain
1	B	17	ASP	Mainchain
1	B	194	LEU	Mainchain
1	B	195	VAL	Mainchain
1	B	2	THR	Mainchain
1	B	204	ARG	Sidechain
1	B	205	ILE	Mainchain
1	B	208	VAL	Mainchain
1	B	209	LYS	Mainchain
1	B	211	VAL	Mainchain
1	B	212	GLN	Mainchain
1	B	219	TYR	Sidechain
1	B	24	GLY	Mainchain
1	B	243	GLN	Sidechain
1	B	246	MET	Mainchain

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Mol	Chain	Res	Type	Group
1	B	249	VAL	Mainchain
1	B	250	LEU	Mainchain
1	B	252	TYR	Mainchain
1	B	255	TYR	Sidechain
1	B	256	TYR	Mainchain
1	B	258	LEU	Mainchain
1	B	259	LEU	Mainchain
1	B	26	THR	Mainchain
1	B	265	THR	Mainchain
1	B	272	LEU	Mainchain
1	B	273	TYR	Mainchain
1	B	278	THR	Mainchain
1	B	282	ASP	Mainchain
1	B	284	PRO	Mainchain
1	B	292	PHE	Mainchain
1	B	294	GLU	Sidechain
1	B	300	ARG	Sidechain,Mainchain
1	B	31	ASN	Mainchain
1	B	310	LEU	Mainchain
1	B	313	ASN	Sidechain
1	B	324	LEU	Mainchain
1	B	325	PRO	Mainchain
1	B	329	ALA	Mainchain
1	B	340	ASP	Mainchain,Peptide
1	B	346	ALA	Mainchain
1	B	347	THR	Mainchain
1	B	35	GLN	Mainchain
1	B	353	PRO	Mainchain
1	B	376	ASP	Mainchain
1	B	39	GLY	Mainchain
1	B	394	ALA	Mainchain
1	B	396	ARG	Sidechain,Mainchain
1	B	404	ILE	Mainchain
1	B	431	GLN	Sidechain
1	B	432	GLN	Sidechain
1	B	435	GLU	Sidechain,Mainchain
1	B	452	VAL	Mainchain
1	B	458	LEU	Peptide
1	B	460	ARG	Sidechain
1	B	461	VAL	Mainchain
1	B	463	TYR	Sidechain
1	B	54	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	B	61	TRP	Mainchain
1	B	66	THR	Mainchain
1	B	68	GLN	Sidechain
1	B	7	ARG	Sidechain
1	B	73	CYS	Mainchain
1	B	74	ALA	Mainchain
1	B	75	TYR	Sidechain
1	B	76	GLY	Mainchain
1	B	79	TYR	Sidechain
1	B	81	GLY	Mainchain
1	B	86	ASP	Mainchain
1	B	87	ILE	Mainchain
1	B	91	ASN	Sidechain,Mainchain
1	B	93	ASN	Mainchain
1	B	94	TYR	Sidechain,Mainchain
1	B	99	ASP	Sidechain
1	C	105	SER	Mainchain
1	C	108	HIS	Mainchain
1	C	123	MET	Mainchain
1	C	13	PHE	Mainchain
1	C	134	TYR	Sidechain
1	C	138	LYS	Mainchain,Peptide
1	C	15	LEU	Mainchain
1	C	157	ASP	Sidechain
1	C	17	ASP	Mainchain
1	C	194	LEU	Mainchain
1	C	195	VAL	Mainchain
1	C	2	THR	Mainchain
1	C	204	ARG	Sidechain
1	C	205	ILE	Mainchain
1	C	208	VAL	Mainchain
1	C	209	LYS	Mainchain
1	C	211	VAL	Mainchain
1	C	212	GLN	Mainchain
1	C	219	TYR	Sidechain
1	C	24	GLY	Mainchain
1	C	243	GLN	Sidechain
1	C	246	MET	Mainchain
1	C	249	VAL	Mainchain
1	C	250	LEU	Mainchain
1	C	252	TYR	Mainchain
1	C	255	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	256	TYR	Mainchain
1	C	258	LEU	Mainchain
1	C	259	LEU	Mainchain
1	C	26	THR	Mainchain
1	C	265	THR	Mainchain
1	C	272	LEU	Mainchain
1	C	273	TYR	Mainchain
1	C	278	THR	Mainchain
1	C	282	ASP	Mainchain
1	C	284	PRO	Mainchain
1	C	292	PHE	Mainchain
1	C	294	GLU	Sidechain
1	C	300	ARG	Sidechain,Mainchain
1	C	31	ASN	Mainchain
1	C	310	LEU	Mainchain
1	C	313	ASN	Sidechain
1	C	324	LEU	Mainchain
1	C	325	PRO	Mainchain
1	C	329	ALA	Mainchain
1	C	340	ASP	Mainchain,Peptide
1	C	346	ALA	Mainchain
1	C	347	THR	Mainchain
1	C	35	GLN	Mainchain
1	C	353	PRO	Mainchain
1	C	376	ASP	Mainchain
1	C	39	GLY	Mainchain
1	C	394	ALA	Mainchain
1	C	396	ARG	Sidechain,Mainchain
1	C	404	ILE	Mainchain
1	C	431	GLN	Sidechain
1	C	432	GLN	Sidechain
1	C	435	GLU	Sidechain,Mainchain
1	C	452	VAL	Mainchain
1	C	458	LEU	Peptide
1	C	460	ARG	Sidechain
1	C	461	VAL	Mainchain
1	C	463	TYR	Sidechain
1	C	54	GLY	Mainchain
1	C	61	TRP	Mainchain
1	C	66	THR	Mainchain
1	C	68	GLN	Sidechain
1	C	7	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	73	CYS	Mainchain
1	C	74	ALA	Mainchain
1	C	75	TYR	Sidechain
1	C	76	GLY	Mainchain
1	C	79	TYR	Sidechain
1	C	81	GLY	Mainchain
1	C	86	ASP	Mainchain
1	C	87	ILE	Mainchain
1	C	91	ASN	Sidechain,Mainchain
1	C	93	ASN	Mainchain
1	C	94	TYR	Sidechain,Mainchain
1	C	99	ASP	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3690	0	3448	1687	135
1	B	3690	0	3414	2177	0
1	C	3690	0	3447	1369	135
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	11073	0	10309	3895	135

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 182.

