



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:54 PM BST

PDB ID : 3ZX8
EMDB ID: : EMD-1863
Title : Cryo-EM reconstruction of native and expanded Turnip Crinkle virus
Authors : Bakker, S.E.; Robottom, J.; Hogle, J.M.; Maeda, A.; Pearson, A.R.; Stockley, P.G.; Ranson, N.A.; Harrison, S.C.
Deposited on : 2011-08-08
Resolution : 11.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

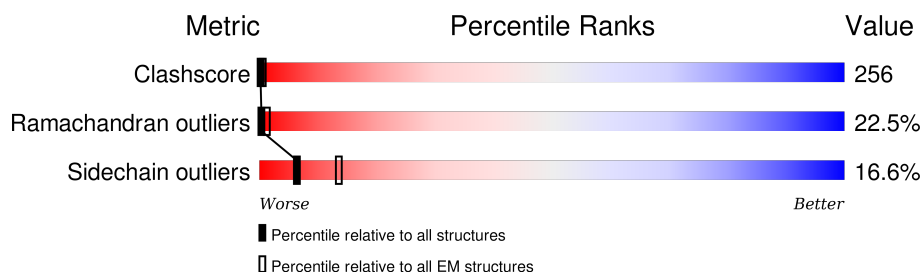
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6290 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	267	Total	C	N	O	S	0	0
			2026	1280	344	397	5		
1	B	267	Total	C	N	O	S	0	0
			2026	1280	344	397	5		
1	C	295	Total	C	N	O	S	0	0
			2238	1410	386	437	5		

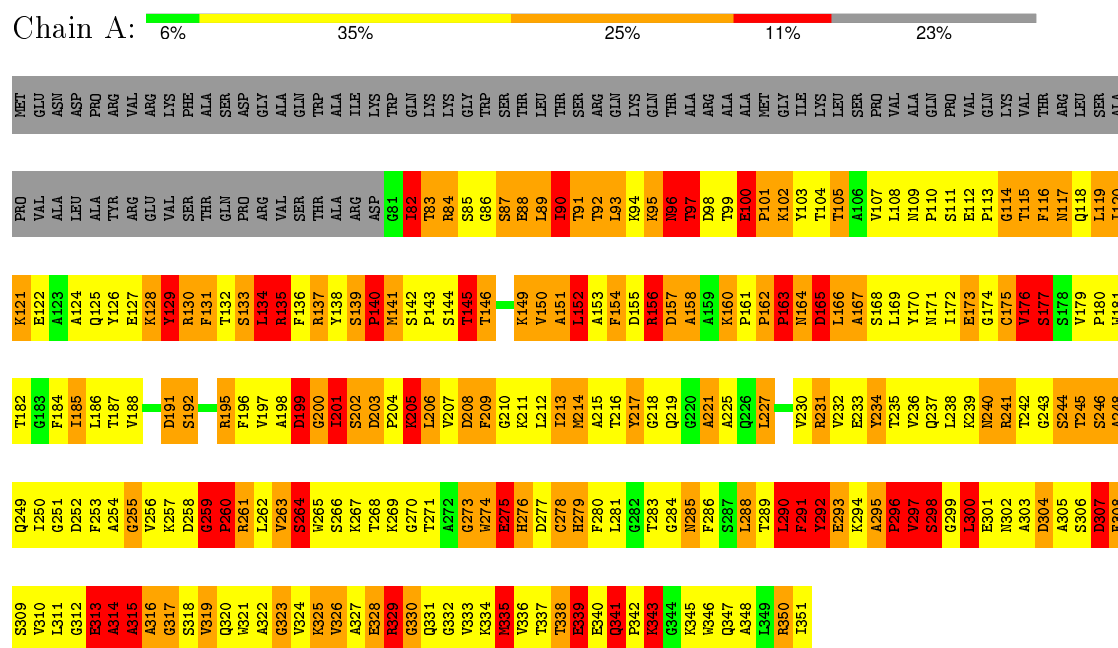
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	ASN	DELETION	UNP P06663
A	.	-	ASP	DELETION	UNP P06663
A	.	-	ALA	DELETION	UNP P06663
A	.	-	ASP	DELETION	UNP P06663
A	346	TRP	LEU	VARIANT	UNP P06663
B	.	-	ASN	DELETION	UNP P06663
B	.	-	ASP	DELETION	UNP P06663
B	.	-	ALA	DELETION	UNP P06663
B	.	-	ASP	DELETION	UNP P06663
B	346	TRP	LEU	VARIANT	UNP P06663
C	.	-	ASN	DELETION	UNP P06663
C	.	-	ASP	DELETION	UNP P06663
C	.	-	ALA	DELETION	UNP P06663
C	.	-	ASP	DELETION	UNP P06663
C	346	TRP	LEU	VARIANT	UNP P06663