All (3895) 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:A:87:ILE:CD1	1:B:374:SER:HB3	1.16	1.63
1:B:445:GLY:CA	1:C:185:ASN:HD22	0.99	1.62
1:A:205:ILE:CG2	1:B:472:LYS:HG3	1.17	1.60
1:A:205:ILE:HG21	1:B:472:LYS:CG	1.31	1.59
1:B:278:THR:HA	1:C:380:VAL:CG2	1.28	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TRP:CZ2	1:B:375:LYS:HD2	1.17	1.59
1:A:219:TYR:HE2	1:B:371:TYR:CB	1.08	1.58
1:A:219:TYR:CE1	1:B:473:ILE:HD12	1.36	1.58
1:A:148:PRO:CA	1:B:107:LEU:HA	1.33	1.57
1:A:221:LYS:HA	1:B:434:THR:CG2	1.25	1.56
1:A:165:TRP:HE1	1:B:110:ARG:CA	0.92	1.56
1:A:190:TRP:CH2	1:B:375:LYS:HD2	1.38	1.56
1:A:222:ALA:CB	1:B:368:ILE:CG1	1.82	1.55
1:A:148:PRO:HA	1:B:107:LEU:CA	1.35	1.55
1:A:186:GLU:HG3	1:B:370:ASN:CB	1.21	1.53
1:A:180:LYS:HD3	1:B:57:PHE:CB	1.39	1.52
1:A:227:CYS:CB	1:B:476:ASP:HB2	1.30	1.52
1:A:222:ALA:CB	1:B:368:ILE:HG13	1.03	1.51
1:A:143:GLN:HG2	1:B:108:HIS:CD2	1.00	1.50
1:A:180:LYS:CA	1:B:55:MET:HB3	1.40	1.49
1:B:422:LEU:HD11	1:C:221:LYS:CG	1.39	1.49
1:B:430:GLY:H	1:C:185:ASN:CG	1.05	1.48
1:A:225:VAL:H	1:B:465:THR:CG2	1.20	1.48
1:B:238:TYR:CA	1:C:376:ASP:C	1.81	1.47
1:B:274:ASN:HA	1:C:286:SER:CB	1.44	1.47
1:A:145:TYR:CG	1:B:9:GLN:OE1	1.65	1.47
1:A:143:GLN:CG	1:B:108:HIS:CD2	1.95	1.46
1:A:87:ILE:HD11	1:B:374:SER:CB	1.03	1.46
1:A:194:LEU:CD2	1:B:375:LYS:HG2	1.44	1.46
1:B:238:TYR:HA	1:C:376:ASP:C	1.16	1.46
1:A:165:TRP:CZ2	1:B:109:GLU:O	1.66	1.45
1:A:221:LYS:CA	1:B:434:THR:HG21	1.43	1.45
1:A:180:LYS:N	1:B:55:MET:CB	1.80	1.45
1:A:190:TRP:CH2	1:B:375:LYS:CD	1.95	1.45
1:B:281:SER:CB	1:C:8:SER:H	1.25	1.45
1:A:463:TYR:CZ	1:A:463:TYR:OH	1.71	1.43
1:A:227:CYS:HB3	1:B:476:ASP:CB	1.48	1.43
1:A:222:ALA:HA	1:B:368:ILE:CD1	1.45	1.43
1:A:87:ILE:CG1	1:B:374:SER:O	1.65	1.43
1:A:180:LYS:HA	1:B:55:MET:CB	1.45	1.42
1:C:463:TYR:OH	1:C:463:TYR:CZ	1.71	1.42
1:B:385:PRO:CA	1:C:3:PRO:HD3	1.46	1.42
1:A:221:LYS:CB	1:B:436:VAL:HA	1.29	1.42
1:A:227:CYS:CB	1:B:476:ASP:CB	1.98	1.42
1:A:180:LYS:N	1:B:55:MET:HB2	1.12	1.42
1:A:180:LYS:HE3	1:B:11:ILE:C	1.40	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLY:CA	1:B:478:SER:CB	1.96	1.41
1:A:194:LEU:HD22	1:B:375:LYS:CG	1.51	1.41
1:B:386:TYR:CE2	1:C:288:LEU:HD13	1.56	1.41
1:B:404:ILE:N	1:B:404:ILE:CA	1.85	1.40
1:B:445:GLY:N	1:C:185:ASN:ND2	1.67	1.40
1:B:400:ASP:CB	1:C:193:SER:O	1.68	1.40
1:A:221:LYS:HB3	1:B:436:VAL:CA	1.11	1.40
1:B:400:ASP:C	1:C:193:SER:HA	1.37	1.39
1:B:383:LYS:HG3	1:C:6:TRP:CD1	1.57	1.39
1:A:185:ASN:CB	1:B:366:ASN:HA	1.26	1.39
1:A:219:TYR:CE2	1:B:371:TYR:CB	1.99	1.38
1:A:193:SER:CA	1:B:403:GLN:HA	1.47	1.38
1:B:445:GLY:CA	1:C:185:ASN:ND2	1.82	1.38
1:B:237:ALA:CB	1:C:379:PHE:N	1.84	1.38
1:A:246:MET:CB	1:B:477:SER:N	1.72	1.37
1:A:87:ILE:CG1	1:B:374:SER:C	1.92	1.37
1:B:238:TYR:HA	1:C:376:ASP:CA	1.54	1.37
1:C:404:ILE:N	1:C:404:ILE:CA	1.85	1.37
1:A:404:ILE:CA	1:A:404:ILE:N	1.84	1.37
1:B:235:ASP:OD2	1:C:399:THR:CG2	1.70	1.36
1:B:387:ILE:HG21	1:C:221:LYS:CE	1.51	1.36
1:A:225:VAL:H	1:B:465:THR:CB	1.34	1.36
1:B:387:ILE:CG2	1:C:221:LYS:HE3	1.52	1.36
1:A:87:ILE:CD1	1:B:374:SER:CB	1.76	1.36
1:B:463:TYR:CZ	1:B:463:TYR:OH	1.71	1.36
1:B:278:THR:HG21	1:C:381:THR:OG1	1.23	1.35
1:A:219:TYR:CD1	1:B:473:ILE:HD12	1.62	1.35
1:B:429:ALA:CB	1:C:182:VAL:O	1.72	1.35
1:B:422:LEU:CD1	1:C:221:LYS:HG2	1.57	1.35
1:A:87:ILE:HG12	1:B:374:SER:C	1.42	1.34
1:B:235:ASP:OD1	1:C:399:THR:CG2	1.75	1.34
1:A:145:TYR:CD1	1:B:9:GLN:OE1	1.80	1.34
1:B:241:PRO:O	1:C:374:SER:CA	1.65	1.34
1:B:383:LYS:NZ	1:C:5:ASP:HB2	1.43	1.33
1:A:222:ALA:CA	1:B:368:ILE:CD1	2.05	1.33
1:A:189:ASP:H	1:B:369:ARG:CA	1.32	1.33
1:A:248:GLY:O	1:B:477:SER:HB3	1.26	1.33
1:B:430:GLY:H	1:C:185:ASN:ND2	1.23	1.33
1:A:229:GLY:CA	1:B:478:SER:HB2	1.53	1.33
1:A:180:LYS:CD	1:B:57:PHE:HB2	1.55	1.32
1:A:190:TRP:CZ3	1:B:371:TYR:CD1	2.14	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TYR:CE2	1:B:373:ILE:C	2.03	1.32
1:B:237:ALA:HB2	1:C:379:PHE:N	0.99	1.31
1:B:235:ASP:CG	1:C:399:THR:HG21	1.47	1.31
1:B:430:GLY:N	1:C:185:ASN:CG	1.84	1.31
1:A:180:LYS:CA	1:B:55:MET:CB	2.00	1.31
1:B:401:GLY:N	1:C:196:SER:HB2	1.46	1.31
1:A:184:LYS:CG	1:B:56:GLY:HA3	1.59	1.31
1:A:205:ILE:HG12	1:B:471:SER:C	1.49	1.30
1:A:249:VAL:HG12	1:B:477:SER:CB	1.60	1.30
1:B:235:ASP:CG	1:C:399:THR:CG2	1.99	1.30
1:B:384:ASN:HA	1:C:2:THR:CG2	1.60	1.30
1:A:219:TYR:CE2	1:B:371:TYR:HB2	1.64	1.30
1:B:238:TYR:HB2	1:C:376:ASP:OD2	1.25	1.30
1:A:190:TRP:HZ3	1:B:371:TYR:CD1	1.46	1.30
1:A:224:GLY:HA2	1:B:434:THR:OG1	1.27	1.29
1:A:88:TYR:CE2	1:B:373:ILE:O	1.83	1.29
1:B:402:SER:H	1:C:193:SER:CB	1.44	1.29
1:B:279:VAL:CG1	1:C:4:ALA:HB1	1.62	1.29
1:B:278:THR:CA	1:C:380:VAL:CG2	2.10	1.28
1:B:385:PRO:CD	1:C:2:THR:HG22	1.61	1.28
1:A:221:LYS:CG	1:B:436:VAL:N	1.96	1.28
1:B:274:ASN:HA	1:C:286:SER:CA	1.63	1.28
1:B:278:THR:HG23	1:C:381:THR:N	1.46	1.28
1:B:449:ASN:HB2	1:C:184:LYS:NZ	1.46	1.27
1:B:278:THR:CA	1:C:380:VAL:HG21	1.61	1.27
1:A:84:GLN:HE22	1:B:375:LYS:NZ	1.32	1.26
1:B:385:PRO:N	1:C:3:PRO:CD	1.89	1.26
1:A:186:GLU:OE1	1:B:373:ILE:HD12	1.15	1.26
1:A:190:TRP:CZ3	1:B:371:TYR:CE1	2.24	1.25
1:A:217:PRO:HG2	1:B:364:SER:OG	1.31	1.25
1:A:188:TYR:N	1:B:367:ALA:O	1.65	1.25
1:A:190:TRP:CZ2	1:B:375:LYS:CD	2.11	1.25
1:A:180:LYS:CD	1:B:57:PHE:CB	2.12	1.25
1:A:190:TRP:CD2	1:B:374:SER:HB2	1.72	1.25
1:B:278:THR:C	1:C:380:VAL:HG21	1.52	1.25
1:B:278:THR:O	1:C:380:VAL:HG21	1.32	1.25
1:A:87:ILE:HG12	1:B:374:SER:CA	1.66	1.25
1:A:180:LYS:HA	1:B:55:MET:CG	1.65	1.24
1:A:165:TRP:HZ2	1:B:109:GLU:C	1.38	1.24
1:A:225:VAL:N	1:B:465:THR:CG2	2.01	1.24
1:A:184:LYS:HG2	1:B:56:GLY:CA	1.67	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASN:CA	1:B:473:ILE:HG23	1.60	1.23
1:A:116:VAL:O	1:B:469:ALA:HB1	1.37	1.23
1:A:227:CYS:CA	1:B:476:ASP:HB2	1.67	1.23
1:B:447:ASP:OD2	1:C:214:ASP:OD2	1.53	1.23
1:B:382:TYR:CD1	1:C:2:THR:HG23	1.72	1.23
1:A:219:TYR:CE2	1:B:371:TYR:CG	1.83	1.23
1:A:165:TRP:NE1	1:B:110:ARG:HA	0.91	1.22
1:A:143:GLN:CD	1:B:108:HIS:HA	1.60	1.22
1:A:229:GLY:HA2	1:B:478:SER:CB	1.59	1.22
1:A:87:ILE:HG12	1:B:374:SER:O	1.25	1.22
1:B:385:PRO:HA	1:C:3:PRO:CD	1.68	1.22
1:B:400:ASP:HB2	1:C:193:SER:O	1.09	1.22
1:B:277:ASN:CB	1:C:286:SER:O	1.85	1.22
1:B:281:SER:HB3	1:C:8:SER:N	1.26	1.22
1:B:274:ASN:CA	1:C:286:SER:CB	2.17	1.22
1:A:192:GLY:O	1:B:464:PRO:HG2	1.39	1.22
1:A:180:LYS:NZ	1:B:57:PHE:HB3	1.55	1.21
1:B:449:ASN:N	1:C:184:LYS:HZ1	1.36	1.21
1:B:404:ILE:CG1	1:C:223:ALA:HA	1.68	1.21
1:A:222:ALA:CA	1:B:368:ILE:HD11	1.67	1.20
1:B:385:PRO:CA	1:C:3:PRO:CD	2.19	1.20
1:B:386:TYR:CE2	1:C:247:ASP:HB3	1.44	1.20
1:B:384:ASN:CA	1:C:2:THR:CG2	2.02	1.19
1:B:382:TYR:HA	1:C:1:ALA:HB3	1.21	1.19
1:A:184:LYS:HE2	1:B:362:ILE:HG22	1.25	1.19
1:A:185:ASN:HB2	1:B:366:ASN:CA	1.72	1.19
1:A:229:GLY:CA	1:B:477:SER:O	1.91	1.18
1:B:237:ALA:HB2	1:C:378:GLY:C	1.61	1.18
1:B:422:LEU:CD2	1:C:221:LYS:NZ	2.05	1.18
1:B:237:ALA:HB2	1:C:379:PHE:CA	1.73	1.18
1:B:424:GLY:CA	1:C:220:ASN:HB3	1.73	1.18
1:A:225:VAL:N	1:B:465:THR:HG23	1.56	1.18
1:B:277:ASN:HB3	1:C:286:SER:O	1.05	1.17
1:B:449:ASN:N	1:C:184:LYS:NZ	1.91	1.17
1:B:383:LYS:NZ	1:C:5:ASP:CB	2.07	1.17
1:A:200:ILE:HD12	1:B:467:LYS:CD	1.74	1.17
1:B:383:LYS:CG	1:C:6:TRP:CD1	2.27	1.17
1:A:186:GLU:CG	1:B:370:ASN:CB	2.10	1.17
1:A:197:ASN:O	1:B:467:LYS:NZ	1.77	1.17
1:A:186:GLU:OE1	1:B:370:ASN:HA	1.42	1.17
1:A:180:LYS:CD	1:B:12:TYR:HB2	1.75	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:SER:CB	1:C:8:SER:N	1.83	1.17
1:A:143:GLN:HG2	1:B:108:HIS:NE2	1.58	1.16
1:A:145:TYR:CD2	1:B:9:GLN:OE1	1.98	1.16
1:B:278:THR:CG2	1:C:381:THR:H	1.58	1.16
1:B:386:TYR:CD2	1:C:288:LEU:HD13	1.81	1.16
1:B:400:ASP:C	1:C:196:SER:HB2	1.51	1.16
1:A:221:LYS:CA	1:B:434:THR:CG2	2.08	1.16
1:B:238:TYR:CD2	1:C:376:ASP:HB2	1.80	1.16
1:A:218:GLY:HA3	1:B:364:SER:O	1.43	1.16
1:A:101:LYS:HG2	1:A:198:TYR:HA	1.27	1.16
1:A:165:TRP:CZ2	1:B:109:GLU:C	2.14	1.16
1:B:9:GLN:HG3	1:B:58:THR:HB	1.28	1.16
1:A:407:ILE:HG23	1:A:461:VAL:HG22	1.19	1.15
1:A:196:SER:OG	1:B:400:ASP:O	1.63	1.15
1:A:229:GLY:HA3	1:B:478:SER:N	1.61	1.15
1:C:230:GLU:HA	1:C:250:LEU:HD23	1.25	1.15
1:B:399:THR:CG2	1:C:196:SER:O	1.95	1.15
1:A:189:ASP:HB2	1:B:369:ARG:HA	1.17	1.14
1:A:223:ALA:N	1:B:468:LEU:HD21	1.37	1.14
1:A:180:LYS:CE	1:B:11:ILE:C	2.15	1.14
1:B:383:LYS:HZ3	1:C:5:ASP:CB	1.58	1.14
1:A:222:ALA:HB2	1:B:368:ILE:CG1	1.57	1.14
1:B:400:ASP:C	1:C:193:SER:CA	2.15	1.14
1:A:116:VAL:O	1:B:469:ALA:CB	1.94	1.14
1:A:229:GLY:HA3	1:B:477:SER:C	1.65	1.14
1:A:225:VAL:H	1:B:465:THR:HG23	1.06	1.14
1:B:401:GLY:N	1:C:193:SER:O	1.79	1.14
1:A:204:ARG:CB	1:B:470:GLY:HA3	1.65	1.14
1:A:230:GLU:HA	1:A:250:LEU:HD23	1.25	1.14
1:B:107:LEU:HA	1:B:110:ARG:HG2	1.26	1.14
1:A:227:CYS:O	1:B:476:ASP:HA	1.44	1.14
1:A:193:SER:CA	1:B:403:GLN:CA	2.19	1.14
1:A:222:ALA:HB1	1:B:368:ILE:CG1	1.56	1.14
1:B:236:PRO:CG	1:C:378:GLY:CA	2.25	1.13
1:A:218:GLY:HA3	1:B:364:SER:C	1.69	1.13
1:B:399:THR:HG21	1:C:196:SER:O	1.47	1.13
1:C:407:ILE:HG23	1:C:461:VAL:HG22	1.18	1.13
1:A:220:ASN:HA	1:B:473:ILE:HG23	1.17	1.13
1:A:229:GLY:HA3	1:B:478:SER:CA	1.79	1.13
1:A:205:ILE:HD13	1:B:472:LYS:CG	1.78	1.13
1:A:219:TYR:CD1	1:B:473:ILE:CD1	2.32	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:SER:HB3	1:C:57:PHE:HA	1.18	1.13
1:A:188:TYR:CD2	1:B:366:ASN:C	2.15	1.13
1:A:146:PHE:N	1:B:112:MET:H	1.24	1.13
1:A:180:LYS:HE3	1:B:11:ILE:O	1.45	1.13
1:A:219:TYR:CD1	1:B:473:ILE:HB	1.50	1.13
1:A:185:ASN:HA	1:A:188:TYR:HD2	1.08	1.13
1:B:400:ASP:CA	1:C:193:SER:O	1.96	1.13
1:A:219:TYR:N	1:B:473:ILE:O	1.71	1.12
1:A:184:LYS:HD2	1:B:363:ALA:CA	1.76	1.12
1:A:225:VAL:CA	1:B:465:THR:HG23	1.78	1.12
1:B:385:PRO:HD3	1:C:2:THR:HG22	1.12	1.12
1:A:219:TYR:CE1	1:B:473:ILE:CD1	2.32	1.12
1:B:386:TYR:CD2	1:C:288:LEU:CD1	2.31	1.12
1:A:9:GLN:HG3	1:A:58:THR:HB	1.28	1.12
1:B:319:ILE:HA	1:B:325:PRO:CB	1.79	1.12
1:B:424:GLY:HA3	1:C:220:ASN:CB	1.79	1.11
1:A:87:ILE:HG13	1:B:374:SER:O	1.43	1.11
1:B:420:LEU:HD23	1:B:452:VAL:HG13	1.21	1.11
1:A:205:ILE:CD1	1:B:478:SER:HB3	1.79	1.11
1:A:189:ASP:N	1:B:369:ARG:HA	1.65	1.11
1:B:387:ILE:N	1:C:247:ASP:OD2	1.83	1.11
1:C:165:TRP:HZ3	1:C:172:SER:HB2	1.14	1.11
1:A:184:LYS:HD2	1:B:363:ALA:HA	1.25	1.11
1:A:144:ASP:O	1:B:58:THR:O	1.66	1.11
1:A:196:SER:CB	1:B:401:GLY:O	1.77	1.11
1:C:9:GLN:HG3	1:C:58:THR:HB	1.28	1.11
1:B:230:GLU:HA	1:B:250:LEU:HD23	1.25	1.11
1:A:186:GLU:OE1	1:B:373:ILE:CD1	1.98	1.11
1:A:145:TYR:CD2	1:B:9:GLN:CD	2.11	1.11
1:A:319:ILE:HA	1:A:325:PRO:CB	1.79	1.11
1:B:274:ASN:C	1:C:286:SER:OG	1.89	1.11
1:A:165:TRP:HZ2	1:B:109:GLU:O	0.76	1.11
1:A:10:SER:HB3	1:A:57:PHE:HA	1.18	1.11
1:B:384:ASN:HA	1:C:2:THR:HG21	1.13	1.11
1:A:217:PRO:HB2	1:B:437:ILE:O	1.50	1.11
1:A:205:ILE:HD12	1:B:478:SER:CB	1.81	1.10
1:C:185:ASN:HA	1:C:188:TYR:HD2	1.08	1.10
1:C:319:ILE:HA	1:C:325:PRO:CB	1.79	1.10
1:A:147:HIS:HA	1:B:112:MET:HE3	1.26	1.10
1:B:45:ILE:HG23	1:B:49:LEU:HD11	1.11	1.10
1:A:191:VAL:HG21	1:B:473:ILE:CD1	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HG13	1:B:476:ASP:OD1	1.49	1.10
1:A:249:VAL:HG12	1:B:477:SER:HB2	1.23	1.10
1:A:205:ILE:HB	1:B:478:SER:OG	1.50	1.10
1:B:429:ALA:HB1	1:C:182:VAL:O	1.50	1.10
1:C:195:VAL:HG23	1:C:200:ILE:HB	1.27	1.10
1:B:445:GLY:HA2	1:C:185:ASN:CB	1.80	1.10
1:A:107:LEU:HA	1:A:110:ARG:HG2	1.26	1.10
1:A:180:LYS:HG2	1:B:327:ILE:CG2	1.81	1.10
1:B:444:VAL:C	1:C:185:ASN:ND2	2.04	1.10
1:C:420:LEU:HD23	1:C:452:VAL:HG13	1.21	1.10
1:C:45:ILE:HG23	1:C:49:LEU:HD11	1.11	1.10
1:A:221:LYS:HG3	1:B:436:VAL:N	1.67	1.10
1:A:191:VAL:CG2	1:B:473:ILE:HD11	1.81	1.09
1:A:45:ILE:HG23	1:A:49:LEU:HD11	1.11	1.09
1:B:422:LEU:CD2	1:C:221:LYS:HZ3	1.62	1.09
1:A:87:ILE:CD1	1:B:374:SER:CA	2.29	1.09
1:B:101:LYS:HG2	1:B:198:TYR:HA	1.27	1.09
1:B:383:LYS:CE	1:C:5:ASP:HB2	1.82	1.09
1:B:422:LEU:HD21	1:C:221:LYS:HZ3	1.02	1.09
1:C:101:LYS:HG2	1:C:198:TYR:HA	1.27	1.09
1:A:196:SER:HB3	1:B:401:GLY:O	1.27	1.09
1:B:195:VAL:HG23	1:B:200:ILE:HB	1.27	1.09
1:C:107:LEU:HA	1:C:110:ARG:HG2	1.26	1.09
1:C:123:MET:HG3	1:C:146:PHE:HE1	1.16	1.09
1:A:227:CYS:C	1:B:476:ASP:CB	2.20	1.09
1:A:229:GLY:HA2	1:B:478:SER:HB3	1.34	1.09
1:B:123:MET:HB3	1:B:137:PHE:CE1	1.87	1.09
1:A:180:LYS:HE3	1:B:12:TYR:N	1.68	1.09
1:A:87:ILE:CG1	1:B:374:SER:CA	2.27	1.09
1:A:189:ASP:N	1:B:369:ARG:CA	2.13	1.09
1:A:227:CYS:C	1:B:476:ASP:HB2	1.72	1.08
1:A:205:ILE:CG1	1:B:478:SER:HB3	1.83	1.08
1:A:145:TYR:CE1	1:B:113:TYR:CE2	2.42	1.08
1:B:123:MET:HB3	1:B:137:PHE:HE1	1.15	1.08
1:B:236:PRO:HG2	1:C:378:GLY:CA	1.83	1.08
1:B:407:ILE:HG23	1:B:461:VAL:HG22	1.19	1.08
1:B:444:VAL:O	1:C:185:ASN:CB	2.01	1.08
1:A:219:TYR:CD1	1:B:473:ILE:CB	2.27	1.08
1:B:319:ILE:HA	1:B:325:PRO:HB3	1.32	1.08
1:A:123:MET:HB3	1:A:137:PHE:CE1	1.87	1.08
1:B:123:MET:HG3	1:B:146:PHE:HE1	1.17	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:GLY:N	1:C:185:ASN:ND2	1.97	1.08
1:C:319:ILE:HG22	1:C:325:PRO:HB2	1.35	1.08
1:B:185:ASN:HA	1:B:188:TYR:HD2	1.08	1.08
1:A:123:MET:HG3	1:A:146:PHE:HE1	1.17	1.08
1:B:444:VAL:O	1:C:185:ASN:CG	1.91	1.08
1:A:319:ILE:HA	1:A:325:PRO:HB3	1.32	1.08
1:C:123:MET:HB3	1:C:137:PHE:HE1	1.15	1.08
1:A:186:GLU:CD	1:B:370:ASN:HA	1.74	1.07
1:A:2:THR:HB	1:A:3:PRO:HD2	1.34	1.07
1:A:116:VAL:O	1:B:470:GLY:N	1.87	1.07
1:A:143:GLN:HG2	1:B:108:HIS:CG	1.88	1.07
1:B:383:LYS:O	1:C:3:PRO:CD	2.01	1.07
1:A:193:SER:C	1:B:403:GLN:HA	1.53	1.07
1:C:123:MET:HB3	1:C:137:PHE:CE1	1.87	1.07
1:B:446:SER:CB	1:C:181:ASP:OD1	1.99	1.07
1:B:429:ALA:HB3	1:C:182:VAL:O	1.53	1.07
1:B:279:VAL:HG13	1:C:4:ALA:CB	1.84	1.07
1:A:205:ILE:CG1	1:B:476:ASP:OD1	2.02	1.07
1:B:2:THR:HB	1:B:3:PRO:HD2	1.34	1.07
1:B:383:LYS:CB	1:C:6:TRP:CD1	2.38	1.07
1:A:319:ILE:HG22	1:A:325:PRO:HB2	1.35	1.07
1:A:180:LYS:CE	1:B:11:ILE:O	2.03	1.07
1:B:445:GLY:HA2	1:C:185:ASN:HD22	0.97	1.07
1:B:236:PRO:CG	1:C:378:GLY:HA2	1.46	1.07
1:B:274:ASN:CA	1:C:286:SER:CA	2.33	1.06
1:A:420:LEU:HD23	1:A:452:VAL:HG13	1.21	1.06
1:B:319:ILE:HG22	1:B:325:PRO:HB2	1.35	1.06
1:A:193:SER:HA	1:B:403:GLN:HA	1.16	1.06
1:B:235:ASP:OD1	1:C:399:THR:HG21	1.37	1.06
1:C:45:ILE:HB	1:C:103:LEU:HD21	1.11	1.06
1:A:190:TRP:CE2	1:B:374:SER:CB	2.35	1.06
1:C:319:ILE:HA	1:C:325:PRO:HB3	1.32	1.06
1:B:387:ILE:HG23	1:C:221:LYS:HE3	1.31	1.06
1:B:422:LEU:HD21	1:C:221:LYS:NZ	1.65	1.06
1:B:45:ILE:HB	1:B:103:LEU:HD21	1.11	1.06
1:B:238:TYR:O	1:C:376:ASP:HA	1.55	1.06
1:A:84:GLN:NE2	1:B:375:LYS:NZ	2.04	1.06
1:A:220:ASN:HA	1:B:473:ILE:CG2	1.84	1.06
1:A:165:TRP:HZ3	1:A:172:SER:HB2	1.14	1.06
1:B:401:GLY:N	1:C:193:SER:CA	2.19	1.06
1:A:219:TYR:CG	1:B:473:ILE:HG13	1.89	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASN:CA	1:C:2:THR:HG21	1.75	1.05
1:A:190:TRP:CH2	1:B:375:LYS:HD3	1.80	1.05
1:A:187:TRP:CE3	1:B:371:TYR:HA	1.91	1.05
1:B:445:GLY:HA2	1:C:185:ASN:ND2	1.54	1.05
1:B:165:TRP:HZ3	1:B:172:SER:HB2	1.14	1.05
1:A:229:GLY:C	1:B:477:SER:O	1.95	1.05
1:B:278:THR:CG2	1:C:381:THR:OG1	2.04	1.05
1:B:278:THR:HA	1:C:380:VAL:HG21	1.21	1.05
1:A:190:TRP:HZ3	1:B:371:TYR:CE1	1.65	1.05
1:A:45:ILE:HB	1:A:103:LEU:HD21	1.11	1.05
1:B:274:ASN:CA	1:C:286:SER:OG	2.01	1.05
1:A:147:HIS:O	1:B:107:LEU:O	1.73	1.05
1:B:278:THR:HG23	1:C:381:THR:H	0.89	1.05
1:A:190:TRP:CE2	1:B:374:SER:HB2	1.91	1.05
1:A:219:TYR:CG	1:B:473:ILE:CG1	2.37	1.05
1:A:224:GLY:HA2	1:B:434:THR:CB	1.87	1.05
1:B:383:LYS:O	1:C:3:PRO:HD2	1.56	1.04
1:A:197:ASN:N	1:B:467:LYS:HE3	1.72	1.04
1:A:204:ARG:HB2	1:B:470:GLY:HA3	1.08	1.04
1:B:404:ILE:CD1	1:C:223:ALA:HA	1.78	1.04
1:A:116:VAL:C	1:B:469:ALA:HB1	1.57	1.04
1:A:205:ILE:HD13	1:B:472:LYS:HG2	1.32	1.04
1:B:445:GLY:N	1:C:185:ASN:HD22	1.39	1.04
1:A:115:MET:HE1	1:A:204:ARG:HB2	1.33	1.04
1:A:83:TRP:HE1	1:A:173:LEU:HD21	1.19	1.04
1:A:187:TRP:HE3	1:B:371:TYR:HA	1.16	1.04
1:B:446:SER:OG	1:C:181:ASP:CG	1.95	1.04
1:B:401:GLY:N	1:C:193:SER:HA	1.73	1.04
1:A:222:ALA:CB	1:B:368:ILE:CD1	2.32	1.04
1:B:235:ASP:OD1	1:C:399:THR:HG23	1.57	1.04
1:A:229:GLY:HA3	1:B:478:SER:CB	1.75	1.04
1:A:180:LYS:HG3	1:B:12:TYR:CD2	1.93	1.04
1:B:402:SER:H	1:C:193:SER:CA	1.71	1.04
1:C:432:GLN:HG2	1:C:465:THR:HG21	1.40	1.04
1:B:402:SER:N	1:C:193:SER:CB	2.20	1.03
1:A:221:LYS:CB	1:B:436:VAL:CA	1.79	1.03
1:A:225:VAL:CG2	1:B:465:THR:HG23	1.86	1.03
1:C:2:THR:HB	1:C:3:PRO:HD2	1.34	1.03
1:A:180:LYS:HD2	1:B:12:TYR:HB2	1.06	1.03
1:A:205:ILE:HD12	1:B:478:SER:OXT	1.57	1.03
1:A:118:VAL:HB	1:B:471:SER:HB2	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:TYR:CA	1:C:1:ALA:HB3	1.82	1.03
1:A:180:LYS:CE	1:B:57:PHE:CB	2.36	1.03
1:B:387:ILE:CG2	1:C:221:LYS:CE	2.21	1.03
1:A:204:ARG:HG3	1:A:228:ILE:HB	1.37	1.03
1:A:146:PHE:N	1:B:112:MET:N	2.07	1.03
1:A:180:LYS:HA	1:B:55:MET:HG3	1.38	1.03
1:C:234:GLY:HA2	1:C:253:PRO:HD3	1.41	1.02
1:A:432:GLN:HG2	1:A:465:THR:HG21	1.40	1.02
1:A:180:LYS:HZ3	1:B:57:PHE:HB3	1.04	1.02
1:A:208:VAL:HG21	1:B:478:SER:N	1.44	1.02
1:A:177:ASP:HB3	1:B:53:GLN:CB	1.90	1.02
1:A:123:MET:HB3	1:A:137:PHE:HE1	1.15	1.02
1:A:204:ARG:O	1:B:471:SER:CA	1.98	1.02
1:A:180:LYS:NZ	1:B:10:SER:O	1.92	1.02
1:B:234:GLY:HA2	1:B:253:PRO:HD3	1.41	1.02
1:A:180:LYS:NZ	1:B:57:PHE:CB	2.22	1.02
1:C:204:ARG:HG3	1:C:228:ILE:HB	1.37	1.02
1:A:246:MET:HB2	1:B:477:SER:N	1.39	1.02
1:A:234:GLY:HA2	1:A:253:PRO:HD3	1.42	1.02
1:B:204:ARG:HG3	1:B:228:ILE:HB	1.37	1.02
1:B:432:GLN:HG2	1:B:465:THR:HG21	1.40	1.02
1:A:249:VAL:CB	1:B:477:SER:OG	2.07	1.02
1:A:87:ILE:HD13	1:B:374:SER:CB	1.89	1.02
1:B:387:ILE:HG21	1:C:221:LYS:HE2	1.36	1.02
1:A:42:TRP:HE1	1:A:62:ILE:HD11	1.24	1.02
1:B:83:TRP:HE1	1:B:173:LEU:HD21	1.19	1.02
1:B:208:VAL:HG12	1:B:231:VAL:HG12	1.42	1.02
1:A:225:VAL:CB	1:B:465:THR:HG23	1.89	1.02
1:C:208:VAL:HG12	1:C:231:VAL:HG12	1.42	1.02
1:A:143:GLN:NE2	1:B:108:HIS:CG	2.27	1.01
1:B:32:THR:HG21	1:B:342:ALA:HA	1.42	1.01
1:C:83:TRP:HE1	1:C:173:LEU:HD21	1.19	1.01
1:A:190:TRP:CE3	1:B:374:SER:HB2	1.94	1.01
1:B:383:LYS:HZ3	1:C:5:ASP:HB2	0.88	1.01
1:B:401:GLY:N	1:C:196:SER:CB	2.22	1.01
1:A:219:TYR:HE1	1:B:471:SER:OG	1.42	1.01
1:C:305:THR:HG21	1:C:310:LEU:HD22	1.01	1.01
1:A:188:TYR:CE2	1:B:367:ALA:N	2.27	1.01
1:B:305:THR:HG21	1:B:310:LEU:HD22	1.01	1.01
1:B:449:ASN:CB	1:C:184:LYS:NZ	2.22	1.01
1:C:42:TRP:HE1	1:C:62:ILE:HD11	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:CA	1:B:370:ASN:ND2	1.78	1.01
1:B:280:LYS:NZ	1:C:226:TYR:HB2	1.74	1.01
1:B:277:ASN:ND2	1:C:286:SER:HB3	1.76	1.01
1:A:248:GLY:C	1:B:477:SER:HB3	1.79	1.01
1:A:230:GLU:N	1:B:478:SER:HB2	1.75	1.01
1:B:42:TRP:HE1	1:B:62:ILE:HD11	1.24	1.01
1:A:189:ASP:H	1:B:369:ARG:HA	0.94	1.00
1:B:402:SER:N	1:C:193:SER:OG	1.93	1.00
1:A:165:TRP:CE2	1:B:110:ARG:HA	1.96	1.00
1:A:194:LEU:CA	1:B:403:GLN:HG2	1.91	1.00
1:C:11:ILE:HG12	1:C:324:LEU:HD23	1.42	1.00
1:A:143:GLN:HG2	1:B:108:HIS:HD2	1.23	1.00
1:A:219:TYR:CD1	1:B:473:ILE:CG1	2.43	1.00
1:B:274:ASN:O	1:C:286:SER:HA	1.61	1.00
1:C:32:THR:HG21	1:C:342:ALA:HA	1.42	1.00
1:A:305:THR:HG21	1:A:310:LEU:HD22	1.01	1.00
1:B:119:VAL:HG23	1:B:206:ASP:HB2	1.44	1.00
1:A:229:GLY:O	1:B:477:SER:O	1.80	1.00
1:B:422:LEU:HD22	1:C:221:LYS:NZ	1.74	1.00
1:A:32:THR:HG21	1:A:342:ALA:HA	1.42	1.00
1:A:87:ILE:HG12	1:B:374:SER:HA	1.42	1.00
1:A:227:CYS:C	1:B:476:ASP:HA	1.80	1.00
1:A:180:LYS:CE	1:B:57:PHE:HB3	1.92	1.00
1:B:274:ASN:HA	1:C:286:SER:HB2	1.41	1.00
1:A:189:ASP:CB	1:B:369:ARG:HA	1.92	1.00
1:A:227:CYS:HB2	1:B:476:ASP:CB	1.91	1.00
1:B:64:PRO:HG3	1:B:82:TYR:HA	1.44	1.00
1:B:11:ILE:HG12	1:B:324:LEU:HD23	1.42	0.99
1:C:433:LEU:HD23	1:C:444:VAL:HG11	1.44	0.99
1:A:433:LEU:HD23	1:A:444:VAL:HG11	1.44	0.99
1:A:165:TRP:CD1	1:B:110:ARG:HA	1.98	0.99
1:B:258:LEU:HD21	1:B:314:VAL:HG23	1.44	0.99
1:C:230:GLU:CA	1:C:250:LEU:HD23	1.92	0.99
1:B:385:PRO:HG3	1:C:224:GLY:O	1.63	0.99
1:A:208:VAL:HG12	1:A:231:VAL:HG12	1.42	0.99
1:B:383:LYS:CB	1:C:6:TRP:HD1	1.73	0.99
1:B:444:VAL:O	1:C:185:ASN:HB2	1.61	0.99
1:A:11:ILE:HG12	1:A:324:LEU:HD23	1.42	0.99
1:A:191:VAL:HG21	1:B:473:ILE:HD11	0.99	0.99
1:B:237:ALA:CB	1:C:378:GLY:C	2.17	0.99
1:A:152:ILE:HD11	1:A:166:LEU:HA	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:MET:HB3	1:B:477:SER:N	1.44	0.98
1:B:429:ALA:HB3	1:C:186:GLU:HB3	1.42	0.98
1:B:230:GLU:CA	1:B:250:LEU:HD23	1.92	0.98
1:A:145:TYR:HE1	1:B:113:TYR:CE2	1.79	0.98
1:C:64:PRO:HG3	1:C:82:TYR:HA	1.44	0.98
1:A:180:LYS:HD3	1:B:57:PHE:CG	1.72	0.98
1:A:219:TYR:HE2	1:B:371:TYR:HB2	0.82	0.98
1:B:383:LYS:CD	1:C:5:ASP:HB2	1.94	0.98
1:A:230:GLU:CA	1:A:250:LEU:HD23	1.92	0.98
1:C:152:ILE:HD11	1:C:166:LEU:HA	1.45	0.98
1:B:387:ILE:CA	1:C:247:ASP:OD2	2.12	0.98
1:A:184:LYS:HE2	1:B:362:ILE:CG2	1.84	0.98
1:A:219:TYR:CE1	1:B:471:SER:OG	2.17	0.98
1:A:225:VAL:N	1:B:465:THR:CB	2.04	0.98
1:A:45:ILE:HG23	1:A:49:LEU:CD1	1.93	0.98
1:A:184:LYS:CD	1:B:363:ALA:HA	1.93	0.98
1:B:185:ASN:HA	1:B:188:TYR:CD2	1.99	0.98
1:A:227:CYS:HB3	1:B:476:ASP:HB3	1.45	0.97
1:A:208:VAL:HB	1:B:478:SER:OG	1.11	0.97
1:B:45:ILE:HG23	1:B:49:LEU:CD1	1.93	0.97
1:A:64:PRO:HG3	1:A:82:TYR:HA	1.44	0.97
1:A:180:LYS:HZ3	1:B:10:SER:C	1.68	0.97
1:B:385:PRO:HA	1:C:3:PRO:HD3	0.99	0.97
1:A:249:VAL:HB	1:B:477:SER:OG	1.64	0.97
1:B:386:TYR:CE2	1:C:247:ASP:CB	2.37	0.97
1:C:258:LEU:HD21	1:C:314:VAL:HG23	1.43	0.97
1:B:188:TYR:HE1	1:B:218:GLY:HA3	1.29	0.97
1:C:45:ILE:HG23	1:C:49:LEU:CD1	1.93	0.97
1:A:119:VAL:HG23	1:A:206:ASP:HB2	1.44	0.97
1:A:186:GLU:HG3	1:B:370:ASN:HB3	0.97	0.97
1:A:225:VAL:CG2	1:B:465:THR:CG2	2.38	0.97
1:B:216:TRP:HB2	1:B:245:VAL:HG22	1.47	0.97
1:C:119:VAL:HG23	1:C:206:ASP:HB2	1.44	0.97
1:A:194:LEU:HD13	1:B:375:LYS:CB	1.94	0.97
1:A:188:TYR:HE1	1:A:218:GLY:HA3	1.29	0.97
1:A:218:GLY:H	1:B:364:SER:HB3	1.30	0.97
1:A:190:TRP:HZ2	1:B:375:LYS:HD2	1.22	0.97
1:B:433:LEU:HD23	1:B:444:VAL:HG11	1.44	0.97
1:A:194:LEU:HD13	1:B:375:LYS:HB3	1.47	0.96
1:C:216:TRP:HB2	1:C:245:VAL:HG22	1.47	0.96
1:B:383:LYS:HB3	1:C:6:TRP:HD1	1.26	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:TYR:CG	1:C:288:LEU:CD1	2.47	0.96
1:A:185:ASN:HA	1:A:188:TYR:CD2	1.99	0.96
1:B:152:ILE:HD11	1:B:166:LEU:HA	1.45	0.96
1:B:400:ASP:O	1:C:193:SER:HA	1.62	0.96
1:A:193:SER:HA	1:B:403:GLN:CA	1.80	0.96
1:A:180:LYS:O	1:B:57:PHE:N	1.84	0.96
1:B:445:GLY:HA3	1:C:185:ASN:HD22	1.30	0.96
1:C:185:ASN:HA	1:C:188:TYR:CD2	1.99	0.96
1:A:186:GLU:CG	1:B:370:ASN:CA	2.43	0.96
1:A:190:TRP:CE3	1:B:371:TYR:CD1	2.53	0.96
1:A:220:ASN:CA	1:B:473:ILE:CG2	2.43	0.96
1:A:10:SER:HB3	1:A:57:PHE:CA	1.96	0.96
1:B:277:ASN:HB2	1:C:286:SER:CB	1.96	0.96
1:A:221:LYS:CA	1:B:474:CYS:SG	2.53	0.96
1:C:10:SER:HB3	1:C:57:PHE:CA	1.96	0.96
1:A:258:LEU:HD21	1:A:314:VAL:HG23	1.44	0.96
1:A:143:GLN:NE2	1:B:108:HIS:ND1	2.12	0.96
1:A:196:SER:HB3	1:B:403:GLN:HG3	1.48	0.96
1:C:208:VAL:HG21	1:C:246:MET:SD	2.06	0.96
1:B:208:VAL:HG21	1:B:246:MET:SD	2.06	0.96
1:B:388:LYS:HA	1:C:244:ASN:O	1.64	0.96
1:A:208:VAL:HG21	1:A:246:MET:SD	2.06	0.96
1:B:238:TYR:HA	1:C:376:ASP:CB	1.94	0.96
1:C:146:PHE:HA	1:C:176:LEU:HA	1.48	0.95
1:C:305:THR:HG21	1:C:310:LEU:CD2	1.96	0.95
1:B:279:VAL:HG13	1:C:4:ALA:HB1	0.98	0.95
1:A:229:GLY:HA2	1:B:478:SER:HB2	1.22	0.95
1:C:45:ILE:CB	1:C:103:LEU:HD21	1.95	0.95
1:A:146:PHE:HA	1:A:176:LEU:HA	1.48	0.95
1:A:436:VAL:HG13	1:A:437:ILE:HG13	1.47	0.95
1:A:45:ILE:CB	1:A:103:LEU:HD21	1.95	0.95
1:B:276:ILE:O	1:C:4:ALA:CB	2.13	0.95
1:B:278:THR:HA	1:C:380:VAL:HG22	0.97	0.95
1:B:449:ASN:H	1:C:184:LYS:HZ1	1.07	0.95
1:B:386:TYR:CZ	1:C:288:LEU:HD13	2.01	0.95
1:A:305:THR:HG21	1:A:310:LEU:CD2	1.96	0.95
1:A:189:ASP:HB2	1:B:369:ARG:CA	1.96	0.95
1:A:186:GLU:HG3	1:B:370:ASN:CA	1.97	0.95
1:B:45:ILE:CB	1:B:103:LEU:HD21	1.95	0.95
1:A:179:THR:C	1:B:55:MET:HB2	1.87	0.95
1:B:382:TYR:O	1:C:2:THR:CG2	2.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASP:OD2	1:C:399:THR:HG22	1.63	0.94
1:B:305:THR:HG21	1:B:310:LEU:CD2	1.96	0.94
1:B:446:SER:OG	1:C:181:ASP:OD1	1.84	0.94
1:A:227:CYS:C	1:B:476:ASP:CA	2.35	0.94
1:C:436:VAL:HG13	1:C:437:ILE:HG13	1.47	0.94
1:A:200:ILE:CD1	1:B:467:LYS:NZ	2.30	0.94
1:A:218:GLY:N	1:B:364:SER:HB3	1.80	0.94
1:A:227:CYS:HB3	1:B:476:ASP:HB2	0.94	0.94
1:A:143:GLN:HE21	1:B:108:HIS:CG	1.84	0.94
1:A:2:THR:CA	1:B:432:GLN:NE2	2.19	0.94
1:C:188:TYR:HE1	1:C:218:GLY:HA3	1.29	0.94
1:B:436:VAL:HG13	1:B:437:ILE:HG13	1.47	0.94
1:A:165:TRP:CZ3	1:A:172:SER:HB2	2.02	0.94
1:A:216:TRP:HB2	1:A:245:VAL:HG22	1.47	0.94
1:A:88:TYR:HE2	1:B:373:ILE:C	1.66	0.94
1:A:188:TYR:CD2	1:B:367:ALA:N	2.35	0.94
1:B:146:PHE:HA	1:B:176:LEU:HA	1.48	0.94
1:B:406:THR:CG2	1:C:221:LYS:O	2.16	0.94
1:A:229:GLY:CA	1:B:478:SER:HB3	1.88	0.94
1:B:165:TRP:CZ3	1:B:172:SER:HB2	2.02	0.94
1:A:217:PRO:CB	1:B:437:ILE:O	2.16	0.94
1:A:198:TYR:HB2	1:B:467:LYS:NZ	1.81	0.94
1:B:11:ILE:HD13	1:B:326:ILE:HG12	1.49	0.94
1:A:200:ILE:HD11	1:B:467:LYS:HZ3	1.33	0.94
1:B:238:TYR:CA	1:C:377:THR:N	2.30	0.93
1:A:190:TRP:CD1	1:B:372:ALA:O	1.92	0.93
1:A:11:ILE:HD13	1:A:326:ILE:HG12	1.49	0.93
1:A:200:ILE:HD12	1:B:467:LYS:CE	1.97	0.93
1:C:11:ILE:HD13	1:C:326:ILE:HG12	1.49	0.93
1:B:404:ILE:HD11	1:C:223:ALA:CA	1.81	0.93
1:A:228:ILE:N	1:B:476:ASP:CB	2.31	0.93
1:A:194:LEU:CD2	1:B:375:LYS:CG	2.24	0.93
1:B:427:TYR:N	1:C:188:TYR:CD1	2.36	0.93
1:B:382:TYR:O	1:C:2:THR:HG23	1.67	0.93
1:A:208:VAL:HG23	1:A:216:TRP:CE2	2.04	0.93
1:C:16:THR:HG1	1:C:94:TYR:HE1	0.95	0.93
1:A:205:ILE:HG23	1:B:472:LYS:N	1.84	0.93
1:A:183:VAL:HA	1:B:370:ASN:ND2	1.82	0.93
1:A:205:ILE:HG12	1:B:471:SER:O	1.66	0.93
1:A:180:LYS:CD	1:B:57:PHE:CG	2.25	0.93
1:A:69:LEU:HB2	1:A:71:GLN:HE21	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LEU:HB2	1:C:71:GLN:HE21	1.34	0.93
1:A:148:PRO:HD3	1:B:49:LEU:HD23	1.49	0.93
1:A:225:VAL:HG23	1:B:465:THR:CG2	1.80	0.93
1:C:165:TRP:CZ3	1:C:172:SER:HB2	2.02	0.93
1:C:208:VAL:HG23	1:C:216:TRP:CE2	2.04	0.93
1:A:248:GLY:O	1:B:477:SER:CB	2.16	0.93
1:B:424:GLY:O	1:C:221:LYS:HB2	1.65	0.93
1:B:386:TYR:CE2	1:C:288:LEU:CD1	2.47	0.92
1:A:216:TRP:O	1:B:473:ILE:O	1.87	0.92
1:B:238:TYR:CA	1:C:376:ASP:CA	2.33	0.92
1:A:180:LYS:NZ	1:B:10:SER:C	2.23	0.92
1:A:143:GLN:OE1	1:B:108:HIS:HA	1.68	0.92
1:A:229:GLY:CA	1:B:477:SER:C	2.34	0.92
1:C:308:ILE:HG22	1:C:312:LYS:HE3	1.50	0.92
1:B:208:VAL:HG23	1:B:216:TRP:CE2	2.04	0.92
1:B:69:LEU:HB2	1:B:71:GLN:HE21	1.34	0.92
1:B:278:THR:O	1:C:380:VAL:CG2	2.18	0.92
1:A:186:GLU:CG	1:B:370:ASN:HB3	1.89	0.92
1:A:230:GLU:H	1:B:478:SER:HB2	1.29	0.92
1:B:383:LYS:HD2	1:C:5:ASP:HB2	1.48	0.92
1:A:197:ASN:O	1:B:467:LYS:CE	2.18	0.92
1:B:277:ASN:CB	1:C:286:SER:HB3	1.99	0.92
1:A:182:VAL:HB	1:B:10:SER:C	1.90	0.91
1:A:147:HIS:HA	1:B:112:MET:CE	2.00	0.91
1:B:444:VAL:C	1:C:185:ASN:CG	2.25	0.91
1:A:205:ILE:HG23	1:B:472:LYS:HG3	1.50	0.91
1:A:182:VAL:H	1:B:57:PHE:CB	1.82	0.91
1:B:400:ASP:C	1:C:193:SER:O	2.08	0.91
1:B:274:ASN:CA	1:C:286:SER:HA	2.01	0.91
1:A:194:LEU:HB2	1:B:375:LYS:HB3	1.53	0.91
1:A:229:GLY:N	1:A:246:MET:HE1	1.85	0.91
1:A:178:THR:HB	1:B:57:PHE:O	1.71	0.91
1:A:145:TYR:CE2	1:B:9:GLN:HB2	2.06	0.91
1:A:185:ASN:CB	1:B:366:ASN:CA	2.21	0.91
1:B:308:ILE:HG22	1:B:312:LYS:HE3	1.50	0.91
1:B:209:LYS:HB3	1:B:231:VAL:HG21	1.52	0.91
1:B:273:TYR:CD1	1:B:389:ASP:HB3	2.05	0.91
1:C:273:TYR:CD1	1:C:389:ASP:HB3	2.06	0.91
1:A:180:LYS:H	1:B:55:MET:CB	1.76	0.91
1:A:208:VAL:HA	1:A:216:TRP:CZ2	2.06	0.91
1:A:180:LYS:HG2	1:B:327:ILE:HG21	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:CA	1:B:368:ILE:HD12	1.99	0.91
1:C:208:VAL:HA	1:C:216:TRP:CZ2	2.06	0.91
1:B:383:LYS:HG3	1:C:6:TRP:NE1	1.84	0.91
1:B:432:GLN:CG	1:B:465:THR:HG21	2.01	0.91
1:B:274:ASN:O	1:C:286:SER:CA	2.19	0.91
1:A:191:VAL:O	1:B:467:LYS:O	1.88	0.91
1:A:308:ILE:HG22	1:A:312:LYS:HE3	1.50	0.90
1:B:305:THR:CG2	1:B:310:LEU:HD22	1.97	0.90
1:A:273:TYR:CD1	1:A:389:ASP:HB3	2.05	0.90
1:B:278:THR:C	1:C:380:VAL:HG11	1.90	0.90
1:A:249:VAL:CG1	1:B:477:SER:CB	2.48	0.90
1:A:180:LYS:CG	1:B:12:TYR:CD2	2.54	0.90
1:B:241:PRO:O	1:C:374:SER:HA	1.11	0.90
1:A:209:LYS:HB3	1:A:231:VAL:HG21	1.52	0.90
1:B:208:VAL:HA	1:B:216:TRP:CZ2	2.06	0.90
1:A:222:ALA:HB2	1:B:368:ILE:HG13	1.19	0.90
1:C:209:LYS:HB3	1:C:231:VAL:HG21	1.52	0.90
1:B:281:SER:HB2	1:C:6:TRP:C	1.92	0.90
1:A:217:PRO:O	1:B:474:CYS:HA	1.72	0.90
1:A:185:ASN:HB2	1:B:366:ASN:HA	0.91	0.90
1:A:145:TYR:CE2	1:B:9:GLN:CB	2.55	0.90
1:C:319:ILE:CG2	1:C:325:PRO:HB2	2.01	0.90
1:A:145:TYR:CE1	1:B:113:TYR:HE2	1.85	0.90
1:A:205:ILE:HD12	1:B:478:SER:HB3	1.42	0.90
1:B:429:ALA:HB3	1:C:186:GLU:CB	2.02	0.90
1:C:191:VAL:HG11	1:C:219:TYR:CZ	2.07	0.90
1:C:432:GLN:CG	1:C:465:THR:HG21	2.01	0.90
1:B:182:VAL:HG13	1:B:183:VAL:H	1.37	0.90
1:B:383:LYS:CE	1:C:5:ASP:CB	2.48	0.90
1:B:382:TYR:CD1	1:C:2:THR:CG2	2.55	0.90
1:C:365:ALA:O	1:C:368:ILE:HG22	1.72	0.90
1:A:190:TRP:HH2	1:B:375:LYS:CD	1.77	0.89
1:B:191:VAL:HG11	1:B:219:TYR:CZ	2.07	0.89
1:B:382:TYR:HD1	1:C:2:THR:HG23	1.15	0.89
1:A:184:LYS:H	1:B:56:GLY:HA2	1.34	0.89
1:B:235:ASP:CG	1:C:399:THR:HG23	1.86	0.89
1:C:433:LEU:HB2	1:C:442:VAL:HG12	1.54	0.89
1:A:190:TRP:CD2	1:B:374:SER:CB	2.55	0.89
1:B:280:LYS:O	1:C:7:ARG:N	2.05	0.89
1:A:229:GLY:C	1:B:478:SER:HB2	1.91	0.89
1:C:257:PRO:HA	1:C:260:ASN:HB2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:CG2	1:A:325:PRO:HB2	2.01	0.89
1:B:293:VAL:HG13	1:B:294:GLU:H	1.36	0.89
1:B:319:ILE:CG2	1:B:325:PRO:HB2	2.01	0.89
1:A:432:GLN:CG	1:A:465:THR:HG21	2.01	0.89
1:C:35:GLN:HB3	1:C:79:TYR:CE1	2.07	0.89
1:B:274:ASN:C	1:C:286:SER:HA	1.93	0.89
1:B:404:ILE:CD1	1:C:223:ALA:CA	2.43	0.89
1:B:404:ILE:HG12	1:C:223:ALA:HA	1.51	0.89
1:B:277:ASN:CG	1:C:286:SER:HB3	1.93	0.89
1:A:192:GLY:O	1:B:464:PRO:CG	2.20	0.89
1:A:257:PRO:HA	1:A:260:ASN:HB2	1.53	0.89
1:A:433:LEU:HB2	1:A:442:VAL:HG12	1.54	0.89
1:A:10:SER:CB	1:A:57:PHE:HA	2.03	0.89
1:B:408:LEU:HD11	1:B:462:LEU:HD21	1.54	0.89
1:A:180:LYS:H	1:B:55:MET:HB2	1.20	0.89
1:B:236:PRO:HB2	1:C:380:VAL:HG12	1.55	0.89
1:C:408:LEU:HD11	1:C:462:LEU:HD21	1.53	0.89
1:C:10:SER:CB	1:C:57:PHE:HA	2.03	0.89
1:A:180:LYS:CA	1:B:55:MET:CG	2.42	0.89
1:A:186:GLU:CG	1:B:370:ASN:HA	2.02	0.89
1:B:449:ASN:ND2	1:C:214:ASP:C	2.25	0.89
1:A:184:LYS:H	1:B:56:GLY:CA	1.85	0.89
1:A:180:LYS:HB3	1:B:12:TYR:CD2	2.08	0.89
1:A:293:VAL:HG13	1:A:294:GLU:H	1.36	0.89
1:A:365:ALA:O	1:A:368:ILE:HG22	1.72	0.89
1:B:396:ARG:C	1:C:224:GLY:HA2	1.91	0.89
1:A:35:GLN:HB3	1:A:79:TYR:CE1	2.07	0.88
1:B:277:ASN:HB2	1:C:286:SER:HB3	1.55	0.88
1:B:445:GLY:HA2	1:C:185:ASN:CG	1.93	0.88
1:C:11:ILE:CD1	1:C:324:LEU:HB3	2.04	0.88
1:B:445:GLY:HA2	1:C:185:ASN:HB3	1.54	0.88
1:B:208:VAL:HG12	1:B:231:VAL:CG1	2.04	0.88
1:A:205:ILE:HG13	1:B:478:SER:HB3	1.54	0.88
1:B:257:PRO:HA	1:B:260:ASN:HB2	1.53	0.88
1:A:200:ILE:HG21	1:B:467:LYS:HA	1.55	0.88
1:C:208:VAL:HG12	1:C:231:VAL:CG1	2.04	0.88
1:B:427:TYR:H	1:C:188:TYR:HD1	1.13	0.88
1:B:387:ILE:HA	1:C:247:ASP:OD2	1.72	0.88
1:A:208:VAL:HG12	1:A:231:VAL:CG1	2.04	0.88
1:B:11:ILE:CD1	1:B:324:LEU:HB3	2.04	0.88
1:A:222:ALA:HB2	1:B:368:ILE:CB	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:VAL:HG13	1:C:183:VAL:H	1.36	0.88
1:B:275:MET:CA	1:C:7:ARG:NH1	2.35	0.88
1:A:165:TRP:HE1	1:B:110:ARG:N	1.72	0.88
1:A:42:TRP:HE1	1:A:62:ILE:CD1	1.86	0.88
1:B:35:GLN:HB3	1:B:79:TYR:CE1	2.07	0.88
1:B:383:LYS:HD3	1:C:5:ASP:OD2	1.73	0.88
1:B:388:LYS:HE2	1:B:390:ASP:HB2	1.55	0.88
1:A:11:ILE:CD1	1:A:324:LEU:HB3	2.04	0.88
1:B:433:LEU:HB2	1:B:442:VAL:HG12	1.54	0.88
1:A:123:MET:HG3	1:A:146:PHE:CE1	2.07	0.88
1:A:408:LEU:HD11	1:A:462:LEU:HD21	1.53	0.88
1:B:276:ILE:O	1:C:4:ALA:CA	2.22	0.88
1:B:422:LEU:CD2	1:C:221:LYS:HZ2	1.83	0.88
1:A:16:THR:HG1	1:A:94:TYR:HE1	0.93	0.88
1:A:57:PHE:CE2	1:A:327:ILE:HG21	2.09	0.88
1:C:293:VAL:HG13	1:C:294:GLU:H	1.36	0.88
1:B:238:TYR:C	1:C:377:THR:N	2.28	0.88
1:A:180:LYS:HE3	1:B:12:TYR:CA	2.04	0.87
1:B:400:ASP:HA	1:C:192:GLY:O	1.74	0.87
1:B:42:TRP:HE1	1:B:62:ILE:CD1	1.86	0.87
1:C:123:MET:HG3	1:C:146:PHE:CE1	2.07	0.87
1:B:383:LYS:NZ	1:C:6:TRP:N	2.23	0.87
1:A:197:ASN:OD1	1:C:193:SER:O	1.92	0.87
1:A:205:ILE:HG21	1:B:472:LYS:HG2	1.56	0.87
1:C:57:PHE:CE2	1:C:327:ILE:HG21	2.09	0.87
1:A:200:ILE:CG2	1:B:467:LYS:HA	2.05	0.87
1:A:249:VAL:CG1	1:B:477:SER:OG	2.22	0.87
1:C:422:LEU:HB3	1:C:450:VAL:HG22	1.55	0.87
1:C:42:TRP:HE1	1:C:62:ILE:CD1	1.86	0.87
1:C:280:LYS:CE	1:C:383:LYS:HB3	2.04	0.87
1:C:305:THR:CG2	1:C:310:LEU:HD22	1.97	0.87
1:C:45:ILE:HB	1:C:103:LEU:CD2	2.03	0.87
1:A:143:GLN:HE21	1:B:108:HIS:CE1	1.92	0.87
1:B:236:PRO:HG2	1:C:378:GLY:C	1.95	0.87
1:B:237:ALA:CA	1:C:379:PHE:N	2.37	0.87
1:B:57:PHE:CE2	1:B:327:ILE:HG21	2.09	0.87
1:B:422:LEU:HB3	1:B:450:VAL:HG22	1.55	0.87
1:A:180:LYS:HZ3	1:A:182:VAL:HB	1.38	0.87
1:A:295:ASN:HB3	1:A:298:ASN:HB2	1.56	0.87
1:A:305:THR:CG2	1:A:310:LEU:HD22	1.97	0.87
1:A:143:GLN:CG	1:B:108:HIS:NE2	2.24	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:THR:HG22	1:C:1:ALA:HB2	1.54	0.87
1:A:215:PHE:HD1	1:A:216:TRP:CE3	1.93	0.87
1:A:422:LEU:HB3	1:A:450:VAL:HG22	1.56	0.87
1:A:87:ILE:HD11	1:B:374:SER:CA	2.00	0.87
1:C:215:PHE:HD1	1:C:216:TRP:CE3	1.93	0.87
1:C:295:ASN:HB3	1:C:298:ASN:HB2	1.56	0.87
1:A:144:ASP:C	1:B:58:THR:O	2.13	0.87
1:A:205:ILE:CG1	1:B:471:SER:C	2.42	0.87
1:B:385:PRO:HD2	1:C:2:THR:HG22	1.56	0.87
1:A:182:VAL:N	1:B:57:PHE:CA	2.31	0.86
1:A:208:VAL:HA	1:A:216:TRP:HZ2	1.40	0.86
1:B:238:TYR:CG	1:C:376:ASP:HB2	2.10	0.86
1:A:180:LYS:HB3	1:B:12:TYR:HD2	1.36	0.86
1:A:223:ALA:H	1:B:468:LEU:CD2	1.87	0.86
1:A:145:TYR:CD2	1:B:9:GLN:CG	2.58	0.86
1:B:295:ASN:HB3	1:B:298:ASN:HB2	1.56	0.86
1:A:280:LYS:CE	1:A:383:LYS:HB3	2.04	0.86
1:B:215:PHE:HD1	1:B:216:TRP:CE3	1.93	0.86
1:A:431:GLN:HE21	1:A:431:GLN:HA	1.41	0.86
1:B:383:LYS:HZ3	1:C:6:TRP:N	1.72	0.86
1:C:431:GLN:HE21	1:C:431:GLN:HA	1.41	0.86
1:B:276:ILE:O	1:C:4:ALA:HA	1.74	0.86
1:A:45:ILE:HB	1:A:103:LEU:CD2	2.03	0.86
1:B:12:TYR:CE1	1:B:14:LEU:HD23	2.11	0.86
1:B:431:GLN:HA	1:B:431:GLN:HE21	1.41	0.86
1:C:388:LYS:HE2	1:C:390:ASP:HB2	1.56	0.86
1:B:400:ASP:CB	1:C:194:LEU:O	2.23	0.86
1:B:449:ASN:ND2	1:C:214:ASP:O	2.09	0.86
1:B:396:ARG:C	1:C:224:GLY:CA	2.44	0.86
1:B:408:LEU:CD2	1:B:452:VAL:HG21	2.06	0.86
1:B:399:THR:HG22	1:C:196:SER:O	1.74	0.86
1:A:205:ILE:HG23	1:B:472:LYS:H	1.40	0.86
1:A:219:TYR:HE1	1:B:471:SER:HG	0.88	0.86
1:B:115:MET:HE1	1:B:204:ARG:HB2	1.54	0.86
1:B:83:TRP:HE1	1:B:173:LEU:CD2	1.89	0.86
1:B:11:ILE:HD13	1:B:326:ILE:CG1	2.06	0.86
1:B:400:ASP:CA	1:C:193:SER:C	2.44	0.86
1:A:408:LEU:CD2	1:A:452:VAL:HG21	2.06	0.86
1:B:386:TYR:CD2	1:C:247:ASP:HB3	2.11	0.86
1:C:83:TRP:HE1	1:C:173:LEU:CD2	1.89	0.86
1:A:223:ALA:H	1:B:468:LEU:HD21	1.03	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:HG13	1:B:374:SER:C	1.85	0.85
1:A:180:LYS:HA	1:B:55:MET:HB3	0.93	0.85
1:A:205:ILE:CG2	1:B:472:LYS:CG	2.13	0.85
1:A:230:GLU:HA	1:A:250:LEU:CD2	2.06	0.85
1:B:139:PRO:HG2	1:B:140:PHE:CD1	2.11	0.85
1:B:16:THR:HG1	1:B:94:TYR:HE1	1.23	0.85
1:B:401:GLY:N	1:C:193:SER:C	2.29	0.85
1:A:11:ILE:HD13	1:A:326:ILE:CG1	2.06	0.85
1:A:83:TRP:HE1	1:A:173:LEU:CD2	1.89	0.85
1:A:219:TYR:CZ	1:B:473:ILE:HD12	2.10	0.85
1:A:147:HIS:CG	1:A:148:PRO:HD2	2.11	0.85
1:A:200:ILE:HD11	1:B:467:LYS:NZ	1.91	0.85
1:B:238:TYR:HB2	1:C:376:ASP:CG	1.96	0.85
1:B:406:THR:HG21	1:C:221:LYS:O	1.75	0.85
1:C:408:LEU:CD2	1:C:452:VAL:HG21	2.06	0.85
1:C:147:HIS:CG	1:C:148:PRO:HD2	2.11	0.85
1:C:208:VAL:HA	1:C:216:TRP:HZ2	1.40	0.85
1:C:230:GLU:HA	1:C:250:LEU:CD2	2.06	0.85
1:A:221:LYS:CA	1:B:434:THR:HG22	2.04	0.85
1:A:88:TYR:CD2	1:B:373:ILE:O	2.29	0.85
1:A:220:ASN:OD1	1:B:439:CYS:SG	2.35	0.85
1:B:241:PRO:HB2	1:C:374:SER:C	1.97	0.85
1:B:123:MET:HG3	1:B:146:PHE:CE1	2.07	0.85
1:B:230:GLU:HA	1:B:250:LEU:CD2	2.06	0.85
1:A:194:LEU:O	1:B:467:LYS:NZ	2.08	0.85
1:B:235:ASP:OD2	1:C:399:THR:HG21	1.47	0.85
1:A:139:PRO:HG2	1:A:140:PHE:CD1	2.11	0.85
1:A:388:LYS:HE2	1:A:390:ASP:HB2	1.56	0.85
1:B:147:HIS:CG	1:B:148:PRO:HD2	2.11	0.85
1:A:180:LYS:C	1:B:55:MET:HB3	1.96	0.85
1:A:455:ALA:HB3	1:A:458:LEU:HD11	1.58	0.85
1:C:200:ILE:HG22	1:C:203:LEU:HD11	1.59	0.84
1:B:237:ALA:HB2	1:C:379:PHE:H	1.39	0.84
1:B:383:LYS:CD	1:C:5:ASP:OD2	2.24	0.84
1:A:163:ASP:CA	1:B:53:GLN:OE1	2.24	0.84
1:A:12:TYR:CE1	1:A:14:LEU:HD23	2.11	0.84
1:A:204:ARG:O	1:B:471:SER:HA	1.58	0.84
1:C:11:ILE:HD13	1:C:326:ILE:CG1	2.06	0.84
1:A:420:LEU:HD23	1:A:452:VAL:CG1	2.07	0.84
1:A:186:GLU:HA	1:B:369:ARG:NH1	1.92	0.84
1:C:12:TYR:CE1	1:C:14:LEU:HD23	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PRO:HG2	1:C:140:PHE:CD1	2.11	0.84
1:B:236:PRO:HG2	1:C:378:GLY:O	1.77	0.84
1:B:281:SER:HB2	1:C:6:TRP:O	1.78	0.84
1:A:187:TRP:C	1:B:367:ALA:O	2.15	0.84
1:A:200:ILE:HG22	1:A:203:LEU:HD11	1.59	0.84
1:B:420:LEU:HD23	1:B:452:VAL:CG1	2.07	0.84
1:B:455:ALA:HB3	1:B:458:LEU:HD11	1.58	0.84
1:B:396:ARG:HB2	1:C:221:LYS:HA	1.57	0.84
1:B:213:LYS:HE2	1:C:375:LYS:HG3	1.57	0.84
1:A:184:LYS:HD2	1:B:363:ALA:C	1.97	0.84
1:A:219:TYR:CE2	1:B:371:TYR:CD2	2.64	0.84
1:A:145:TYR:HE1	1:B:113:TYR:HE2	1.14	0.84
1:B:386:TYR:CD1	1:C:288:LEU:HD12	2.11	0.84
1:B:449:ASN:HB2	1:C:184:LYS:HZ3	1.05	0.84
1:A:195:VAL:HG22	1:B:466:GLU:CG	2.07	0.84
1:B:208:VAL:HA	1:B:216:TRP:HZ2	1.40	0.84
1:B:387:ILE:HG22	1:B:395:MET:HA	1.60	0.84
1:A:148:PRO:CD	1:B:49:LEU:HD23	2.07	0.83
1:A:227:CYS:O	1:B:476:ASP:CA	2.26	0.83
1:B:211:VAL:HB	1:B:216:TRP:CZ2	2.13	0.83
1:A:180:LYS:HG2	1:B:327:ILE:HG22	1.58	0.83
1:B:385:PRO:HA	1:C:3:PRO:CG	2.07	0.83
1:C:420:LEU:HD23	1:C:452:VAL:CG1	2.07	0.83
1:A:236:PRO:O	1:A:240:CYS:HB2	1.78	0.83
1:A:211:VAL:HB	1:A:216:TRP:CZ2	2.13	0.83
1:A:229:GLY:CA	1:A:246:MET:HE1	2.08	0.83
1:B:281:SER:HB2	1:C:8:SER:H	1.41	0.83
1:A:222:ALA:CA	1:B:368:ILE:CG1	2.50	0.83
1:B:385:PRO:HD3	1:C:2:THR:CG2	2.03	0.83
1:B:385:PRO:N	1:C:3:PRO:HD3	1.72	0.83
1:C:455:ALA:HB3	1:C:458:LEU:HD11	1.58	0.83
1:C:14:LEU:HD12	1:C:62:ILE:HG22	1.61	0.83
1:C:211:VAL:HB	1:C:216:TRP:CZ2	2.13	0.83
1:A:200:ILE:HD12	1:B:467:LYS:HD2	1.60	0.83
1:A:221:LYS:HB3	1:B:436:VAL:N	1.93	0.83
1:A:249:VAL:HG12	1:B:477:SER:OG	1.79	0.83
1:C:236:PRO:O	1:C:240:CYS:HB2	1.78	0.82
1:A:195:VAL:HG22	1:B:466:GLU:HG3	1.59	0.82
1:A:195:VAL:HA	1:A:200:ILE:HD12	1.60	0.82
1:A:214:ASP:OD1	1:B:360:LYS:O	1.95	0.82
1:A:432:GLN:HG2	1:A:465:THR:CG2	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:CB	1:C:379:PHE:H	1.92	0.82
1:C:387:ILE:HG22	1:C:395:MET:HA	1.60	0.82
1:B:200:ILE:HG22	1:B:203:LEU:HD11	1.59	0.82
1:C:7:ARG:HG2	1:C:287:THR:OG1	1.79	0.82
1:A:180:LYS:CB	1:B:12:TYR:HD2	1.92	0.82
1:A:225:VAL:HG23	1:B:465:THR:HG22	1.62	0.82
1:A:14:LEU:HD12	1:A:62:ILE:HG22	1.61	0.82
1:B:275:MET:C	1:C:7:ARG:NH1	2.19	0.82
1:A:208:VAL:CA	1:B:472:LYS:HE2	2.09	0.82
1:A:280:LYS:HE3	1:A:383:LYS:HB3	1.62	0.82
1:A:229:GLY:N	1:B:477:SER:O	2.13	0.82
1:C:35:GLN:HB3	1:C:79:TYR:HE1	1.44	0.82
1:B:365:ALA:O	1:B:368:ILE:HG22	1.72	0.82
1:B:422:LEU:HB3	1:B:450:VAL:CG2	2.09	0.82
1:A:200:ILE:HD12	1:B:467:LYS:NZ	1.93	0.82
1:C:195:VAL:HA	1:C:200:ILE:HD12	1.60	0.82
1:A:115:MET:CE	1:A:204:ARG:HB2	2.09	0.82
1:A:223:ALA:N	1:B:468:LEU:CD2	2.32	0.82
1:B:7:ARG:HG2	1:B:287:THR:OG1	1.79	0.82
1:C:280:LYS:HE3	1:C:383:LYS:HB3	1.62	0.82
1:A:315:ALA:HA	1:A:318:ILE:HG23	1.62	0.82
1:B:195:VAL:HA	1:B:200:ILE:HD12	1.60	0.82
1:B:35:GLN:HB3	1:B:79:TYR:HE1	1.44	0.82
1:B:14:LEU:HD12	1:B:62:ILE:HG22	1.61	0.82
1:B:115:MET:CE	1:B:204:ARG:HB2	2.09	0.81
1:A:198:TYR:HB2	1:B:467:LYS:HZ3	1.42	0.81
1:B:385:PRO:CA	1:C:3:PRO:CG	2.57	0.81
1:A:243:GLN:HB3	1:A:284:PRO:HG2	1.62	0.81
1:A:194:LEU:CD1	1:B:375:LYS:HB3	2.10	0.81
1:B:213:LYS:HE2	1:C:375:LYS:CG	2.11	0.81
1:C:115:MET:CE	1:C:204:ARG:HB2	2.09	0.81
1:B:238:TYR:CB	1:C:376:ASP:OD2	2.19	0.81
1:C:422:LEU:HB3	1:C:450:VAL:CG2	2.09	0.81
1:C:432:GLN:HG2	1:C:465:THR:CG2	2.09	0.81
1:B:379:PHE:CE1	1:B:397:LYS:HE3	2.16	0.81
1:C:468:LEU:HD23	1:C:473:ILE:HG12	1.60	0.81
1:A:200:ILE:HD12	1:B:467:LYS:CG	2.10	0.81
1:A:7:ARG:HG2	1:A:287:THR:OG1	1.80	0.81
1:A:180:LYS:CG	1:B:12:TYR:HD2	1.92	0.81
1:B:341:PRO:HD2	1:B:342:ALA:N	1.88	0.81
1:C:379:PHE:CE1	1:C:397:LYS:HE3	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PRO:HD3	1:A:245:VAL:HG23	1.62	0.81
1:A:379:PHE:CE1	1:A:397:LYS:HE3	2.16	0.81
1:A:422:LEU:HB3	1:A:450:VAL:CG2	2.09	0.81
1:A:200:ILE:CB	1:B:467:LYS:HA	2.10	0.81
1:C:217:PRO:HD3	1:C:245:VAL:CG2	2.10	0.81
1:A:137:PHE:HB3	1:A:140:PHE:HB2	1.63	0.81
1:A:35:GLN:HB3	1:A:79:TYR:HE1	1.44	0.81
1:B:468:LEU:HD23	1:B:473:ILE:HG12	1.60	0.81
1:A:217:PRO:HD3	1:A:245:VAL:CG2	2.10	0.81
1:B:217:PRO:HD3	1:B:245:VAL:CG2	2.10	0.81
1:B:278:THR:C	1:C:380:VAL:CG2	2.41	0.81
1:B:426:SER:HA	1:C:188:TYR:HD1	1.46	0.81
1:A:2:THR:CA	1:B:432:GLN:HE22	1.34	0.81
1:C:263:LYS:HD2	1:C:304:TYR:CD2	2.16	0.81
1:A:180:LYS:HZ1	1:B:11:ILE:CA	1.94	0.81
1:B:45:ILE:HB	1:B:103:LEU:CD2	2.03	0.81
1:A:468:LEU:HD23	1:A:473:ILE:HG12	1.60	0.81
1:A:87:ILE:CD1	1:B:374:SER:OG	2.29	0.81
1:B:188:TYR:CE1	1:B:218:GLY:HA3	2.15	0.81
1:B:402:SER:H	1:C:193:SER:HB2	1.46	0.81
1:B:432:GLN:HG2	1:B:465:THR:CG2	2.09	0.81
1:C:137:PHE:HB3	1:C:140:PHE:HB2	1.63	0.81
1:B:428:THR:HA	1:C:186:GLU:C	2.01	0.81
1:C:188:TYR:CE1	1:C:218:GLY:HA3	2.15	0.81
1:C:315:ALA:HA	1:C:318:ILE:HG23	1.62	0.81
1:B:263:LYS:HD2	1:B:304:TYR:CD2	2.16	0.80
1:A:194:LEU:CB	1:B:375:LYS:HB3	2.12	0.80
1:C:217:PRO:HD3	1:C:245:VAL:HG23	1.62	0.80
1:A:185:ASN:CG	1:B:369:ARG:HD3	2.02	0.80
1:B:382:TYR:CA	1:C:1:ALA:CB	2.52	0.80
1:A:180:LYS:HD3	1:B:57:PHE:HB2	0.81	0.80
1:B:137:PHE:HB3	1:B:140:PHE:HB2	1.63	0.80
1:B:185:ASN:CA	1:B:188:TYR:HD2	1.91	0.80
1:B:400:ASP:C	1:C:193:SER:C	2.40	0.80
1:B:424:GLY:O	1:C:218:GLY:CA	2.30	0.80
1:B:243:GLN:HB3	1:B:284:PRO:HG2	1.62	0.80
1:A:88:TYR:CZ	1:B:373:ILE:C	2.55	0.80
1:C:115:MET:HE1	1:C:204:ARG:HB2	1.61	0.80
1:A:387:ILE:HG22	1:A:395:MET:HA	1.60	0.80
1:A:177:ASP:HB3	1:B:53:GLN:HB3	1.61	0.80
1:A:206:ASP:HA	1:A:230:GLU:HG3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:HE22	1:B:375:LYS:HZ2	1.28	0.80
1:B:192:GLY:O	1:B:195:VAL:HG12	1.82	0.80
1:A:410:ASN:HB3	1:A:454:MET:HE1	1.61	0.80
1:B:206:ASP:HA	1:B:230:GLU:HG3	1.64	0.80
1:A:197:ASN:C	1:B:467:LYS:CE	2.50	0.80
1:A:205:ILE:CD1	1:B:478:SER:OXT	2.30	0.80
1:A:143:GLN:CD	1:B:108:HIS:CA	2.46	0.80
1:A:148:PRO:CG	1:B:49:LEU:HD23	2.11	0.80
1:A:200:ILE:HB	1:B:467:LYS:HA	1.64	0.80
1:B:428:THR:CB	1:C:186:GLU:O	2.29	0.80
1:A:204:ARG:HB2	1:B:470:GLY:CA	1.90	0.80
1:A:263:LYS:HD2	1:A:304:TYR:CD2	2.16	0.80
1:C:192:GLY:O	1:C:195:VAL:HG12	1.82	0.80
1:A:219:TYR:HD1	1:B:473:ILE:HB	1.00	0.80
1:B:204:ARG:HG3	1:B:228:ILE:CB	2.12	0.80
1:B:408:LEU:HD21	1:B:452:VAL:HG21	1.64	0.80
1:B:278:THR:CA	1:C:380:VAL:HG22	1.94	0.80
1:A:185:ASN:CA	1:A:188:TYR:HD2	1.92	0.79
1:A:204:ARG:HG3	1:A:228:ILE:CB	2.12	0.79
1:A:214:ASP:HB2	1:B:360:LYS:HA	1.63	0.79
1:C:152:ILE:HD11	1:C:166:LEU:CA	2.12	0.79
1:C:206:ASP:HA	1:C:230:GLU:HG3	1.64	0.79
1:A:205:ILE:HG13	1:A:229:GLY:HA2	1.65	0.79
1:B:208:VAL:CA	1:B:216:TRP:CZ2	2.65	0.79
1:A:224:GLY:N	1:B:465:THR:HA	1.98	0.79
1:B:465:THR:HA	1:B:468:LEU:HD12	1.65	0.79
1:B:424:GLY:HA2	1:C:216:TRP:O	1.81	0.79
1:C:243:GLN:HB3	1:C:284:PRO:HG2	1.62	0.79
1:B:236:PRO:CB	1:C:380:VAL:HG12	2.11	0.79
1:A:192:GLY:O	1:A:195:VAL:HG12	1.82	0.79
1:C:205:ILE:HG13	1:C:229:GLY:HA2	1.65	0.79
1:C:465:THR:HA	1:C:468:LEU:HD12	1.65	0.79
1:B:420:LEU:CD2	1:B:452:VAL:HG13	2.11	0.79
1:C:204:ARG:HG3	1:C:228:ILE:CB	2.12	0.79
1:C:208:VAL:CA	1:C:216:TRP:CZ2	2.65	0.79
1:A:208:VAL:CA	1:A:216:TRP:CZ2	2.65	0.79
1:A:205:ILE:CD1	1:B:472:LYS:HG2	2.11	0.79
1:A:465:THR:HA	1:A:468:LEU:HD12	1.65	0.79
1:A:84:GLN:HE22	1:B:375:LYS:HZ1	1.30	0.79
1:C:408:LEU:HD21	1:C:452:VAL:HG21	1.64	0.79
1:A:175:ASP:O	1:B:110:ARG:O	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:HIS:HD2	1:B:177:ASP:O	1.66	0.79
1:B:205:ILE:HG13	1:B:229:GLY:HA2	1.65	0.79
1:A:139:PRO:HG2	1:A:140:PHE:CE1	2.18	0.79
1:B:400:ASP:HB3	1:C:194:LEU:O	1.83	0.79
1:B:428:THR:HA	1:C:186:GLU:O	1.83	0.79
1:B:11:ILE:HD11	1:B:324:LEU:HB3	1.65	0.79
1:A:217:PRO:CG	1:B:364:SER:OG	2.25	0.79
1:C:139:PRO:HG2	1:C:140:PHE:CE1	2.18	0.79
1:A:152:ILE:HD11	1:A:166:LEU:CA	2.12	0.78
1:A:420:LEU:CD2	1:A:452:VAL:HG22	2.13	0.78
1:B:217:PRO:HD3	1:B:245:VAL:HG23	1.62	0.78
1:A:227:CYS:HB2	1:B:476:ASP:CA	2.13	0.78
1:A:224:GLY:N	1:B:465:THR:CA	2.43	0.78
1:A:408:LEU:HD21	1:A:452:VAL:HG21	1.64	0.78
1:B:315:ALA:HA	1:B:318:ILE:HG23	1.62	0.78
1:A:211:VAL:HB	1:B:472:LYS:NZ	1.98	0.78
1:A:216:TRP:O	1:B:473:ILE:C	2.22	0.78
1:B:446:SER:O	1:C:182:VAL:N	2.12	0.78
1:C:185:ASN:CA	1:C:188:TYR:HD2	1.92	0.78
1:C:420:LEU:CD2	1:C:452:VAL:HG22	2.13	0.78
1:A:205:ILE:HD13	1:B:472:LYS:HA	1.64	0.78
1:A:455:ALA:HB3	1:A:458:LEU:CD1	2.13	0.78
1:C:55:MET:HG3	1:C:57:PHE:HE2	1.48	0.78
1:A:205:ILE:HB	1:B:478:SER:HG	1.44	0.78
1:A:186:GLU:HA	1:B:369:ARG:HH11	1.47	0.78
1:B:152:ILE:HD11	1:B:166:LEU:CA	2.12	0.78
1:A:218:GLY:CA	1:B:364:SER:O	2.30	0.78
1:C:341:PRO:HD2	1:C:342:ALA:N	1.87	0.78
1:A:143:GLN:CG	1:B:108:HIS:CG	2.56	0.78
1:C:11:ILE:HD11	1:C:324:LEU:HB3	1.65	0.78
1:C:455:ALA:HB3	1:C:458:LEU:CD1	2.13	0.78
1:A:16:THR:HG21	1:A:42:TRP:CD1	2.19	0.78
1:A:191:VAL:HG13	1:B:371:TYR:C	2.03	0.78
1:B:455:ALA:HB3	1:B:458:LEU:CD1	2.13	0.78
1:C:16:THR:HG21	1:C:42:TRP:CD1	2.19	0.78
1:B:449:ASN:CA	1:C:184:LYS:HZ1	1.96	0.78
1:B:402:SER:N	1:C:193:SER:CA	2.44	0.78
1:A:180:LYS:CB	1:B:12:TYR:CD2	2.67	0.78
1:A:182:VAL:N	1:B:57:PHE:CB	2.46	0.78
1:A:61:TRP:CZ3	1:A:326:ILE:HG21	2.19	0.78
1:B:122:HIS:ND1	1:B:173:LEU:HD22	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TRP:CZ3	1:B:326:ILE:HG21	2.19	0.78
1:B:139:PRO:HG2	1:B:140:PHE:CE1	2.18	0.78
1:B:427:TYR:N	1:C:188:TYR:HD1	1.75	0.78
1:B:16:THR:HG21	1:B:42:TRP:NE1	1.99	0.78
1:B:420:LEU:CD2	1:B:452:VAL:HG22	2.13	0.77
1:B:445:GLY:CA	1:C:185:ASN:CB	2.61	0.77
1:C:61:TRP:CZ3	1:C:326:ILE:HG21	2.19	0.77
1:C:407:ILE:CG2	1:C:461:VAL:HG22	2.10	0.77
1:A:185:ASN:OD1	1:B:369:ARG:HD3	1.83	0.77
1:C:147:HIS:HD2	1:C:177:ASP:O	1.66	0.77
1:B:385:PRO:HG3	1:C:224:GLY:C	2.04	0.77
1:A:64:PRO:HD2	1:A:81:GLY:O	1.84	0.77
1:B:16:THR:HG21	1:B:42:TRP:CD1	2.19	0.77
1:A:189:ASP:O	1:B:463:TYR:CE2	2.37	0.77
1:C:122:HIS:ND1	1:C:173:LEU:HD22	1.99	0.77
1:C:16:THR:HG21	1:C:42:TRP:NE1	2.00	0.77
1:A:227:CYS:CB	1:B:476:ASP:HB3	2.04	0.77
1:B:68:GLN:HA	1:B:85:THR:HG22	1.67	0.77
1:C:64:PRO:HD2	1:C:81:GLY:O	1.84	0.77
1:A:180:LYS:CG	1:B:327:ILE:CG2	2.61	0.77
1:B:64:PRO:HD2	1:B:81:GLY:O	1.84	0.77
1:C:147:HIS:CE1	1:C:163:ASP:HB3	2.19	0.77
1:A:177:ASP:HB3	1:B:53:GLN:CA	2.14	0.77
1:A:420:LEU:CD2	1:A:452:VAL:HG13	2.11	0.77
1:A:52:ILE:HD12	1:A:112:MET:SD	2.25	0.77
1:B:52:ILE:HD12	1:B:112:MET:SD	2.25	0.77
1:C:420:LEU:HD21	1:C:452:VAL:HG22	1.66	0.77
1:A:129:GLY:O	1:B:109:GLU:HG2	1.85	0.77
1:A:55:MET:HG3	1:A:57:PHE:HE2	1.48	0.77
1:A:11:ILE:HD11	1:A:324:LEU:HB3	1.65	0.77
1:A:88:TYR:CZ	1:B:373:ILE:O	2.38	0.77
1:B:11:ILE:HD11	1:B:324:LEU:CB	2.15	0.77
1:A:145:TYR:CE2	1:B:9:GLN:CG	2.53	0.77
1:A:147:HIS:CE1	1:A:163:ASP:HB3	2.19	0.77
1:A:243:GLN:HA	1:A:249:VAL:HG11	1.67	0.77
1:A:420:LEU:HD21	1:A:452:VAL:HG22	1.66	0.77
1:B:147:HIS:CE1	1:B:163:ASP:HB3	2.19	0.77
1:A:11:ILE:HD11	1:A:324:LEU:CB	2.15	0.77
1:B:243:GLN:HA	1:B:249:VAL:HG11	1.67	0.77
1:B:249:VAL:HG22	1:B:289:LEU:HD12	1.67	0.77
1:A:194:LEU:HA	1:B:403:GLN:HG2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLN:HA	1:C:85:THR:HG22	1.67	0.77
1:A:122:HIS:ND1	1:A:173:LEU:HD22	1.99	0.76
1:A:380:VAL:HG13	1:A:381:THR:H	1.50	0.76
1:B:42:TRP:NE1	1:B:62:ILE:HD11	2.00	0.76
1:C:11:ILE:HD11	1:C:324:LEU:CB	2.14	0.76
1:A:85:THR:O	1:A:85:THR:HG23	1.84	0.76
1:A:84:GLN:NE2	1:B:375:LYS:HZ1	1.81	0.76
1:A:219:TYR:CD2	1:B:473:ILE:HG13	2.20	0.76
1:B:400:ASP:HB2	1:C:194:LEU:O	1.84	0.76
1:A:68:GLN:HA	1:A:85:THR:HG22	1.67	0.76
1:B:422:LEU:HD11	1:C:221:LYS:CD	2.14	0.76
1:C:243:GLN:HA	1:C:249:VAL:HG11	1.68	0.76
1:C:85:THR:HG23	1:C:85:THR:O	1.84	0.76
1:C:129:GLY:O	1:C:132:VAL:HB	1.86	0.76
1:B:129:GLY:O	1:B:132:VAL:HB	1.86	0.76
1:B:51:TYR:OH	1:B:332:GLU:HG3	1.86	0.76
1:B:85:THR:HG23	1:B:85:THR:O	1.84	0.76
1:C:188:TYR:HE1	1:C:218:GLY:CA	1.98	0.76
1:C:249:VAL:HG22	1:C:289:LEU:HD12	1.67	0.76
1:A:16:THR:HG21	1:A:42:TRP:NE1	2.00	0.76
1:A:436:VAL:HG13	1:A:437:ILE:CG1	2.16	0.76
1:A:87:ILE:HD13	1:B:374:SER:OG	1.84	0.76
1:B:188:TYR:HE1	1:B:218:GLY:CA	1.98	0.76
1:B:55:MET:HG3	1:B:57:PHE:HE2	1.48	0.76
1:A:60:ILE:HD12	1:A:107:LEU:HD13	1.68	0.76
1:A:341:PRO:HD2	1:A:342:ALA:N	1.88	0.76
1:A:196:SER:O	1:B:466:GLU:OE1	2.02	0.76
1:C:52:ILE:HD12	1:C:112:MET:SD	2.25	0.76
1:B:389:ASP:N	1:C:244:ASN:OD1	2.18	0.76
1:A:219:TYR:CD1	1:B:473:ILE:N	2.40	0.76
1:B:383:LYS:HG2	1:C:113:TYR:CE1	2.21	0.76
1:B:399:THR:HG22	1:C:196:SER:CA	2.16	0.76
1:B:449:ASN:N	1:C:184:LYS:HZ2	1.82	0.76
1:B:277:ASN:CB	1:C:7:ARG:CZ	2.46	0.76
1:B:380:VAL:HG13	1:B:381:THR:H	1.50	0.76
1:A:197:ASN:C	1:B:467:LYS:HE3	2.06	0.76
1:C:60:ILE:HD12	1:C:107:LEU:HD13	1.68	0.76
1:C:436:VAL:HG13	1:C:437:ILE:CG1	2.16	0.76
1:C:465:THR:HA	1:C:468:LEU:CD1	2.16	0.76
1:A:129:GLY:O	1:A:132:VAL:HB	1.86	0.75
1:A:205:ILE:CA	1:B:471:SER:HA	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LEU:HD22	1:C:407:ILE:CD1	2.16	0.75
1:C:42:TRP:NE1	1:C:62:ILE:HD11	2.00	0.75
1:A:190:TRP:CZ2	1:B:375:LYS:CB	2.58	0.75
1:A:435:GLU:HB2	1:A:440:THR:HB	1.67	0.75
1:B:161:VAL:HG23	1:B:210:HIS:CD2	2.22	0.75
1:A:182:VAL:HB	1:B:10:SER:O	1.86	0.75
1:A:188:TYR:HE1	1:A:218:GLY:CA	1.98	0.75
1:A:188:TYR:CE1	1:A:218:GLY:HA3	2.15	0.75
1:A:249:VAL:HG22	1:A:289:LEU:HD12	1.67	0.75
1:C:51:TYR:OH	1:C:332:GLU:HG3	1.86	0.75
1:A:215:PHE:HE1	1:B:472:LYS:HB2	1.51	0.75
1:A:222:ALA:HB2	1:B:368:ILE:CD1	2.06	0.75
1:A:42:TRP:NE1	1:A:62:ILE:HD11	2.00	0.75
1:B:410:ASN:HB3	1:B:454:MET:HE1	1.66	0.75
1:B:420:LEU:HD21	1:B:452:VAL:HG22	1.66	0.75
1:C:307:ASP:HB2	1:C:413:ALA:HB2	1.67	0.75
1:C:68:GLN:HA	1:C:85:THR:CG2	2.16	0.75
1:A:51:TYR:OH	1:A:332:GLU:HG3	1.86	0.75
1:B:399:THR:HB	1:C:196:SER:HA	1.67	0.75
1:B:436:VAL:HG13	1:B:437:ILE:CG1	2.16	0.75
1:A:179:THR:OG1	1:B:52:ILE:HG13	1.87	0.75
1:A:319:ILE:HA	1:A:325:PRO:HB2	1.66	0.75
1:A:396:ARG:NH1	1:A:404:ILE:HD11	2.01	0.75
1:A:465:THR:HA	1:A:468:LEU:CD1	2.16	0.75
1:B:382:TYR:O	1:C:2:THR:CB	2.34	0.75
1:B:307:ASP:HB2	1:B:413:ALA:HB2	1.67	0.75
1:B:320:LEU:HD22	1:B:407:ILE:CD1	2.17	0.75
1:C:123:MET:HE3	1:C:140:PHE:HE1	1.50	0.75
1:C:161:VAL:HG23	1:C:210:HIS:CD2	2.21	0.75
1:B:449:ASN:CA	1:C:184:LYS:NZ	2.49	0.75
1:C:435:GLU:HB2	1:C:440:THR:HB	1.67	0.75
1:A:180:LYS:CE	1:B:57:PHE:CG	2.68	0.75
1:A:194:LEU:HD22	1:B:375:LYS:CB	2.17	0.75
1:A:212:GLN:HE22	1:B:53:GLN:C	1.61	0.75
1:B:195:VAL:CG2	1:B:200:ILE:HB	2.13	0.75
1:B:68:GLN:HA	1:B:85:THR:CG2	2.16	0.75
1:A:190:TRP:CZ2	1:B:374:SER:CB	2.70	0.74
1:A:307:ASP:HB2	1:A:413:ALA:HB2	1.67	0.74
1:A:320:LEU:HD22	1:A:407:ILE:CD1	2.16	0.74
1:B:206:ASP:HA	1:B:230:GLU:CG	2.17	0.74
1:A:84:GLN:NE2	1:B:375:LYS:HZ2	1.77	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:THR:HA	1:B:468:LEU:CD1	2.16	0.74
1:B:60:ILE:HD12	1:B:107:LEU:HD13	1.68	0.74
1:A:145:TYR:HE2	1:B:9:GLN:HB2	1.47	0.74
1:A:68:GLN:HA	1:A:85:THR:CG2	2.16	0.74
1:B:191:VAL:HG11	1:B:219:TYR:OH	1.86	0.74
1:C:396:ARG:NH1	1:C:404:ILE:HD11	2.01	0.74
1:A:188:TYR:N	1:B:367:ALA:C	2.32	0.74
1:B:310:LEU:O	1:B:314:VAL:HG12	1.87	0.74
1:A:196:SER:HB3	1:B:403:GLN:CG	2.13	0.74
1:A:205:ILE:HD13	1:B:472:LYS:CA	2.18	0.74
1:B:56:GLY:HA3	1:B:366:ASN:HB3	1.69	0.74
1:C:410:ASN:HB3	1:C:454:MET:HE1	1.68	0.74
1:B:383:LYS:CG	1:C:6:TRP:NE1	2.45	0.74
1:A:373:ILE:CG2	1:A:377:THR:HG22	2.18	0.74
1:C:14:LEU:HD12	1:C:62:ILE:CG2	2.17	0.74
1:B:238:TYR:CA	1:C:376:ASP:CB	2.65	0.74
1:B:277:ASN:HB2	1:C:7:ARG:CZ	2.15	0.74
1:A:161:VAL:HG23	1:A:210:HIS:CD2	2.22	0.74
1:B:435:GLU:HB2	1:B:440:THR:HB	1.67	0.74
1:C:373:ILE:CG2	1:C:377:THR:HG22	2.18	0.74
1:B:14:LEU:HD12	1:B:62:ILE:CG2	2.17	0.74
1:A:310:LEU:O	1:A:314:VAL:HG12	1.88	0.74
1:C:152:ILE:CD1	1:C:166:LEU:HG	2.18	0.74
1:A:180:LYS:HZ1	1:B:11:ILE:HA	1.51	0.74
1:A:190:TRP:HH2	1:B:375:LYS:HZ2	1.35	0.74
1:A:200:ILE:CD1	1:B:467:LYS:HZ3	1.96	0.74
1:B:55:MET:HG3	1:B:57:PHE:CE2	2.23	0.74
1:B:276:ILE:O	1:C:4:ALA:HB2	1.88	0.74
1:A:206:ASP:HA	1:A:230:GLU:CG	2.17	0.74
1:A:194:LEU:CG	1:B:375:LYS:HB3	2.18	0.74
1:B:386:TYR:CD2	1:C:288:LEU:HD11	2.21	0.74
1:A:197:ASN:O	1:B:467:LYS:HE3	1.86	0.74
1:A:163:ASP:HA	1:B:53:GLN:OE1	1.87	0.74
1:C:191:VAL:HG11	1:C:219:TYR:OH	1.87	0.74
1:C:55:MET:HG3	1:C:57:PHE:CE2	2.22	0.74
1:C:56:GLY:HA3	1:C:366:ASN:HB3	1.68	0.74
1:A:163:ASP:HB3	1:B:53:GLN:OE1	1.87	0.74
1:A:216:TRP:CZ2	1:B:478:SER:OXT	2.41	0.74
1:A:218:GLY:H	1:B:364:SER:CB	2.00	0.74
1:B:274:ASN:HA	1:C:286:SER:N	2.02	0.73
1:A:205:ILE:CD1	1:B:472:LYS:HA	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:THR:CA	1:C:186:GLU:O	2.36	0.73
1:A:200:ILE:HG21	1:B:467:LYS:C	2.09	0.73
1:B:468:LEU:HD23	1:B:473:ILE:CG1	2.18	0.73
1:C:206:ASP:HA	1:C:230:GLU:CG	2.17	0.73
1:C:468:LEU:HD23	1:C:473:ILE:CG1	2.18	0.73
1:A:11:ILE:HB	1:A:326:ILE:HA	1.70	0.73
1:B:152:ILE:CD1	1:B:166:LEU:HG	2.18	0.73
1:B:277:ASN:HD22	1:C:286:SER:HB3	1.52	0.73
1:B:319:ILE:HA	1:B:325:PRO:HB2	1.66	0.73
1:B:383:LYS:HZ3	1:C:6:TRP:H	1.33	0.73
1:C:12:TYR:HE1	1:C:14:LEU:HD23	1.54	0.73
1:B:422:LEU:CD1	1:C:221:LYS:CG	2.35	0.73
1:B:11:ILE:HB	1:B:326:ILE:HA	1.70	0.73
1:A:14:LEU:HD12	1:A:62:ILE:CG2	2.17	0.73
1:A:204:ARG:CG	1:A:228:ILE:HB	2.18	0.73
1:A:55:MET:HG3	1:A:57:PHE:CE2	2.23	0.73
1:B:83:TRP:CH2	1:B:171:VAL:HG21	2.24	0.73
1:C:204:ARG:CG	1:C:228:ILE:HB	2.18	0.73
1:C:310:LEU:O	1:C:314:VAL:HG12	1.88	0.73
1:C:382:TYR:CD1	1:C:397:LYS:HA	2.24	0.73
1:B:213:LYS:CE	1:C:375:LYS:CG	2.66	0.73
1:A:222:ALA:HA	1:B:368:ILE:HD11	0.76	0.73
1:B:381:THR:HG21	1:C:201:ASP:OD1	1.88	0.73
1:B:407:ILE:CG2	1:B:461:VAL:HG22	2.10	0.73
1:A:115:MET:CE	1:B:470:GLY:HA3	2.17	0.73
1:A:152:ILE:CD1	1:A:166:LEU:HG	2.18	0.73
1:A:56:GLY:HA3	1:A:366:ASN:HB3	1.69	0.73
1:C:123:MET:CB	1:C:174:PRO:HG2	2.19	0.73
1:C:234:GLY:HA2	1:C:253:PRO:CD	2.18	0.73
1:B:383:LYS:NZ	1:C:5:ASP:HB3	2.00	0.73
1:A:123:MET:CB	1:A:174:PRO:HG2	2.19	0.73
1:A:143:GLN:CD	1:B:108:HIS:CG	2.61	0.73
1:A:316:ALA:O	1:A:320:LEU:HB2	1.89	0.73
1:B:238:TYR:C	1:C:376:ASP:HA	2.08	0.73
1:B:382:TYR:CD1	1:B:397:LYS:HA	2.24	0.73
1:C:319:ILE:HA	1:C:325:PRO:HB2	1.66	0.73
1:C:11:ILE:HB	1:C:326:ILE:HA	1.70	0.73
1:C:57:PHE:CZ	1:C:327:ILE:HG21	2.24	0.73
1:A:420:LEU:HD21	1:A:452:VAL:CG2	2.19	0.73
1:B:201:ASP:C	1:B:225:VAL:HG13	2.09	0.73
1:B:238:TYR:C	1:C:376:ASP:C	2.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLY:CA	1:B:478:SER:CA	2.52	0.73
1:A:468:LEU:HD23	1:A:473:ILE:CG1	2.18	0.73
1:A:57:PHE:CZ	1:A:327:ILE:HG21	2.24	0.73
1:B:123:MET:HE1	1:B:140:PHE:HE1	1.54	0.73
1:C:316:ALA:O	1:C:320:LEU:HB2	1.89	0.73
1:B:316:ALA:O	1:B:320:LEU:HB2	1.89	0.72
1:B:422:LEU:HD22	1:C:221:LYS:HZ2	1.46	0.72
1:A:83:TRP:CH2	1:A:171:VAL:HG21	2.24	0.72
1:A:219:TYR:HD1	1:B:472:LYS:C	1.91	0.72
1:A:201:ASP:C	1:A:225:VAL:HG13	2.09	0.72
1:A:234:GLY:HA2	1:A:253:PRO:CD	2.18	0.72
1:B:123:MET:CB	1:B:174:PRO:HG2	2.19	0.72
1:B:382:TYR:HD1	1:C:2:THR:CG2	1.93	0.72
1:C:49:LEU:HD23	1:C:110:ARG:HD2	1.70	0.72
1:A:189:ASP:O	1:B:463:TYR:HE2	1.72	0.72
1:A:211:VAL:HG13	1:A:212:GLN:N	2.04	0.72
1:A:382:TYR:CD1	1:A:397:LYS:HA	2.24	0.72
1:B:400:ASP:CA	1:C:192:GLY:O	2.37	0.72
1:C:201:ASP:C	1:C:225:VAL:HG13	2.09	0.72
1:C:83:TRP:CH2	1:C:171:VAL:HG21	2.24	0.72
1:B:422:LEU:CD1	1:C:221:LYS:HZ2	2.02	0.72
1:A:187:TRP:CZ3	1:B:374:SER:OG	2.43	0.72
1:A:188:TYR:OH	1:B:363:ALA:C	2.28	0.72
1:A:247:ASP:HA	1:B:475:SER:OG	1.89	0.72
1:B:57:PHE:CZ	1:B:327:ILE:HG21	2.24	0.72
1:A:373:ILE:HG23	1:A:377:THR:HG22	1.72	0.72
1:B:195:VAL:HG23	1:B:200:ILE:CB	2.15	0.72
1:B:280:LYS:O	1:C:7:ARG:HB2	1.89	0.72
1:B:371:TYR:CE2	1:B:473:ILE:HD11	2.25	0.72
1:A:143:GLN:O	1:B:112:MET:N	2.23	0.72
1:B:234:GLY:HA2	1:B:253:PRO:CD	2.18	0.72
1:B:408:LEU:O	1:B:408:LEU:HD22	1.90	0.72
1:C:195:VAL:HG23	1:C:200:ILE:CB	2.15	0.72
1:A:406:THR:HG21	1:A:425:ALA:CB	2.20	0.72
1:A:408:LEU:HD22	1:A:408:LEU:O	1.90	0.72
1:A:371:TYR:CE2	1:A:473:ILE:HD11	2.25	0.72
1:C:211:VAL:HG13	1:C:212:GLN:N	2.04	0.72
1:C:406:THR:HG21	1:C:425:ALA:CB	2.20	0.72
1:A:407:ILE:CG2	1:A:461:VAL:HG22	2.10	0.72
1:C:420:LEU:HD21	1:C:452:VAL:CG2	2.19	0.72
1:A:49:LEU:HD23	1:A:110:ARG:HD2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:HD2	1:B:12:TYR:CB	2.02	0.71
1:B:21:ARG:HG3	1:B:40:GLY:HA2	1.72	0.71
1:B:241:PRO:HB2	1:C:375:LYS:N	2.04	0.71
1:A:194:LEU:HD21	1:B:375:LYS:HG2	1.67	0.71
1:A:194:LEU:CA	1:B:403:GLN:CG	2.67	0.71
1:C:371:TYR:CE2	1:C:473:ILE:HD11	2.25	0.71
1:A:190:TRP:HZ3	1:B:371:TYR:HD1	1.33	0.71
1:B:12:TYR:HE1	1:B:14:LEU:HD23	1.53	0.71
1:B:208:VAL:CA	1:B:216:TRP:HZ2	2.03	0.71
1:A:205:ILE:HD12	1:B:478:SER:CA	2.21	0.71
1:C:373:ILE:HG23	1:C:377:THR:HG22	1.72	0.71
1:C:408:LEU:O	1:C:408:LEU:HD22	1.90	0.71
1:C:21:ARG:HG3	1:C:40:GLY:HA2	1.72	0.71
1:B:211:VAL:HG13	1:B:212:GLN:N	2.04	0.71
1:A:187:TRP:O	1:B:368:ILE:O	2.07	0.71
1:B:446:SER:HB2	1:C:181:ASP:OD1	1.90	0.71
1:A:294:GLU:OE2	1:A:300:ARG:HG3	1.90	0.71
1:B:229:GLY:CA	1:B:246:MET:HE1	2.19	0.71
1:B:382:TYR:HA	1:C:1:ALA:CB	2.10	0.71
1:B:406:THR:HG21	1:B:425:ALA:CB	2.20	0.71
1:B:45:ILE:CG2	1:B:103:LEU:HD21	2.21	0.71
1:B:49:LEU:HD23	1:B:110:ARG:HD2	1.70	0.71
1:A:468:LEU:HD23	1:A:473:ILE:CD1	2.21	0.71
1:A:180:LYS:HE2	1:B:11:ILE:O	1.86	0.71
1:B:294:GLU:OE2	1:B:300:ARG:HG3	1.90	0.71
1:B:420:LEU:HD21	1:B:452:VAL:CG2	2.19	0.71
1:A:178:THR:HA	1:B:52:ILE:HD12	1.73	0.71
1:C:468:LEU:HD23	1:C:473:ILE:CD1	2.21	0.71
1:C:61:TRP:HZ3	1:C:326:ILE:HG21	1.54	0.71
1:A:12:TYR:HE1	1:A:14:LEU:HD23	1.54	0.71
1:A:101:LYS:CG	1:A:198:TYR:HA	2.16	0.71
1:A:205:ILE:CG1	1:B:478:SER:CB	2.66	0.71
1:B:16:THR:OG1	1:B:94:TYR:HE1	1.73	0.71
1:B:399:THR:HG22	1:C:196:SER:C	2.11	0.71
1:A:224:GLY:CA	1:B:434:THR:OG1	2.23	0.71
1:B:381:THR:CG2	1:C:1:ALA:HB2	2.21	0.71
1:A:209:LYS:HB3	1:A:231:VAL:CG2	2.21	0.71
1:A:215:PHE:CD1	1:A:216:TRP:CE3	2.79	0.71
1:A:473:ILE:HG23	1:A:474:CYS:H	1.56	0.71
1:B:215:PHE:CD1	1:B:216:TRP:CE3	2.79	0.71
1:B:382:TYR:C	1:C:2:THR:HG23	2.11	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:HA	1:A:292:PHE:HZ	1.56	0.70
1:A:61:TRP:HZ3	1:A:326:ILE:HG21	1.54	0.70
1:C:294:GLU:OE2	1:C:300:ARG:HG3	1.90	0.70
1:A:200:ILE:HG21	1:B:467:LYS:CA	2.21	0.70
1:A:21:ARG:HG3	1:A:40:GLY:HA2	1.72	0.70
1:B:14:LEU:CD1	1:B:62:ILE:HG22	2.21	0.70
1:C:45:ILE:CG2	1:C:103:LEU:HD21	2.21	0.70
1:A:195:VAL:HA	1:A:200:ILE:CD1	2.20	0.70
1:A:211:VAL:HG11	1:A:216:TRP:NE1	2.06	0.70
1:B:209:LYS:HB3	1:B:231:VAL:CG2	2.21	0.70
1:B:274:ASN:C	1:C:286:SER:CB	2.57	0.70
1:C:215:PHE:CD1	1:C:216:TRP:CE3	2.79	0.70
1:C:473:ILE:HG23	1:C:474:CYS:H	1.56	0.70
1:A:14:LEU:CD1	1:A:62:ILE:HG22	2.22	0.70
1:A:227:CYS:CB	1:B:476:ASP:CA	2.69	0.70
1:B:116:VAL:HG11	1:B:200:ILE:HG23	1.73	0.70
1:A:180:LYS:C	1:B:57:PHE:H	1.93	0.70
1:C:179:THR:O	1:C:180:LYS:HB3	1.91	0.70
1:C:195:VAL:HA	1:C:200:ILE:CD1	2.20	0.70
1:B:386:TYR:CG	1:C:288:LEU:HD12	2.26	0.70
1:B:204:ARG:CG	1:B:228:ILE:HB	2.18	0.70
1:C:209:LYS:HB3	1:C:231:VAL:CG2	2.21	0.70
1:C:252:TYR:HA	1:C:292:PHE:HZ	1.56	0.70
1:C:341:PRO:CD	1:C:342:ALA:N	2.54	0.70
1:A:179:THR:O	1:A:180:LYS:HB3	1.91	0.70
1:A:45:ILE:CG2	1:A:103:LEU:HD21	2.21	0.70
1:A:64:PRO:HG3	1:A:82:TYR:CA	2.21	0.70
1:B:195:VAL:HA	1:B:200:ILE:CD1	2.20	0.70
1:B:209:LYS:HD2	1:B:232:LEU:O	1.92	0.70
1:B:11:ILE:HD13	1:B:324:LEU:HB3	1.73	0.70
1:C:258:LEU:HD21	1:C:314:VAL:CG2	2.21	0.70
1:C:11:ILE:HD13	1:C:324:LEU:HB3	1.73	0.70
1:A:165:TRP:HE1	1:B:110:ARG:CB	1.99	0.70
1:B:382:TYR:HE1	1:B:385:PRO:CD	2.04	0.70
1:C:211:VAL:HG11	1:C:216:TRP:NE1	2.07	0.70
1:A:116:VAL:HG11	1:A:200:ILE:HG23	1.73	0.70
1:A:209:LYS:HD2	1:A:232:LEU:O	1.92	0.70
1:A:11:ILE:HD13	1:A:324:LEU:HB3	1.73	0.70
1:A:189:ASP:CA	1:B:369:ARG:HA	2.21	0.70
1:A:221:LYS:HB2	1:B:436:VAL:CA	2.10	0.70
1:A:205:ILE:HB	1:B:478:SER:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:CA	1:A:216:TRP:HZ2	2.03	0.69
1:B:468:LEU:HD23	1:B:473:ILE:CD1	2.21	0.69
1:B:381:THR:HG22	1:C:1:ALA:CB	2.22	0.69
1:C:116:VAL:HG11	1:C:200:ILE:HG23	1.74	0.69
1:B:238:TYR:CA	1:C:376:ASP:HA	2.22	0.69
1:A:185:ASN:HB3	1:B:366:ASN:OD1	1.92	0.69
1:A:188:TYR:H	1:B:367:ALA:C	1.92	0.69
1:B:149:PHE:HA	1:B:165:TRP:CD1	2.27	0.69
1:C:12:TYR:CD2	1:C:52:ILE:HG22	2.27	0.69
1:B:447:ASP:CG	1:C:214:ASP:OD2	2.31	0.69
1:C:420:LEU:CD2	1:C:452:VAL:HG13	2.11	0.69
1:A:12:TYR:CD2	1:A:52:ILE:HG22	2.28	0.69
1:A:190:TRP:CZ2	1:B:374:SER:HB3	2.26	0.69
1:A:205:ILE:HD12	1:B:478:SER:C	2.11	0.69
1:A:221:LYS:CB	1:B:436:VAL:N	2.36	0.69
1:A:88:TYR:HE2	1:B:374:SER:N	1.90	0.69
1:B:152:ILE:HD13	1:B:166:LEU:HG	1.74	0.69
1:B:277:ASN:ND2	1:C:285:ASP:O	2.25	0.69
1:B:399:THR:O	1:C:192:GLY:O	2.09	0.69
1:B:422:LEU:HD11	1:C:221:LYS:CB	2.21	0.69
1:C:14:LEU:CD1	1:C:62:ILE:HG22	2.21	0.69
1:C:101:LYS:CG	1:C:198:TYR:HA	2.16	0.69
1:C:209:LYS:HD2	1:C:232:LEU:O	1.92	0.69
1:A:341:PRO:CD	1:A:342:ALA:N	2.54	0.69
1:A:87:ILE:O	1:A:88:TYR:HD2	1.75	0.69
1:A:215:PHE:HE1	1:B:472:LYS:CB	2.05	0.69
1:C:382:TYR:HE1	1:C:385:PRO:CD	2.04	0.69
1:A:146:PHE:H	1:B:112:MET:H	1.33	0.69
1:C:311:ALA:O	1:C:314:VAL:HG13	1.93	0.69
1:C:16:THR:OG1	1:C:94:TYR:HE1	1.73	0.69
1:B:216:TRP:HA	1:B:216:TRP:HE3	1.57	0.69
1:B:252:TYR:HA	1:B:292:PHE:HZ	1.56	0.69
1:B:341:PRO:CD	1:B:342:ALA:N	2.54	0.69
1:B:408:LEU:HD13	1:B:408:LEU:H	1.58	0.69
1:B:12:TYR:CD2	1:B:52:ILE:HG22	2.27	0.69
1:B:179:THR:O	1:B:180:LYS:HB3	1.91	0.69
1:B:386:TYR:CD1	1:C:288:LEU:CD1	2.74	0.69
1:C:229:GLY:CA	1:C:246:MET:HE1	2.22	0.69
1:A:216:TRP:HE3	1:A:216:TRP:HA	1.57	0.69
1:B:87:ILE:O	1:B:88:TYR:HD2	1.74	0.69
1:B:9:GLN:HG3	1:B:58:THR:CB	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ILE:HG21	1:C:103:LEU:HD11	1.75	0.69
1:A:382:TYR:HE1	1:A:385:PRO:CD	2.04	0.69
1:B:45:ILE:HG21	1:B:103:LEU:HD11	1.75	0.69
1:C:52:ILE:HG13	1:C:53:GLN:H	1.56	0.69
1:C:87:ILE:O	1:C:88:TYR:HD2	1.75	0.69
1:A:149:PHE:HA	1:A:165:TRP:CD1	2.27	0.69
1:A:182:VAL:CG2	1:B:10:SER:O	2.41	0.69
1:A:184:LYS:HD2	1:B:363:ALA:O	1.91	0.69
1:A:221:LYS:HG2	1:B:436:VAL:N	1.81	0.69
1:A:258:LEU:HD21	1:A:314:VAL:CG2	2.21	0.69
1:A:269:MET:HG3	1:A:393:ILE:HD11	1.75	0.69
1:A:52:ILE:HG13	1:A:53:GLN:N	2.08	0.69
1:A:52:ILE:HG13	1:A:53:GLN:H	1.56	0.69
1:B:123:MET:SD	1:B:137:PHE:HD1	2.16	0.69
1:B:294:GLU:CD	1:B:300:ARG:HG3	2.13	0.69
1:B:400:ASP:CB	1:C:194:LEU:C	2.62	0.69
1:C:216:TRP:CB	1:C:245:VAL:HG22	2.23	0.69
1:C:69:LEU:HB2	1:C:71:GLN:NE2	2.06	0.69
1:A:406:THR:HG21	1:A:425:ALA:HB1	1.75	0.69
1:B:311:ALA:O	1:B:314:VAL:HG13	1.93	0.69
1:A:198:TYR:HB2	1:B:467:LYS:HZ1	1.56	0.69
1:C:152:ILE:HD13	1:C:166:LEU:HG	1.74	0.69
1:C:294:GLU:CD	1:C:300:ARG:HG3	2.13	0.69
1:C:269:MET:HG3	1:C:393:ILE:HD11	1.75	0.69
1:C:406:THR:HG21	1:C:425:ALA:HB1	1.75	0.69
1:A:200:ILE:HD12	1:B:467:LYS:HG3	1.75	0.68
1:A:215:PHE:CD1	1:A:216:TRP:CZ3	2.82	0.68
1:B:273:TYR:CE1	1:B:386:TYR:HB2	2.28	0.68
1:B:269:MET:HG3	1:B:393:ILE:HD11	1.75	0.68
1:A:107:LEU:CA	1:A:110:ARG:HG2	2.14	0.68
1:A:179:THR:OG1	1:B:49:LEU:O	2.12	0.68
1:A:246:MET:CE	1:B:476:ASP:CG	2.62	0.68
1:A:311:ALA:O	1:A:314:VAL:HG13	1.93	0.68
1:A:69:LEU:HB2	1:A:71:GLN:NE2	2.06	0.68
1:B:161:VAL:HG23	1:B:210:HIS:HD2	1.58	0.68
1:B:215:PHE:CD1	1:B:216:TRP:CZ3	2.82	0.68
1:B:61:TRP:HZ3	1:B:326:ILE:HG21	1.54	0.68
1:B:426:SER:HA	1:C:188:TYR:CD1	2.28	0.68
1:C:215:PHE:CD1	1:C:216:TRP:CZ3	2.82	0.68
1:A:151:PHE:O	1:A:153:GLN:HG2	1.93	0.68
1:A:294:GLU:CD	1:A:300:ARG:HG3	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:OG1	1:A:94:TYR:HE1	1.73	0.68
1:B:211:VAL:HG11	1:B:216:TRP:NE1	2.06	0.68
1:B:386:TYR:CZ	1:C:288:LEU:CD1	2.76	0.68
1:C:149:PHE:HA	1:C:165:TRP:CD1	2.27	0.68
1:C:216:TRP:HA	1:C:216:TRP:HE3	1.57	0.68
1:C:408:LEU:H	1:C:408:LEU:HD13	1.58	0.68
1:C:52:ILE:HG13	1:C:53:GLN:N	2.08	0.68
1:A:116:VAL:O	1:B:469:ALA:HB3	1.91	0.68
1:A:152:ILE:HD13	1:A:166:LEU:HG	1.74	0.68
1:A:315:ALA:O	1:A:319:ILE:HG12	1.93	0.68
1:C:195:VAL:CG2	1:C:200:ILE:HB	2.13	0.68
1:C:273:TYR:CE1	1:C:386:TYR:HB2	2.29	0.68
1:A:382:TYR:OH	1:A:396:ARG:HG2	1.93	0.68
1:B:400:ASP:HA	1:C:193:SER:C	2.14	0.68
1:B:400:ASP:HB2	1:C:194:LEU:C	2.14	0.68
1:B:406:THR:HG21	1:B:425:ALA:HB1	1.75	0.68
1:A:208:VAL:N	1:B:472:LYS:CE	2.50	0.68
1:C:87:ILE:HG23	1:C:139:PRO:HG3	1.75	0.68
1:A:118:VAL:HB	1:B:471:SER:CB	2.18	0.68
1:A:178:THR:CA	1:B:52:ILE:HD12	2.22	0.68
1:A:205:ILE:N	1:B:471:SER:HA	1.81	0.68
1:A:216:TRP:CB	1:A:245:VAL:HG22	2.23	0.68
1:A:219:TYR:CD1	1:B:472:LYS:C	2.66	0.68
1:A:225:VAL:CG2	1:B:465:THR:HG22	2.22	0.68
1:A:321:ASN:CG	1:A:322:ASP:H	1.97	0.68
1:A:45:ILE:HG21	1:A:103:LEU:HD11	1.75	0.68
1:A:87:ILE:HG23	1:A:139:PRO:HG3	1.75	0.68
1:A:89:SER:O	1:A:90:LEU:HB2	1.92	0.68
1:A:180:LYS:HG3	1:B:12:TYR:CG	2.28	0.68
1:B:315:ALA:O	1:B:319:ILE:HG12	1.93	0.68
1:C:107:LEU:CA	1:C:110:ARG:HG2	2.14	0.68
1:B:446:SER:HB3	1:C:181:ASP:N	2.08	0.68
1:C:382:TYR:OH	1:C:396:ARG:HG2	1.93	0.68
1:A:227:CYS:HB2	1:B:476:ASP:N	2.08	0.68
1:B:151:PHE:O	1:B:153:GLN:HG2	1.93	0.68
1:B:28:ALA:HB3	1:B:348:TRP:HZ2	1.58	0.68
1:B:369:ARG:HB3	1:B:369:ARG:HH11	1.57	0.68
1:A:228:ILE:N	1:B:476:ASP:HB2	1.99	0.68
1:C:123:MET:SD	1:C:137:PHE:HD1	2.16	0.68
1:C:208:VAL:CG2	1:C:216:TRP:CE2	2.76	0.68
1:A:177:ASP:C	1:B:53:GLN:HA	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:C	1:B:467:LYS:HE3	2.14	0.68
1:A:408:LEU:H	1:A:408:LEU:HD13	1.58	0.68
1:A:408:LEU:HD21	1:A:452:VAL:CG2	2.23	0.68
1:A:88:TYR:CZ	1:B:373:ILE:CA	2.65	0.68
1:B:216:TRP:CB	1:B:245:VAL:HG22	2.23	0.68
1:B:69:LEU:HB2	1:B:71:GLN:NE2	2.06	0.68
1:C:151:PHE:O	1:C:153:GLN:HG2	1.93	0.68
1:B:385:PRO:HB3	1:C:226:TYR:N	2.09	0.68
1:B:180:LYS:HZ1	1:B:182:VAL:HB	1.58	0.68
1:A:200:ILE:CG2	1:B:467:LYS:CA	2.72	0.68
1:A:208:VAL:CG2	1:A:216:TRP:CE2	2.76	0.68
1:A:273:TYR:CE1	1:A:386:TYR:HB2	2.28	0.68
1:A:165:TRP:NE1	1:B:110:ARG:N	2.34	0.68
1:B:251:ASN:O	1:B:254:ILE:HG22	1.94	0.68
1:B:89:SER:O	1:B:90:LEU:HB2	1.92	0.68
1:C:251:ASN:O	1:C:254:ILE:HG22	1.94	0.68
1:C:321:ASN:CG	1:C:322:ASP:H	1.97	0.68
1:A:123:MET:SD	1:A:137:PHE:HD1	2.16	0.67
1:B:408:LEU:HD21	1:B:452:VAL:CG2	2.23	0.67
1:B:52:ILE:HG13	1:B:53:GLN:N	2.08	0.67
1:B:402:SER:N	1:C:193:SER:HA	2.08	0.67
1:C:408:LEU:HD21	1:C:452:VAL:CG2	2.23	0.67
1:A:385:PRO:HD2	1:A:396:ARG:O	1.94	0.67
1:C:161:VAL:HG23	1:C:210:HIS:HD2	1.58	0.67
1:A:251:ASN:O	1:A:254:ILE:HG22	1.94	0.67
1:B:205:ILE:HD12	1:B:208:VAL:CG2	2.25	0.67
1:A:215:PHE:CE2	1:B:367:ALA:HB1	2.29	0.67
1:B:87:ILE:HG23	1:B:139:PRO:HG3	1.75	0.67
1:C:111:GLY:O	1:C:112:MET:HB2	1.94	0.67
1:A:221:LYS:O	1:B:434:THR:HG22	1.93	0.67
1:B:424:GLY:HA3	1:C:220:ASN:HB3	0.83	0.67
1:C:385:PRO:HD2	1:C:396:ARG:O	1.94	0.67
1:C:64:PRO:HG3	1:C:82:TYR:CA	2.21	0.67
1:B:101:LYS:CG	1:B:198:TYR:HA	2.16	0.67
1:B:396:ARG:C	1:C:224:GLY:HA3	2.15	0.67
1:C:315:ALA:O	1:C:319:ILE:HG12	1.93	0.67
1:C:369:ARG:HB3	1:C:369:ARG:HH11	1.57	0.67
1:A:177:ASP:OD1	1:B:53:GLN:O	2.12	0.67
1:A:145:TYR:CE1	1:B:9:GLN:OE1	2.23	0.67
1:B:280:LYS:O	1:C:6:TRP:C	2.32	0.67
1:A:239:THR:HG21	1:A:253:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HB3	1:A:369:ARG:HH11	1.57	0.67
1:C:205:ILE:HD12	1:C:208:VAL:CG2	2.24	0.67
1:B:274:ASN:C	1:C:286:SER:CA	2.59	0.67
1:B:64:PRO:HG3	1:B:82:TYR:CA	2.21	0.67
1:C:28:ALA:HB3	1:C:348:TRP:HZ2	1.58	0.67
1:A:190:TRP:CE3	1:A:191:VAL:CG1	2.78	0.67
1:A:251:ASN:OD1	1:A:254:ILE:HD12	1.95	0.67
1:B:208:VAL:CG2	1:B:216:TRP:CE2	2.76	0.67
1:B:321:ASN:CG	1:B:322:ASP:H	1.97	0.67
1:B:449:ASN:HB2	1:C:184:LYS:HZ2	1.57	0.67
1:C:89:SER:O	1:C:90:LEU:HB2	1.92	0.67
1:A:165:TRP:NE1	1:B:110:ARG:CB	2.58	0.66
1:A:184:LYS:HB2	1:B:363:ALA:O	1.94	0.66
1:B:176:LEU:HD22	1:B:187:TRP:HE1	1.59	0.66
1:B:182:VAL:O	1:B:186:GLU:HB3	1.95	0.66
1:A:180:LYS:CG	1:B:327:ILE:HG21	2.23	0.66
1:C:211:VAL:CB	1:C:216:TRP:CZ2	2.78	0.66
1:B:238:TYR:HA	1:C:376:ASP:CG	2.14	0.66
1:A:147:HIS:ND1	1:A:148:PRO:HD2	2.10	0.66
1:A:153:GLN:O	1:A:154:ASN:HB3	1.95	0.66
1:A:200:ILE:HG22	1:A:203:LEU:CD1	2.25	0.66
1:C:382:TYR:CE1	1:C:397:LYS:HA	2.30	0.66
1:B:385:PRO:CD	1:C:3:PRO:HD2	2.25	0.66
1:B:200:ILE:HG22	1:B:203:LEU:CD1	2.25	0.66
1:C:236:PRO:HG3	1:C:278:THR:HG21	1.77	0.66
1:C:399:THR:HG22	1:C:400:ASP:H	1.60	0.66
1:A:140:PHE:CE2	1:A:176:LEU:HD21	2.31	0.66
1:A:194:LEU:HD13	1:B:375:LYS:CG	2.25	0.66
1:A:28:ALA:HB3	1:A:348:TRP:HZ2	1.58	0.66
1:C:147:HIS:ND1	1:C:148:PRO:HD2	2.10	0.66
1:C:182:VAL:O	1:C:186:GLU:HB3	1.95	0.66
1:A:176:LEU:HD22	1:A:187:TRP:HE1	1.59	0.66
1:A:205:ILE:HD12	1:A:208:VAL:CG2	2.25	0.66
1:A:211:VAL:CB	1:A:216:TRP:CZ2	2.78	0.66
1:B:385:PRO:HD2	1:B:396:ARG:O	1.94	0.66
1:C:200:ILE:HG22	1:C:203:LEU:CD1	2.25	0.66
1:C:362:ILE:O	1:C:366:ASN:HB2	1.96	0.66
1:A:111:GLY:O	1:A:112:MET:HB2	1.94	0.66
1:A:346:ALA:HB1	1:A:348:TRP:CE3	2.31	0.66
1:A:399:THR:HG22	1:A:400:ASP:H	1.60	0.66
1:B:111:GLY:O	1:B:112:MET:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:PHE:CE2	1:B:176:LEU:HD21	2.31	0.66
1:B:194:LEU:HG	1:B:200:ILE:HD13	1.78	0.66
1:B:258:LEU:O	1:B:262:PHE:HB2	1.95	0.66
1:C:140:PHE:CE2	1:C:176:LEU:HD21	2.31	0.66
1:C:239:THR:HG21	1:C:253:PRO:HD3	1.77	0.66
1:C:346:ALA:HB1	1:C:348:TRP:CE3	2.31	0.66
1:B:236:PRO:CB	1:C:380:VAL:CG1	2.74	0.66
1:A:258:LEU:O	1:A:262:PHE:HB2	1.95	0.66
1:B:190:TRP:CE3	1:B:191:VAL:CG1	2.78	0.66
1:B:211:VAL:CG2	1:B:215:PHE:HB3	2.26	0.66
1:C:83:TRP:NE1	1:C:173:LEU:HD21	2.03	0.66
1:C:251:ASN:OD1	1:C:254:ILE:HD12	1.95	0.66
1:A:185:ASN:OD1	1:B:369:ARG:CD	2.44	0.66
1:A:236:PRO:HG3	1:A:278:THR:HG21	1.77	0.66
1:A:379:PHE:CZ	1:A:397:LYS:HE3	2.31	0.66
1:B:187:TRP:CZ3	1:B:190:TRP:CZ3	2.84	0.66
1:B:382:TYR:CE1	1:B:397:LYS:HA	2.31	0.66
1:C:11:ILE:CG1	1:C:324:LEU:HD23	2.24	0.66
1:C:55:MET:O	1:C:362:ILE:HG22	1.96	0.66
1:A:182:VAL:O	1:A:186:GLU:HB3	1.95	0.66
1:B:379:PHE:CZ	1:B:397:LYS:HE3	2.31	0.66
1:A:208:VAL:CB	1:B:478:SER:OG	2.05	0.66
1:B:55:MET:O	1:B:362:ILE:HG22	1.96	0.66
1:A:180:LYS:CD	1:B:12:TYR:CB	2.65	0.66
1:A:211:VAL:CG2	1:A:215:PHE:HB3	2.26	0.66
1:C:153:GLN:O	1:C:154:ASN:HB3	1.95	0.66
1:C:211:VAL:CG2	1:C:215:PHE:HB3	2.26	0.66
1:A:55:MET:O	1:A:362:ILE:HG22	1.96	0.65
1:A:362:ILE:O	1:A:366:ASN:HB2	1.96	0.65
1:B:211:VAL:CB	1:B:216:TRP:CZ2	2.78	0.65
1:B:239:THR:HG21	1:B:253:PRO:HD3	1.76	0.65
1:B:243:GLN:HB3	1:B:284:PRO:CG	2.25	0.65
1:B:346:ALA:HB1	1:B:348:TRP:CE3	2.31	0.65
1:C:176:LEU:HD22	1:C:187:TRP:HE1	1.59	0.65
1:C:190:TRP:CE3	1:C:191:VAL:CG1	2.78	0.65
1:C:243:GLN:HB3	1:C:284:PRO:CG	2.25	0.65
1:B:251:ASN:OD1	1:B:254:ILE:HD12	1.95	0.65
1:A:222:ALA:HB1	1:B:368:ILE:HG13	0.65	0.65
1:A:195:VAL:HG11	1:B:464:PRO:O	1.96	0.65
1:A:147:HIS:CA	1:B:110:ARG:C	2.48	0.65
1:B:410:ASN:HB3	1:B:454:MET:CE	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ILE:HG21	1:C:326:ILE:HG12	1.78	0.65
1:A:115:MET:HE1	1:B:470:GLY:HA3	1.78	0.65
1:A:243:GLN:HB3	1:A:284:PRO:CG	2.25	0.65
1:A:305:THR:HG23	1:A:307:ASP:OD2	1.97	0.65
1:B:236:PRO:HG3	1:B:278:THR:HG21	1.77	0.65
1:B:305:THR:HG23	1:B:307:ASP:OD2	1.97	0.65
1:B:385:PRO:HA	1:C:3:PRO:CB	2.27	0.65
1:B:472:LYS:O	1:B:473:ILE:HG22	1.97	0.65
1:A:332:GLU:HG2	1:A:333:GLN:H	1.62	0.65
1:B:124:GLY:N	1:B:174:PRO:HD2	2.12	0.65
1:B:147:HIS:ND1	1:B:148:PRO:HD2	2.10	0.65
1:B:153:GLN:O	1:B:154:ASN:HB3	1.95	0.65
1:A:87:ILE:CG1	1:B:374:SER:HA	2.11	0.65
1:A:191:VAL:O	1:B:467:LYS:HB3	1.97	0.65
1:A:186:GLU:CA	1:B:369:ARG:HH11	2.10	0.65
1:A:194:LEU:HG	1:A:200:ILE:HD13	1.78	0.65
1:A:213:LYS:O	1:A:214:ASP:HB3	1.97	0.65
1:A:341:PRO:HD2	1:A:342:ALA:H	1.59	0.65
1:C:194:LEU:HG	1:C:200:ILE:HD13	1.78	0.65
1:A:148:PRO:HA	1:B:107:LEU:N	2.09	0.65
1:A:218:GLY:CA	1:B:364:SER:HB3	2.27	0.65
1:A:11:ILE:HG21	1:A:326:ILE:HG12	1.78	0.65
1:C:379:PHE:CZ	1:C:397:LYS:HE3	2.31	0.65
1:A:187:TRP:CZ3	1:A:190:TRP:CZ3	2.84	0.65
1:B:385:PRO:HB3	1:C:226:TYR:HA	1.79	0.65
1:B:238:TYR:CD2	1:C:403:GLN:NE2	2.64	0.65
1:A:352:TYR:C	1:A:354:THR:H	1.99	0.65
1:A:410:ASN:HB3	1:A:454:MET:CE	2.26	0.65
1:C:187:TRP:CZ3	1:C:190:TRP:CZ3	2.84	0.65
1:C:258:LEU:O	1:C:262:PHE:HB2	1.95	0.65
1:A:382:TYR:CE1	1:A:397:LYS:HA	2.30	0.65
1:B:11:ILE:HD12	1:B:325:PRO:C	2.17	0.65
1:A:205:ILE:CG2	1:B:472:LYS:N	2.59	0.65
1:C:124:GLY:N	1:C:174:PRO:HD2	2.12	0.65
1:A:11:ILE:CG1	1:A:324:LEU:HD23	2.24	0.64
1:B:258:LEU:HD21	1:B:314:VAL:CG2	2.21	0.64
1:C:332:GLU:HG2	1:C:333:GLN:H	1.62	0.64
1:C:410:ASN:HB3	1:C:454:MET:CE	2.26	0.64
1:A:145:TYR:CE1	1:B:113:TYR:CD2	2.84	0.64
1:A:161:VAL:HG23	1:A:210:HIS:HD2	1.58	0.64
1:A:226:TYR:HA	1:A:247:ASP:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:TYR:CE2	1:C:139:PRO:HB3	2.32	0.64
1:C:341:PRO:HD2	1:C:342:ALA:H	1.59	0.64
1:C:78:ALA:O	1:C:81:GLY:HA2	1.97	0.64
1:A:11:ILE:HD11	1:A:324:LEU:CA	2.28	0.64
1:A:88:TYR:CE2	1:A:139:PRO:HB3	2.32	0.64
1:B:385:PRO:CA	1:C:3:PRO:HG3	2.27	0.64
1:A:124:GLY:N	1:A:174:PRO:HD2	2.12	0.64
1:A:229:GLY:HA3	1:A:246:MET:HE1	1.73	0.64
1:B:88:TYR:CE2	1:B:139:PRO:HB3	2.32	0.64
1:C:87:ILE:O	1:C:88:TYR:CD2	2.51	0.64
1:A:216:TRP:CE3	1:A:216:TRP:HA	2.33	0.64
1:B:213:LYS:O	1:B:214:ASP:HB3	1.97	0.64
1:A:220:ASN:C	1:B:473:ILE:HG23	2.18	0.64
1:B:87:ILE:O	1:B:88:TYR:CD2	2.51	0.64
1:A:197:ASN:ND2	1:C:196:SER:OG	2.19	0.64
1:B:213:LYS:CE	1:C:375:LYS:HG3	2.27	0.64
1:A:83:TRP:NE1	1:A:173:LEU:HD21	2.03	0.64
1:A:196:SER:OG	1:C:193:SER:HA	1.97	0.64
1:B:226:TYR:HA	1:B:247:ASP:OD1	1.98	0.64
1:B:11:ILE:HG21	1:B:326:ILE:HG12	1.78	0.64
1:C:11:ILE:HD11	1:C:324:LEU:CA	2.27	0.64
1:C:11:ILE:HD12	1:C:325:PRO:C	2.17	0.64
1:B:237:ALA:CA	1:C:379:PHE:H	2.06	0.64
1:B:332:GLU:HG2	1:B:333:GLN:H	1.62	0.64
1:C:216:TRP:HA	1:C:216:TRP:CE3	2.33	0.64
1:B:422:LEU:HD13	1:C:221:LYS:HZ2	1.62	0.64
1:B:388:LYS:CA	1:C:244:ASN:O	2.42	0.64
1:B:11:ILE:HD11	1:B:324:LEU:CA	2.28	0.64
1:B:216:TRP:HA	1:B:216:TRP:CE3	2.33	0.64
1:B:385:PRO:N	1:C:3:PRO:HD2	1.65	0.64
1:B:78:ALA:O	1:B:81:GLY:HA2	1.97	0.64
1:C:115:MET:HE1	1:C:228:ILE:HG13	1.80	0.64
1:C:226:TYR:HA	1:C:247:ASP:OD1	1.97	0.64
1:C:383:LYS:O	1:C:385:PRO:HD3	1.97	0.64
1:A:252:TYR:HA	1:A:292:PHE:CZ	2.33	0.64
1:A:11:ILE:CD1	1:A:326:ILE:HG12	2.26	0.64
1:A:55:MET:SD	1:A:362:ILE:HD13	2.38	0.64
1:A:458:LEU:HD13	1:A:460:ARG:HH22	1.62	0.64
1:A:11:ILE:HB	1:A:326:ILE:HG12	1.79	0.64
1:A:190:TRP:CE3	1:B:371:TYR:CG	2.86	0.64
1:A:292:PHE:O	1:A:293:VAL:HG12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:O	1:A:81:GLY:HA2	1.96	0.64
1:A:87:ILE:O	1:A:88:TYR:CD2	2.51	0.64
1:B:83:TRP:NE1	1:B:173:LEU:HD21	2.03	0.64
1:B:11:ILE:CD1	1:B:326:ILE:HG12	2.26	0.64
1:B:430:GLY:CA	1:C:185:ASN:ND2	2.61	0.64
1:C:208:VAL:CA	1:C:216:TRP:HZ2	2.03	0.64
1:C:213:LYS:O	1:C:214:ASP:HB3	1.97	0.64
1:C:305:THR:HG23	1:C:307:ASP:OD2	1.97	0.64
1:B:383:LYS:CD	1:C:5:ASP:CB	2.73	0.64
1:A:383:LYS:O	1:A:385:PRO:HD3	1.97	0.63
1:B:172:SER:O	1:B:174:PRO:HD3	1.97	0.63
1:B:251:ASN:HB3	1:B:254:ILE:CG2	2.28	0.63
1:B:274:ASN:O	1:C:286:SER:OG	2.15	0.63
1:A:221:LYS:C	1:B:434:THR:CG2	2.66	0.63
1:C:11:ILE:HB	1:C:326:ILE:HG12	1.79	0.63
1:C:292:PHE:O	1:C:293:VAL:HG12	1.98	0.63
1:B:280:LYS:HB2	1:C:3:PRO:O	1.95	0.63
1:C:472:LYS:O	1:C:473:ILE:HG22	1.97	0.63
1:A:11:ILE:HD12	1:A:325:PRO:C	2.17	0.63
1:A:225:VAL:O	1:A:225:VAL:HG12	1.98	0.63
1:B:292:PHE:O	1:B:293:VAL:HG12	1.98	0.63
1:B:11:ILE:HB	1:B:326:ILE:HG12	1.79	0.63
1:A:182:VAL:N	1:B:57:PHE:CG	2.58	0.63
1:C:252:TYR:HA	1:C:292:PHE:CZ	2.33	0.63
1:C:473:ILE:CG2	1:C:474:CYS:H	2.10	0.63
1:C:45:ILE:CG2	1:C:49:LEU:HD11	2.06	0.63
1:B:252:TYR:HA	1:B:292:PHE:CZ	2.33	0.63
1:C:55:MET:SD	1:C:362:ILE:HD13	2.38	0.63
1:A:473:ILE:CG2	1:A:474:CYS:H	2.10	0.63
1:A:68:GLN:HE22	1:A:81:GLY:HA2	1.62	0.63
1:A:165:TRP:NE1	1:B:110:ARG:CA	1.78	0.63
1:B:383:LYS:O	1:B:385:PRO:HD3	1.97	0.63
1:B:458:LEU:HD13	1:B:460:ARG:HH22	1.62	0.63
1:C:75:TYR:HE1	1:C:170:THR:CG2	2.12	0.63
1:A:75:TYR:HE1	1:A:170:THR:CG2	2.12	0.63
1:A:472:LYS:O	1:A:473:ILE:HG22	1.97	0.63
1:A:68:GLN:O	1:A:85:THR:HG21	1.99	0.63
1:B:371:TYR:CD2	1:B:473:ILE:HD11	2.34	0.63
1:C:11:ILE:CD1	1:C:326:ILE:HG12	2.26	0.63
1:B:238:TYR:N	1:C:376:ASP:C	2.34	0.63
1:B:75:TYR:CE1	1:B:170:THR:HG21	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ILE:HG23	1:B:388:LYS:H	1.63	0.63
1:A:200:ILE:HG22	1:B:468:LEU:N	2.14	0.63
1:C:387:ILE:HG23	1:C:388:LYS:H	1.63	0.63
1:C:458:LEU:HD13	1:C:460:ARG:HH22	1.62	0.63
1:A:55:MET:HB3	1:A:57:PHE:CE2	2.34	0.63
1:A:187:TRP:CB	1:B:367:ALA:O	2.47	0.63
1:A:224:GLY:CA	1:B:434:THR:CB	2.72	0.63
1:B:55:MET:SD	1:B:362:ILE:HD13	2.38	0.63
1:C:172:SER:O	1:C:174:PRO:HD3	1.98	0.63
1:A:287:THR:HG21	1:A:380:VAL:C	2.20	0.63
1:A:387:ILE:HG23	1:A:388:LYS:H	1.63	0.63
1:B:383:LYS:C	1:C:3:PRO:CD	2.59	0.63
1:B:75:TYR:HE1	1:B:170:THR:CG2	2.12	0.63
1:C:371:TYR:CD2	1:C:473:ILE:HD11	2.34	0.63
1:A:177:ASP:CB	1:B:53:GLN:HG2	2.27	0.63
1:A:194:LEU:HD22	1:B:375:LYS:HG2	0.68	0.63
1:A:214:ASP:CG	1:B:360:LYS:O	2.36	0.63
1:A:143:GLN:NE2	1:B:108:HIS:HA	2.12	0.63
1:B:2:THR:HB	1:B:3:PRO:CD	2.22	0.63
1:B:341:PRO:HD2	1:B:342:ALA:H	1.59	0.63
1:A:197:ASN:CA	1:B:467:LYS:HE3	2.28	0.63
1:B:45:ILE:CG2	1:B:49:LEU:HD11	2.06	0.63
1:C:225:VAL:O	1:C:225:VAL:HG12	1.98	0.63
1:C:287:THR:HG21	1:C:380:VAL:C	2.20	0.63
1:B:238:TYR:CB	1:C:376:ASP:CG	2.65	0.63
1:C:55:MET:HB3	1:C:57:PHE:CE2	2.34	0.63
1:C:68:GLN:O	1:C:85:THR:HG21	1.99	0.63
1:C:68:GLN:HE22	1:C:81:GLY:HA2	1.62	0.63
1:A:45:ILE:CG2	1:A:49:LEU:HD11	2.06	0.62
1:A:143:GLN:OE1	1:B:112:MET:O	2.16	0.62
1:B:208:VAL:HG23	1:B:216:TRP:CZ2	2.34	0.62
1:B:238:TYR:CB	1:C:376:ASP:CB	2.76	0.62
1:B:229:GLY:HA3	1:B:246:MET:HE1	1.80	0.62
1:B:341:PRO:CD	1:B:342:ALA:H	2.12	0.62
1:A:208:VAL:CG2	1:B:478:SER:N	2.33	0.62
1:A:144:ASP:OD1	1:B:6:TRP:HH2	1.81	0.62
1:C:341:PRO:CD	1:C:342:ALA:H	2.12	0.62
1:A:217:PRO:C	1:B:473:ILE:O	2.37	0.62
1:A:341:PRO:CD	1:A:342:ALA:H	2.12	0.62
1:B:225:VAL:HG12	1:B:225:VAL:O	1.98	0.62
1:B:281:SER:CB	1:C:6:TRP:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLN:HE22	1:B:81:GLY:HA2	1.62	0.62
1:C:352:TYR:C	1:C:354:THR:H	1.99	0.62
1:A:418:TYR:CD1	1:A:454:MET:HE3	2.34	0.62
1:B:11:ILE:HD12	1:B:325:PRO:O	1.99	0.62
1:A:172:SER:O	1:A:174:PRO:HD3	1.98	0.62
1:A:177:ASP:HB3	1:B:53:GLN:CG	2.29	0.62
1:B:430:GLY:N	1:C:185:ASN:CB	2.58	0.62
1:C:208:VAL:HG23	1:C:216:TRP:CZ2	2.34	0.62
1:A:208:VAL:HG23	1:A:216:TRP:CZ2	2.34	0.62
1:A:217:PRO:HB2	1:B:437:ILE:C	2.20	0.62
1:A:371:TYR:CD2	1:A:473:ILE:HD11	2.34	0.62
1:A:52:ILE:O	1:A:55:MET:HB2	2.00	0.62
1:B:287:THR:HG21	1:B:380:VAL:C	2.20	0.62
1:B:383:LYS:HD2	1:C:5:ASP:CB	2.25	0.62
1:B:79:TYR:CE2	1:B:344:ARG:HG2	2.35	0.62
1:C:180:LYS:HD3	1:C:180:LYS:O	2.00	0.62
1:C:75:TYR:CE1	1:C:170:THR:HG21	2.34	0.62
1:A:186:GLU:CD	1:B:370:ASN:CA	2.59	0.62
1:A:11:ILE:HD12	1:A:325:PRO:O	1.99	0.62
1:B:274:ASN:O	1:C:286:SER:CB	2.46	0.62
1:B:69:LEU:CB	1:B:71:GLN:HE21	2.12	0.62
1:C:251:ASN:HB3	1:C:254:ILE:CG2	2.29	0.62
1:A:218:GLY:HA2	1:B:437:ILE:H	1.65	0.62
1:A:251:ASN:HB3	1:A:254:ILE:CG2	2.28	0.62
1:C:48:LYS:O	1:C:49:LEU:HB2	2.00	0.62
1:A:428:THR:HG23	1:A:431:GLN:HB2	1.82	0.62
1:B:180:LYS:O	1:B:180:LYS:HD3	2.00	0.62
1:B:383:LYS:HB3	1:C:6:TRP:CD1	2.15	0.62
1:A:75:TYR:CE1	1:A:170:THR:HG21	2.34	0.62
1:A:143:GLN:HG3	1:B:108:HIS:NE2	2.13	0.62
1:B:327:ILE:O	1:B:327:ILE:HG23	2.00	0.62
1:B:352:TYR:C	1:B:354:THR:H	1.99	0.62
1:A:148:PRO:HG3	1:B:49:LEU:HD23	1.82	0.62
1:B:238:TYR:N	1:C:377:THR:N	2.38	0.62
1:A:187:TRP:CZ3	1:B:374:SER:CB	2.82	0.62
1:B:387:ILE:CG2	1:B:395:MET:HA	2.28	0.62
1:B:428:THR:HG23	1:B:431:GLN:HB2	1.82	0.62
1:A:179:THR:CG2	1:B:50:ASP:O	2.48	0.62
1:B:381:THR:CG2	1:C:201:ASP:OD1	2.48	0.62
1:C:428:THR:HG23	1:C:431:GLN:HB2	1.82	0.62
1:A:180:LYS:NZ	1:B:11:ILE:CA	2.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:GLY:C	1:C:184:LYS:NZ	2.53	0.61
1:C:472:LYS:HG2	1:C:478:SER:OXT	2.01	0.61
1:A:79:TYR:CE2	1:A:344:ARG:HG2	2.35	0.61
1:B:332:GLU:HA	1:B:358:LEU:HB3	1.82	0.61
1:B:68:GLN:O	1:B:85:THR:HG21	1.99	0.61
1:C:258:LEU:HG	1:C:262:PHE:CD2	2.34	0.61
1:C:11:ILE:HD12	1:C:325:PRO:O	1.99	0.61
1:A:258:LEU:HG	1:A:262:PHE:CD2	2.34	0.61
1:A:2:THR:HB	1:A:3:PRO:CD	2.22	0.61
1:B:13:PHE:CD2	1:B:328:TYR:HD2	2.19	0.61
1:B:316:ALA:HA	1:B:319:ILE:HD11	1.82	0.61
1:A:217:PRO:HG2	1:B:364:SER:CB	2.28	0.61
1:A:239:THR:HG21	1:A:253:PRO:CD	2.31	0.61
1:A:48:LYS:O	1:A:49:LEU:HB2	2.00	0.61
1:B:258:LEU:HG	1:B:262:PHE:CD2	2.34	0.61
1:A:184:LYS:CE	1:B:362:ILE:HG22	2.17	0.61
1:B:472:LYS:HG2	1:B:478:SER:OXT	2.01	0.61
1:A:144:ASP:HB3	1:B:58:THR:O	1.99	0.61
1:C:52:ILE:CD1	1:C:112:MET:SD	2.88	0.61
1:B:385:PRO:HB3	1:C:226:TYR:H	1.65	0.61
1:B:382:TYR:CE1	1:C:2:THR:HG23	2.32	0.61
1:C:79:TYR:CE2	1:C:344:ARG:HG2	2.35	0.61
1:C:79:TYR:HE2	1:C:344:ARG:HG2	1.64	0.61
1:B:237:ALA:CB	1:C:379:PHE:CA	2.62	0.61
1:C:52:ILE:O	1:C:55:MET:HB2	2.00	0.61
1:A:11:ILE:HG22	1:A:326:ILE:HG23	1.83	0.61
1:A:200:ILE:HB	1:B:467:LYS:CA	2.23	0.61
1:B:52:ILE:CD1	1:B:112:MET:SD	2.88	0.61
1:B:6:TRP:CH2	1:B:113:TYR:HB3	2.36	0.61
1:B:239:THR:HG21	1:B:253:PRO:CD	2.31	0.61
1:B:79:TYR:HE2	1:B:344:ARG:HG2	1.64	0.61
1:C:6:TRP:CH2	1:C:113:TYR:HB3	2.36	0.61
1:C:9:GLN:HG3	1:C:58:THR:CB	2.17	0.61
1:A:104:SER:O	1:A:108:HIS:HB2	2.00	0.61
1:A:472:LYS:HG2	1:A:478:SER:OXT	2.01	0.61
1:B:104:SER:O	1:B:108:HIS:HB2	2.00	0.61
1:C:104:SER:O	1:C:108:HIS:HB2	2.00	0.61
1:A:6:TRP:CH2	1:A:113:TYR:HB3	2.36	0.61
1:A:387:ILE:CG2	1:A:395:MET:HA	2.28	0.61
1:B:11:ILE:HG22	1:B:326:ILE:HG23	1.83	0.61
1:B:238:TYR:HD2	1:C:403:GLN:CD	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:CA	1:B:369:ARG:NH1	2.63	0.61
1:B:280:LYS:CE	1:B:383:LYS:HB3	2.04	0.61
1:C:13:PHE:CD2	1:C:328:TYR:HD2	2.19	0.61
1:C:472:LYS:O	1:C:473:ILE:HB	2.01	0.61
1:A:13:PHE:CD2	1:A:328:TYR:HD2	2.19	0.61
1:A:185:ASN:CB	1:B:366:ASN:OD1	2.49	0.61
1:C:332:GLU:HA	1:C:358:LEU:HB3	1.82	0.61
1:A:84:GLN:HE22	1:B:375:LYS:HZ3	1.40	0.61
1:B:55:MET:HB3	1:B:57:PHE:CE2	2.34	0.61
1:C:11:ILE:HG22	1:C:326:ILE:HG23	1.83	0.61
1:A:184:LYS:CG	1:B:56:GLY:CA	2.48	0.61
1:A:79:TYR:HE2	1:A:344:ARG:HG2	1.64	0.61
1:B:422:LEU:HD11	1:C:221:LYS:HG2	0.65	0.61
1:B:383:LYS:HZ1	1:C:5:ASP:HB3	1.66	0.61
1:A:52:ILE:CD1	1:A:112:MET:SD	2.88	0.60
1:A:145:TYR:HE2	1:B:9:GLN:CB	2.06	0.60
1:B:444:VAL:HG23	1:C:185:ASN:OD1	2.01	0.60
1:A:163:ASP:CB	1:B:53:GLN:OE1	2.48	0.60
1:C:327:ILE:O	1:C:327:ILE:HG23	2.00	0.60
1:A:147:HIS:CA	1:B:111:GLY:O	2.50	0.60
1:A:195:VAL:HG11	1:B:464:PRO:C	2.22	0.60
1:A:327:ILE:HG23	1:A:327:ILE:O	2.00	0.60
1:A:13:PHE:O	1:A:329:ALA:HB2	2.01	0.60
1:A:332:GLU:HA	1:A:358:LEU:HB3	1.82	0.60
1:A:194:LEU:CD1	1:B:375:LYS:CB	2.73	0.60
1:B:382:TYR:CE1	1:C:2:THR:CG2	2.83	0.60
1:B:236:PRO:HB3	1:C:380:VAL:CG1	2.30	0.60
1:C:69:LEU:CB	1:C:71:GLN:HE21	2.12	0.60
1:C:258:LEU:CD1	1:C:317:PHE:CE1	2.85	0.60
1:A:223:ALA:C	1:B:465:THR:HA	2.21	0.60
1:A:251:ASN:HB2	1:A:290:GLY:O	2.01	0.60
1:A:468:LEU:HD22	1:A:473:ILE:HG21	1.83	0.60
1:A:9:GLN:HG3	1:A:58:THR:CB	2.18	0.60
1:B:258:LEU:CD1	1:B:317:PHE:CE1	2.84	0.60
1:A:194:LEU:CD1	1:B:375:LYS:CG	2.78	0.60
1:A:183:VAL:HG13	1:A:184:LYS:H	1.66	0.60
1:A:243:GLN:HA	1:A:249:VAL:CG1	2.31	0.60
1:A:194:LEU:O	1:B:467:LYS:CE	2.50	0.60
1:A:212:GLN:NE2	1:B:53:GLN:C	2.38	0.60
1:C:387:ILE:CG2	1:C:395:MET:HA	2.28	0.60
1:A:316:ALA:HA	1:A:319:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LYS:HZ3	1:C:5:ASP:C	2.05	0.60
1:B:430:GLY:N	1:C:185:ASN:OD1	2.29	0.60
1:B:459:PRO:O	1:B:460:ARG:HB2	2.01	0.60
1:C:195:VAL:CA	1:C:200:ILE:HD12	2.30	0.60
1:C:239:THR:HG21	1:C:253:PRO:CD	2.31	0.60
1:C:255:TYR:CG	1:C:292:PHE:HE2	2.20	0.60
1:C:2:THR:HB	1:C:3:PRO:CD	2.22	0.60
1:A:243:GLN:CA	1:A:249:VAL:HG11	2.31	0.60
1:A:255:TYR:CG	1:A:292:PHE:HE2	2.20	0.60
1:B:255:TYR:CG	1:B:292:PHE:HE2	2.19	0.60
1:C:28:ALA:HB3	1:C:348:TRP:CZ2	2.36	0.60
1:A:221:LYS:HA	1:B:474:CYS:SG	2.39	0.60
1:B:243:GLN:CA	1:B:249:VAL:HG11	2.31	0.60
1:B:251:ASN:HB2	1:B:290:GLY:O	2.01	0.60
1:B:28:ALA:HB3	1:B:348:TRP:CZ2	2.37	0.60
1:A:188:TYR:OH	1:B:363:ALA:O	2.19	0.60
1:B:399:THR:CG2	1:C:196:SER:C	2.69	0.60
1:B:48:LYS:O	1:B:49:LEU:HB2	2.00	0.60
1:B:52:ILE:O	1:B:55:MET:HB2	2.00	0.60
1:C:183:VAL:HG13	1:C:184:LYS:H	1.66	0.60
1:C:468:LEU:HD22	1:C:473:ILE:HG21	1.83	0.60
1:A:58:THR:HG22	1:A:112:MET:HA	1.84	0.60
1:A:205:ILE:HG12	1:B:472:LYS:N	2.14	0.60
1:A:88:TYR:CE2	1:B:374:SER:N	2.66	0.60
1:B:115:MET:HE1	1:B:228:ILE:HG13	1.84	0.60
1:B:383:LYS:HZ3	1:C:5:ASP:CA	2.15	0.60
1:B:472:LYS:O	1:B:473:ILE:HB	2.01	0.60
1:C:316:ALA:HA	1:C:319:ILE:HD11	1.82	0.60
1:C:11:ILE:CG2	1:C:326:ILE:HG12	2.32	0.60
1:A:144:ASP:O	1:B:58:THR:C	2.41	0.60
1:B:258:LEU:HD11	1:B:317:PHE:CE1	2.37	0.60
1:C:243:GLN:CA	1:C:249:VAL:HG11	2.31	0.60
1:C:243:GLN:HA	1:C:249:VAL:CG1	2.31	0.60
1:A:200:ILE:CD1	1:B:467:LYS:HZ2	2.12	0.59
1:A:180:LYS:HE2	1:B:57:PHE:CG	2.37	0.59
1:C:229:GLY:HA3	1:C:246:MET:HE1	1.82	0.59
1:C:435:GLU:OE1	1:C:436:VAL:HG12	2.02	0.59
1:A:11:ILE:CG2	1:A:326:ILE:HG12	2.32	0.59
1:A:258:LEU:HD11	1:A:317:PHE:CE1	2.37	0.59
1:A:87:ILE:HD11	1:A:190:TRP:CZ2	2.37	0.59
1:B:312:LYS:HG2	1:B:361:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:CG1	1:B:324:LEU:HD23	2.24	0.59
1:A:188:TYR:CE1	1:B:367:ALA:HB3	2.37	0.59
1:C:251:ASN:HB2	1:C:290:GLY:O	2.01	0.59
1:C:258:LEU:HD11	1:C:317:PHE:CE1	2.37	0.59
1:C:87:ILE:HD11	1:C:190:TRP:CZ2	2.37	0.59
1:A:258:LEU:CD1	1:A:317:PHE:CE1	2.85	0.59
1:A:435:GLU:OE1	1:A:436:VAL:HG12	2.02	0.59
1:B:213:LYS:CG	1:C:375:LYS:HG3	2.31	0.59
1:B:236:PRO:HB3	1:B:278:THR:HG22	1.84	0.59
1:B:11:ILE:CB	1:B:326:ILE:HG12	2.32	0.59
1:A:222:ALA:HB2	1:B:368:ILE:HB	1.83	0.59
1:A:11:ILE:CB	1:A:326:ILE:HG12	2.32	0.59
1:A:182:VAL:HG13	1:A:183:VAL:N	2.17	0.59
1:A:262:PHE:O	1:A:263:LYS:HG2	2.03	0.59
1:A:312:LYS:HG2	1:A:361:LEU:HD13	1.85	0.59
1:A:472:LYS:O	1:A:473:ILE:HB	2.01	0.59
1:B:280:LYS:NZ	1:C:226:TYR:CB	2.58	0.59
1:B:435:GLU:OE1	1:B:436:VAL:HG12	2.02	0.59
1:C:58:THR:HG22	1:C:112:MET:HA	1.83	0.59
1:C:258:LEU:HG	1:C:262:PHE:CE2	2.37	0.59
1:C:312:LYS:HG2	1:C:361:LEU:HD13	1.85	0.59
1:B:383:LYS:HB2	1:C:6:TRP:CD1	2.34	0.59
1:A:187:TRP:CG	1:B:370:ASN:CB	2.81	0.59
1:B:243:GLN:HA	1:B:249:VAL:CG1	2.31	0.59
1:B:243:GLN:HB3	1:B:284:PRO:HD2	1.85	0.59
1:B:262:PHE:O	1:B:263:LYS:HG2	2.03	0.59
1:B:386:TYR:HD2	1:C:3:PRO:HB3	1.68	0.59
1:A:187:TRP:HZ3	1:A:190:TRP:CZ3	2.21	0.59
1:A:258:LEU:HG	1:A:262:PHE:CE2	2.38	0.59
1:A:205:ILE:CB	1:B:478:SER:CB	2.81	0.59
1:C:13:PHE:O	1:C:329:ALA:HB2	2.01	0.59
1:A:251:ASN:HB3	1:A:254:ILE:HG22	1.84	0.59
1:B:183:VAL:HG13	1:B:184:LYS:H	1.67	0.59
1:B:216:TRP:HB2	1:B:245:VAL:CG2	2.29	0.59
1:B:208:VAL:CG2	1:B:246:MET:SD	2.88	0.59
1:A:228:ILE:HA	1:B:476:ASP:O	2.02	0.59
1:C:315:ALA:CA	1:C:318:ILE:HG23	2.31	0.59
1:A:211:VAL:HG11	1:A:216:TRP:CE2	2.38	0.59
1:A:280:LYS:HE3	1:A:383:LYS:CB	2.33	0.59
1:B:152:ILE:CD1	1:B:166:LEU:HA	2.28	0.59
1:B:195:VAL:CA	1:B:200:ILE:HD12	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:HG11	1:B:216:TRP:CE2	2.38	0.59
1:B:300:ARG:NH1	1:B:328:TYR:CE1	2.69	0.59
1:A:222:ALA:N	1:B:368:ILE:HD12	2.18	0.59
1:B:406:THR:HG21	1:C:221:LYS:C	2.23	0.59
1:B:399:THR:HG22	1:C:195:VAL:C	2.23	0.59
1:B:422:LEU:CG	1:C:221:LYS:HG2	2.30	0.59
1:C:243:GLN:HB3	1:C:284:PRO:HD2	1.84	0.59
1:A:28:ALA:HB3	1:A:348:TRP:CZ2	2.36	0.59
1:A:459:PRO:O	1:A:460:ARG:HB2	2.01	0.59
1:B:11:ILE:CG2	1:B:326:ILE:HG12	2.32	0.59
1:A:187:TRP:HB3	1:B:371:TYR:CA	2.31	0.59
1:A:221:LYS:O	1:B:434:THR:CG2	2.51	0.59
1:A:193:SER:O	1:B:467:LYS:HG2	2.03	0.59
1:C:101:LYS:HE2	1:C:198:TYR:CD2	2.38	0.59
1:C:11:ILE:CB	1:C:326:ILE:HG12	2.32	0.59
1:C:300:ARG:NH1	1:C:328:TYR:CE1	2.69	0.59
1:A:229:GLY:HA3	1:B:477:SER:O	1.71	0.59
1:A:236:PRO:HB3	1:A:278:THR:HG22	1.84	0.59
1:A:48:LYS:HA	1:A:48:LYS:HE3	1.85	0.59
1:B:187:TRP:HZ3	1:B:190:TRP:CZ3	2.21	0.59
1:B:258:LEU:HG	1:B:262:PHE:CE2	2.37	0.59
1:B:315:ALA:CA	1:B:318:ILE:HG23	2.31	0.59
1:A:200:ILE:CD1	1:B:467:LYS:CE	2.74	0.59
1:B:280:LYS:CB	1:C:3:PRO:O	2.43	0.59
1:A:101:LYS:HE2	1:A:198:TYR:CD2	2.38	0.58
1:A:179:THR:OG1	1:B:52:ILE:CG1	2.49	0.58
1:A:143:GLN:NE2	1:B:108:HIS:CA	2.66	0.58
1:B:13:PHE:O	1:B:329:ALA:HB2	2.01	0.58
1:C:187:TRP:HZ3	1:C:190:TRP:CZ3	2.21	0.58
1:C:28:ALA:CB	1:C:348:TRP:HZ2	2.16	0.58
1:A:182:VAL:H	1:B:57:PHE:HB3	1.65	0.58
1:A:194:LEU:O	1:B:403:GLN:OE1	2.21	0.58
1:A:28:ALA:CB	1:A:348:TRP:HZ2	2.16	0.58
1:A:221:LYS:CB	1:B:434:THR:CG2	2.79	0.58
1:B:468:LEU:HD22	1:B:473:ILE:HG21	1.83	0.58
1:A:145:TYR:CD2	1:B:9:GLN:HG3	2.38	0.58
1:C:137:PHE:CB	1:C:140:PHE:HB2	2.33	0.58
1:C:262:PHE:O	1:C:263:LYS:HG2	2.03	0.58
1:A:188:TYR:CD2	1:B:366:ASN:O	2.53	0.58
1:A:60:ILE:CD1	1:A:107:LEU:HD13	2.32	0.58
1:B:101:LYS:HE2	1:B:198:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:O	1:B:106:ALA:HB3	2.03	0.58
1:B:60:ILE:CD1	1:B:107:LEU:HD13	2.32	0.58
1:B:137:PHE:CB	1:B:140:PHE:HB2	2.32	0.58
1:B:308:ILE:CG2	1:B:312:LYS:HE3	2.30	0.58
1:B:28:ALA:CB	1:B:348:TRP:HZ2	2.17	0.58
1:A:194:LEU:HA	1:B:403:GLN:CG	2.33	0.58
1:B:429:ALA:HB1	1:C:181:ASP:O	2.03	0.58
1:C:208:VAL:CG2	1:C:246:MET:SD	2.88	0.58
1:B:238:TYR:HD2	1:C:376:ASP:HB2	1.61	0.58
1:A:15:LEU:O	1:A:16:THR:HG23	2.03	0.58
1:A:204:ARG:HG3	1:A:228:ILE:CG2	2.34	0.58
1:A:315:ALA:CA	1:A:318:ILE:HG23	2.31	0.58
1:B:48:LYS:HE3	1:B:48:LYS:HA	1.85	0.58
1:C:431:GLN:O	1:C:444:VAL:HG13	2.04	0.58
1:C:91:ASN:C	1:C:92:GLU:HG3	2.20	0.58
1:A:182:VAL:CB	1:B:10:SER:O	2.52	0.58
1:B:251:ASN:HB3	1:B:254:ILE:HG22	1.84	0.58
1:B:278:THR:CG2	1:C:381:THR:N	2.32	0.58
1:B:24:GLY:O	1:B:348:TRP:CD1	2.56	0.58
1:A:188:TYR:CE1	1:B:365:ALA:HA	2.39	0.58
1:C:103:LEU:O	1:C:106:ALA:HB3	2.03	0.58
1:C:236:PRO:HB3	1:C:278:THR:HG22	1.84	0.58
1:C:459:PRO:O	1:C:460:ARG:HB2	2.01	0.58
1:A:58:THR:CG2	1:A:112:MET:HA	2.33	0.58
1:A:159:THR:O	1:A:160:GLN:HG3	2.03	0.58
1:B:19:PHE:CD1	1:B:347:THR:HB	2.39	0.58
1:B:243:GLN:OE1	1:B:289:LEU:HD12	2.04	0.58
1:B:401:GLY:C	1:C:193:SER:OG	1.96	0.58
1:B:91:ASN:C	1:B:92:GLU:HG3	2.20	0.58
1:C:48:LYS:HE3	1:C:48:LYS:HA	1.85	0.58
1:A:243:GLN:HB3	1:A:284:PRO:HD2	1.84	0.58
1:A:300:ARG:NH1	1:A:328:TYR:CE1	2.69	0.58
1:A:24:GLY:O	1:A:348:TRP:CD1	2.56	0.58
1:A:364:SER:HB2	1:A:437:ILE:CG2	2.33	0.58
1:A:431:GLN:O	1:A:444:VAL:HG13	2.04	0.58
1:B:278:THR:C	1:C:380:VAL:CG1	2.69	0.58
1:B:293:VAL:HG11	1:B:331:GLN:NE2	2.19	0.58
1:B:87:ILE:HD11	1:B:190:TRP:CZ2	2.37	0.58
1:C:24:GLY:O	1:C:348:TRP:CD1	2.56	0.58
1:A:137:PHE:CB	1:A:140:PHE:HB2	2.32	0.58
1:A:19:PHE:CD1	1:A:347:THR:HB	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:HG22	1:B:468:LEU:H	1.68	0.58
1:A:293:VAL:HG11	1:A:331:GLN:NE2	2.19	0.58
1:B:443:THR:HG22	1:B:451:PRO:HG3	1.86	0.58
1:C:319:ILE:CB	1:C:325:PRO:HB2	2.33	0.58
1:C:293:VAL:HG11	1:C:331:GLN:NE2	2.19	0.58
1:A:249:VAL:CA	1:B:477:SER:OG	2.51	0.58
1:C:58:THR:CG2	1:C:112:MET:HA	2.33	0.58
1:C:251:ASN:HB3	1:C:254:ILE:HG22	1.84	0.58
1:B:385:PRO:CD	1:C:3:PRO:CD	2.76	0.58
1:B:319:ILE:CB	1:B:325:PRO:HB2	2.33	0.58
1:B:364:SER:HB2	1:B:437:ILE:CG2	2.33	0.58
1:B:406:THR:HG23	1:C:221:LYS:O	2.01	0.58
1:B:431:GLN:O	1:B:444:VAL:HG13	2.03	0.58
1:C:243:GLN:OE1	1:C:289:LEU:HD12	2.04	0.58
1:C:364:SER:HB2	1:C:437:ILE:CG2	2.33	0.58
1:A:123:MET:SD	1:A:137:PHE:CD1	2.97	0.57
1:A:219:TYR:HD1	1:B:472:LYS:O	1.87	0.57
1:B:125:TYR:CE1	1:B:133:ASP:HB2	2.39	0.57
1:B:159:THR:O	1:B:160:GLN:HG3	2.03	0.57
1:B:204:ARG:HG3	1:B:228:ILE:CG2	2.34	0.57
1:B:327:ILE:HA	1:B:331:GLN:OE1	2.04	0.57
1:C:61:TRP:HZ2	1:C:204:ARG:NE	2.02	0.57
1:C:211:VAL:HG11	1:C:216:TRP:CE2	2.38	0.57
1:C:443:THR:HG22	1:C:451:PRO:HG3	1.86	0.57
1:A:184:LYS:HB2	1:B:367:ALA:CB	2.32	0.57
1:A:205:ILE:HD11	1:A:246:MET:HE3	1.85	0.57
1:A:379:PHE:CZ	1:A:397:LYS:CE	2.87	0.57
1:A:418:TYR:CD1	1:A:454:MET:CE	2.87	0.57
1:A:443:THR:HG22	1:A:451:PRO:HG3	1.86	0.57
1:A:191:VAL:HG13	1:B:372:ALA:N	2.16	0.57
1:B:418:TYR:CD1	1:B:454:MET:HE3	2.39	0.57
1:C:308:ILE:CG2	1:C:312:LYS:HE3	2.30	0.57
1:C:379:PHE:CZ	1:C:397:LYS:CE	2.87	0.57
1:C:60:ILE:CD1	1:C:107:LEU:HD13	2.32	0.57
1:A:118:VAL:HG22	1:B:375:LYS:HE2	1.85	0.57
1:A:194:LEU:HA	1:B:403:GLN:OE1	2.04	0.57
1:A:243:GLN:OE1	1:A:289:LEU:HD12	2.04	0.57
1:B:15:LEU:O	1:B:16:THR:HG23	2.03	0.57
1:B:187:TRP:CE3	1:B:190:TRP:CZ3	2.92	0.57
1:B:444:VAL:CG2	1:C:185:ASN:OD1	2.52	0.57
1:C:123:MET:SD	1:C:137:PHE:CD1	2.97	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LYS:HE3	1:C:383:LYS:CB	2.33	0.57
1:C:418:TYR:CD1	1:C:454:MET:CE	2.87	0.57
1:A:103:LEU:O	1:A:106:ALA:HB3	2.03	0.57
1:A:182:VAL:HG21	1:B:58:THR:CB	2.34	0.57
1:A:208:VAL:CG2	1:A:246:MET:SD	2.88	0.57
1:A:319:ILE:CB	1:A:325:PRO:HB2	2.33	0.57
1:A:147:HIS:CA	1:B:112:MET:HE3	2.16	0.57
1:B:190:TRP:CE3	1:B:191:VAL:HG12	2.40	0.57
1:B:57:PHE:CZ	1:B:327:ILE:HD13	2.40	0.57
1:A:204:ARG:O	1:B:471:SER:CB	2.53	0.57
1:A:57:PHE:CZ	1:A:327:ILE:HD13	2.40	0.57
1:B:418:TYR:CD1	1:B:454:MET:CE	2.87	0.57
1:A:200:ILE:CD1	1:B:467:LYS:HG3	2.34	0.57
1:C:15:LEU:O	1:C:16:THR:HG23	2.03	0.57
1:C:279:VAL:HG13	1:C:280:LYS:H	1.69	0.57
1:B:277:ASN:HB2	1:C:286:SER:OG	2.05	0.57
1:C:19:PHE:CD1	1:C:347:THR:HB	2.39	0.57
1:A:215:PHE:CE2	1:B:367:ALA:CB	2.88	0.57
1:A:252:TYR:N	1:A:253:PRO:HD2	2.20	0.57
1:A:116:VAL:C	1:B:470:GLY:H	1.96	0.57
1:C:136:VAL:HG12	1:C:136:VAL:O	2.05	0.57
1:C:204:ARG:HG3	1:C:228:ILE:CG2	2.34	0.57
1:C:252:TYR:N	1:C:253:PRO:HD2	2.20	0.57
1:C:57:PHE:CZ	1:C:327:ILE:HD13	2.40	0.57
1:A:136:VAL:O	1:A:136:VAL:HG12	2.05	0.57
1:A:182:VAL:HG13	1:B:56:GLY:O	2.04	0.57
1:A:200:ILE:CG2	1:B:468:LEU:N	2.68	0.57
1:A:327:ILE:HA	1:A:331:GLN:OE1	2.04	0.57
1:B:60:ILE:HD12	1:B:107:LEU:CD1	2.35	0.57
1:B:136:VAL:HG12	1:B:136:VAL:O	2.05	0.57
1:B:61:TRP:HZ2	1:B:204:ARG:NE	2.03	0.57
1:B:213:LYS:HG2	1:C:375:LYS:HE2	1.87	0.57
1:B:211:VAL:HB	1:B:216:TRP:CH2	2.40	0.57
1:B:52:ILE:HD11	1:B:112:MET:HE1	1.87	0.57
1:C:159:THR:O	1:C:160:GLN:HG3	2.03	0.57
1:C:187:TRP:CE3	1:C:190:TRP:CZ3	2.92	0.57
1:A:436:VAL:HG22	1:A:437:ILE:H	1.70	0.57
1:A:184:LYS:CE	1:B:366:ASN:HD22	2.18	0.57
1:A:195:VAL:HG12	1:B:464:PRO:HG2	1.85	0.57
1:C:10:SER:HB3	1:C:57:PHE:CB	2.35	0.57
1:A:125:TYR:CE1	1:A:133:ASP:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TRP:CE3	1:A:190:TRP:CZ3	2.92	0.57
1:A:187:TRP:CE3	1:B:374:SER:OG	2.53	0.57
1:A:190:TRP:CE3	1:A:191:VAL:HG12	2.40	0.57
1:A:222:ALA:HB3	1:B:473:ILE:HG12	1.86	0.57
1:A:165:TRP:CD1	1:B:110:ARG:CB	2.88	0.57
1:B:400:ASP:HB2	1:C:193:SER:C	2.10	0.57
1:B:407:ILE:HG12	1:B:461:VAL:HG13	1.87	0.57
1:C:123:MET:HE3	1:C:140:PHE:CE1	2.37	0.57
1:C:125:TYR:CE1	1:C:133:ASP:HB2	2.39	0.57
1:C:216:TRP:HB2	1:C:217:PRO:HD3	1.86	0.57
1:B:386:TYR:CE1	1:C:288:LEU:HD12	2.39	0.57
1:A:279:VAL:HG13	1:A:280:LYS:H	1.69	0.57
1:B:216:TRP:HB2	1:B:217:PRO:HD3	1.86	0.57
1:C:190:TRP:CE3	1:C:191:VAL:HG12	2.40	0.57
1:C:211:VAL:HB	1:C:216:TRP:CH2	2.40	0.57
1:A:123:MET:HE1	1:A:140:PHE:HE1	1.69	0.56
1:A:230:GLU:C	1:A:250:LEU:HD23	2.25	0.56
1:A:165:TRP:CD1	1:B:110:ARG:HB2	2.40	0.56
1:B:238:TYR:CB	1:C:376:ASP:HB2	2.35	0.56
1:B:386:TYR:CG	1:C:288:LEU:HD11	2.35	0.56
1:B:213:LYS:CE	1:C:375:LYS:HG2	2.34	0.56
1:A:187:TRP:CE3	1:A:190:TRP:CE3	2.94	0.56
1:A:69:LEU:CB	1:A:71:GLN:HE21	2.12	0.56
1:B:401:GLY:N	1:C:193:SER:CB	2.68	0.56
1:B:383:LYS:HG2	1:C:113:TYR:HE1	1.66	0.56
1:C:263:LYS:HA	1:C:310:LEU:HD23	1.86	0.56
1:C:407:ILE:HG12	1:C:461:VAL:HG13	1.87	0.56
1:A:190:TRP:CZ2	1:B:375:LYS:CG	2.88	0.56
1:A:204:ARG:NH1	1:A:230:GLU:HG2	2.21	0.56
1:A:407:ILE:HG12	1:A:461:VAL:HG13	1.87	0.56
1:A:61:TRP:HZ2	1:A:204:ARG:NE	2.03	0.56
1:A:91:ASN:C	1:A:92:GLU:HG3	2.20	0.56
1:B:182:VAL:HG13	1:B:183:VAL:HG12	1.87	0.56
1:B:445:GLY:CA	1:C:185:ASN:HB2	2.35	0.56
1:C:327:ILE:HA	1:C:331:GLN:OE1	2.04	0.56
1:B:230:GLU:C	1:B:250:LEU:HD23	2.25	0.56
1:B:263:LYS:HA	1:B:310:LEU:HD23	1.86	0.56
1:B:379:PHE:CZ	1:B:397:LYS:CE	2.87	0.56
1:B:400:ASP:HA	1:C:195:VAL:N	2.19	0.56
1:C:152:ILE:CD1	1:C:166:LEU:HA	2.28	0.56
1:B:446:SER:CB	1:C:181:ASP:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:TRP:CE3	1:C:190:TRP:CE3	2.94	0.56
1:C:230:GLU:C	1:C:250:LEU:HD23	2.25	0.56
1:A:215:PHE:CE1	1:B:472:LYS:CB	2.88	0.56
1:A:216:TRP:HB2	1:A:217:PRO:HD3	1.86	0.56
1:B:2:THR:CB	1:B:3:PRO:HD2	2.18	0.56
1:A:205:ILE:HG12	1:B:476:ASP:OD1	2.02	0.56
1:A:205:ILE:CD1	1:B:478:SER:CB	2.52	0.56
1:A:60:ILE:HD12	1:A:107:LEU:CD1	2.35	0.56
1:A:218:GLY:HA3	1:B:364:SER:CA	2.33	0.56
1:A:25:SER:HB3	1:A:28:ALA:HB2	1.87	0.56
1:A:379:PHE:CE1	1:A:397:LYS:CE	2.88	0.56
1:B:321:ASN:HA	1:B:384:ASN:ND2	2.21	0.56
1:C:180:LYS:NZ	1:C:182:VAL:HB	2.20	0.56
1:C:295:ASN:O	1:C:298:ASN:HB2	2.05	0.56
1:A:295:ASN:O	1:A:298:ASN:HB2	2.05	0.56
1:B:123:MET:SD	1:B:137:PHE:CD1	2.97	0.56
1:B:187:TRP:CE3	1:B:190:TRP:CE3	2.93	0.56
1:B:295:ASN:O	1:B:298:ASN:HB2	2.05	0.56
1:A:178:THR:HB	1:B:58:THR:HA	1.88	0.56
1:A:382:TYR:HE1	1:A:385:PRO:HD3	1.70	0.56
1:A:401:GLY:O	1:A:467:LYS:HE3	2.06	0.56
1:A:180:LYS:CE	1:B:11:ILE:CA	2.84	0.56
1:B:252:TYR:N	1:B:253:PRO:HD2	2.20	0.56
1:C:204:ARG:NH1	1:C:230:GLU:HG2	2.20	0.56
1:C:418:TYR:CD1	1:C:454:MET:HE3	2.41	0.56
1:C:60:ILE:HD12	1:C:107:LEU:CD1	2.35	0.56
1:A:199:SER:C	1:A:200:ILE:HG13	2.16	0.56
1:B:185:ASN:O	1:B:188:TYR:HB2	2.06	0.56
1:B:216:TRP:CE3	1:B:216:TRP:CA	2.89	0.56
1:B:255:TYR:HD2	1:B:256:TYR:N	2.04	0.56
1:B:468:LEU:CD2	1:B:473:ILE:HG21	2.36	0.56
1:B:99:ASP:O	1:B:102:ALA:HB3	2.05	0.56
1:C:115:MET:HE2	1:C:204:ARG:HB2	1.85	0.56
1:C:152:ILE:HD11	1:C:166:LEU:HG	1.87	0.56
1:C:137:PHE:HZ	1:C:174:PRO:HG3	1.71	0.56
1:C:401:GLY:O	1:C:467:LYS:HE3	2.06	0.56
1:A:263:LYS:HA	1:A:310:LEU:HD23	1.86	0.56
1:A:10:SER:HB3	1:A:57:PHE:CB	2.35	0.56
1:B:209:LYS:CB	1:B:231:VAL:HG11	2.36	0.56
1:A:187:TRP:CA	1:B:367:ALA:O	2.53	0.56
1:B:383:LYS:NZ	1:C:6:TRP:H	1.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:TYR:HD2	1:C:256:TYR:N	2.04	0.56
1:C:321:ASN:HA	1:C:384:ASN:ND2	2.21	0.56
1:C:379:PHE:CE1	1:C:397:LYS:CE	2.88	0.56
1:C:468:LEU:CD2	1:C:473:ILE:HG21	2.36	0.56
1:C:468:LEU:CD2	1:C:473:ILE:HG12	2.34	0.56
1:A:137:PHE:HZ	1:A:174:PRO:HG3	1.71	0.56
1:A:180:LYS:NZ	1:B:11:ILE:N	2.53	0.56
1:A:209:LYS:N	1:A:231:VAL:HG11	2.21	0.56
1:A:216:TRP:CE3	1:A:216:TRP:CA	2.89	0.56
1:B:25:SER:HB3	1:B:28:ALA:HB2	1.87	0.56
1:A:205:ILE:CB	1:B:478:SER:OG	2.39	0.56
1:C:209:LYS:N	1:C:231:VAL:HG11	2.21	0.56
1:B:386:TYR:CE1	1:C:288:LEU:CD1	2.89	0.56
1:C:436:VAL:HG22	1:C:437:ILE:H	1.70	0.56
1:A:211:VAL:HB	1:A:216:TRP:CH2	2.40	0.55
1:B:137:PHE:HZ	1:B:174:PRO:HG3	1.71	0.55
1:B:193:SER:O	1:B:196:SER:HB3	2.07	0.55
1:C:73:CYS:HB3	1:C:126:ASP:OD1	2.06	0.55
1:B:424:GLY:O	1:C:218:GLY:HA2	2.05	0.55
1:C:209:LYS:CB	1:C:231:VAL:HG11	2.36	0.55
1:A:12:TYR:CE1	1:A:14:LEU:CD2	2.89	0.55
1:A:152:ILE:HD11	1:A:166:LEU:HG	1.87	0.55
1:B:152:ILE:HD11	1:B:166:LEU:HG	1.87	0.55
1:B:403:GLN:NE2	1:C:196:SER:OG	2.39	0.55
1:B:436:VAL:HG22	1:B:437:ILE:H	1.70	0.55
1:A:192:GLY:C	1:B:464:PRO:CG	2.74	0.55
1:C:382:TYR:HE1	1:C:385:PRO:HD3	1.70	0.55
1:A:147:HIS:NE2	1:A:163:ASP:HB3	2.20	0.55
1:A:73:CYS:HB3	1:A:126:ASP:OD1	2.06	0.55
1:B:73:CYS:HB3	1:B:126:ASP:OD1	2.06	0.55
1:C:216:TRP:CE3	1:C:216:TRP:CA	2.89	0.55
1:B:282:ASP:OD1	1:C:379:PHE:HD2	1.89	0.55
1:C:418:TYR:CE1	1:C:454:MET:HE2	2.42	0.55
1:A:182:VAL:N	1:B:57:PHE:N	2.54	0.55
1:B:448:GLY:C	1:C:184:LYS:HZ2	2.08	0.55
1:C:25:SER:HB3	1:C:28:ALA:HB2	1.87	0.55
1:A:75:TYR:HE1	1:A:170:THR:HG21	1.71	0.55
1:A:185:ASN:N	1:B:366:ASN:HB3	2.16	0.55
1:A:99:ASP:O	1:A:102:ALA:HB3	2.06	0.55
1:B:147:HIS:NE2	1:B:163:ASP:HB3	2.20	0.55
1:B:209:LYS:N	1:B:231:VAL:HG11	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:TYR:HE1	1:B:385:PRO:HD3	1.70	0.55
1:A:221:LYS:NZ	1:B:436:VAL:O	2.35	0.55
1:A:222:ALA:HB2	1:B:368:ILE:HD12	1.83	0.55
1:A:255:TYR:CD2	1:A:256:TYR:N	2.75	0.55
1:A:255:TYR:HD2	1:A:256:TYR:N	2.04	0.55
1:C:182:VAL:HG13	1:C:183:VAL:HG12	1.87	0.55
1:A:212:GLN:OE1	1:B:53:GLN:O	2.24	0.55
1:A:184:LYS:CB	1:B:363:ALA:O	2.54	0.55
1:A:193:SER:HB3	1:B:376:ASP:OD1	2.07	0.55
1:A:254:ILE:HD11	1:A:321:ASN:HD21	1.72	0.55
1:A:321:ASN:HA	1:A:384:ASN:ND2	2.21	0.55
1:A:468:LEU:CD2	1:A:473:ILE:HG21	2.36	0.55
1:B:230:GLU:O	1:B:250:LEU:HD23	2.07	0.55
1:B:294:GLU:HB3	1:B:300:ARG:HA	1.89	0.55
1:A:225:VAL:N	1:B:465:THR:CA	2.67	0.55
1:B:401:GLY:O	1:B:467:LYS:HE3	2.06	0.55
1:A:208:VAL:N	1:B:472:LYS:HE2	2.19	0.55
1:A:249:VAL:N	1:B:477:SER:HB3	2.22	0.55
1:C:254:ILE:HD11	1:C:321:ASN:HD21	1.72	0.55
1:A:180:LYS:HZ3	1:B:57:PHE:CB	1.91	0.55
1:A:182:VAL:HG13	1:A:183:VAL:HG12	1.88	0.55
1:A:185:ASN:ND2	1:B:319:ILE:CG1	2.70	0.55
1:A:190:TRP:HH2	1:B:375:LYS:NZ	2.02	0.55
1:A:385:PRO:HG2	1:A:396:ARG:H	1.72	0.55
1:B:137:PHE:O	1:B:139:PRO:HD3	2.07	0.55
1:C:138:LYS:HA	1:C:140:PHE:H	1.72	0.55
1:C:199:SER:C	1:C:200:ILE:HG13	2.16	0.55
1:A:209:LYS:CB	1:A:231:VAL:HG11	2.36	0.55
1:A:308:ILE:CG2	1:A:312:LYS:HE3	2.30	0.55
1:B:238:TYR:CA	1:C:376:ASP:CG	2.75	0.55
1:B:254:ILE:HD11	1:B:321:ASN:HD21	1.72	0.55
1:B:385:PRO:HG2	1:B:396:ARG:H	1.72	0.55
1:B:418:TYR:CE1	1:B:454:MET:HE2	2.42	0.55
1:B:431:GLN:HA	1:B:431:GLN:NE2	2.18	0.55
1:A:221:LYS:C	1:B:434:THR:HG22	2.27	0.55
1:B:468:LEU:CD2	1:B:473:ILE:HG12	2.34	0.55
1:B:424:GLY:O	1:C:218:GLY:C	2.44	0.55
1:B:204:ARG:NH1	1:B:230:GLU:HG2	2.21	0.54
1:B:255:TYR:CD1	1:B:292:PHE:CD2	2.96	0.54
1:B:428:THR:HB	1:C:186:GLU:O	2.06	0.54
1:C:147:HIS:NE2	1:C:163:ASP:HB3	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HA	1:A:140:PHE:H	1.72	0.54
1:A:230:GLU:O	1:A:250:LEU:HD23	2.07	0.54
1:A:294:GLU:HB3	1:A:300:ARG:HA	1.89	0.54
1:B:236:PRO:HG3	1:C:381:THR:OG1	2.07	0.54
1:B:255:TYR:CD2	1:B:256:TYR:N	2.75	0.54
1:B:385:PRO:HA	1:C:3:PRO:HB3	1.88	0.54
1:B:426:SER:N	1:C:219:TYR:O	2.23	0.54
1:B:205:ILE:O	1:B:230:GLU:HG3	2.07	0.54
1:A:180:LYS:CA	1:B:55:MET:HG3	2.21	0.54
1:A:180:LYS:HZ2	1:B:57:PHE:CB	2.20	0.54
1:C:185:ASN:CA	1:C:188:TYR:CD2	2.79	0.54
1:C:57:PHE:HZ	1:C:327:ILE:HD13	1.73	0.54
1:A:205:ILE:O	1:A:230:GLU:HG3	2.07	0.54
1:B:379:PHE:CE1	1:B:397:LYS:CE	2.89	0.54
1:C:32:THR:CG2	1:C:342:ALA:HA	2.28	0.54
1:C:420:LEU:CD2	1:C:452:VAL:CG2	2.83	0.54
1:C:99:ASP:O	1:C:102:ALA:HB3	2.06	0.54
1:A:137:PHE:O	1:A:139:PRO:HD3	2.07	0.54
1:A:250:LEU:CD1	1:A:292:PHE:CE1	2.91	0.54
1:B:137:PHE:CG	1:B:146:PHE:CZ	2.95	0.54
1:B:180:LYS:NZ	1:B:182:VAL:HB	2.21	0.54
1:B:399:THR:CG2	1:C:196:SER:CA	2.84	0.54
1:A:115:MET:CE	1:B:470:GLY:CA	2.84	0.54
1:A:205:ILE:HD12	1:B:478:SER:OG	2.06	0.54
1:A:144:ASP:OD1	1:B:6:TRP:CH2	2.59	0.54
1:B:280:LYS:HZ1	1:C:226:TYR:HB2	1.67	0.54
1:C:255:TYR:CD2	1:C:256:TYR:N	2.75	0.54
1:C:294:GLU:HB3	1:C:300:ARG:HA	1.89	0.54
1:B:238:TYR:O	1:C:377:THR:N	2.40	0.54
1:C:313:ASN:ND2	1:C:410:ASN:O	2.40	0.54
1:A:255:TYR:CD1	1:A:292:PHE:CD2	2.96	0.54
1:B:12:TYR:CE1	1:B:14:LEU:CD2	2.89	0.54
1:B:138:LYS:HA	1:B:140:PHE:H	1.72	0.54
1:B:313:ASN:ND2	1:B:410:ASN:O	2.40	0.54
1:C:216:TRP:HB2	1:C:217:PRO:CD	2.38	0.54
1:C:250:LEU:CD1	1:C:292:PHE:CE1	2.91	0.54
1:A:313:ASN:ND2	1:A:410:ASN:O	2.40	0.54
1:A:182:VAL:HG21	1:B:58:THR:CA	2.13	0.54
1:C:214:ASP:O	1:C:217:PRO:HG2	2.07	0.54
1:C:230:GLU:O	1:C:250:LEU:HD23	2.07	0.54
1:C:255:TYR:CD1	1:C:292:PHE:CD2	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:PRO:HG2	1:C:396:ARG:H	1.72	0.54
1:A:248:GLY:C	1:B:477:SER:CB	2.68	0.54
1:B:148:PRO:O	1:B:165:TRP:CD1	2.61	0.54
1:B:250:LEU:CD1	1:B:292:PHE:CE1	2.91	0.54
1:B:385:PRO:HB3	1:C:226:TYR:CA	2.37	0.54
1:B:387:ILE:HG13	1:B:424:GLY:HA3	1.89	0.54
1:A:197:ASN:C	1:B:467:LYS:NZ	2.57	0.54
1:C:148:PRO:O	1:C:165:TRP:CD1	2.61	0.54
1:B:241:PRO:CA	1:C:374:SER:CA	2.59	0.54
1:A:221:LYS:HG3	1:B:434:THR:HG23	1.90	0.54
1:A:420:LEU:CD2	1:A:452:VAL:CG2	2.83	0.54
1:A:165:TRP:CE2	1:B:110:ARG:CA	2.75	0.54
1:B:147:HIS:CE1	1:B:163:ASP:CB	2.90	0.54
1:B:16:THR:CG2	1:B:42:TRP:CD1	2.91	0.54
1:B:229:GLY:N	1:B:246:MET:HE1	2.22	0.54
1:A:221:LYS:HB2	1:B:436:VAL:HA	1.65	0.54
1:A:200:ILE:CD1	1:B:467:LYS:HD2	2.36	0.54
1:C:137:PHE:CG	1:C:146:PHE:CZ	2.95	0.54
1:C:205:ILE:O	1:C:230:GLU:HG3	2.07	0.54
1:B:213:LYS:NZ	1:C:375:LYS:HG2	2.23	0.54
1:A:137:PHE:CG	1:A:146:PHE:CZ	2.95	0.54
1:A:148:PRO:O	1:A:165:TRP:CD1	2.61	0.54
1:A:216:TRP:HB2	1:A:217:PRO:CD	2.38	0.54
1:A:57:PHE:HZ	1:A:327:ILE:HD13	1.73	0.54
1:A:428:THR:CG2	1:A:431:GLN:HG2	2.39	0.54
1:B:214:ASP:O	1:B:217:PRO:HG2	2.07	0.54
1:B:238:TYR:CD2	1:C:376:ASP:CB	2.73	0.54
1:A:184:LYS:CB	1:B:367:ALA:HB2	2.38	0.54
1:B:45:ILE:O	1:B:49:LEU:HD13	2.08	0.54
1:C:75:TYR:HE1	1:C:170:THR:HG21	1.71	0.54
1:A:75:TYR:CE1	1:A:170:THR:CG2	2.91	0.53
1:A:188:TYR:CE1	1:B:365:ALA:CA	2.70	0.53
1:A:180:LYS:CE	1:B:12:TYR:HB2	2.37	0.53
1:B:137:PHE:O	1:B:140:PHE:CD1	2.62	0.53
1:B:395:MET:SD	1:B:407:ILE:HD12	2.49	0.53
1:C:137:PHE:O	1:C:140:PHE:CD1	2.61	0.53
1:C:147:HIS:CE1	1:C:163:ASP:CB	2.90	0.53
1:A:468:LEU:CD2	1:A:473:ILE:HG12	2.34	0.53
1:B:75:TYR:HE1	1:B:170:THR:HG21	1.71	0.53
1:B:190:TRP:CZ3	1:B:191:VAL:HG12	2.43	0.53
1:B:29:THR:O	1:B:30:CYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PHE:CZ	1:A:362:ILE:CG2	2.91	0.53
1:A:395:MET:SD	1:A:407:ILE:HD12	2.49	0.53
1:B:32:THR:CG2	1:B:342:ALA:HA	2.28	0.53
1:C:137:PHE:O	1:C:139:PRO:HD3	2.07	0.53
1:C:215:PHE:CE1	1:C:216:TRP:CZ3	2.96	0.53
1:B:213:LYS:HG2	1:C:375:LYS:CE	2.39	0.53
1:C:395:MET:SD	1:C:407:ILE:HD12	2.49	0.53
1:A:143:GLN:CG	1:B:108:HIS:CE1	2.91	0.53
1:A:193:SER:O	1:A:196:SER:HB3	2.07	0.53
1:A:215:PHE:CE1	1:A:216:TRP:CZ3	2.96	0.53
1:A:243:GLN:HB3	1:A:284:PRO:CD	2.39	0.53
1:B:137:PHE:O	1:B:140:PHE:HD1	1.92	0.53
1:A:215:PHE:HA	1:B:364:SER:HA	1.90	0.53
1:B:382:TYR:CE1	1:B:396:ARG:O	2.62	0.53
1:A:184:LYS:HG2	1:B:56:GLY:HA3	0.70	0.53
1:C:188:TYR:CE1	1:C:218:GLY:CA	2.85	0.53
1:C:254:ILE:HD11	1:C:321:ASN:ND2	2.23	0.53
1:C:250:LEU:CD1	1:C:292:PHE:HE1	2.22	0.53
1:A:45:ILE:HG21	1:A:103:LEU:CD1	2.38	0.53
1:A:254:ILE:HD11	1:A:321:ASN:ND2	2.23	0.53
1:A:194:LEU:CD1	1:B:375:LYS:HG3	2.38	0.53
1:A:200:ILE:CG2	1:B:467:LYS:C	2.76	0.53
1:A:145:TYR:OH	1:B:6:TRP:HA	2.09	0.53
1:B:91:ASN:OD1	1:B:94:TYR:HD2	1.92	0.53
1:C:348:TRP:CD1	1:C:348:TRP:O	2.62	0.53
1:C:66:THR:CG2	1:C:86:ASP:HB3	2.39	0.53
1:A:320:LEU:HD22	1:A:407:ILE:HD13	1.90	0.53
1:A:91:ASN:OD1	1:A:94:TYR:HD2	1.92	0.53
1:B:216:TRP:HB2	1:B:217:PRO:CD	2.38	0.53
1:B:21:ARG:CG	1:B:21:ARG:HH21	2.22	0.53
1:C:157:ASP:OD2	1:C:159:THR:HB	2.08	0.53
1:C:386:TYR:O	1:C:388:LYS:N	2.42	0.53
1:C:16:THR:CG2	1:C:42:TRP:CD1	2.91	0.53
1:A:191:VAL:HG21	1:B:473:ILE:CG1	2.37	0.53
1:A:218:GLY:N	1:B:437:ILE:HA	2.24	0.53
1:A:382:TYR:C	1:A:382:TYR:CD1	2.81	0.53
1:A:382:TYR:CE1	1:A:396:ARG:O	2.62	0.53
1:A:387:ILE:HG13	1:A:424:GLY:HA3	1.89	0.53
1:B:332:GLU:HA	1:B:358:LEU:CB	2.39	0.53
1:B:57:PHE:HZ	1:B:327:ILE:HD13	1.73	0.53
1:B:66:THR:CG2	1:B:86:ASP:HB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:CG	1:C:21:ARG:HH21	2.22	0.53
1:C:243:GLN:HB3	1:C:284:PRO:CD	2.39	0.53
1:C:428:THR:CG2	1:C:431:GLN:HG2	2.39	0.53
1:B:383:LYS:NZ	1:C:5:ASP:C	2.61	0.53
1:A:315:ALA:HA	1:A:318:ILE:CG2	2.36	0.53
1:A:332:GLU:HA	1:A:358:LEU:CB	2.39	0.53
1:A:386:TYR:O	1:A:388:LYS:N	2.42	0.53
1:A:45:ILE:O	1:A:49:LEU:HD13	2.08	0.53
1:A:68:GLN:C	1:A:85:THR:HG21	2.29	0.53
1:B:11:ILE:HD13	1:B:326:ILE:HG13	1.89	0.53
1:B:122:HIS:CB	1:B:173:LEU:HB3	2.39	0.53
1:B:237:ALA:HB2	1:C:379:PHE:CB	2.38	0.53
1:A:190:TRP:CD2	1:B:374:SER:N	2.64	0.53
1:A:29:THR:O	1:A:30:CYS:HB2	2.08	0.53
1:A:273:TYR:CE1	1:A:389:ASP:HB3	2.44	0.53
1:A:16:THR:CG2	1:A:42:TRP:CD1	2.91	0.53
1:A:66:THR:CG2	1:A:86:ASP:HB3	2.39	0.53
1:B:157:ASP:OD2	1:B:159:THR:HB	2.08	0.53
1:B:191:VAL:HG11	1:B:219:TYR:CE2	2.44	0.53
1:B:215:PHE:CE1	1:B:216:TRP:CZ3	2.96	0.53
1:A:87:ILE:C	1:B:374:SER:O	2.47	0.53
1:B:382:TYR:CD1	1:B:382:TYR:C	2.81	0.53
1:B:68:GLN:C	1:B:85:THR:HG21	2.29	0.53
1:C:147:HIS:CD2	1:C:177:ASP:O	2.56	0.53
1:C:57:PHE:CZ	1:C:362:ILE:CG2	2.91	0.53
1:A:6:TRP:CZ2	1:A:113:TYR:CD1	2.98	0.53
1:A:250:LEU:CD1	1:A:292:PHE:HE1	2.22	0.53
1:B:238:TYR:CD1	1:B:238:TYR:C	2.83	0.53
1:B:300:ARG:HH11	1:B:328:TYR:HE1	1.53	0.53
1:B:399:THR:CB	1:C:196:SER:HA	2.38	0.53
1:C:91:ASN:OD1	1:C:94:TYR:HD2	1.92	0.53
1:A:137:PHE:O	1:A:140:PHE:CD1	2.62	0.52
1:A:122:HIS:CB	1:A:173:LEU:HB3	2.39	0.52
1:A:279:VAL:O	1:A:283:CYS:HB2	2.09	0.52
1:A:348:TRP:O	1:A:348:TRP:CD1	2.62	0.52
1:B:428:THR:CG2	1:B:431:GLN:HG2	2.39	0.52
1:A:163:ASP:C	1:B:53:GLN:OE1	2.47	0.52
1:C:122:HIS:CB	1:C:173:LEU:HB3	2.39	0.52
1:C:190:TRP:CZ3	1:C:191:VAL:HG12	2.43	0.52
1:C:191:VAL:HG11	1:C:219:TYR:CE2	2.44	0.52
1:C:279:VAL:O	1:C:283:CYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PRO:HA	1:C:373:ILE:HG22	1.91	0.52
1:C:382:TYR:C	1:C:382:TYR:CD1	2.81	0.52
1:C:387:ILE:HG13	1:C:424:GLY:HA3	1.89	0.52
1:C:382:TYR:CE1	1:C:396:ARG:O	2.62	0.52
1:A:163:ASP:O	1:B:53:GLN:OE1	2.27	0.52
1:A:220:ASN:HA	1:B:473:ILE:HG22	1.86	0.52
1:A:382:TYR:CE1	1:A:385:PRO:HD3	2.45	0.52
1:B:217:PRO:HD3	1:B:245:VAL:HG22	1.91	0.52
1:B:243:GLN:HB3	1:B:284:PRO:CD	2.39	0.52
1:B:254:ILE:HD11	1:B:321:ASN:ND2	2.23	0.52
1:A:221:LYS:HG3	1:B:434:THR:CG2	2.39	0.52
1:B:75:TYR:CE1	1:B:170:THR:CG2	2.91	0.52
1:B:91:ASN:OD1	1:B:94:TYR:CD2	2.63	0.52
1:C:6:TRP:CZ2	1:C:113:TYR:CD1	2.98	0.52
1:C:137:PHE:O	1:C:140:PHE:HD1	1.92	0.52
1:C:332:GLU:HA	1:C:358:LEU:CB	2.39	0.52
1:C:405:VAL:HB	1:C:463:TYR:CD2	2.44	0.52
1:C:45:ILE:O	1:C:49:LEU:HD13	2.08	0.52
1:C:68:GLN:C	1:C:85:THR:HG21	2.29	0.52
1:A:123:MET:HB2	1:A:174:PRO:HG2	1.91	0.52
1:A:137:PHE:O	1:A:140:PHE:HD1	1.92	0.52
1:A:157:ASP:OD2	1:A:159:THR:HB	2.08	0.52
1:A:197:ASN:HD21	1:C:196:SER:CB	2.18	0.52
1:A:21:ARG:CG	1:A:21:ARG:HH21	2.22	0.52
1:A:238:TYR:CD1	1:A:238:TYR:C	2.83	0.52
1:A:394:ALA:HA	1:A:408:LEU:HA	1.92	0.52
1:B:279:VAL:O	1:B:283:CYS:HB2	2.09	0.52
1:B:348:TRP:O	1:B:348:TRP:CD1	2.62	0.52
1:B:45:ILE:HG21	1:B:103:LEU:CD1	2.38	0.52
1:A:192:GLY:C	1:B:464:PRO:HG2	2.23	0.52
1:B:57:PHE:CZ	1:B:362:ILE:CG2	2.91	0.52
1:A:144:ASP:O	1:B:58:THR:CG2	2.42	0.52
1:C:45:ILE:HG21	1:C:103:LEU:CD1	2.38	0.52
1:C:18:ARG:CZ	1:C:79:TYR:CD2	2.92	0.52
1:A:144:ASP:O	1:B:58:THR:HG22	1.88	0.52
1:A:147:HIS:CE1	1:A:163:ASP:CB	2.90	0.52
1:A:187:TRP:CH2	1:B:374:SER:OG	2.61	0.52
1:A:190:TRP:CZ3	1:A:191:VAL:HG12	2.43	0.52
1:A:188:TYR:CE1	1:A:218:GLY:CA	2.85	0.52
1:B:274:ASN:HD21	1:C:285:ASP:H	1.58	0.52
1:B:405:VAL:HB	1:B:463:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:TYR:C	1:C:238:TYR:CD1	2.83	0.52
1:A:468:LEU:HD23	1:A:473:ILE:HD13	1.91	0.52
1:A:91:ASN:OD1	1:A:94:TYR:CD2	2.63	0.52
1:A:178:THR:HA	1:B:112:MET:CE	2.40	0.52
1:B:101:LYS:HE2	1:B:198:TYR:CE2	2.45	0.52
1:B:299:PRO:HB2	1:B:303:SER:HB2	1.92	0.52
1:B:308:ILE:O	1:B:311:ALA:HB3	2.10	0.52
1:B:445:GLY:CA	1:C:185:ASN:CG	2.60	0.52
1:C:185:ASN:O	1:C:188:TYR:HB2	2.06	0.52
1:C:193:SER:O	1:C:196:SER:HB3	2.06	0.52
1:C:458:LEU:CD1	1:C:460:ARG:HH22	2.23	0.52
1:A:319:ILE:CA	1:A:325:PRO:HB2	2.39	0.52
1:B:250:LEU:CD1	1:B:292:PHE:HE1	2.21	0.52
1:B:279:VAL:HG21	1:B:289:LEU:HD21	1.91	0.52
1:B:13:PHE:HB3	1:B:328:TYR:HA	1.92	0.52
1:B:426:SER:CA	1:C:188:TYR:HD1	2.20	0.52
1:C:262:PHE:CZ	1:C:314:VAL:HB	2.45	0.52
1:C:394:ALA:HA	1:C:408:LEU:HA	1.92	0.52
1:A:246:MET:HE1	1:B:476:ASP:CG	2.30	0.52
1:A:279:VAL:HG21	1:A:289:LEU:HD21	1.91	0.52
1:A:299:PRO:HB2	1:A:303:SER:HB2	1.92	0.52
1:A:205:ILE:HG21	1:B:472:LYS:HG3	0.54	0.52
1:C:101:LYS:HE2	1:C:198:TYR:CE2	2.45	0.52
1:C:29:THR:O	1:C:30:CYS:HB2	2.07	0.52
1:C:404:ILE:CB	1:C:404:ILE:N	2.73	0.52
1:C:320:LEU:HD22	1:C:407:ILE:HD13	1.90	0.52
1:B:281:SER:HB3	1:C:8:SER:H	0.69	0.52
1:C:91:ASN:OD1	1:C:94:TYR:CD2	2.63	0.52
1:A:101:LYS:HE2	1:A:198:TYR:CE2	2.45	0.52
1:A:123:MET:CA	1:A:174:PRO:HG2	2.40	0.52
1:A:185:ASN:HA	1:B:365:ALA:O	2.04	0.52
1:A:216:TRP:HB3	1:A:246:MET:HG2	1.91	0.52
1:A:32:THR:CG2	1:A:342:ALA:HA	2.28	0.52
1:A:465:THR:HA	1:A:468:LEU:HD11	1.92	0.52
1:B:123:MET:CA	1:B:174:PRO:HG2	2.40	0.52
1:B:286:SER:HB3	1:B:288:LEU:HG	1.92	0.52
1:C:299:PRO:HB2	1:C:303:SER:HB2	1.92	0.52
1:C:13:PHE:HB3	1:C:328:TYR:HA	1.92	0.52
1:A:18:ARG:CZ	1:A:79:TYR:CD2	2.92	0.52
1:B:6:TRP:CZ2	1:B:113:TYR:CD1	2.97	0.52
1:B:458:LEU:CD1	1:B:460:ARG:HH22	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HD3	1:C:221:LYS:C	2.31	0.52
1:C:279:VAL:HG21	1:C:289:LEU:HD21	1.91	0.52
1:C:2:THR:CB	1:C:3:PRO:HD2	2.18	0.52
1:C:468:LEU:HD23	1:C:473:ILE:HD13	1.91	0.52
1:A:182:VAL:HG21	1:B:58:THR:HB	1.92	0.52
1:A:431:GLN:NE2	1:A:431:GLN:HA	2.18	0.52
1:A:458:LEU:CD1	1:A:460:ARG:HH22	2.23	0.52
1:B:83:TRP:NE1	1:B:173:LEU:CD2	2.68	0.52
1:B:18:ARG:CZ	1:B:79:TYR:CD2	2.92	0.52
1:B:187:TRP:HE3	1:B:190:TRP:CE3	2.28	0.52
1:B:382:TYR:CE1	1:B:385:PRO:HD3	2.44	0.52
1:C:11:ILE:HD13	1:C:326:ILE:HG13	1.89	0.52
1:C:308:ILE:O	1:C:311:ALA:HB3	2.10	0.52
1:A:262:PHE:CZ	1:A:314:VAL:HB	2.45	0.51
1:A:405:VAL:HB	1:A:463:TYR:CD2	2.45	0.51
1:B:87:ILE:CG2	1:B:139:PRO:HG3	2.40	0.51
1:B:262:PHE:CZ	1:B:314:VAL:HB	2.45	0.51
1:A:185:ASN:HD22	1:B:319:ILE:HB	1.75	0.51
1:B:386:TYR:O	1:B:388:LYS:N	2.42	0.51
1:B:468:LEU:HD23	1:B:473:ILE:HD13	1.91	0.51
1:C:123:MET:CA	1:C:174:PRO:HG2	2.40	0.51
1:C:12:TYR:CE1	1:C:14:LEU:CD2	2.89	0.51
1:C:200:ILE:O	1:C:225:VAL:HG11	2.10	0.51
1:A:152:ILE:CD1	1:A:166:LEU:HA	2.28	0.51
1:A:216:TRP:HB2	1:A:245:VAL:CG2	2.29	0.51
1:A:301:PHE:CD2	1:A:301:PHE:C	2.83	0.51
1:A:308:ILE:O	1:A:311:ALA:HB3	2.10	0.51
1:A:13:PHE:HB3	1:A:328:TYR:HA	1.92	0.51
1:A:382:TYR:CD2	1:A:398:GLY:O	2.64	0.51
1:B:199:SER:C	1:B:200:ILE:HG13	2.16	0.51
1:B:68:GLN:HB2	1:B:69:LEU:HD23	1.92	0.51
1:C:300:ARG:HH11	1:C:328:TYR:HE1	1.53	0.51
1:C:301:PHE:C	1:C:301:PHE:CD2	2.83	0.51
1:C:380:VAL:CG1	1:C:381:THR:H	2.22	0.51
1:C:382:TYR:CD2	1:C:398:GLY:O	2.64	0.51
1:C:427:TYR:CE1	1:C:433:LEU:HD11	2.45	0.51
1:A:286:SER:HB3	1:A:288:LEU:HG	1.92	0.51
1:A:49:LEU:O	1:A:52:ILE:HG12	2.11	0.51
1:A:189:ASP:HB2	1:B:369:ARG:CG	2.41	0.51
1:B:394:ALA:HA	1:B:408:LEU:HA	1.92	0.51
1:B:418:TYR:HD1	1:B:454:MET:CE	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ALA:HA	1:C:318:ILE:CG2	2.36	0.51
1:C:382:TYR:CE1	1:C:385:PRO:HD3	2.44	0.51
1:C:473:ILE:HG23	1:C:474:CYS:N	2.25	0.51
1:A:200:ILE:O	1:A:225:VAL:HG11	2.10	0.51
1:A:238:TYR:O	1:A:241:PRO:HG2	2.11	0.51
1:A:2:THR:CB	1:A:3:PRO:HD2	2.18	0.51
1:B:315:ALA:HA	1:B:318:ILE:CG2	2.36	0.51
1:B:427:TYR:CE1	1:B:433:LEU:HD11	2.46	0.51
1:B:443:THR:O	1:B:451:PRO:HD2	2.11	0.51
1:C:250:LEU:HD12	1:C:292:PHE:CE1	2.46	0.51
1:C:280:LYS:O	1:C:281:SER:HB2	2.11	0.51
1:A:190:TRP:CD2	1:B:374:SER:CA	2.83	0.51
1:A:217:PRO:HA	1:B:474:CYS:O	2.10	0.51
1:A:404:ILE:N	1:A:404:ILE:CB	2.73	0.51
1:B:201:ASP:O	1:B:225:VAL:HG13	2.10	0.51
1:B:250:LEU:HD12	1:B:292:PHE:CE1	2.45	0.51
1:B:7:ARG:NE	1:B:286:SER:O	2.44	0.51
1:B:428:THR:CA	1:C:186:GLU:C	2.77	0.51
1:C:238:TYR:O	1:C:241:PRO:HG2	2.11	0.51
1:A:123:MET:CE	1:A:140:PHE:HE1	2.24	0.51
1:B:134:TYR:CE1	1:B:143:GLN:CB	2.94	0.51
1:B:301:PHE:C	1:B:301:PHE:CD2	2.83	0.51
1:B:420:LEU:CD2	1:B:452:VAL:CG2	2.83	0.51
1:A:177:ASP:HB3	1:B:53:GLN:HG2	1.90	0.51
1:C:243:GLN:HG2	1:C:284:PRO:O	2.11	0.51
1:B:238:TYR:HD2	1:C:403:GLN:NE2	2.07	0.51
1:A:278:THR:O	1:A:282:ASP:HB2	2.11	0.51
1:B:117:ASP:CG	1:B:204:ARG:NH1	2.65	0.51
1:B:14:LEU:HD22	1:B:19:PHE:CE2	2.46	0.51
1:B:216:TRP:HB3	1:B:246:MET:HG2	1.91	0.51
1:B:280:LYS:O	1:C:6:TRP:CA	2.54	0.51
1:B:280:LYS:O	1:C:7:ARG:CB	2.59	0.51
1:B:320:LEU:HD22	1:B:407:ILE:HD13	1.90	0.51
1:B:434:THR:C	1:B:435:GLU:O	2.47	0.51
1:A:182:VAL:CG2	1:B:58:THR:CB	2.89	0.51
1:C:134:TYR:CE1	1:C:143:GLN:CB	2.94	0.51
1:C:217:PRO:HD3	1:C:245:VAL:HG22	1.91	0.51
1:C:225:VAL:CG1	1:C:225:VAL:O	2.59	0.51
1:C:229:GLY:N	1:C:246:MET:HE1	2.25	0.51
1:A:181:ASP:OD1	1:B:319:ILE:HD13	2.11	0.51
1:A:380:VAL:CG1	1:A:381:THR:H	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:TYR:HD1	1:A:454:MET:CE	2.23	0.51
1:A:418:TYR:CE1	1:A:454:MET:HE2	2.46	0.51
1:A:68:GLN:HB2	1:A:69:LEU:HD23	1.92	0.51
1:B:200:ILE:O	1:B:225:VAL:HG11	2.10	0.51
1:B:406:THR:HG21	1:C:221:LYS:CB	2.41	0.51
1:B:449:ASN:CB	1:C:184:LYS:HZ2	2.13	0.51
1:C:14:LEU:HD22	1:C:19:PHE:CE2	2.46	0.51
1:C:101:LYS:HE3	1:C:198:TYR:CZ	2.46	0.51
1:C:200:ILE:CG2	1:C:203:LEU:HD11	2.38	0.51
1:C:216:TRP:HB3	1:C:246:MET:HG2	1.91	0.51
1:C:418:TYR:HD1	1:C:454:MET:CE	2.23	0.51
1:C:443:THR:O	1:C:451:PRO:HD2	2.11	0.51
1:C:465:THR:HA	1:C:468:LEU:HD11	1.92	0.51
1:A:187:TRP:HE3	1:A:190:TRP:CE3	2.28	0.51
1:A:250:LEU:HD12	1:A:292:PHE:CE1	2.46	0.51
1:B:137:PHE:CZ	1:B:174:PRO:HG3	2.46	0.51
1:C:216:TRP:HB2	1:C:245:VAL:CG2	2.29	0.51
1:C:431:GLN:NE2	1:C:431:GLN:HA	2.18	0.51
1:C:68:GLN:HB2	1:C:69:LEU:HD23	1.92	0.51
1:A:101:LYS:HE3	1:A:198:TYR:CZ	2.46	0.50
1:A:134:TYR:CE1	1:A:143:GLN:CB	2.94	0.50
1:A:229:GLY:H	1:A:246:MET:HE1	1.71	0.50
1:A:280:LYS:O	1:A:281:SER:HB2	2.11	0.50
1:A:427:TYR:CE1	1:A:433:LEU:HD11	2.45	0.50
1:A:7:ARG:NE	1:A:286:SER:O	2.44	0.50
1:B:255:TYR:CD1	1:B:292:PHE:CE2	2.99	0.50
1:C:187:TRP:HE3	1:C:190:TRP:CE3	2.29	0.50
1:C:295:ASN:CB	1:C:298:ASN:HB2	2.37	0.50
1:C:434:THR:C	1:C:435:GLU:O	2.47	0.50
1:B:192:GLY:HA2	1:B:223:ALA:HB2	1.94	0.50
1:B:243:GLN:HG2	1:B:284:PRO:O	2.11	0.50
1:B:295:ASN:CB	1:B:298:ASN:HB2	2.36	0.50
1:B:359:TYR:HA	1:B:362:ILE:HD12	1.93	0.50
1:B:382:TYR:CD2	1:B:398:GLY:O	2.64	0.50
1:A:148:PRO:HB3	1:B:49:LEU:CD2	2.41	0.50
1:C:208:VAL:HG23	1:C:216:TRP:CD2	2.46	0.50
1:C:278:THR:O	1:C:282:ASP:HB2	2.11	0.50
1:A:443:THR:O	1:A:451:PRO:HD2	2.11	0.50
1:B:188:TYR:CE1	1:B:218:GLY:CA	2.85	0.50
1:B:465:THR:HA	1:B:468:LEU:HD11	1.92	0.50
1:A:145:TYR:N	1:B:9:GLN:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:VAL:HG23	1:C:206:ASP:CB	2.31	0.50
1:B:237:ALA:HB3	1:C:399:THR:OG1	2.11	0.50
1:C:49:LEU:O	1:C:52:ILE:HG12	2.11	0.50
1:A:11:ILE:HD13	1:A:326:ILE:HG13	1.89	0.50
1:A:200:ILE:HD12	1:B:467:LYS:HZ2	1.75	0.50
1:A:215:PHE:CD1	1:A:215:PHE:C	2.85	0.50
1:A:347:THR:CG2	1:A:348:TRP:N	2.73	0.50
1:B:278:THR:O	1:B:282:ASP:HB2	2.10	0.50
1:B:243:GLN:HE22	1:B:289:LEU:HD13	1.77	0.50
1:A:185:ASN:N	1:B:366:ASN:CB	2.36	0.50
1:C:201:ASP:O	1:C:225:VAL:HG13	2.10	0.50
1:C:243:GLN:HE22	1:C:289:LEU:HD13	1.77	0.50
1:A:117:ASP:CG	1:A:204:ARG:NH1	2.65	0.50
1:A:87:ILE:HG21	1:A:123:MET:HE1	1.93	0.50
1:A:183:VAL:HG22	1:A:184:LYS:N	2.27	0.50
1:A:201:ASP:O	1:A:225:VAL:HG13	2.10	0.50
1:A:255:TYR:CD1	1:A:292:PHE:CE2	2.99	0.50
1:A:57:PHE:CZ	1:A:362:ILE:HG23	2.47	0.50
1:A:45:ILE:CG2	1:A:49:LEU:CD1	2.80	0.50
1:B:327:ILE:HG13	1:B:331:GLN:CD	2.32	0.50
1:A:188:TYR:CZ	1:B:367:ALA:N	2.78	0.50
1:B:385:PRO:CD	1:B:396:ARG:O	2.60	0.50
1:B:385:PRO:CB	1:C:3:PRO:HD3	2.34	0.50
1:C:87:ILE:CG2	1:C:139:PRO:HG3	2.40	0.50
1:A:14:LEU:HD22	1:A:19:PHE:CE2	2.46	0.50
1:A:262:PHE:CZ	1:A:314:VAL:HA	2.47	0.50
1:A:364:SER:HB2	1:A:437:ILE:HG22	1.93	0.50
1:A:436:VAL:HG22	1:A:437:ILE:N	2.26	0.50
1:A:165:TRP:CE2	1:B:109:GLU:C	2.80	0.50
1:B:225:VAL:O	1:B:225:VAL:CG1	2.59	0.50
1:B:273:TYR:CE1	1:B:389:ASP:HB3	2.44	0.50
1:B:392:THR:CG2	1:B:410:ASN:HB2	2.42	0.50
1:B:49:LEU:O	1:B:52:ILE:HG12	2.11	0.50
1:B:57:PHE:CZ	1:B:362:ILE:HG23	2.47	0.50
1:A:147:HIS:O	1:B:110:ARG:N	2.30	0.50
1:A:180:LYS:HE3	1:B:12:TYR:HA	1.91	0.50
1:A:194:LEU:O	1:B:403:GLN:CG	2.59	0.50
1:A:373:ILE:HG22	1:A:377:THR:HG22	1.92	0.50
1:B:242:TYR:CA	1:B:245:VAL:HG12	2.42	0.50
1:B:243:GLN:NE2	1:B:284:PRO:O	2.42	0.50
1:B:262:PHE:CZ	1:B:314:VAL:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:VAL:HG22	1:B:437:ILE:N	2.26	0.50
1:C:300:ARG:HG2	1:C:335:TYR:O	2.12	0.50
1:C:347:THR:CG2	1:C:348:TRP:N	2.73	0.50
1:C:57:PHE:CZ	1:C:362:ILE:HG23	2.47	0.50
1:C:42:TRP:CD2	1:C:94:TYR:CD1	3.00	0.50
1:B:238:TYR:O	1:B:241:PRO:HG2	2.11	0.50
1:B:300:ARG:HG2	1:B:335:TYR:O	2.12	0.50
1:C:117:ASP:CG	1:C:204:ARG:NH1	2.65	0.50
1:C:215:PHE:C	1:C:215:PHE:CD1	2.85	0.50
1:B:277:ASN:HB2	1:C:286:SER:O	2.00	0.50
1:C:307:ASP:HB2	1:C:413:ALA:CB	2.40	0.50
1:C:364:SER:HB2	1:C:437:ILE:HG22	1.93	0.50
1:C:369:ARG:HG2	1:C:379:PHE:CZ	2.47	0.50
1:C:273:TYR:CE1	1:C:389:ASP:HB3	2.44	0.50
1:A:18:ARG:HD3	1:A:344:ARG:HB3	1.94	0.50
1:A:194:LEU:O	1:B:403:GLN:HG3	2.11	0.50
1:A:243:GLN:HE22	1:A:289:LEU:HD13	1.76	0.50
1:A:262:PHE:CE2	1:A:314:VAL:HB	2.47	0.50
1:A:280:LYS:HE3	1:A:383:LYS:C	2.31	0.50
1:A:300:ARG:HG2	1:A:335:TYR:O	2.12	0.50
1:B:158:GLN:HA	1:B:161:VAL:CG1	2.42	0.50
1:B:101:LYS:HE3	1:B:198:TYR:CZ	2.46	0.50
1:B:208:VAL:HG23	1:B:216:TRP:CD2	2.46	0.50
1:B:215:PHE:CD1	1:B:215:PHE:C	2.85	0.50
1:C:13:PHE:CD2	1:C:328:TYR:CD2	2.99	0.50
1:C:7:ARG:NE	1:C:286:SER:O	2.44	0.50
1:C:255:TYR:CD1	1:C:292:PHE:CE2	2.99	0.50
1:C:385:PRO:CD	1:C:396:ARG:O	2.60	0.50
1:C:392:THR:CG2	1:C:410:ASN:HB2	2.42	0.50
1:A:123:MET:N	1:A:174:PRO:HG2	2.27	0.49
1:A:177:ASP:HB3	1:B:53:GLN:HA	1.94	0.49
1:A:184:LYS:HB2	1:B:367:ALA:HB2	1.94	0.49
1:A:189:ASP:CB	1:B:369:ARG:O	2.60	0.49
1:A:300:ARG:HH11	1:A:328:TYR:HE1	1.53	0.49
1:A:434:THR:C	1:A:435:GLU:O	2.47	0.49
1:A:432:GLN:HG3	1:A:465:THR:HG21	1.90	0.49
1:B:134:TYR:CE1	1:B:143:GLN:HB2	2.47	0.49
1:B:420:LEU:CD2	1:B:452:VAL:CG1	2.82	0.49
1:B:42:TRP:CD2	1:B:94:TYR:CD1	3.00	0.49
1:C:158:GLN:HA	1:C:161:VAL:CG1	2.42	0.49
1:C:183:VAL:HG22	1:C:184:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLY:HA2	1:C:223:ALA:HB2	1.94	0.49
1:C:327:ILE:HG13	1:C:331:GLN:CD	2.32	0.49
1:A:192:GLY:HA2	1:A:223:ALA:HB2	1.94	0.49
1:A:295:ASN:CB	1:A:298:ASN:HB2	2.36	0.49
1:A:327:ILE:HG13	1:A:331:GLN:OE1	2.12	0.49
1:A:369:ARG:HG2	1:A:379:PHE:CZ	2.47	0.49
1:A:34:ASP:O	1:A:36:LYS:HG3	2.12	0.49
1:A:392:THR:CG2	1:A:410:ASN:HB2	2.42	0.49
1:B:123:MET:N	1:B:174:PRO:HG2	2.27	0.49
1:B:229:GLY:HA3	1:B:246:MET:CE	2.42	0.49
1:B:347:THR:CG2	1:B:348:TRP:N	2.73	0.49
1:B:34:ASP:O	1:B:36:LYS:HG3	2.12	0.49
1:C:137:PHE:CZ	1:C:174:PRO:HG3	2.47	0.49
1:B:428:THR:HA	1:C:188:TYR:N	2.28	0.49
1:C:280:LYS:HE3	1:C:383:LYS:C	2.31	0.49
1:C:243:GLN:NE2	1:C:284:PRO:O	2.42	0.49
1:C:432:GLN:HG3	1:C:465:THR:HG21	1.90	0.49
1:A:158:GLN:HA	1:A:161:VAL:CG1	2.42	0.49
1:A:137:PHE:CZ	1:A:174:PRO:HG3	2.47	0.49
1:A:263:LYS:CA	1:A:310:LEU:HD23	2.42	0.49
1:A:243:GLN:HG2	1:A:284:PRO:O	2.11	0.49
1:A:243:GLN:NE2	1:A:284:PRO:O	2.42	0.49
1:A:418:TYR:HD1	1:A:454:MET:HE3	1.73	0.49
1:A:88:TYR:CZ	1:B:373:ILE:HA	2.45	0.49
1:B:369:ARG:HG2	1:B:379:PHE:CZ	2.47	0.49
1:C:262:PHE:CZ	1:C:314:VAL:HA	2.47	0.49
1:C:436:VAL:HG22	1:C:437:ILE:N	2.26	0.49
1:A:186:GLU:HB2	1:B:369:ARG:HH12	1.77	0.49
1:A:19:PHE:HD1	1:A:347:THR:HB	1.77	0.49
1:A:227:CYS:SG	1:B:473:ILE:HG22	2.53	0.49
1:A:240:CYS:CB	1:A:241:PRO:CD	2.89	0.49
1:A:42:TRP:CD2	1:A:94:TYR:CD1	3.00	0.49
1:A:87:ILE:CG2	1:A:139:PRO:HG3	2.40	0.49
1:B:183:VAL:HG22	1:B:184:LYS:N	2.27	0.49
1:B:13:PHE:CD2	1:B:328:TYR:CD2	2.99	0.49
1:C:463:TYR:OH	1:C:463:TYR:CE2	2.51	0.49
1:A:214:ASP:O	1:A:217:PRO:HG2	2.07	0.49
1:A:327:ILE:HG13	1:A:331:GLN:CD	2.32	0.49
1:B:19:PHE:HD1	1:B:347:THR:HB	1.77	0.49
1:C:161:VAL:O	1:C:210:HIS:HB3	2.12	0.49
1:C:123:MET:N	1:C:174:PRO:HG2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:GLY:HA3	1:C:246:MET:CE	2.42	0.49
1:C:263:LYS:CA	1:C:310:LEU:HD23	2.42	0.49
1:C:327:ILE:HG13	1:C:331:GLN:OE1	2.12	0.49
1:C:359:TYR:HA	1:C:362:ILE:HD12	1.93	0.49
1:B:383:LYS:HE2	1:C:5:ASP:CB	2.39	0.49
1:A:197:ASN:OD1	1:B:400:ASP:OD1	2.30	0.49
1:A:225:VAL:CG1	1:A:225:VAL:O	2.59	0.49
1:A:236:PRO:CB	1:A:278:THR:HG22	2.43	0.49
1:A:259:LEU:HD21	1:A:304:TYR:OH	2.12	0.49
1:A:385:PRO:CD	1:A:396:ARG:O	2.60	0.49
1:A:79:TYR:HE2	1:A:344:ARG:CD	2.25	0.49
1:A:79:TYR:HE2	1:A:344:ARG:CG	2.26	0.49
1:B:119:VAL:HG23	1:B:206:ASP:CB	2.31	0.49
1:B:123:MET:HB2	1:B:174:PRO:HG2	1.91	0.49
1:B:263:LYS:CA	1:B:310:LEU:HD23	2.42	0.49
1:B:364:SER:HB2	1:B:437:ILE:HG22	1.93	0.49
1:B:385:PRO:HG2	1:B:396:ARG:N	2.28	0.49
1:B:79:TYR:HE2	1:B:344:ARG:CD	2.25	0.49
1:C:123:MET:HB2	1:C:174:PRO:HG2	1.91	0.49
1:C:180:LYS:O	1:C:182:VAL:HG12	2.13	0.49
1:C:262:PHE:CE2	1:C:314:VAL:HB	2.47	0.49
1:C:236:PRO:CB	1:C:278:THR:HG22	2.43	0.49
1:B:384:ASN:CA	1:C:2:THR:HG22	2.05	0.49
1:C:273:TYR:HB2	1:C:389:ASP:OD1	2.13	0.49
1:A:434:THR:HG21	1:A:474:CYS:SG	2.53	0.49
1:B:262:PHE:CE2	1:B:314:VAL:HB	2.47	0.49
1:B:327:ILE:HG13	1:B:331:GLN:OE1	2.12	0.49
1:A:219:TYR:CZ	1:B:371:TYR:CD2	2.71	0.49
1:B:45:ILE:CG2	1:B:49:LEU:CD1	2.80	0.49
1:C:134:TYR:CE1	1:C:143:GLN:HB2	2.47	0.49
1:C:13:PHE:CE2	1:C:296:HIS:CD2	3.01	0.49
1:C:83:TRP:NE1	1:C:173:LEU:CD2	2.68	0.49
1:C:242:TYR:CA	1:C:245:VAL:HG12	2.42	0.49
1:A:11:ILE:HB	1:A:326:ILE:CA	2.41	0.49
1:A:204:ARG:HG2	1:A:228:ILE:O	2.12	0.49
1:A:246:MET:CE	1:B:476:ASP:OD1	2.61	0.49
1:A:147:HIS:HA	1:B:111:GLY:O	2.12	0.49
1:A:180:LYS:CE	1:B:12:TYR:N	2.55	0.49
1:A:221:LYS:CG	1:B:434:THR:CG2	2.91	0.49
1:C:204:ARG:NH1	1:C:230:GLU:HB3	2.28	0.49
1:A:180:LYS:NZ	1:B:57:PHE:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:CE	1:A:198:TYR:CE2	2.96	0.49
1:A:204:ARG:NH1	1:A:230:GLU:HB3	2.28	0.49
1:A:246:MET:N	1:B:474:CYS:O	2.46	0.49
1:A:394:ALA:HA	1:A:407:ILE:O	2.13	0.49
1:B:147:HIS:CD2	1:B:177:ASP:O	2.56	0.49
1:B:307:ASP:HB2	1:B:413:ALA:CB	2.40	0.49
1:C:79:TYR:HE2	1:C:344:ARG:CG	2.25	0.49
1:A:13:PHE:CD2	1:A:328:TYR:CD2	2.99	0.49
1:A:13:PHE:CE2	1:A:296:HIS:CD2	3.01	0.49
1:A:205:ILE:HA	1:B:471:SER:HA	1.94	0.49
1:A:161:VAL:O	1:A:210:HIS:HB3	2.12	0.49
1:A:242:TYR:CA	1:A:245:VAL:HG12	2.42	0.49
1:A:273:TYR:HB2	1:A:389:ASP:OD1	2.13	0.49
1:A:307:ASP:HB2	1:A:413:ALA:CB	2.40	0.49
1:B:154:ASN:O	1:B:157:ASP:HB3	2.13	0.49
1:B:161:VAL:O	1:B:210:HIS:HB3	2.12	0.49
1:A:187:TRP:CD1	1:B:370:ASN:CB	2.96	0.49
1:A:203:LEU:HB3	1:B:471:SER:H	1.77	0.49
1:C:434:THR:HG21	1:C:474:CYS:SG	2.53	0.49
1:A:177:ASP:CG	1:B:53:GLN:O	2.52	0.48
1:A:196:SER:OG	1:B:400:ASP:C	2.45	0.48
1:A:216:TRP:N	1:A:217:PRO:HD2	2.28	0.48
1:A:359:TYR:HA	1:A:362:ILE:HD12	1.93	0.48
1:B:180:LYS:O	1:B:182:VAL:HG12	2.13	0.48
1:B:185:ASN:CA	1:B:188:TYR:CD2	2.79	0.48
1:B:204:ARG:CZ	1:B:230:GLU:HB2	2.43	0.48
1:B:273:TYR:HB2	1:B:389:ASP:OD1	2.13	0.48
1:B:436:VAL:HG13	1:B:437:ILE:CD1	2.43	0.48
1:A:133:ASP:O	1:A:134:TYR:HB2	2.13	0.48
1:A:193:SER:O	1:A:196:SER:CB	2.61	0.48
1:A:194:LEU:HD13	1:B:375:LYS:HG3	1.93	0.48
1:A:204:ARG:CZ	1:A:230:GLU:HB2	2.43	0.48
1:A:382:TYR:OH	1:A:385:PRO:HG3	2.13	0.48
1:B:204:ARG:NH1	1:B:230:GLU:HB3	2.28	0.48
1:B:321:ASN:OD1	1:B:384:ASN:ND2	2.47	0.48
1:B:434:THR:HG21	1:B:474:CYS:SG	2.53	0.48
1:C:154:ASN:O	1:C:157:ASP:HB3	2.13	0.48
1:C:193:SER:O	1:C:196:SER:CB	2.61	0.48
1:C:21:ARG:HH21	1:C:21:ARG:HG2	1.78	0.48
1:C:240:CYS:CB	1:C:241:PRO:CD	2.89	0.48
1:C:259:LEU:HD21	1:C:304:TYR:OH	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ALA:HA	1:C:407:ILE:O	2.13	0.48
1:C:75:TYR:CE1	1:C:170:THR:CG2	2.91	0.48
1:A:147:HIS:HB2	1:A:175:ASP:O	2.13	0.48
1:A:208:VAL:HG23	1:A:216:TRP:CD2	2.46	0.48
1:A:21:ARG:HH21	1:A:21:ARG:HG2	1.78	0.48
1:A:255:TYR:CG	1:A:292:PHE:CE2	3.00	0.48
1:A:436:VAL:HG13	1:A:437:ILE:CD1	2.43	0.48
1:B:399:THR:CG2	1:C:196:SER:HA	2.44	0.48
1:B:394:ALA:HA	1:B:407:ILE:O	2.13	0.48
1:B:392:THR:HG21	1:B:410:ASN:HB2	1.94	0.48
1:C:11:ILE:HB	1:C:326:ILE:CA	2.41	0.48
1:C:147:HIS:HB2	1:C:175:ASP:O	2.12	0.48
1:C:346:ALA:O	1:C:349:LEU:HB2	2.14	0.48
1:A:119:VAL:HG23	1:A:206:ASP:CB	2.31	0.48
1:A:165:TRP:CE2	1:B:110:ARG:N	2.80	0.48
1:A:221:LYS:O	1:B:463:TYR:HB3	2.13	0.48
1:A:473:ILE:HG23	1:A:474:CYS:N	2.25	0.48
1:B:134:TYR:CD1	1:B:143:GLN:HB3	2.49	0.48
1:B:147:HIS:HB2	1:B:175:ASP:O	2.13	0.48
1:C:134:TYR:CD1	1:C:143:GLN:HB3	2.49	0.48
1:C:101:LYS:CE	1:C:198:TYR:CE2	2.96	0.48
1:C:455:ALA:HB3	1:C:458:LEU:HD12	1.95	0.48
1:C:79:TYR:HE2	1:C:344:ARG:CD	2.25	0.48
1:A:189:ASP:HB3	1:B:369:ARG:O	2.13	0.48
1:A:225:VAL:HG11	1:B:466:GLU:HA	1.95	0.48
1:A:246:MET:HE3	1:B:476:ASP:OD1	2.13	0.48
1:A:256:TYR:N	1:A:257:PRO:HD2	2.28	0.48
1:B:256:TYR:N	1:B:257:PRO:HD2	2.28	0.48
1:B:404:ILE:CB	1:B:404:ILE:N	2.73	0.48
1:B:455:ALA:HB3	1:B:458:LEU:HD12	1.95	0.48
1:B:428:THR:OG1	1:C:186:GLU:O	2.31	0.48
1:C:18:ARG:HD3	1:C:344:ARG:HB3	1.95	0.48
1:C:204:ARG:HH11	1:C:204:ARG:CG	2.20	0.48
1:B:241:PRO:HB2	1:C:376:ASP:H	1.79	0.48
1:C:385:PRO:HG2	1:C:396:ARG:N	2.28	0.48
1:A:392:THR:HG21	1:A:410:ASN:HB2	1.94	0.48
1:A:385:PRO:HG2	1:A:396:ARG:N	2.28	0.48
1:B:18:ARG:HD3	1:B:344:ARG:HB3	1.94	0.48
1:B:193:SER:O	1:B:196:SER:CB	2.61	0.48
1:B:101:LYS:CE	1:B:198:TYR:CE2	2.96	0.48
1:B:259:LEU:HD21	1:B:304:TYR:OH	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ILE:CA	1:B:325:PRO:HB2	2.39	0.48
1:B:346:ALA:O	1:B:349:LEU:HB2	2.14	0.48
1:B:237:ALA:O	1:C:376:ASP:OD1	2.30	0.48
1:A:134:TYR:CE1	1:A:143:GLN:HB2	2.47	0.48
1:A:122:HIS:HB2	1:A:173:LEU:HB3	1.96	0.48
1:A:204:ARG:CB	1:B:470:GLY:CA	2.23	0.48
1:A:346:ALA:O	1:A:349:LEU:HB2	2.14	0.48
1:B:123:MET:HE1	1:B:140:PHE:CE1	2.41	0.48
1:B:216:TRP:N	1:B:217:PRO:HD2	2.28	0.48
1:A:180:LYS:CB	1:B:55:MET:CG	2.92	0.48
1:B:428:THR:HB	1:C:190:TRP:H	1.78	0.48
1:C:204:ARG:CZ	1:C:230:GLU:HB2	2.43	0.48
1:C:216:TRP:N	1:C:217:PRO:HD2	2.28	0.48
1:C:255:TYR:CG	1:C:292:PHE:CE2	3.00	0.48
1:C:321:ASN:OD1	1:C:384:ASN:ND2	2.46	0.48
1:C:436:VAL:HG13	1:C:437:ILE:CD1	2.43	0.48
1:A:190:TRP:CE3	1:A:191:VAL:HG13	2.49	0.48
1:A:294:GLU:OE1	1:A:331:GLN:HA	2.14	0.48
1:A:35:GLN:HG3	1:A:76:GLY:HA3	1.95	0.48
1:A:42:TRP:CE3	1:A:94:TYR:CG	3.01	0.48
1:B:133:ASP:O	1:B:134:TYR:HB2	2.13	0.48
1:B:190:TRP:CE3	1:B:191:VAL:HG13	2.49	0.48
1:A:180:LYS:HZ2	1:B:57:PHE:HB2	1.77	0.48
1:C:286:SER:C	1:C:287:THR:HG23	2.33	0.48
1:C:392:THR:HG21	1:C:410:ASN:HB2	1.94	0.48
1:C:42:TRP:CE3	1:C:94:TYR:CG	3.01	0.48
1:A:180:LYS:HG3	1:B:12:TYR:CB	2.43	0.48
1:B:122:HIS:CE1	1:B:173:LEU:HD22	2.48	0.48
1:B:182:VAL:HG13	1:B:183:VAL:N	2.18	0.48
1:B:205:ILE:HD13	1:B:205:ILE:HG21	1.47	0.48
1:B:238:TYR:CD2	1:C:403:GLN:OE1	2.67	0.48
1:B:13:PHE:CE2	1:B:296:HIS:CD2	3.01	0.48
1:B:364:SER:HB2	1:B:437:ILE:HG23	1.96	0.48
1:A:194:LEU:CG	1:B:375:LYS:CG	2.90	0.48
1:A:196:SER:CB	1:B:403:GLN:HG3	2.33	0.48
1:A:180:LYS:HE2	1:B:57:PHE:HB3	1.91	0.48
1:B:79:TYR:HE2	1:B:344:ARG:CG	2.26	0.48
1:C:122:HIS:HB2	1:C:173:LEU:HB3	1.96	0.48
1:C:34:ASP:O	1:C:36:LYS:HG3	2.13	0.48
1:C:433:LEU:O	1:C:442:VAL:HB	2.14	0.48
1:A:134:TYR:CD1	1:A:143:GLN:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PRO:HG2	1:A:396:ARG:CA	2.44	0.48
1:A:91:ASN:C	1:A:92:GLU:CG	2.82	0.48
1:B:286:SER:C	1:B:287:THR:HG23	2.33	0.48
1:B:383:LYS:CG	1:C:113:TYR:CE1	2.95	0.48
1:B:463:TYR:CE2	1:B:463:TYR:OH	2.51	0.48
1:A:227:CYS:CA	1:B:476:ASP:HA	2.43	0.48
1:B:13:PHE:CD2	1:B:61:TRP:CZ3	3.02	0.48
1:C:133:ASP:O	1:C:134:TYR:HB2	2.13	0.48
1:C:272:LEU:O	1:C:275:MET:HB3	2.14	0.48
1:B:382:TYR:C	1:C:2:THR:CG2	2.77	0.48
1:C:308:ILE:H	1:C:308:ILE:HG13	1.19	0.48
1:C:385:PRO:HG2	1:C:396:ARG:CA	2.44	0.48
1:A:88:TYR:CD2	1:A:139:PRO:HB3	2.49	0.47
1:A:215:PHE:CE1	1:B:472:LYS:HB3	2.49	0.47
1:A:286:SER:C	1:A:287:THR:HG23	2.33	0.47
1:A:321:ASN:OD1	1:A:384:ASN:ND2	2.47	0.47
1:A:420:LEU:CD1	1:A:454:MET:HE2	2.44	0.47
1:B:204:ARG:HG2	1:B:228:ILE:O	2.12	0.47
1:B:250:LEU:HD12	1:B:292:PHE:HE1	1.79	0.47
1:B:42:TRP:CE3	1:B:94:TYR:CG	3.01	0.47
1:C:180:LYS:HZ3	1:C:182:VAL:HB	1.77	0.47
1:C:35:GLN:HG3	1:C:76:GLY:HA3	1.95	0.47
1:C:382:TYR:OH	1:C:385:PRO:HG3	2.13	0.47
1:C:45:ILE:CG2	1:C:49:LEU:CD1	2.80	0.47
1:A:208:VAL:C	1:A:216:TRP:HZ2	2.17	0.47
1:A:249:VAL:CA	1:B:477:SER:CB	2.92	0.47
1:A:272:LEU:O	1:A:275:MET:HB3	2.14	0.47
1:A:433:LEU:O	1:A:442:VAL:HB	2.14	0.47
1:B:122:HIS:HB2	1:B:173:LEU:HB3	1.96	0.47
1:B:447:ASP:OD1	1:C:184:LYS:HD2	2.15	0.47
1:C:122:HIS:CE1	1:C:173:LEU:HD22	2.48	0.47
1:C:208:VAL:C	1:C:216:TRP:HZ2	2.17	0.47
1:C:373:ILE:HG22	1:C:377:THR:HG22	1.92	0.47
1:B:237:ALA:HA	1:C:379:PHE:H	1.77	0.47
1:C:418:TYR:CD1	1:C:454:MET:HE2	2.49	0.47
1:C:88:TYR:CD2	1:C:139:PRO:HB3	2.49	0.47
1:A:122:HIS:CE1	1:A:173:LEU:HD22	2.48	0.47
1:A:250:LEU:HD12	1:A:292:PHE:HE1	1.80	0.47
1:A:455:ALA:HB3	1:A:458:LEU:HD12	1.95	0.47
1:B:123:MET:CE	1:B:140:PHE:HE1	2.24	0.47
1:B:195:VAL:HG23	1:B:200:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLN:HG3	1:B:76:GLY:HA3	1.95	0.47
1:C:13:PHE:CD2	1:C:61:TRP:CZ3	3.02	0.47
1:A:120:ALA:HA	1:A:187:TRP:CH2	2.49	0.47
1:A:232:LEU:HD23	1:A:232:LEU:H	1.78	0.47
1:A:43:GLN:NE2	1:A:99:ASP:OD1	2.46	0.47
1:B:120:ALA:HA	1:B:187:TRP:CH2	2.49	0.47
1:B:205:ILE:HD12	1:B:208:VAL:HG21	1.96	0.47
1:A:188:TYR:N	1:B:369:ARG:C	2.68	0.47
1:C:184:LYS:C	1:C:188:TYR:CD2	2.88	0.47
1:C:190:TRP:CE3	1:C:191:VAL:HG13	2.49	0.47
1:C:204:ARG:HG2	1:C:228:ILE:O	2.12	0.47
1:A:154:ASN:O	1:A:157:ASP:HB3	2.13	0.47
1:A:13:PHE:CD2	1:A:61:TRP:CZ3	3.02	0.47
1:B:232:LEU:N	1:B:232:LEU:HD23	2.30	0.47
1:A:180:LYS:CE	1:B:57:PHE:HB2	2.22	0.47
1:C:250:LEU:HD12	1:C:292:PHE:HE1	1.80	0.47
1:C:294:GLU:OE1	1:C:331:GLN:HA	2.14	0.47
1:C:49:LEU:HD23	1:C:110:ARG:CD	2.41	0.47
1:A:364:SER:HB2	1:A:437:ILE:HG23	1.96	0.47
1:B:11:ILE:HB	1:B:326:ILE:CA	2.40	0.47
1:B:12:TYR:C	1:B:12:TYR:CD1	2.88	0.47
1:B:185:ASN:N	1:B:188:TYR:CD2	2.83	0.47
1:B:187:TRP:HZ3	1:B:190:TRP:CH2	2.33	0.47
1:B:241:PRO:HB2	1:C:376:ASP:N	2.29	0.47
1:B:255:TYR:CG	1:B:292:PHE:CE2	3.00	0.47
1:A:190:TRP:CZ3	1:B:374:SER:HB2	2.43	0.47
1:B:433:LEU:O	1:B:442:VAL:HB	2.14	0.47
1:C:12:TYR:C	1:C:12:TYR:CD1	2.88	0.47
1:C:120:ALA:HA	1:C:187:TRP:CH2	2.49	0.47
1:C:187:TRP:HZ3	1:C:190:TRP:CH2	2.33	0.47
1:C:232:LEU:N	1:C:232:LEU:HD23	2.30	0.47
1:C:256:TYR:N	1:C:257:PRO:HD2	2.28	0.47
1:B:213:LYS:HZ3	1:C:375:LYS:HG2	1.80	0.47
1:B:238:TYR:CD2	1:C:403:GLN:CD	2.84	0.47
1:A:12:TYR:CD1	1:A:12:TYR:C	2.88	0.47
1:A:83:TRP:NE1	1:A:173:LEU:CD2	2.68	0.47
1:A:180:LYS:H	1:B:55:MET:CA	2.25	0.47
1:A:249:VAL:CA	1:B:477:SER:HB3	2.45	0.47
1:A:129:GLY:C	1:B:109:GLU:OE2	2.52	0.47
1:B:88:TYR:CD2	1:B:139:PRO:HB3	2.49	0.47
1:B:184:LYS:C	1:B:188:TYR:CD2	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:HH21	1:B:21:ARG:HG2	1.79	0.47
1:B:232:LEU:H	1:B:232:LEU:HD23	1.78	0.47
1:B:385:PRO:HG2	1:B:396:ARG:CA	2.44	0.47
1:B:420:LEU:CD1	1:B:454:MET:HE2	2.44	0.47
1:A:178:THR:CB	1:B:57:PHE:O	2.54	0.47
1:C:319:ILE:CA	1:C:325:PRO:HB2	2.39	0.47
1:C:364:SER:HB2	1:C:437:ILE:HG23	1.96	0.47
1:C:43:GLN:NE2	1:C:99:ASP:OD1	2.46	0.47
1:A:404:ILE:N	1:A:404:ILE:HG22	2.30	0.47
1:A:56:GLY:HA3	1:A:366:ASN:CB	2.42	0.47
1:B:115:MET:HE2	1:B:204:ARG:HB2	1.93	0.47
1:B:237:ALA:CB	1:C:379:PHE:CB	2.93	0.47
1:A:181:ASP:N	1:B:362:ILE:CG2	2.77	0.47
1:A:187:TRP:HB3	1:B:371:TYR:HB2	1.96	0.47
1:B:399:THR:HG22	1:C:196:SER:N	2.29	0.47
1:C:83:TRP:HH2	1:C:171:VAL:HG21	1.74	0.47
1:C:195:VAL:HG23	1:C:200:ILE:O	2.14	0.47
1:B:397:LYS:N	1:C:224:GLY:HA3	2.30	0.47
1:C:404:ILE:N	1:C:404:ILE:HG22	2.30	0.47
1:A:123:MET:CB	1:A:137:PHE:CE1	2.79	0.47
1:A:229:GLY:HA3	1:A:246:MET:CE	2.42	0.47
1:A:232:LEU:HD23	1:A:232:LEU:N	2.30	0.47
1:A:146:PHE:HB2	1:B:111:GLY:HA2	1.03	0.47
1:B:432:GLN:HG3	1:B:465:THR:HG21	1.90	0.47
1:C:123:MET:CG	1:C:146:PHE:HE1	2.07	0.47
1:C:55:MET:HG3	1:C:362:ILE:HG21	1.97	0.47
1:C:420:LEU:CD1	1:C:454:MET:HE2	2.45	0.47
1:A:147:HIS:CE1	1:B:110:ARG:NH1	2.83	0.47
1:A:387:ILE:HD11	1:A:424:GLY:C	2.35	0.47
1:A:387:ILE:HD13	1:A:387:ILE:HG21	1.37	0.47
1:A:62:ILE:HD13	1:A:62:ILE:HG21	1.43	0.47
1:B:204:ARG:CZ	1:B:230:GLU:CB	2.93	0.47
1:B:243:GLN:NE2	1:B:285:ASP:HA	2.30	0.47
1:B:252:TYR:CA	1:B:292:PHE:HZ	2.27	0.47
1:A:187:TRP:CD1	1:B:370:ASN:HB3	2.49	0.47
1:B:387:ILE:HD11	1:B:424:GLY:C	2.36	0.47
1:C:408:LEU:HD13	1:C:460:ARG:O	2.15	0.47
1:A:143:GLN:NE2	1:B:108:HIS:CB	2.77	0.47
1:A:148:PRO:HG3	1:B:49:LEU:CD2	2.45	0.47
1:A:205:ILE:CG1	1:B:472:LYS:N	2.75	0.47
1:A:49:LEU:HD23	1:A:110:ARG:CD	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLU:OE1	1:B:331:GLN:HA	2.14	0.47
1:C:185:ASN:N	1:C:188:TYR:CD2	2.83	0.47
1:A:147:HIS:HB3	1:B:110:ARG:O	2.14	0.46
1:A:187:TRP:HZ3	1:A:190:TRP:CH2	2.33	0.46
1:A:217:PRO:HD3	1:A:245:VAL:HG22	1.91	0.46
1:A:221:LYS:CB	1:B:434:THR:HG22	2.44	0.46
1:A:243:GLN:NE2	1:A:285:ASP:HA	2.30	0.46
1:A:422:LEU:HD11	1:A:425:ALA:HB2	1.97	0.46
1:A:418:TYR:CE1	1:A:454:MET:CE	2.98	0.46
1:B:147:HIS:N	1:B:175:ASP:O	2.48	0.46
1:C:232:LEU:HD23	1:C:232:LEU:H	1.78	0.46
1:B:282:ASP:HA	1:C:373:ILE:HD13	1.97	0.46
1:C:387:ILE:HD11	1:C:424:GLY:C	2.35	0.46
1:C:78:ALA:O	1:C:81:GLY:CA	2.61	0.46
1:A:292:PHE:C	1:A:293:VAL:HG12	2.36	0.46
1:A:463:TYR:CE2	1:A:463:TYR:OH	2.51	0.46
1:A:147:HIS:N	1:B:110:ARG:O	2.39	0.46
1:B:272:LEU:O	1:B:275:MET:HB3	2.14	0.46
1:B:317:PHE:C	1:B:317:PHE:CD1	2.89	0.46
1:B:458:LEU:CD1	1:B:460:ARG:NH2	2.79	0.46
1:C:19:PHE:HD1	1:C:347:THR:HB	1.77	0.46
1:C:205:ILE:HD12	1:C:208:VAL:HG21	1.96	0.46
1:C:204:ARG:CZ	1:C:230:GLU:CB	2.93	0.46
1:C:243:GLN:NE2	1:C:285:ASP:HA	2.30	0.46
1:A:192:GLY:N	1:B:463:TYR:OH	2.41	0.46
1:A:215:PHE:CD2	1:B:367:ALA:HB2	2.51	0.46
1:A:458:LEU:CD1	1:A:460:ARG:NH2	2.79	0.46
1:B:208:VAL:C	1:B:216:TRP:HZ2	2.17	0.46
1:B:292:PHE:C	1:B:293:VAL:HG12	2.36	0.46
1:C:476:ASP:O	1:C:477:SER:HB3	2.15	0.46
1:A:242:TYR:HA	1:A:245:VAL:HG12	1.97	0.46
1:A:243:GLN:CB	1:A:249:VAL:HG11	2.45	0.46
1:A:368:ILE:HG21	1:A:368:ILE:HD13	1.44	0.46
1:B:107:LEU:HG	1:B:108:HIS:N	2.30	0.46
1:B:19:PHE:CE1	1:B:347:THR:HG21	2.50	0.46
1:B:400:ASP:CB	1:C:195:VAL:N	2.78	0.46
1:B:446:SER:HG	1:C:181:ASP:CG	1.96	0.46
1:C:148:PRO:O	1:C:165:TRP:NE1	2.48	0.46
1:B:394:ALA:HB1	1:C:221:LYS:NZ	2.30	0.46
1:C:240:CYS:N	1:C:241:PRO:HD2	2.30	0.46
1:C:422:LEU:HD11	1:C:425:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TRP:HH2	1:A:171:VAL:HG21	1.74	0.46
1:A:300:ARG:NH1	1:A:329:ALA:O	2.49	0.46
1:A:280:LYS:NZ	1:A:383:LYS:HB3	2.31	0.46
1:A:75:TYR:HE1	1:A:170:THR:CB	2.29	0.46
1:B:148:PRO:O	1:B:165:TRP:NE1	2.49	0.46
1:B:408:LEU:HD13	1:B:460:ARG:O	2.15	0.46
1:A:218:GLY:HA2	1:B:437:ILE:N	2.30	0.46
1:B:75:TYR:HE1	1:B:170:THR:CB	2.29	0.46
1:C:292:PHE:C	1:C:293:VAL:HG12	2.36	0.46
1:C:451:PRO:O	1:C:453:PRO:HD3	2.16	0.46
1:A:185:ASN:ND2	1:B:319:ILE:HD12	2.30	0.46
1:A:204:ARG:CZ	1:A:230:GLU:CB	2.93	0.46
1:A:216:TRP:O	1:B:474:CYS:N	2.49	0.46
1:A:19:PHE:CE1	1:A:347:THR:HG21	2.50	0.46
1:B:242:TYR:HA	1:B:245:VAL:HG12	1.97	0.46
1:B:340:ASP:OD1	1:B:341:PRO:N	2.48	0.46
1:B:55:MET:HG3	1:B:362:ILE:HG21	1.97	0.46
1:B:62:ILE:HG21	1:B:62:ILE:HD13	1.42	0.46
1:B:68:GLN:NE2	1:B:81:GLY:HA2	2.29	0.46
1:B:78:ALA:O	1:B:81:GLY:CA	2.61	0.46
1:C:75:TYR:HE1	1:C:170:THR:CB	2.29	0.46
1:C:61:TRP:HZ2	1:C:204:ARG:CZ	2.29	0.46
1:C:418:TYR:CE1	1:C:454:MET:CE	2.98	0.46
1:C:68:GLN:NE2	1:C:81:GLY:HA2	2.29	0.46
1:A:123:MET:CE	1:A:140:PHE:CE1	2.98	0.46
1:A:211:VAL:HG12	1:A:211:VAL:H	1.05	0.46
1:A:340:ASP:OD1	1:A:341:PRO:N	2.48	0.46
1:A:408:LEU:HD13	1:A:460:ARG:O	2.15	0.46
1:B:188:TYR:HE1	1:B:218:GLY:C	2.18	0.46
1:B:332:GLU:O	1:B:358:LEU:HB2	2.15	0.46
1:B:451:PRO:O	1:B:453:PRO:HD3	2.16	0.46
1:C:188:TYR:HE1	1:C:218:GLY:C	2.18	0.46
1:C:56:GLY:HA3	1:C:366:ASN:CB	2.42	0.46
1:A:332:GLU:O	1:A:358:LEU:HB2	2.15	0.46
1:A:451:PRO:O	1:A:453:PRO:HD3	2.16	0.46
1:A:78:ALA:O	1:A:81:GLY:CA	2.61	0.46
1:B:404:ILE:HG22	1:B:404:ILE:N	2.30	0.46
1:B:83:TRP:HH2	1:B:171:VAL:HG21	1.74	0.46
1:C:18:ARG:CD	1:C:344:ARG:HB3	2.46	0.46
1:C:263:LYS:H	1:C:310:LEU:HD23	1.81	0.46
1:C:317:PHE:CD1	1:C:317:PHE:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:GLU:O	1:C:358:LEU:HB2	2.15	0.46
1:A:188:TYR:HE1	1:A:218:GLY:C	2.18	0.46
1:A:55:MET:HG3	1:A:362:ILE:HG21	1.97	0.46
1:C:147:HIS:N	1:C:175:ASP:O	2.48	0.46
1:B:422:LEU:HD21	1:C:221:LYS:HG2	1.98	0.46
1:C:243:GLN:CB	1:C:249:VAL:HG11	2.45	0.46
1:C:300:ARG:NH1	1:C:329:ALA:O	2.49	0.46
1:C:25:SER:C	1:C:348:TRP:HE1	2.20	0.46
1:C:388:LYS:CE	1:C:390:ASP:HB2	2.39	0.46
1:A:143:GLN:N	1:B:113:TYR:CD2	2.84	0.46
1:A:123:MET:CG	1:A:146:PHE:HE1	2.07	0.46
1:A:165:TRP:CZ2	1:B:110:ARG:N	2.77	0.46
1:A:194:LEU:CG	1:B:375:LYS:CB	2.91	0.46
1:A:246:MET:HB2	1:B:476:ASP:C	2.26	0.46
1:A:55:MET:HE3	1:A:332:GLU:HB3	1.97	0.46
1:A:61:TRP:HZ2	1:A:204:ARG:CZ	2.29	0.46
1:A:180:LYS:CG	1:B:12:TYR:HB2	2.42	0.46
1:B:243:GLN:CB	1:B:249:VAL:HG11	2.45	0.46
1:C:188:TYR:CE1	1:C:218:GLY:C	2.89	0.46
1:B:381:THR:HG22	1:C:1:ALA:CA	2.46	0.46
1:C:42:TRP:NE1	1:C:62:ILE:CD1	2.68	0.46
1:A:147:HIS:N	1:A:175:ASP:O	2.48	0.45
1:A:21:ARG:NH2	1:A:21:ARG:HG2	2.32	0.45
1:A:263:LYS:H	1:A:310:LEU:HD23	1.81	0.45
1:A:317:PHE:CD1	1:A:317:PHE:C	2.89	0.45
1:A:476:ASP:O	1:A:477:SER:HB3	2.15	0.45
1:A:88:TYR:CE2	1:B:373:ILE:CA	2.88	0.45
1:B:176:LEU:O	1:B:177:ASP:HB2	2.16	0.45
1:B:400:ASP:C	1:C:192:GLY:O	2.55	0.45
1:B:404:ILE:HG21	1:B:404:ILE:HD12	1.03	0.45
1:B:418:TYR:CD1	1:B:454:MET:HE2	2.51	0.45
1:C:100:LEU:O	1:C:103:LEU:HB3	2.16	0.45
1:C:205:ILE:HG21	1:C:205:ILE:HD13	1.47	0.45
1:C:19:PHE:CE1	1:C:347:THR:HG21	2.50	0.45
1:C:62:ILE:HD13	1:C:62:ILE:HG21	1.42	0.45
1:A:18:ARG:CD	1:A:344:ARG:HB3	2.46	0.45
1:A:205:ILE:HD12	1:A:208:VAL:HG21	1.96	0.45
1:A:31:ASN:ND2	1:A:33:ALA:HB3	2.31	0.45
1:B:18:ARG:CD	1:B:344:ARG:HB3	2.46	0.45
1:A:185:ASN:HD22	1:B:319:ILE:CB	2.29	0.45
1:C:21:ARG:NH2	1:C:21:ARG:HG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:TYR:HA	1:C:245:VAL:HG12	1.97	0.45
1:A:68:GLN:NE2	1:A:81:GLY:HA2	2.29	0.45
1:B:408:LEU:HD11	1:B:462:LEU:CD2	2.36	0.45
1:B:426:SER:C	1:C:188:TYR:HA	2.37	0.45
1:B:445:GLY:N	1:C:185:ASN:HD21	1.96	0.45
1:A:246:MET:HE3	1:B:476:ASP:CG	2.34	0.45
1:C:177:ASP:OD1	1:C:183:VAL:HG21	2.16	0.45
1:C:19:PHE:CD1	1:C:347:THR:CB	3.00	0.45
1:C:354:THR:O	1:C:359:TYR:CD1	2.70	0.45
1:C:280:LYS:NZ	1:C:383:LYS:HB3	2.31	0.45
1:B:281:SER:HB2	1:C:8:SER:N	2.08	0.45
1:A:185:ASN:ND2	1:B:319:ILE:HB	2.31	0.45
1:A:191:VAL:HG11	1:A:219:TYR:CZ	2.07	0.45
1:A:144:ASP:N	1:B:113:TYR:CG	2.84	0.45
1:B:123:MET:CE	1:B:140:PHE:CE1	2.98	0.45
1:B:132:VAL:HG11	1:B:134:TYR:HE2	1.81	0.45
1:B:19:PHE:CD1	1:B:347:THR:CB	3.00	0.45
1:B:21:ARG:HG2	1:B:21:ARG:NH2	2.32	0.45
1:B:31:ASN:ND2	1:B:33:ALA:HB3	2.31	0.45
1:B:43:GLN:NE2	1:B:99:ASP:OD1	2.46	0.45
1:C:123:MET:CE	1:C:140:PHE:CE1	2.98	0.45
1:C:31:ASN:ND2	1:C:33:ALA:HB3	2.31	0.45
1:C:64:PRO:CG	1:C:82:TYR:HA	2.31	0.45
1:A:194:LEU:HD13	1:B:375:LYS:CA	2.44	0.45
1:A:25:SER:C	1:A:348:TRP:HE1	2.20	0.45
1:A:320:LEU:HD22	1:A:407:ILE:HD11	1.98	0.45
1:B:100:LEU:O	1:B:103:LEU:HB3	2.16	0.45
1:A:145:TYR:CD1	1:B:113:TYR:CE2	3.01	0.45
1:B:61:TRP:HZ2	1:B:204:ARG:CZ	2.29	0.45
1:B:188:TYR:CE1	1:B:218:GLY:C	2.89	0.45
1:B:255:TYR:CB	1:B:292:PHE:CE2	3.00	0.45
1:B:300:ARG:NH1	1:B:329:ALA:O	2.49	0.45
1:B:418:TYR:CE1	1:B:454:MET:CE	2.98	0.45
1:B:66:THR:HB	1:B:67:ALA:H	1.23	0.45
1:A:176:LEU:O	1:A:177:ASP:HB2	2.16	0.45
1:A:188:TYR:CE1	1:A:218:GLY:C	2.89	0.45
1:B:238:TYR:HD2	1:C:403:GLN:OE1	1.99	0.45
1:B:251:ASN:HA	1:B:251:ASN:HD22	1.53	0.45
1:B:82:TYR:OH	1:B:296:HIS:CE1	2.70	0.45
1:A:185:ASN:ND2	1:B:319:ILE:CB	2.79	0.45
1:C:176:LEU:O	1:C:177:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASP:OD2	1:C:5:ASP:OD2	2.30	0.45
1:C:87:ILE:HG23	1:C:87:ILE:O	2.16	0.45
1:A:177:ASP:OD1	1:A:183:VAL:HG21	2.17	0.45
1:A:240:CYS:N	1:A:241:PRO:HD2	2.30	0.45
1:A:87:ILE:O	1:A:87:ILE:HG23	2.16	0.45
1:B:177:ASP:OD1	1:B:183:VAL:HG11	2.17	0.45
1:B:205:ILE:HD12	1:B:208:VAL:CB	2.46	0.45
1:B:204:ARG:HH12	1:B:230:GLU:HG2	1.82	0.45
1:B:232:LEU:O	1:B:233:ASP:HB2	2.17	0.45
1:B:241:PRO:CB	1:C:376:ASP:N	2.77	0.45
1:B:263:LYS:H	1:B:310:LEU:HD23	1.81	0.45
1:A:188:TYR:CZ	1:B:367:ALA:HB3	2.52	0.45
1:A:188:TYR:C	1:B:368:ILE:HG12	2.37	0.45
1:B:396:ARG:O	1:C:224:GLY:CA	2.65	0.45
1:C:229:GLY:N	1:C:246:MET:CE	2.80	0.45
1:C:317:PHE:CD1	1:C:318:ILE:N	2.85	0.45
1:C:340:ASP:OD1	1:C:341:PRO:N	2.48	0.45
1:B:386:TYR:H	1:C:3:PRO:HB3	1.82	0.45
1:A:180:LYS:CA	1:B:55:MET:HG2	2.42	0.45
1:A:184:LYS:CE	1:B:366:ASN:ND2	2.80	0.45
1:A:242:TYR:O	1:A:245:VAL:HG12	2.17	0.45
1:A:332:GLU:CG	1:A:333:GLN:H	2.30	0.45
1:A:19:PHE:CD1	1:A:347:THR:CB	3.00	0.45
1:B:229:GLY:N	1:B:246:MET:CE	2.80	0.45
1:B:380:VAL:CG1	1:B:381:THR:H	2.22	0.45
1:B:418:TYR:HD1	1:B:454:MET:HE3	1.79	0.45
1:A:227:CYS:SG	1:B:473:ILE:CG2	3.05	0.45
1:B:401:GLY:CA	1:C:196:SER:HB2	2.39	0.45
1:B:424:GLY:C	1:C:218:GLY:C	2.76	0.45
1:C:424:GLY:O	1:C:425:ALA:HB3	2.17	0.45
1:A:148:PRO:CA	1:B:107:LEU:CB	2.94	0.45
1:A:317:PHE:CD1	1:A:318:ILE:N	2.85	0.45
1:A:424:GLY:O	1:A:425:ALA:HB3	2.17	0.45
1:A:66:THR:O	1:A:67:ALA:HB2	2.17	0.45
1:B:25:SER:C	1:B:348:TRP:HE1	2.20	0.45
1:A:182:VAL:CG2	1:B:58:THR:HB	2.47	0.45
1:C:123:MET:HG3	1:C:176:LEU:HD11	1.99	0.45
1:C:177:ASP:OD1	1:C:183:VAL:HG11	2.17	0.45
1:C:400:ASP:OD1	1:C:401:GLY:N	2.50	0.45
1:A:107:LEU:HG	1:A:108:HIS:N	2.30	0.45
1:A:246:MET:CB	1:B:476:ASP:C	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD12	1:A:317:PHE:CE1	2.52	0.45
1:A:82:TYR:OH	1:A:296:HIS:CE1	2.70	0.45
1:A:354:THR:O	1:A:359:TYR:CD1	2.70	0.45
1:A:55:MET:CG	1:A:57:PHE:HE2	2.26	0.45
1:B:107:LEU:HD12	1:B:111:GLY:O	2.17	0.45
1:B:277:ASN:CB	1:C:286:SER:CB	2.69	0.45
1:B:424:GLY:O	1:B:425:ALA:HB3	2.17	0.45
1:C:158:GLN:HA	1:C:161:VAL:HG11	1.99	0.45
1:C:242:TYR:O	1:C:245:VAL:HG12	2.17	0.45
1:C:373:ILE:HA	1:C:377:THR:HA	1.99	0.45
1:C:458:LEU:CD1	1:C:460:ARG:NH2	2.79	0.45
1:A:373:ILE:HA	1:A:377:THR:HA	1.99	0.44
1:B:123:MET:HG3	1:B:176:LEU:HD11	1.99	0.44
1:B:236:PRO:CB	1:B:278:THR:HG22	2.43	0.44
1:B:241:PRO:CA	1:C:374:SER:HA	2.28	0.44
1:B:373:ILE:HA	1:B:377:THR:HA	1.99	0.44
1:B:387:ILE:HG23	1:B:388:LYS:N	2.32	0.44
1:B:428:THR:O	1:C:185:ASN:OD1	2.35	0.44
1:B:453:PRO:O	1:B:460:ARG:NE	2.50	0.44
1:C:182:VAL:HG13	1:C:183:VAL:N	2.17	0.44
1:C:472:LYS:O	1:C:473:ILE:CB	2.65	0.44
1:C:66:THR:O	1:C:67:ALA:HB2	2.17	0.44
1:C:91:ASN:C	1:C:92:GLU:CG	2.82	0.44
1:A:158:GLN:HA	1:A:161:VAL:HG11	1.99	0.44
1:A:400:ASP:OD1	1:A:401:GLY:N	2.50	0.44
1:B:277:ASN:ND2	1:C:286:SER:CB	2.66	0.44
1:B:368:ILE:HD13	1:B:368:ILE:HG21	1.44	0.44
1:A:188:TYR:N	1:B:370:ASN:N	2.62	0.44
1:A:179:THR:HG23	1:B:50:ASP:O	2.16	0.44
1:C:258:LEU:HD12	1:C:317:PHE:CE1	2.52	0.44
1:C:252:TYR:CA	1:C:292:PHE:HZ	2.27	0.44
1:C:318:ILE:HG12	1:C:319:ILE:N	2.33	0.44
1:A:177:ASP:OD1	1:A:183:VAL:HG11	2.17	0.44
1:A:191:VAL:HG23	1:A:192:GLY:N	2.33	0.44
1:A:422:LEU:HD12	1:A:424:GLY:O	2.18	0.44
1:B:66:THR:O	1:B:67:ALA:HB2	2.17	0.44
1:B:64:PRO:CG	1:B:82:TYR:HA	2.31	0.44
1:C:107:LEU:HD12	1:C:111:GLY:O	2.17	0.44
1:C:159:THR:O	1:C:159:THR:HG22	2.17	0.44
1:C:152:ILE:HD11	1:C:166:LEU:CG	2.48	0.44
1:C:205:ILE:HD12	1:C:208:VAL:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ARG:HH12	1:C:230:GLU:HG2	1.82	0.44
1:C:232:LEU:O	1:C:233:ASP:HB2	2.16	0.44
1:B:213:LYS:HG2	1:C:375:LYS:HG3	1.99	0.44
1:A:100:LEU:O	1:A:103:LEU:HB3	2.17	0.44
1:A:188:TYR:C	1:B:368:ILE:CG1	2.86	0.44
1:B:123:MET:H	1:B:174:PRO:HG2	1.82	0.44
1:B:123:MET:CG	1:B:146:PHE:HE1	2.07	0.44
1:B:354:THR:O	1:B:359:TYR:CD1	2.70	0.44
1:A:187:TRP:HB2	1:B:370:ASN:HB2	1.14	0.44
1:A:179:THR:HA	1:B:54:GLY:N	2.30	0.44
1:B:87:ILE:O	1:B:87:ILE:HG23	2.16	0.44
1:B:91:ASN:C	1:B:92:GLU:CG	2.82	0.44
1:C:107:LEU:HG	1:C:108:HIS:N	2.31	0.44
1:A:107:LEU:HD12	1:A:111:GLY:O	2.17	0.44
1:A:152:ILE:HD11	1:A:166:LEU:CG	2.48	0.44
1:A:255:TYR:CB	1:A:292:PHE:CE2	3.00	0.44
1:A:453:PRO:O	1:A:460:ARG:NE	2.50	0.44
1:B:177:ASP:OD1	1:B:183:VAL:HG21	2.16	0.44
1:C:123:MET:H	1:C:174:PRO:HG2	1.82	0.44
1:C:21:ARG:NH2	1:C:39:GLY:O	2.51	0.44
1:C:255:TYR:CB	1:C:292:PHE:CE2	3.00	0.44
1:C:320:LEU:HD22	1:C:407:ILE:HD11	1.98	0.44
1:C:82:TYR:OH	1:C:296:HIS:CE1	2.70	0.44
1:A:21:ARG:NH2	1:A:39:GLY:O	2.51	0.44
1:A:232:LEU:O	1:A:233:ASP:HB2	2.16	0.44
1:A:318:ILE:HG12	1:A:319:ILE:N	2.33	0.44
1:B:242:TYR:O	1:B:245:VAL:HG12	2.17	0.44
1:B:472:LYS:HE2	1:B:478:SER:OXT	2.18	0.44
1:A:184:LYS:N	1:B:56:GLY:CA	2.67	0.44
1:C:132:VAL:HG11	1:C:134:TYR:HE2	1.82	0.44
1:C:420:LEU:CD2	1:C:452:VAL:CG1	2.83	0.44
1:C:49:LEU:O	1:C:52:ILE:CG1	2.66	0.44
1:A:123:MET:H	1:A:174:PRO:HG2	1.82	0.44
1:A:73:CYS:CB	1:A:126:ASP:OD1	2.65	0.44
1:A:472:LYS:HE2	1:A:478:SER:OXT	2.18	0.44
1:B:317:PHE:CD1	1:B:318:ILE:N	2.85	0.44
1:B:258:LEU:HD12	1:B:317:PHE:CE1	2.52	0.44
1:B:318:ILE:HG12	1:B:319:ILE:N	2.33	0.44
1:A:246:MET:HB3	1:B:476:ASP:CA	2.46	0.44
1:B:55:MET:CE	1:B:332:GLU:HB3	2.48	0.44
1:A:123:MET:HG3	1:A:176:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:HG21	1:B:109:GLU:HA	2.00	0.44
1:A:143:GLN:O	1:B:112:MET:CA	2.64	0.44
1:A:144:ASP:N	1:B:113:TYR:CD2	2.85	0.44
1:A:238:TYR:CD1	1:A:239:THR:N	2.86	0.44
1:A:49:LEU:O	1:A:52:ILE:CG1	2.66	0.44
1:B:158:GLN:HA	1:B:161:VAL:HG11	1.99	0.44
1:B:20:ALA:O	1:B:21:ARG:HB2	2.18	0.44
1:B:246:MET:HE3	1:B:246:MET:HB3	0.97	0.44
1:B:251:ASN:HB3	1:B:254:ILE:HG21	2.00	0.44
1:C:191:VAL:HG23	1:C:192:GLY:N	2.33	0.44
1:C:117:ASP:HA	1:C:204:ARG:HB3	2.00	0.44
1:C:353:PRO:O	1:C:355:ASP:N	2.51	0.44
1:C:453:PRO:O	1:C:460:ARG:NE	2.50	0.44
1:B:383:LYS:HZ2	1:C:6:TRP:N	2.10	0.44
1:A:132:VAL:HG11	1:A:134:TYR:HE2	1.82	0.44
1:A:137:PHE:CD1	1:A:146:PHE:CZ	3.06	0.44
1:A:197:ASN:OD1	1:C:193:SER:C	2.50	0.44
1:A:353:PRO:O	1:A:355:ASP:N	2.51	0.44
1:A:369:ARG:HH11	1:A:369:ARG:CB	2.29	0.44
1:B:162:GLU:HA	1:B:210:HIS:O	2.18	0.44
1:B:353:PRO:O	1:B:355:ASP:N	2.51	0.44
1:B:21:ARG:NH2	1:B:39:GLY:O	2.51	0.44
1:B:48:LYS:CE	1:B:48:LYS:HA	2.46	0.44
1:A:145:TYR:OH	1:B:6:TRP:N	2.51	0.44
1:C:238:TYR:CD1	1:C:239:THR:N	2.86	0.44
1:C:55:MET:SD	1:C:362:ILE:CD1	3.06	0.44
1:C:46:ILE:HD13	1:C:46:ILE:HG21	1.78	0.44
1:C:472:LYS:HE2	1:C:478:SER:OXT	2.18	0.44
1:A:159:THR:O	1:A:159:THR:HG22	2.17	0.43
1:A:117:ASP:HA	1:A:204:ARG:HB3	2.00	0.43
1:A:223:ALA:CA	1:B:463:TYR:CD1	2.97	0.43
1:A:420:LEU:CD2	1:A:452:VAL:CG1	2.82	0.43
1:A:57:PHE:CZ	1:A:327:ILE:CG2	2.99	0.43
1:B:73:CYS:CB	1:B:126:ASP:OD1	2.65	0.43
1:B:255:TYR:CD1	1:B:292:PHE:HD2	2.36	0.43
1:B:253:PRO:HB2	1:B:275:MET:CE	2.48	0.43
1:B:293:VAL:HG13	1:B:294:GLU:N	2.19	0.43
1:B:348:TRP:C	1:B:350:SER:N	2.72	0.43
1:A:187:TRP:HB2	1:B:367:ALA:O	2.17	0.43
1:B:429:ALA:HB1	1:C:182:VAL:C	2.32	0.43
1:C:162:GLU:HA	1:C:210:HIS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:O	1:A:139:PRO:CD	2.66	0.43
1:A:178:THR:HA	1:B:52:ILE:CD1	2.45	0.43
1:A:253:PRO:HB2	1:A:275:MET:CE	2.49	0.43
1:B:7:ARG:HG3	1:B:288:LEU:HD23	2.00	0.43
1:A:187:TRP:CD1	1:B:370:ASN:HB2	2.53	0.43
1:B:403:GLN:HG3	1:B:467:LYS:HG2	2.00	0.43
1:B:49:LEU:O	1:B:52:ILE:CG1	2.66	0.43
1:A:182:VAL:HB	1:B:57:PHE:HB3	1.54	0.43
1:B:62:ILE:HG13	1:B:63:THR:N	2.32	0.43
1:C:73:CYS:CB	1:C:126:ASP:OD1	2.65	0.43
1:C:205:ILE:HG21	1:C:216:TRP:CZ3	2.53	0.43
1:C:369:ARG:HH11	1:C:369:ARG:CB	2.29	0.43
1:C:422:LEU:HD12	1:C:424:GLY:O	2.18	0.43
1:A:185:ASN:HD21	1:B:319:ILE:HG13	1.83	0.43
1:A:162:GLU:HA	1:A:210:HIS:O	2.18	0.43
1:A:55:MET:CG	1:A:362:ILE:HG21	2.49	0.43
1:A:403:GLN:HG3	1:A:467:LYS:HG2	2.00	0.43
1:B:137:PHE:O	1:B:139:PRO:CD	2.66	0.43
1:B:278:THR:HG23	1:C:380:VAL:C	2.22	0.43
1:B:319:ILE:CA	1:B:325:PRO:CB	2.73	0.43
1:B:382:TYR:CE1	1:C:2:THR:HG22	2.51	0.43
1:A:218:GLY:C	1:B:473:ILE:O	2.47	0.43
1:B:55:MET:HE3	1:B:332:GLU:HB3	2.00	0.43
1:C:137:PHE:CD1	1:C:146:PHE:CZ	3.06	0.43
1:C:149:PHE:CD1	1:C:165:TRP:CD2	3.07	0.43
1:C:209:LYS:HB2	1:C:231:VAL:HG11	2.01	0.43
1:C:55:MET:CE	1:C:332:GLU:HB3	2.48	0.43
1:A:130:SER:N	1:B:109:GLU:OE2	2.51	0.43
1:A:180:LYS:HZ1	1:B:11:ILE:N	2.16	0.43
1:A:220:ASN:OD1	1:B:474:CYS:SG	2.73	0.43
1:A:307:ASP:N	1:A:307:ASP:OD2	2.51	0.43
1:A:388:LYS:HE2	1:A:390:ASP:CB	2.39	0.43
1:B:205:ILE:HG21	1:B:216:TRP:CZ3	2.53	0.43
1:B:209:LYS:HB2	1:B:231:VAL:HG11	2.01	0.43
1:B:353:PRO:C	1:B:355:ASP:N	2.71	0.43
1:C:101:LYS:O	1:C:105:SER:HB2	2.19	0.43
1:C:388:LYS:HE2	1:C:390:ASP:CB	2.40	0.43
1:C:66:THR:O	1:C:91:ASN:N	2.52	0.43
1:A:149:PHE:CD1	1:A:165:TRP:CD2	3.07	0.43
1:A:201:ASP:HA	1:B:466:GLU:HA	1.99	0.43
1:A:222:ALA:HB3	1:B:473:ILE:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:O	1:B:105:SER:HB2	2.19	0.43
1:B:149:PHE:CD1	1:B:165:TRP:CD2	3.07	0.43
1:B:339:ASN:O	1:B:340:ASP:HB2	2.19	0.43
1:A:227:CYS:CA	1:B:476:ASP:CA	2.92	0.43
1:A:249:VAL:HA	1:B:477:SER:HB3	1.99	0.43
1:C:132:VAL:HG11	1:C:134:TYR:CE2	2.54	0.43
1:C:61:TRP:CZ2	1:C:204:ARG:NE	2.85	0.43
1:C:204:ARG:NH1	1:C:230:GLU:CB	2.82	0.43
1:C:387:ILE:HG23	1:C:388:LYS:N	2.32	0.43
1:C:385:PRO:CG	1:C:396:ARG:O	2.67	0.43
1:A:101:LYS:O	1:A:105:SER:HB2	2.19	0.43
1:A:121:ASN:C	1:A:121:ASN:HD22	2.22	0.43
1:A:187:TRP:HB3	1:B:371:TYR:CB	2.49	0.43
1:A:252:TYR:CA	1:A:292:PHE:HZ	2.27	0.43
1:A:7:ARG:HG3	1:A:288:LEU:HD23	2.00	0.43
1:B:11:ILE:HD11	1:B:324:LEU:C	2.39	0.43
1:A:180:LYS:CE	1:B:12:TYR:CA	2.88	0.43
1:B:132:VAL:HG11	1:B:134:TYR:CE2	2.54	0.43
1:B:159:THR:O	1:B:159:THR:HG22	2.18	0.43
1:B:307:ASP:N	1:B:307:ASP:OD2	2.51	0.43
1:B:450:VAL:HA	1:B:451:PRO:HD2	1.82	0.43
1:B:46:ILE:HG21	1:B:46:ILE:HD13	1.78	0.43
1:C:430:GLY:N	1:C:445:GLY:HA2	2.34	0.43
1:A:211:VAL:HG21	1:A:215:PHE:HB3	2.00	0.43
1:A:55:MET:CE	1:A:332:GLU:HB3	2.48	0.43
1:A:348:TRP:C	1:A:350:SER:N	2.72	0.43
1:B:137:PHE:CD1	1:B:146:PHE:CZ	3.06	0.43
1:B:191:VAL:HG23	1:B:192:GLY:N	2.33	0.43
1:B:255:TYR:CD2	1:B:255:TYR:C	2.92	0.43
1:B:315:ALA:O	1:B:318:ILE:HG23	2.19	0.43
1:B:320:LEU:HD22	1:B:407:ILE:HD11	1.98	0.43
1:A:177:ASP:CB	1:B:53:GLN:CG	2.92	0.43
1:C:137:PHE:O	1:C:139:PRO:CD	2.66	0.43
1:A:132:VAL:HG11	1:A:134:TYR:CE2	2.54	0.43
1:A:204:ARG:HH12	1:A:230:GLU:HG2	1.82	0.43
1:B:204:ARG:HH11	1:B:204:ARG:HG2	1.84	0.43
1:B:211:VAL:HG12	1:B:211:VAL:H	1.06	0.43
1:B:236:PRO:CG	1:C:378:GLY:C	2.71	0.43
1:B:332:GLU:CG	1:B:333:GLN:H	2.30	0.43
1:B:388:LYS:CE	1:B:390:ASP:HB2	2.39	0.43
1:B:472:LYS:O	1:B:473:ILE:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ASN:HA	1:C:251:ASN:HD22	1.53	0.43
1:B:274:ASN:CG	1:C:286:SER:H	2.21	0.43
1:C:315:ALA:O	1:C:318:ILE:HG23	2.19	0.43
1:A:20:ALA:O	1:A:21:ARG:HB2	2.18	0.43
1:A:251:ASN:HB3	1:A:254:ILE:HG21	2.00	0.43
1:A:280:LYS:HE3	1:A:383:LYS:CA	2.48	0.43
1:A:315:ALA:O	1:A:318:ILE:HG23	2.19	0.43
1:A:430:GLY:N	1:A:445:GLY:HA2	2.33	0.43
1:A:64:PRO:CG	1:A:82:TYR:HA	2.31	0.43
1:B:190:TRP:CZ3	1:B:191:VAL:CG1	3.01	0.43
1:B:200:ILE:CG2	1:B:203:LEU:HD11	2.38	0.43
1:B:204:ARG:HH11	1:B:204:ARG:CG	2.20	0.43
1:B:238:TYR:CD1	1:B:239:THR:N	2.86	0.43
1:B:317:PHE:O	1:B:321:ASN:CB	2.67	0.43
1:B:382:TYR:HD2	1:B:398:GLY:O	2.02	0.43
1:C:11:ILE:HD11	1:C:324:LEU:C	2.39	0.43
1:C:307:ASP:OD2	1:C:307:ASP:N	2.51	0.43
1:A:137:PHE:O	1:A:140:PHE:HB2	2.19	0.43
1:A:145:TYR:CD1	1:B:113:TYR:CD2	3.06	0.43
1:A:204:ARG:NH1	1:A:230:GLU:CB	2.82	0.43
1:A:251:ASN:HA	1:A:251:ASN:HD22	1.53	0.43
1:A:317:PHE:O	1:A:321:ASN:CB	2.67	0.43
1:A:387:ILE:HG23	1:A:388:LYS:N	2.32	0.43
1:A:444:VAL:H	1:A:444:VAL:HG13	1.30	0.43
1:A:55:MET:CG	1:A:57:PHE:CE2	2.98	0.43
1:A:87:ILE:O	1:A:88:TYR:CB	2.67	0.43
1:A:180:LYS:NZ	1:B:11:ILE:C	2.66	0.43
1:B:140:PHE:CZ	1:B:176:LEU:HD21	2.54	0.43
1:A:218:GLY:CA	1:B:364:SER:C	2.62	0.43
1:B:408:LEU:N	1:B:408:LEU:HD13	2.30	0.43
1:B:422:LEU:HD12	1:B:424:GLY:O	2.18	0.43
1:B:435:GLU:CB	1:B:440:THR:HB	2.46	0.43
1:B:87:ILE:HD11	1:B:190:TRP:CE2	2.54	0.43
1:C:253:PRO:HB2	1:C:275:MET:CE	2.49	0.43
1:C:346:ALA:C	1:C:348:TRP:N	2.71	0.43
1:C:353:PRO:C	1:C:355:ASP:N	2.71	0.43
1:C:280:LYS:HE3	1:C:383:LYS:CA	2.48	0.43
1:C:12:TYR:CG	1:C:52:ILE:HG22	2.54	0.43
1:A:279:VAL:HG23	1:A:283:CYS:SG	2.59	0.42
1:A:300:ARG:HB2	1:A:336:ALA:O	2.19	0.42
1:A:353:PRO:C	1:A:355:ASP:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:THR:O	1:A:91:ASN:N	2.52	0.42
1:B:117:ASP:HA	1:B:204:ARG:HB3	2.00	0.42
1:B:137:PHE:O	1:B:140:PHE:HB2	2.19	0.42
1:B:204:ARG:NH1	1:B:230:GLU:CB	2.82	0.42
1:B:385:PRO:HD2	1:C:2:THR:CG2	2.39	0.42
1:B:385:PRO:CG	1:B:396:ARG:O	2.67	0.42
1:B:422:LEU:CD1	1:C:221:LYS:CB	2.91	0.42
1:B:443:THR:O	1:B:451:PRO:CD	2.67	0.42
1:B:433:LEU:HD13	1:B:464:PRO:HA	2.01	0.42
1:A:148:PRO:CB	1:B:49:LEU:HD23	2.46	0.42
1:C:18:ARG:HG2	1:C:345:GLU:H	1.84	0.42
1:C:190:TRP:CZ3	1:C:191:VAL:CG1	3.01	0.42
1:C:208:VAL:HG12	1:C:231:VAL:HG11	1.97	0.42
1:C:7:ARG:HG3	1:C:288:LEU:HD23	2.00	0.42
1:C:55:MET:CG	1:C:362:ILE:HG21	2.49	0.42
1:C:57:PHE:CZ	1:C:327:ILE:CG2	2.99	0.42
1:A:190:TRP:CZ3	1:B:371:TYR:HD1	2.09	0.42
1:A:255:TYR:HB3	1:A:292:PHE:CE2	2.54	0.42
1:A:321:ASN:CG	1:A:322:ASP:N	2.69	0.42
1:A:12:TYR:CG	1:A:52:ILE:HG22	2.54	0.42
1:B:11:ILE:HA	1:B:59:ALA:HB3	2.01	0.42
1:B:213:LYS:CD	1:C:375:LYS:HG2	2.49	0.42
1:A:190:TRP:N	1:B:369:ARG:O	2.52	0.42
1:C:137:PHE:O	1:C:140:PHE:HB2	2.19	0.42
1:C:20:ALA:O	1:C:21:ARG:HB2	2.18	0.42
1:C:55:MET:HE3	1:C:332:GLU:HB3	2.00	0.42
1:C:400:ASP:O	1:C:403:GLN:HB2	2.19	0.42
1:A:13:PHE:HD1	1:A:14:LEU:N	2.18	0.42
1:A:190:TRP:CZ3	1:A:191:VAL:CG1	3.01	0.42
1:A:400:ASP:O	1:A:403:GLN:HB2	2.19	0.42
1:A:443:THR:O	1:A:451:PRO:CD	2.67	0.42
1:B:116:VAL:O	1:B:116:VAL:HG13	2.20	0.42
1:B:121:ASN:C	1:B:121:ASN:HD22	2.22	0.42
1:B:142:SER:HB2	1:B:145:TYR:CE1	2.55	0.42
1:B:300:ARG:HB2	1:B:336:ALA:O	2.19	0.42
1:B:400:ASP:O	1:B:403:GLN:HB2	2.19	0.42
1:B:401:GLY:O	1:B:403:GLN:HG3	2.20	0.42
1:B:57:PHE:CZ	1:B:362:ILE:HG21	2.54	0.42
1:C:13:PHE:HD1	1:C:14:LEU:N	2.17	0.42
1:C:251:ASN:HB3	1:C:254:ILE:HG21	2.00	0.42
1:C:255:TYR:HB3	1:C:292:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ILE:HD13	1:C:52:ILE:HG21	1.75	0.42
1:A:190:TRP:NE1	1:B:376:ASP:N	2.65	0.42
1:A:193:SER:CB	1:B:403:GLN:HB3	2.50	0.42
1:A:200:ILE:CG2	1:A:203:LEU:HD11	2.38	0.42
1:A:346:ALA:C	1:A:348:TRP:N	2.71	0.42
1:B:236:PRO:HB3	1:B:278:THR:CG2	2.49	0.42
1:B:279:VAL:HG13	1:B:280:LYS:N	2.35	0.42
1:B:346:ALA:C	1:B:348:TRP:N	2.71	0.42
1:B:348:TRP:O	1:B:350:SER:N	2.53	0.42
1:B:66:THR:O	1:B:91:ASN:N	2.52	0.42
1:C:121:ASN:HD22	1:C:121:ASN:C	2.22	0.42
1:C:450:VAL:HA	1:C:451:PRO:HD2	1.82	0.42
1:C:403:GLN:HG3	1:C:467:LYS:HG2	2.00	0.42
1:C:48:LYS:CE	1:C:48:LYS:HA	2.46	0.42
1:B:383:LYS:HZ1	1:C:5:ASP:CB	2.12	0.42
1:C:87:ILE:HD11	1:C:190:TRP:CE2	2.54	0.42
1:A:209:LYS:HB2	1:A:231:VAL:HG11	2.01	0.42
1:A:255:TYR:CD2	1:A:255:TYR:C	2.92	0.42
1:A:312:LYS:CG	1:A:361:LEU:HD13	2.49	0.42
1:A:42:TRP:CZ3	1:A:94:TYR:CD2	3.07	0.42
1:B:369:ARG:HH11	1:B:369:ARG:CB	2.29	0.42
1:B:382:TYR:CG	1:B:398:GLY:N	2.85	0.42
1:B:446:SER:OG	1:C:181:ASP:CB	2.38	0.42
1:C:140:PHE:CZ	1:C:176:LEU:HD21	2.54	0.42
1:C:211:VAL:HG21	1:C:215:PHE:HB3	2.00	0.42
1:C:401:GLY:O	1:C:403:GLN:HG3	2.20	0.42
1:C:433:LEU:HD13	1:C:464:PRO:HA	2.02	0.42
1:A:140:PHE:CZ	1:A:176:LEU:HD21	2.54	0.42
1:A:190:TRP:HH2	1:B:375:LYS:CE	2.31	0.42
1:A:61:TRP:CZ2	1:A:204:ARG:NE	2.85	0.42
1:A:385:PRO:CG	1:A:396:ARG:O	2.67	0.42
1:B:55:MET:CG	1:B:362:ILE:HG21	2.49	0.42
1:A:190:TRP:CZ2	1:B:374:SER:HB2	2.44	0.42
1:B:428:THR:HB	1:C:190:TRP:N	2.34	0.42
1:C:279:VAL:HG23	1:C:283:CYS:SG	2.59	0.42
1:C:348:TRP:C	1:C:350:SER:N	2.72	0.42
1:C:87:ILE:O	1:C:88:TYR:CB	2.67	0.42
1:C:16:THR:OG1	1:C:94:TYR:CE1	2.58	0.42
1:A:185:ASN:HD22	1:B:319:ILE:HD12	1.85	0.42
1:A:348:TRP:O	1:A:350:SER:N	2.53	0.42
1:A:382:TYR:HD2	1:A:398:GLY:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:O	1:A:403:GLN:HG3	2.20	0.42
1:A:433:LEU:HD13	1:A:464:PRO:HA	2.02	0.42
1:B:107:LEU:O	1:B:111:GLY:N	2.51	0.42
1:B:280:LYS:O	1:B:281:SER:HB2	2.11	0.42
1:B:255:TYR:HB3	1:B:292:PHE:CE2	2.54	0.42
1:B:308:ILE:H	1:B:308:ILE:HG13	1.20	0.42
1:B:400:ASP:OD1	1:B:401:GLY:N	2.50	0.42
1:B:87:ILE:HG21	1:B:123:MET:HE1	2.02	0.42
1:C:300:ARG:HB2	1:C:336:ALA:O	2.19	0.42
1:A:339:ASN:O	1:A:340:ASP:HB2	2.19	0.42
1:A:427:TYR:CZ	1:A:433:LEU:HD11	2.55	0.42
1:B:12:TYR:OH	1:B:19:PHE:HE1	2.03	0.42
1:B:132:VAL:CG1	1:B:134:TYR:CE2	3.02	0.42
1:B:18:ARG:HG2	1:B:345:GLU:H	1.84	0.42
1:B:256:TYR:CB	1:B:257:PRO:CD	2.98	0.42
1:B:277:ASN:HD22	1:C:286:SER:CB	2.28	0.42
1:A:194:LEU:HA	1:B:376:ASP:HB3	2.00	0.42
1:A:194:LEU:C	1:B:403:GLN:CG	2.88	0.42
1:B:430:GLY:N	1:B:445:GLY:HA2	2.33	0.42
1:B:447:ASP:HB3	1:C:184:LYS:HE2	1.67	0.42
1:A:229:GLY:CA	1:B:476:ASP:OD1	2.68	0.42
1:B:55:MET:SD	1:B:362:ILE:CD1	3.06	0.42
1:B:422:LEU:CD2	1:C:221:LYS:HG2	2.49	0.42
1:C:348:TRP:O	1:C:350:SER:N	2.53	0.42
1:B:213:LYS:CD	1:C:375:LYS:CG	2.98	0.42
1:C:408:LEU:HD11	1:C:462:LEU:CD2	2.35	0.42
1:C:444:VAL:HG13	1:C:444:VAL:H	1.30	0.42
1:C:7:ARG:HG2	1:C:287:THR:HG1	1.81	0.42
1:C:42:TRP:CZ3	1:C:94:TYR:CD2	3.07	0.42
1:A:11:ILE:HA	1:A:59:ALA:HB3	2.01	0.42
1:A:180:LYS:NZ	1:A:182:VAL:HB	2.21	0.42
1:A:11:ILE:HD11	1:A:324:LEU:C	2.39	0.42
1:A:407:ILE:HA	1:A:461:VAL:HA	2.02	0.42
1:A:57:PHE:CZ	1:A:362:ILE:HG21	2.54	0.42
1:B:152:ILE:HD11	1:B:166:LEU:CG	2.48	0.42
1:B:279:VAL:HG23	1:B:283:CYS:SG	2.59	0.42
1:B:295:ASN:O	1:B:298:ASN:N	2.53	0.42
1:B:13:PHE:CB	1:B:328:TYR:HA	2.50	0.42
1:A:193:SER:CB	1:B:403:GLN:CB	2.94	0.42
1:B:42:TRP:CZ3	1:B:94:TYR:CD2	3.07	0.42
1:B:458:LEU:HA	1:B:459:PRO:HD2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:MET:CE	1:B:476:ASP:CB	2.97	0.42
1:C:317:PHE:O	1:C:321:ASN:CB	2.67	0.42
1:C:407:ILE:HA	1:C:461:VAL:HA	2.02	0.42
1:C:418:TYR:HD1	1:C:454:MET:HE3	1.81	0.42
1:C:432:GLN:O	1:C:465:THR:HB	2.20	0.42
1:C:79:TYR:C	1:C:81:GLY:N	2.73	0.42
1:A:132:VAL:CG1	1:A:134:TYR:CE2	3.02	0.42
1:A:293:VAL:HG11	1:A:331:GLN:CD	2.40	0.42
1:A:380:VAL:HG13	1:A:381:THR:N	2.28	0.42
1:B:136:VAL:CG1	1:B:136:VAL:O	2.68	0.42
1:B:241:PRO:CB	1:C:376:ASP:H	2.33	0.42
1:B:293:VAL:HG11	1:B:331:GLN:CD	2.41	0.42
1:B:380:VAL:HG13	1:B:381:THR:N	2.28	0.42
1:A:199:SER:O	1:B:466:GLU:HG3	2.20	0.42
1:C:136:VAL:CG1	1:C:136:VAL:O	2.68	0.42
1:C:12:TYR:CD1	1:C:14:LEU:HD23	2.53	0.42
1:C:255:TYR:C	1:C:255:TYR:CD2	2.92	0.42
1:C:330:GLY:HA3	1:C:335:TYR:HD1	1.85	0.42
1:C:368:ILE:HD13	1:C:368:ILE:HG21	1.44	0.42
1:C:265:THR:O	1:C:411:LYS:HD2	2.20	0.42
1:B:173:LEU:HA	1:B:174:PRO:HD2	1.82	0.41
1:B:255:TYR:HD1	1:B:292:PHE:HD2	1.68	0.41
1:B:287:THR:HG21	1:B:380:VAL:O	2.19	0.41
1:B:11:ILE:CD1	1:B:324:LEU:C	2.89	0.41
1:B:383:LYS:CD	1:C:5:ASP:CG	2.86	0.41
1:C:12:TYR:OH	1:C:19:PHE:HE1	2.03	0.41
1:C:427:TYR:CZ	1:C:433:LEU:HD11	2.55	0.41
1:C:57:PHE:CZ	1:C:362:ILE:HG21	2.54	0.41
1:A:221:LYS:HB3	1:B:436:VAL:HA	0.43	0.41
1:A:330:GLY:HA3	1:A:335:TYR:HD1	1.85	0.41
1:A:408:LEU:HD11	1:A:462:LEU:CD2	2.36	0.41
1:B:87:ILE:O	1:B:88:TYR:CB	2.67	0.41
1:C:255:TYR:CD1	1:C:292:PHE:HD2	2.36	0.41
1:C:293:VAL:HG11	1:C:331:GLN:CD	2.40	0.41
1:C:339:ASN:O	1:C:340:ASP:HB2	2.19	0.41
1:C:382:TYR:HD2	1:C:398:GLY:O	2.02	0.41
1:C:434:THR:CG2	1:C:474:CYS:SG	3.08	0.41
1:C:443:THR:O	1:C:451:PRO:CD	2.67	0.41
1:A:189:ASP:O	1:B:463:TYR:OH	2.30	0.41
1:A:205:ILE:CD1	1:B:472:LYS:CA	2.86	0.41
1:A:224:GLY:CA	1:B:434:THR:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TYR:CD1	1:A:292:PHE:HD2	2.36	0.41
1:A:400:ASP:CG	1:A:401:GLY:N	2.74	0.41
1:A:265:THR:O	1:A:411:LYS:HD2	2.20	0.41
1:B:228:ILE:HG21	1:B:228:ILE:HD12	1.72	0.41
1:B:238:TYR:O	1:C:376:ASP:CA	2.46	0.41
1:C:11:ILE:CD1	1:C:324:LEU:C	2.89	0.41
1:C:400:ASP:CG	1:C:401:GLY:N	2.74	0.41
1:C:66:THR:HG22	1:C:86:ASP:HB3	2.03	0.41
1:C:87:ILE:HG21	1:C:87:ILE:HD13	1.82	0.41
1:A:11:ILE:CD1	1:A:324:LEU:C	2.89	0.41
1:A:12:TYR:OH	1:A:19:PHE:HE1	2.03	0.41
1:A:18:ARG:HG2	1:A:345:GLU:H	1.84	0.41
1:A:287:THR:HG21	1:A:380:VAL:O	2.19	0.41
1:A:262:PHE:CZ	1:A:314:VAL:CA	3.03	0.41
1:A:432:GLN:O	1:A:465:THR:HB	2.20	0.41
1:A:55:MET:SD	1:A:362:ILE:CD1	3.06	0.41
1:A:185:ASN:ND2	1:B:319:ILE:HG13	2.34	0.41
1:B:319:ILE:HG22	1:B:325:PRO:CB	2.27	0.41
1:B:330:GLY:CA	1:B:335:TYR:HD1	2.34	0.41
1:B:344:ARG:N	1:B:344:ARG:HD2	2.36	0.41
1:B:381:THR:CB	1:C:1:ALA:HB2	2.50	0.41
1:B:385:PRO:O	1:B:395:MET:CB	2.68	0.41
1:B:427:TYR:CZ	1:B:433:LEU:HD11	2.55	0.41
1:B:432:GLN:O	1:B:465:THR:HB	2.20	0.41
1:C:262:PHE:CZ	1:C:314:VAL:CA	3.03	0.41
1:B:384:ASN:HA	1:C:2:THR:HG22	1.59	0.41
1:C:346:ALA:HB3	1:C:349:LEU:HB2	2.03	0.41
1:A:136:VAL:CG1	1:A:136:VAL:O	2.68	0.41
1:A:379:PHE:CZ	1:A:397:LYS:HE2	2.56	0.41
1:A:434:THR:CG2	1:A:474:CYS:SG	3.08	0.41
1:B:243:GLN:HE21	1:B:285:ASP:HA	1.85	0.41
1:B:42:TRP:NE1	1:B:62:ILE:CD1	2.68	0.41
1:B:79:TYR:C	1:B:81:GLY:N	2.73	0.41
1:C:142:SER:HB2	1:C:145:TYR:CE1	2.55	0.41
1:B:429:ALA:CB	1:C:186:GLU:HB3	2.30	0.41
1:C:236:PRO:HB3	1:C:278:THR:CG2	2.49	0.41
1:C:379:PHE:CZ	1:C:397:LYS:HE2	2.56	0.41
1:A:194:LEU:HA	1:B:403:GLN:CD	2.41	0.41
1:A:216:TRP:HE3	1:B:472:LYS:HB3	1.38	0.41
1:A:208:VAL:HG22	1:A:216:TRP:NE1	2.36	0.41
1:A:295:ASN:O	1:A:298:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:HA3	1:A:403:GLN:NE2	2.36	0.41
1:A:408:LEU:N	1:A:408:LEU:HD13	2.30	0.41
1:A:48:LYS:CE	1:A:48:LYS:HA	2.46	0.41
1:B:134:TYR:CZ	1:B:143:GLN:HB2	2.55	0.41
1:B:12:TYR:CD1	1:B:14:LEU:HD23	2.54	0.41
1:B:191:VAL:HG23	1:B:192:GLY:H	1.85	0.41
1:B:19:PHE:CD1	1:B:347:THR:CG2	3.04	0.41
1:B:199:SER:HB2	1:B:200:ILE:H	1.27	0.41
1:B:399:THR:HG22	1:B:400:ASP:N	2.36	0.41
1:B:66:THR:HG22	1:B:86:ASP:HB3	2.03	0.41
1:C:117:ASP:OD2	1:C:204:ARG:NH1	2.54	0.41
1:C:11:ILE:HA	1:C:59:ALA:HB3	2.02	0.41
1:C:122:HIS:ND1	1:C:173:LEU:CD2	2.78	0.41
1:C:132:VAL:CG1	1:C:134:TYR:CE2	3.03	0.41
1:C:137:PHE:CG	1:C:146:PHE:HZ	2.39	0.41
1:C:134:TYR:CZ	1:C:143:GLN:HB2	2.55	0.41
1:C:191:VAL:HG13	1:C:191:VAL:H	1.24	0.41
1:B:399:THR:HG22	1:C:195:VAL:O	2.20	0.41
1:C:330:GLY:CA	1:C:335:TYR:HD1	2.34	0.41
1:C:338:GLY:O	1:C:340:ASP:N	2.53	0.41
1:C:408:LEU:N	1:C:408:LEU:HD13	2.31	0.41
1:A:190:TRP:CZ2	1:B:375:LYS:HB2	2.35	0.41
1:A:344:ARG:N	1:A:344:ARG:HD2	2.36	0.41
1:A:66:THR:HG22	1:A:86:ASP:HB3	2.03	0.41
1:B:253:PRO:HB2	1:B:275:MET:HE3	2.02	0.41
1:B:301:PHE:O	1:B:304:TYR:HD1	2.04	0.41
1:B:407:ILE:HA	1:B:461:VAL:HA	2.02	0.41
1:B:434:THR:CG2	1:B:474:CYS:SG	3.09	0.41
1:C:116:VAL:HG13	1:C:116:VAL:O	2.20	0.41
1:C:208:VAL:HG22	1:C:216:TRP:NE1	2.36	0.41
1:C:66:THR:HG21	1:C:87:ILE:N	2.35	0.41
1:A:228:ILE:HG21	1:A:228:ILE:HD12	1.72	0.41
1:A:52:ILE:HG12	1:A:52:ILE:H	1.59	0.41
1:B:13:PHE:HD1	1:B:14:LEU:N	2.18	0.41
1:B:472:LYS:O	1:B:473:ILE:CB	2.66	0.41
1:B:400:ASP:HB3	1:C:194:LEU:C	2.34	0.41
1:C:256:TYR:CB	1:C:257:PRO:CD	2.98	0.41
1:C:13:PHE:CB	1:C:328:TYR:HA	2.50	0.41
1:C:344:ARG:N	1:C:344:ARG:HD2	2.36	0.41
1:B:279:VAL:HG11	1:C:4:ALA:HB1	1.83	0.41
1:C:68:GLN:O	1:C:85:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:MET:HA	1:C:7:ARG:NH1	2.29	0.41
1:A:117:ASP:OD2	1:A:204:ARG:NH1	2.53	0.41
1:A:194:LEU:O	1:B:403:GLN:CD	2.59	0.41
1:A:246:MET:HB3	1:B:476:ASP:C	2.27	0.41
1:A:293:VAL:HG13	1:A:294:GLU:N	2.19	0.41
1:A:301:PHE:O	1:A:304:TYR:HD1	2.04	0.41
1:A:318:ILE:HG21	1:A:318:ILE:HD13	1.14	0.41
1:A:13:PHE:CB	1:A:328:TYR:HA	2.50	0.41
1:A:346:ALA:HB3	1:A:349:LEU:HB2	2.03	0.41
1:A:371:TYR:O	1:A:374:SER:HB2	2.21	0.41
1:A:87:ILE:HD11	1:B:374:SER:C	2.36	0.41
1:A:66:THR:HG21	1:A:87:ILE:N	2.35	0.41
1:B:117:ASP:OD2	1:B:204:ARG:NH1	2.53	0.41
1:B:330:GLY:HA3	1:B:335:TYR:HD1	1.85	0.41
1:B:353:PRO:C	1:B:355:ASP:H	2.24	0.41
1:B:452:VAL:O	1:B:452:VAL:HG22	2.16	0.41
1:A:219:TYR:CG	1:B:473:ILE:CD1	2.87	0.41
1:C:10:SER:HB3	1:C:57:PHE:HB3	2.03	0.41
1:C:287:THR:HG21	1:C:380:VAL:O	2.19	0.41
1:C:385:PRO:O	1:C:395:MET:CB	2.68	0.41
1:C:401:GLY:HA3	1:C:403:GLN:NE2	2.35	0.41
1:C:465:THR:O	1:C:465:THR:HG23	2.21	0.41
1:A:191:VAL:HG23	1:A:192:GLY:H	1.85	0.41
1:A:208:VAL:CG2	1:A:216:TRP:NE1	2.84	0.41
1:A:272:LEU:HA	1:A:275:MET:HB3	2.02	0.41
1:A:283:CYS:SG	1:A:289:LEU:HD11	2.61	0.41
1:A:19:PHE:CD1	1:A:347:THR:CG2	3.04	0.41
1:A:381:THR:O	1:A:382:TYR:C	2.59	0.41
1:A:385:PRO:O	1:A:395:MET:CB	2.68	0.41
1:A:465:THR:O	1:A:465:THR:HG23	2.21	0.41
1:B:123:MET:CB	1:B:137:PHE:CE1	2.80	0.41
1:B:255:TYR:CE1	1:B:293:VAL:O	2.74	0.41
1:B:262:PHE:CZ	1:B:314:VAL:CA	3.04	0.41
1:B:265:THR:O	1:B:411:LYS:HD2	2.20	0.41
1:B:66:THR:HG21	1:B:87:ILE:N	2.35	0.41
1:C:19:PHE:CD1	1:C:347:THR:CG2	3.04	0.41
1:C:301:PHE:O	1:C:304:TYR:HD1	2.04	0.41
1:C:381:THR:O	1:C:382:TYR:C	2.59	0.41
1:A:137:PHE:CG	1:A:146:PHE:HZ	2.39	0.41
1:A:134:TYR:CZ	1:A:143:GLN:HB2	2.55	0.41
1:A:256:TYR:CB	1:A:257:PRO:CD	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TYR:HD1	1:A:292:PHE:HD2	1.68	0.41
1:A:330:GLY:CA	1:A:335:TYR:HD1	2.34	0.41
1:A:338:GLY:O	1:A:340:ASP:N	2.53	0.41
1:A:79:TYR:C	1:A:81:GLY:N	2.73	0.41
1:B:134:TYR:CG	1:B:143:GLN:HB3	2.56	0.41
1:B:61:TRP:CZ2	1:B:204:ARG:NE	2.85	0.41
1:B:208:VAL:CG2	1:B:216:TRP:NE1	2.84	0.41
1:B:338:GLY:O	1:B:340:ASP:N	2.53	0.41
1:B:346:ALA:HB3	1:B:349:LEU:HB2	2.03	0.41
1:B:382:TYR:CE1	1:B:385:PRO:CD	2.94	0.41
1:C:295:ASN:O	1:C:298:ASN:N	2.53	0.41
1:C:371:TYR:O	1:C:374:SER:HB2	2.21	0.41
1:C:385:PRO:O	1:C:395:MET:HB3	2.20	0.41
1:C:55:MET:CG	1:C:57:PHE:CE2	2.97	0.41
1:A:188:TYR:CD1	1:B:368:ILE:CG2	2.52	0.40
1:A:450:VAL:HA	1:A:451:PRO:HD2	1.82	0.40
1:B:191:VAL:HG13	1:B:191:VAL:H	1.25	0.40
1:B:208:VAL:HG22	1:B:216:TRP:NE1	2.36	0.40
1:B:211:VAL:HG21	1:B:215:PHE:HB3	2.00	0.40
1:B:279:VAL:HG13	1:C:4:ALA:CA	2.44	0.40
1:B:273:TYR:OH	1:C:244:ASN:HA	2.21	0.40
1:C:283:CYS:SG	1:C:289:LEU:HD11	2.61	0.40
1:A:245:VAL:C	1:A:246:MET:CG	2.90	0.40
1:A:353:PRO:C	1:A:355:ASP:H	2.24	0.40
1:A:46:ILE:HD13	1:A:46:ILE:HG21	1.78	0.40
1:B:106:ALA:O	1:B:109:GLU:HB2	2.21	0.40
1:A:197:ASN:ND2	1:B:400:ASP:OD1	2.50	0.40
1:A:193:SER:HA	1:B:404:ILE:N	2.22	0.40
1:B:12:TYR:CG	1:B:52:ILE:HG22	2.54	0.40
1:C:134:TYR:CG	1:C:143:GLN:HB3	2.56	0.40
1:C:184:LYS:HG3	1:C:185:ASN:H	1.86	0.40
1:C:238:TYR:HA	1:C:241:PRO:HG3	2.04	0.40
1:C:319:ILE:CA	1:C:325:PRO:CB	2.72	0.40
1:C:312:LYS:CG	1:C:361:LEU:HD13	2.49	0.40
1:A:180:LYS:HB3	1:B:12:TYR:CE2	2.52	0.40
1:A:190:TRP:CH2	1:B:375:LYS:NZ	2.84	0.40
1:A:221:LYS:HA	1:B:434:THR:HG21	0.47	0.40
1:A:204:ARG:CG	1:A:228:ILE:O	2.70	0.40
1:A:249:VAL:CB	1:B:477:SER:CB	2.94	0.40
1:A:249:VAL:HA	1:B:477:SER:CB	2.51	0.40
1:A:255:TYR:CE1	1:A:293:VAL:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PRO:O	1:A:395:MET:HB3	2.20	0.40
1:A:472:LYS:O	1:A:473:ILE:CB	2.66	0.40
1:B:272:LEU:HA	1:B:275:MET:HB3	2.02	0.40
1:B:448:GLY:HA3	1:C:184:LYS:HB2	0.96	0.40
1:C:123:MET:CE	1:C:140:PHE:HE1	2.24	0.40
1:C:186:GLU:HG3	1:C:187:TRP:N	2.36	0.40
1:C:208:VAL:CG2	1:C:216:TRP:NE1	2.84	0.40
1:C:262:PHE:CE1	1:C:314:VAL:HB	2.57	0.40
1:C:458:LEU:HD13	1:C:460:ARG:NH2	2.33	0.40
1:A:134:TYR:CG	1:A:143:GLN:HB3	2.56	0.40
1:A:205:ILE:HG13	1:A:229:GLY:CA	2.44	0.40
1:A:458:LEU:HA	1:A:459:PRO:HD2	1.65	0.40
1:A:190:TRP:HH2	1:B:375:LYS:HD3	1.57	0.40
1:B:401:GLY:HA3	1:B:403:GLN:NE2	2.36	0.40
1:B:458:LEU:HD13	1:B:460:ARG:NH2	2.33	0.40
1:C:106:ALA:O	1:C:109:GLU:HB2	2.21	0.40
1:C:190:TRP:HZ3	1:C:219:TYR:OH	2.05	0.40
1:C:204:ARG:HH11	1:C:204:ARG:HG2	1.84	0.40
1:C:255:TYR:HD1	1:C:292:PHE:HD2	1.68	0.40
1:C:255:TYR:CE1	1:C:293:VAL:O	2.74	0.40
1:C:321:ASN:CG	1:C:322:ASP:N	2.69	0.40
1:C:332:GLU:CG	1:C:333:GLN:H	2.30	0.40
1:C:387:ILE:HD13	1:C:387:ILE:HG21	1.37	0.40
1:A:10:SER:HB3	1:A:57:PHE:HB3	2.03	0.40
1:A:224:GLY:N	1:B:434:THR:HB	2.36	0.40
1:A:452:VAL:O	1:A:452:VAL:HG22	2.17	0.40
1:B:1:ALA:HB1	1:B:113:TYR:HE1	1.86	0.40
1:B:122:HIS:ND1	1:B:173:LEU:CD2	2.77	0.40
1:B:262:PHE:CE1	1:B:314:VAL:HB	2.57	0.40
1:B:283:CYS:SG	1:B:289:LEU:HD11	2.61	0.40
1:B:385:PRO:O	1:B:395:MET:HB3	2.20	0.40
1:C:152:ILE:HD11	1:C:166:LEU:CB	2.52	0.40
1:C:205:ILE:HG13	1:C:229:GLY:CA	2.44	0.40
1:C:245:VAL:C	1:C:246:MET:CG	2.90	0.40
1:C:353:PRO:C	1:C:355:ASP:H	2.24	0.40
1:C:472:LYS:O	1:C:473:ILE:CG2	2.66	0.40

All (135) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PHE:C	1:C:25:SER:O[2_646]	0.53	1.67
1:A:149:PHE:CB	1:C:29:THR:OG1[2_646]	0.66	1.54
1:A:149:PHE:CD2	1:C:29:THR:CA[2_646]	0.70	1.50
1:A:165:TRP:O	1:C:27:THR:CA[2_646]	0.72	1.48
1:A:152:ILE:CA	1:C:26:THR:N[2_646]	0.76	1.44
1:A:152:ILE:CB	1:C:26:THR:OG1[2_646]	0.76	1.44
1:A:153:GLN:CG	1:C:24:GLY:O[2_646]	0.82	1.38
1:A:151:PHE:C	1:C:25:SER:C[2_646]	0.95	1.25
1:A:152:ILE:CB	1:C:26:THR:CB[2_646]	0.95	1.25
1:A:153:GLN:C	1:C:24:GLY:CA[2_646]	0.97	1.23
1:A:153:GLN:CB	1:C:24:GLY:O[2_646]	0.99	1.21
1:A:165:TRP:CB	1:C:27:THR:O[2_646]	0.99	1.21
1:A:165:TRP:CA	1:C:27:THR:CG2[2_646]	1.00	1.20
1:A:152:ILE:N	1:C:26:THR:N[2_646]	1.04	1.16
1:A:152:ILE:CG1	1:C:26:THR:OG1[2_646]	1.06	1.14
1:A:165:TRP:CA	1:C:27:THR:CB[2_646]	1.07	1.13
1:A:151:PHE:N	1:C:28:ALA:CB[2_646]	1.09	1.11
1:A:151:PHE:CZ	1:C:349:LEU:CG[2_646]	1.09	1.11
1:A:165:TRP:C	1:C:27:THR:CB[2_646]	1.10	1.10
1:A:149:PHE:CG	1:C:29:THR:CA[2_646]	1.11	1.09
1:A:152:ILE:N	1:C:25:SER:C[2_646]	1.13	1.07
1:A:153:GLN:CA	1:C:24:GLY:CA[2_646]	1.18	1.02
1:A:150:CYS:C	1:C:28:ALA:CA[2_646]	1.19	1.01
1:A:151:PHE:O	1:C:25:SER:C[2_646]	1.19	1.01
1:A:151:PHE:CE1	1:C:349:LEU:CG[2_646]	1.22	0.98
1:A:149:PHE:CD2	1:C:29:THR:C[2_646]	1.23	0.97
1:A:149:PHE:CB	1:C:29:THR:CB[2_646]	1.25	0.95
1:A:153:GLN:CA	1:C:24:GLY:C[2_646]	1.29	0.91
1:A:151:PHE:CA	1:C:25:SER:O[2_646]	1.30	0.90
1:A:165:TRP:C	1:C:27:THR:CA[2_646]	1.30	0.90
1:A:149:PHE:CA	1:C:29:THR:OG1[2_646]	1.32	0.88
1:A:165:TRP:O	1:C:27:THR:N[2_646]	1.32	0.88
1:A:150:CYS:O	1:C:28:ALA:N[2_646]	1.33	0.87
1:A:153:GLN:CB	1:C:24:GLY:C[2_646]	1.37	0.83
1:A:150:CYS:C	1:C:28:ALA:N[2_646]	1.42	0.78
1:A:150:CYS:CA	1:C:28:ALA:CA[2_646]	1.42	0.78
1:A:152:ILE:CG2	1:C:26:THR:OG1[2_646]	1.46	0.74
1:A:151:PHE:CE1	1:C:349:LEU:CB[2_646]	1.47	0.73
1:A:149:PHE:CE2	1:C:30:CYS:N[2_646]	1.48	0.72
1:A:151:PHE:O	1:C:25:SER:CA[2_646]	1.48	0.72
1:A:151:PHE:CZ	1:C:349:LEU:CD1[2_646]	1.48	0.72
1:A:152:ILE:N	1:C:25:SER:O[2_646]	1.49	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:CYS:C	1:C:28:ALA:CB[2_646]	1.50	0.70
1:A:151:PHE:O	1:C:25:SER:O[2_646]	1.50	0.70
1:A:153:GLN:O	1:C:23:ASP:O[2_646]	1.53	0.67
1:A:160:GLN:OE1	1:C:23:ASP:O[2_646]	1.54	0.66
1:A:153:GLN:N	1:C:25:SER:N[2_646]	1.55	0.65
1:A:152:ILE:CG1	1:C:26:THR:CB[2_646]	1.55	0.65
1:A:152:ILE:N	1:C:26:THR:CA[2_646]	1.58	0.62
1:A:128:ALA:CB	1:C:31:ASN:CB[2_646]	1.59	0.61
1:A:165:TRP:N	1:C:27:THR:CB[2_646]	1.61	0.59
1:A:152:ILE:C	1:C:26:THR:N[2_646]	1.62	0.58
1:A:153:GLN:O	1:C:24:GLY:CA[2_646]	1.63	0.57
1:A:165:TRP:C	1:C:27:THR:CG2[2_646]	1.64	0.56
1:A:153:GLN:O	1:C:24:GLY:N[2_646]	1.65	0.55
1:A:151:PHE:CD1	1:C:349:LEU:CA[2_646]	1.66	0.54
1:A:153:GLN:O	1:C:23:ASP:C[2_646]	1.66	0.54
1:A:130:SER:CB	1:C:31:ASN:OD1[2_646]	1.67	0.53
1:A:153:GLN:N	1:C:24:GLY:C[2_646]	1.67	0.53
1:A:165:TRP:C	1:C:27:THR:OG1[2_646]	1.69	0.51
1:A:152:ILE:CD1	1:C:26:THR:CB[2_646]	1.71	0.49
1:A:152:ILE:CA	1:C:25:SER:C[2_646]	1.72	0.48
1:A:151:PHE:O	1:C:25:SER:CB[2_646]	1.72	0.48
1:A:153:GLN:NE2	1:C:21:ARG:CD[2_646]	1.72	0.48
1:A:153:GLN:CG	1:C:24:GLY:C[2_646]	1.74	0.46
1:A:153:GLN:CB	1:C:24:GLY:CA[2_646]	1.75	0.45
1:A:152:ILE:CB	1:C:26:THR:CA[2_646]	1.76	0.44
1:A:149:PHE:CD2	1:C:29:THR:N[2_646]	1.76	0.44
1:A:165:TRP:CB	1:C:27:THR:C[2_646]	1.77	0.43
1:A:149:PHE:CE2	1:C:29:THR:C[2_646]	1.78	0.42
1:A:153:GLN:OE1	1:C:348:TRP:CD2[2_646]	1.80	0.40
1:A:152:ILE:CB	1:C:26:THR:CG2[2_646]	1.81	0.39
1:A:151:PHE:CE1	1:C:349:LEU:CA[2_646]	1.81	0.39
1:A:165:TRP:O	1:C:27:THR:CB[2_646]	1.81	0.39
1:A:151:PHE:N	1:C:28:ALA:CA[2_646]	1.82	0.38
1:A:149:PHE:C	1:C:29:THR:N[2_646]	1.83	0.37
1:A:149:PHE:CG	1:C:29:THR:CB[2_646]	1.84	0.36
1:A:152:ILE:CA	1:C:26:THR:CA[2_646]	1.84	0.36
1:A:130:SER:O	1:C:34:ASP:OD1[2_646]	1.85	0.35
1:A:150:CYS:CA	1:C:28:ALA:CB[2_646]	1.86	0.34
1:A:153:GLN:C	1:C:24:GLY:N[2_646]	1.86	0.34
1:A:152:ILE:CA	1:C:26:THR:OG1[2_646]	1.87	0.33
1:A:151:PHE:C	1:C:26:THR:N[2_646]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TRP:CA	1:C:27:THR:CA[2_646]	1.88	0.32
1:A:149:PHE:CB	1:C:29:THR:CA[2_646]	1.88	0.32
1:A:154:ASN:N	1:C:24:GLY:CA[2_646]	1.89	0.31
1:A:149:PHE:CD2	1:C:30:CYS:N[2_646]	1.90	0.30
1:A:152:ILE:CB	1:C:26:THR:N[2_646]	1.91	0.29
1:A:128:ALA:O	1:C:31:ASN:ND2[2_646]	1.91	0.29
1:A:151:PHE:CB	1:C:348:TRP:CE2[2_646]	1.91	0.29
1:A:152:ILE:N	1:C:26:THR:C[2_646]	1.93	0.27
1:A:166:LEU:N	1:C:27:THR:CG2[2_646]	1.93	0.27
1:A:150:CYS:O	1:C:27:THR:C[2_646]	1.93	0.27
1:A:151:PHE:N	1:C:28:ALA:N[2_646]	1.93	0.27
1:A:167:GLY:O	1:C:349:LEU:O[2_646]	1.94	0.26
1:A:153:GLN:OE1	1:C:348:TRP:CG[2_646]	1.94	0.26
1:A:154:ASN:CB	1:C:22:THR:O[2_646]	1.96	0.24
1:A:151:PHE:CB	1:C:348:TRP:CZ2[2_646]	1.96	0.24
1:A:130:SER:CA	1:C:31:ASN:OD1[2_646]	1.97	0.23
1:A:149:PHE:CG	1:C:29:THR:N[2_646]	1.97	0.23
1:A:149:PHE:N	1:C:29:THR:OG1[2_646]	1.97	0.23
1:A:150:CYS:N	1:C:28:ALA:CA[2_646]	2.01	0.19
1:A:149:PHE:O	1:C:29:THR:N[2_646]	2.03	0.17
1:A:166:LEU:N	1:C:27:THR:OG1[2_646]	2.04	0.16
1:A:165:TRP:CG	1:C:27:THR:O[2_646]	2.04	0.16
1:A:153:GLN:CA	1:C:24:GLY:O[2_646]	2.07	0.13
1:A:165:TRP:CA	1:C:27:THR:O[2_646]	2.07	0.13
1:A:150:CYS:O	1:C:28:ALA:CA[2_646]	2.07	0.13
1:A:165:TRP:CB	1:C:27:THR:CG2[2_646]	2.09	0.11
1:A:151:PHE:O	1:C:348:TRP:NE1[2_646]	2.09	0.11
1:A:165:TRP:O	1:C:26:THR:C[2_646]	2.09	0.11
1:A:152:ILE:CG2	1:C:26:THR:CG2[2_646]	2.09	0.11
1:A:152:ILE:N	1:C:27:THR:N[2_646]	2.10	0.10
1:A:151:PHE:CB	1:C:348:TRP:NE1[2_646]	2.10	0.10
1:A:149:PHE:CE2	1:C:29:THR:CA[2_646]	2.11	0.09
1:A:152:ILE:CG1	1:C:27:THR:N[2_646]	2.11	0.09
1:A:130:SER:N	1:C:31:ASN:OD1[2_646]	2.11	0.09
1:A:153:GLN:CD	1:C:348:TRP:NE1[2_646]	2.12	0.08
1:A:149:PHE:CD2	1:C:29:THR:CB[2_646]	2.13	0.07
1:A:153:GLN:CD	1:C:348:TRP:CE2[2_646]	2.14	0.06
1:A:166:LEU:N	1:C:27:THR:CB[2_646]	2.14	0.06
1:A:153:GLN:NE2	1:C:348:TRP:CE2[2_646]	2.15	0.05
1:A:152:ILE:CG2	1:C:26:THR:CB[2_646]	2.15	0.05
1:A:152:ILE:CG1	1:C:26:THR:CA[2_646]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:CG	1:C:29:THR:OG1[2_646]	2.16	0.04
1:A:151:PHE:N	1:C:25:SER:O[2_646]	2.17	0.03
1:A:130:SER:O	1:C:34:ASP:CG[2_646]	2.17	0.03
1:A:152:ILE:CA	1:C:26:THR:CB[2_646]	2.17	0.03
1:A:151:PHE:CZ	1:C:349:LEU:CB[2_646]	2.18	0.02
1:A:153:GLN:CD	1:C:24:GLY:O[2_646]	2.18	0.02
1:A:165:TRP:O	1:C:27:THR:C[2_646]	2.19	0.01
1:A:128:ALA:C	1:C:31:ASN:CB[2_646]	2.19	0.01
1:A:165:TRP:CA	1:C:27:THR:C[2_646]	2.19	0.01
1:A:150:CYS:N	1:C:29:THR:N[2_646]	2.19	0.01
1:A:152:ILE:O	1:C:26:THR:N[2_646]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/478 (100%)	237 (50%)	117 (25%)	122 (26%)	0	0
1	B	476/478 (100%)	237 (50%)	117 (25%)	122 (26%)	0	0
1	C	476/478 (100%)	237 (50%)	117 (25%)	122 (26%)	0	0
All	All	1428/1434 (100%)	711 (50%)	351 (25%)	366 (26%)	0	0

All (366) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	7	ARG
1	A	16	THR
1	A	19	PHE
1	A	21	ARG
1	A	30	CYS
1	A	32	THR
1	A	33	ALA

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Mol	Chain	Res	Type
1	A	63	THR
1	A	66	THR
1	A	67	ALA
1	A	68	GLN
1	A	72	ASP
1	A	74	ALA
1	A	83	TRP
1	A	84	GLN
1	A	87	ILE
1	A	88	TYR
1	A	90	LEU
1	A	91	ASN
1	A	120	ALA
1	A	139	PRO
1	A	144	ASP
1	A	155	TYR
1	A	161	VAL
1	A	164	CYS
1	A	169	ASN
1	A	173	LEU
1	A	177	ASP
1	A	180	LYS
1	A	181	ASP
1	A	182	VAL
1	A	199	SER
1	A	214	ASP
1	A	225	VAL
1	A	226	TYR
1	A	231	VAL
1	A	233	ASP
1	A	247	ASP
1	A	263	LYS
1	A	268	SER
1	A	280	LYS
1	A	281	SER
1	A	293	VAL
1	A	295	ASN
1	A	296	HIS
1	A	301	PHE
1	A	341	PRO
1	A	344	ARG
1	A	345	GLU

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Mol	Chain	Res	Type
1	A	346	ALA
1	A	354	THR
1	A	382	TYR
1	A	387	ILE
1	A	426	SER
1	A	436	VAL
1	A	437	ILE
1	A	440	THR
1	A	460	ARG
1	A	472	LYS
1	A	473	ILE
1	B	2	THR
1	B	7	ARG
1	B	16	THR
1	B	19	PHE
1	B	21	ARG
1	B	30	CYS
1	B	32	THR
1	B	33	ALA
1	B	63	THR
1	B	66	THR
1	B	67	ALA
1	B	68	GLN
1	B	72	ASP
1	B	74	ALA
1	B	83	TRP
1	B	84	GLN
1	B	87	ILE
1	B	88	TYR
1	B	90	LEU
1	B	91	ASN
1	B	120	ALA
1	B	139	PRO
1	B	144	ASP
1	B	155	TYR
1	B	161	VAL
1	B	164	CYS
1	B	169	ASN
1	B	173	LEU
1	B	177	ASP
1	B	180	LYS
1	B	181	ASP

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Mol	Chain	Res	Type
1	B	182	VAL
1	B	199	SER
1	B	214	ASP
1	B	225	VAL
1	B	226	TYR
1	B	231	VAL
1	B	233	ASP
1	B	247	ASP
1	B	263	LYS
1	B	268	SER
1	B	280	LYS
1	B	281	SER
1	B	293	VAL
1	B	295	ASN
1	B	296	HIS
1	B	301	PHE
1	B	341	PRO
1	B	344	ARG
1	B	345	GLU
1	B	346	ALA
1	B	354	THR
1	B	382	TYR
1	B	387	ILE
1	B	426	SER
1	B	436	VAL
1	B	437	ILE
1	B	440	THR
1	B	460	ARG
1	B	472	LYS
1	B	473	ILE
1	C	2	THR
1	C	7	ARG
1	C	16	THR
1	C	19	PHE
1	C	21	ARG
1	C	30	CYS
1	C	32	THR
1	C	33	ALA
1	C	63	THR
1	C	66	THR
1	C	67	ALA
1	C	68	GLN

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Mol	Chain	Res	Type
1	C	72	ASP
1	C	74	ALA
1	C	83	TRP
1	C	84	GLN
1	C	87	ILE
1	C	88	TYR
1	C	90	LEU
1	C	91	ASN
1	C	120	ALA
1	C	139	PRO
1	C	144	ASP
1	C	155	TYR
1	C	161	VAL
1	C	164	CYS
1	C	169	ASN
1	C	173	LEU
1	C	177	ASP
1	C	180	LYS
1	C	181	ASP
1	C	182	VAL
1	C	199	SER
1	C	214	ASP
1	C	225	VAL
1	C	226	TYR
1	C	231	VAL
1	C	233	ASP
1	C	247	ASP
1	C	263	LYS
1	C	268	SER
1	C	280	LYS
1	C	281	SER
1	C	293	VAL
1	C	295	ASN
1	C	296	HIS
1	C	301	PHE
1	C	341	PRO
1	C	344	ARG
1	C	345	GLU
1	C	346	ALA
1	C	354	THR
1	C	382	TYR
1	C	387	ILE

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Mol	Chain	Res	Type
1	C	426	SER
1	C	436	VAL
1	C	437	ILE
1	C	440	THR
1	C	460	ARG
1	C	472	LYS
1	C	473	ILE
1	A	6	TRP
1	A	22	THR
1	A	39	GLY
1	A	44	GLY
1	A	71	GLN
1	A	75	TYR
1	A	79	TYR
1	A	86	ASP
1	A	97	ALA
1	A	124	GLY
1	A	141	SER
1	A	170	THR
1	A	190	TRP
1	A	198	TYR
1	A	224	GLY
1	A	234	GLY
1	A	267	GLY
1	A	294	GLU
1	A	302	ALA
1	A	329	ALA
1	A	332	GLU
1	A	339	ASN
1	A	377	THR
1	A	383	LYS
1	A	400	ASP
1	A	416	ASP
1	A	417	SER
1	A	423	SER
1	A	429	ALA
1	A	477	SER
1	B	22	THR
1	B	39	GLY
1	B	44	GLY
1	B	71	GLN
1	B	75	TYR

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Mol	Chain	Res	Type
1	B	79	TYR
1	B	86	ASP
1	B	97	ALA
1	B	124	GLY
1	B	141	SER
1	B	170	THR
1	B	190	TRP
1	B	198	TYR
1	B	224	GLY
1	B	234	GLY
1	B	267	GLY
1	B	294	GLU
1	B	302	ALA
1	B	329	ALA
1	B	332	GLU
1	B	339	ASN
1	B	377	THR
1	B	383	LYS
1	B	400	ASP
1	B	416	ASP
1	B	417	SER
1	B	423	SER
1	B	429	ALA
1	B	477	SER
1	C	22	THR
1	C	39	GLY
1	C	44	GLY
1	C	71	GLN
1	C	75	TYR
1	C	79	TYR
1	C	86	ASP
1	C	97	ALA
1	C	124	GLY
1	C	141	SER
1	C	170	THR
1	C	190	TRP
1	C	198	TYR
1	C	224	GLY
1	C	234	GLY
1	C	267	GLY
1	C	294	GLU
1	C	302	ALA

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Mol	Chain	Res	Type
1	C	329	ALA
1	C	332	GLU
1	C	339	ASN
1	C	377	THR
1	C	383	LYS
1	C	400	ASP
1	C	416	ASP
1	C	417	SER
1	C	423	SER
1	C	429	ALA
1	C	477	SER
1	A	3	PRO
1	A	26	THR
1	A	70	PRO
1	A	77	ASP
1	A	112	MET
1	A	183	VAL
1	A	196	SER
1	A	349	LEU
1	A	446	SER
1	B	3	PRO
1	B	6	TRP
1	B	26	THR
1	B	70	PRO
1	B	77	ASP
1	B	112	MET
1	B	183	VAL
1	B	196	SER
1	B	349	LEU
1	B	446	SER
1	C	3	PRO
1	C	6	TRP
1	C	26	THR
1	C	70	PRO
1	C	77	ASP
1	C	112	MET
1	C	183	VAL
1	C	196	SER
1	C	349	LEU
1	C	446	SER
1	A	106	ALA
1	A	134	TYR

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Mol	Chain	Res	Type
1	A	241	PRO
1	A	297	ASP
1	A	380	VAL
1	A	381	THR
1	A	450	VAL
1	A	456	GLY
1	B	134	TYR
1	B	241	PRO
1	B	297	ASP
1	B	380	VAL
1	B	381	THR
1	B	450	VAL
1	B	456	GLY
1	C	134	TYR
1	C	241	PRO
1	C	297	ASP
1	C	380	VAL
1	C	381	THR
1	C	450	VAL
1	C	456	GLY
1	A	36	LYS
1	A	240	CYS
1	A	252	TYR
1	A	299	PRO
1	A	321	ASN
1	A	340	ASP
1	A	352	TYR
1	A	384	ASN
1	B	36	LYS
1	B	106	ALA
1	B	240	CYS
1	B	252	TYR
1	B	299	PRO
1	B	321	ASN
1	B	340	ASP
1	B	352	TYR
1	B	384	ASN
1	C	36	LYS
1	C	106	ALA
1	C	240	CYS
1	C	252	TYR
1	C	299	PRO

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Mol	Chain	Res	Type
1	C	321	ASN
1	C	340	ASP
1	C	352	TYR
1	C	384	ASN
1	A	276	ILE
1	B	276	ILE
1	C	276	ILE
1	A	152	ILE
1	A	457	GLY
1	B	152	ILE
1	B	457	GLY
1	C	152	ILE
1	C	236	PRO
1	C	457	GLY
1	C	459	PRO
1	A	236	PRO
1	A	459	PRO
1	B	236	PRO
1	B	459	PRO
1	A	451	PRO
1	B	451	PRO
1	C	451	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	400/400 (100%)	256 (64%)	144 (36%)	0 1
1	B	400/400 (100%)	256 (64%)	144 (36%)	0 1
1	C	400/400 (100%)	256 (64%)	144 (36%)	0 1
All	All	1200/1200 (100%)	768 (64%)	432 (36%)	0 1

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	SER
1	A	9	GLN
1	A	10	SER
1	A	12	TYR
1	A	13	PHE
1	A	14	LEU
1	A	15	LEU
1	A	17	ASP
1	A	21	ARG
1	A	23	ASP
1	A	27	THR
1	A	31	ASN
1	A	35	GLN
1	A	42	TRP
1	A	48	LYS
1	A	50	ASP
1	A	55	MET
1	A	57	PHE
1	A	62	ILE
1	A	68	GLN
1	A	69	LEU
1	A	77	ASP
1	A	80	THR
1	A	84	GLN
1	A	90	LEU
1	A	91	ASN
1	A	92	GLU
1	A	96	THR
1	A	105	SER
1	A	107	LEU
1	A	108	HIS
1	A	110	ARG
1	A	114	LEU
1	A	115	MET
1	A	121	ASN
1	A	122	HIS
1	A	123	MET
1	A	126	ASP
1	A	139	PRO
1	A	157	ASP
1	A	161	VAL
1	A	163	ASP

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Mol	Chain	Res	Type
1	A	164	CYS
1	A	166	LEU
1	A	176	LEU
1	A	178	THR
1	A	180	LYS
1	A	181	ASP
1	A	183	VAL
1	A	184	LYS
1	A	186	GLU
1	A	193	SER
1	A	194	LEU
1	A	195	VAL
1	A	197	ASN
1	A	199	SER
1	A	205	ILE
1	A	206	ASP
1	A	207	THR
1	A	210	HIS
1	A	212	GLN
1	A	214	ASP
1	A	216	TRP
1	A	228	ILE
1	A	230	GLU
1	A	235	ASP
1	A	238	TYR
1	A	246	MET
1	A	249	VAL
1	A	250	LEU
1	A	251	ASN
1	A	252	TYR
1	A	255	TYR
1	A	259	LEU
1	A	264	SER
1	A	266	SER
1	A	268	SER
1	A	269	MET
1	A	271	ASP
1	A	272	LEU
1	A	275	MET
1	A	276	ILE
1	A	283	CYS
1	A	285	ASP

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Mol	Chain	Res	Type
1	A	286	SER
1	A	287	THR
1	A	291	THR
1	A	292	PHE
1	A	300	ARG
1	A	305	THR
1	A	306	ASN
1	A	307	ASP
1	A	308	ILE
1	A	314	VAL
1	A	317	PHE
1	A	318	ILE
1	A	320	LEU
1	A	322	ASP
1	A	324	LEU
1	A	325	PRO
1	A	333	GLN
1	A	341	PRO
1	A	347	THR
1	A	348	TRP
1	A	349	LEU
1	A	359	TYR
1	A	361	LEU
1	A	369	ARG
1	A	370	ASN
1	A	375	LYS
1	A	376	ASP
1	A	379	PHE
1	A	381	THR
1	A	389	ASP
1	A	395	MET
1	A	399	THR
1	A	404	ILE
1	A	407	ILE
1	A	408	LEU
1	A	417	SER
1	A	419	THR
1	A	420	LEU
1	A	421	SER
1	A	422	LEU
1	A	431	GLN
1	A	432	GLN

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Mol	Chain	Res	Type
1	A	434	THR
1	A	437	ILE
1	A	442	VAL
1	A	443	THR
1	A	444	VAL
1	A	447	ASP
1	A	449	ASN
1	A	452	VAL
1	A	454	MET
1	A	462	LEU
1	A	464	PRO
1	A	465	THR
1	A	466	GLU
1	A	471	SER
1	A	473	ILE
1	A	474	CYS
1	A	476	ASP
1	B	7	ARG
1	B	8	SER
1	B	9	GLN
1	B	10	SER
1	B	12	TYR
1	B	13	PHE
1	B	14	LEU
1	B	15	LEU
1	B	17	ASP
1	B	21	ARG
1	B	23	ASP
1	B	27	THR
1	B	31	ASN
1	B	35	GLN
1	B	42	TRP
1	B	48	LYS
1	B	50	ASP
1	B	55	MET
1	B	57	PHE
1	B	62	ILE
1	B	68	GLN
1	B	69	LEU
1	B	77	ASP
1	B	80	THR
1	B	84	GLN

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Mol	Chain	Res	Type
1	B	90	LEU
1	B	91	ASN
1	B	92	GLU
1	B	96	THR
1	B	105	SER
1	B	107	LEU
1	B	108	HIS
1	B	110	ARG
1	B	114	LEU
1	B	115	MET
1	B	121	ASN
1	B	122	HIS
1	B	123	MET
1	B	126	ASP
1	B	139	PRO
1	B	157	ASP
1	B	161	VAL
1	B	163	ASP
1	B	164	CYS
1	B	166	LEU
1	B	176	LEU
1	B	178	THR
1	B	180	LYS
1	B	181	ASP
1	B	183	VAL
1	B	184	LYS
1	B	186	GLU
1	B	193	SER
1	B	194	LEU
1	B	195	VAL
1	B	197	ASN
1	B	199	SER
1	B	205	ILE
1	B	206	ASP
1	B	207	THR
1	B	210	HIS
1	B	212	GLN
1	B	214	ASP
1	B	216	TRP
1	B	228	ILE
1	B	230	GLU
1	B	235	ASP

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Mol	Chain	Res	Type
1	B	238	TYR
1	B	246	MET
1	B	249	VAL
1	B	250	LEU
1	B	251	ASN
1	B	252	TYR
1	B	255	TYR
1	B	259	LEU
1	B	264	SER
1	B	266	SER
1	B	268	SER
1	B	269	MET
1	B	271	ASP
1	B	272	LEU
1	B	275	MET
1	B	276	ILE
1	B	283	CYS
1	B	285	ASP
1	B	286	SER
1	B	287	THR
1	B	291	THR
1	B	292	PHE
1	B	300	ARG
1	B	305	THR
1	B	306	ASN
1	B	307	ASP
1	B	308	ILE
1	B	314	VAL
1	B	317	PHE
1	B	318	ILE
1	B	320	LEU
1	B	322	ASP
1	B	324	LEU
1	B	325	PRO
1	B	333	GLN
1	B	341	PRO
1	B	347	THR
1	B	348	TRP
1	B	349	LEU
1	B	359	TYR
1	B	361	LEU
1	B	369	ARG

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Mol	Chain	Res	Type
1	B	370	ASN
1	B	375	LYS
1	B	376	ASP
1	B	379	PHE
1	B	381	THR
1	B	389	ASP
1	B	395	MET
1	B	399	THR
1	B	404	ILE
1	B	407	ILE
1	B	408	LEU
1	B	417	SER
1	B	419	THR
1	B	420	LEU
1	B	421	SER
1	B	422	LEU
1	B	431	GLN
1	B	432	GLN
1	B	434	THR
1	B	437	ILE
1	B	442	VAL
1	B	443	THR
1	B	444	VAL
1	B	447	ASP
1	B	449	ASN
1	B	452	VAL
1	B	454	MET
1	B	462	LEU
1	B	464	PRO
1	B	465	THR
1	B	466	GLU
1	B	471	SER
1	B	473	ILE
1	B	474	CYS
1	B	476	ASP
1	C	7	ARG
1	C	8	SER
1	C	9	GLN
1	C	10	SER
1	C	12	TYR
1	C	13	PHE
1	C	14	LEU

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Mol	Chain	Res	Type
1	C	15	LEU
1	C	17	ASP
1	C	21	ARG
1	C	23	ASP
1	C	27	THR
1	C	31	ASN
1	C	35	GLN
1	C	42	TRP
1	C	48	LYS
1	C	50	ASP
1	C	55	MET
1	C	57	PHE
1	C	62	ILE
1	C	68	GLN
1	C	69	LEU
1	C	77	ASP
1	C	80	THR
1	C	84	GLN
1	C	90	LEU
1	C	91	ASN
1	C	92	GLU
1	C	96	THR
1	C	105	SER
1	C	107	LEU
1	C	108	HIS
1	C	110	ARG
1	C	114	LEU
1	C	115	MET
1	C	121	ASN
1	C	122	HIS
1	C	123	MET
1	C	126	ASP
1	C	139	PRO
1	C	157	ASP
1	C	161	VAL
1	C	163	ASP
1	C	164	CYS
1	C	166	LEU
1	C	176	LEU
1	C	178	THR
1	C	180	LYS
1	C	181	ASP

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Mol	Chain	Res	Type
1	C	183	VAL
1	C	184	LYS
1	C	186	GLU
1	C	193	SER
1	C	194	LEU
1	C	195	VAL
1	C	197	ASN
1	C	199	SER
1	C	205	ILE
1	C	206	ASP
1	C	207	THR
1	C	210	HIS
1	C	212	GLN
1	C	214	ASP
1	C	216	TRP
1	C	228	ILE
1	C	230	GLU
1	C	235	ASP
1	C	238	TYR
1	C	246	MET
1	C	249	VAL
1	C	250	LEU
1	C	251	ASN
1	C	252	TYR
1	C	255	TYR
1	C	259	LEU
1	C	264	SER
1	C	266	SER
1	C	268	SER
1	C	269	MET
1	C	271	ASP
1	C	272	LEU
1	C	275	MET
1	C	276	ILE
1	C	283	CYS
1	C	285	ASP
1	C	286	SER
1	C	287	THR
1	C	291	THR
1	C	292	PHE
1	C	300	ARG
1	C	305	THR

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Mol	Chain	Res	Type
1	C	306	ASN
1	C	307	ASP
1	C	308	ILE
1	C	314	VAL
1	C	317	PHE
1	C	318	ILE
1	C	320	LEU
1	C	322	ASP
1	C	324	LEU
1	C	325	PRO
1	C	333	GLN
1	C	341	PRO
1	C	347	THR
1	C	348	TRP
1	C	349	LEU
1	C	359	TYR
1	C	361	LEU
1	C	369	ARG
1	C	370	ASN
1	C	375	LYS
1	C	376	ASP
1	C	379	PHE
1	C	381	THR
1	C	389	ASP
1	C	395	MET
1	C	399	THR
1	C	404	ILE
1	C	407	ILE
1	C	408	LEU
1	C	417	SER
1	C	419	THR
1	C	420	LEU
1	C	421	SER
1	C	422	LEU
1	C	431	GLN
1	C	432	GLN
1	C	434	THR
1	C	437	ILE
1	C	442	VAL
1	C	443	THR
1	C	444	VAL
1	C	447	ASP

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Mol	Chain	Res	Type
1	C	449	ASN
1	C	452	VAL
1	C	454	MET
1	C	462	LEU
1	C	464	PRO
1	C	465	THR
1	C	466	GLU
1	C	471	SER
1	C	473	ILE
1	C	474	CYS
1	C	476	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	35	GLN
1	A	68	GLN
1	A	71	GLN
1	A	84	GLN
1	A	91	ASN
1	A	143	GLN
1	A	147	HIS
1	A	185	ASN
1	A	210	HIS
1	A	212	GLN
1	A	296	HIS
1	A	298	ASN
1	A	306	ASN
1	A	321	ASN
1	A	334	HIS
1	A	384	ASN
1	A	403	GLN
1	A	410	ASN
1	A	431	GLN
1	B	31	ASN
1	B	35	GLN
1	B	68	GLN
1	B	71	GLN
1	B	91	ASN
1	B	147	HIS
1	B	158	GLN

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Mol	Chain	Res	Type
1	B	210	HIS
1	B	220	ASN
1	B	274	ASN
1	B	296	HIS
1	B	298	ASN
1	B	306	ASN
1	B	321	ASN
1	B	334	HIS
1	B	384	ASN
1	B	403	GLN
1	B	410	ASN
1	B	431	GLN
1	C	31	ASN
1	C	35	GLN
1	C	68	GLN
1	C	71	GLN
1	C	91	ASN
1	C	147	HIS
1	C	185	ASN
1	C	210	HIS
1	C	212	GLN
1	C	296	HIS
1	C	298	ASN
1	C	306	ASN
1	C	321	ASN
1	C	334	HIS
1	C	384	ASN
1	C	403	GLN
1	C	410	ASN
1	C	431	GLN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	208:VAL	C	209:LYS	N	1.17
1	A	458:LEU	C	459:PRO	N	1.17
1	B	208:VAL	C	209:LYS	N	1.17
1	B	458:LEU	C	459:PRO	N	1.17
1	C	208:VAL	C	209:LYS	N	1.17
1	C	458:LEU	C	459:PRO	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.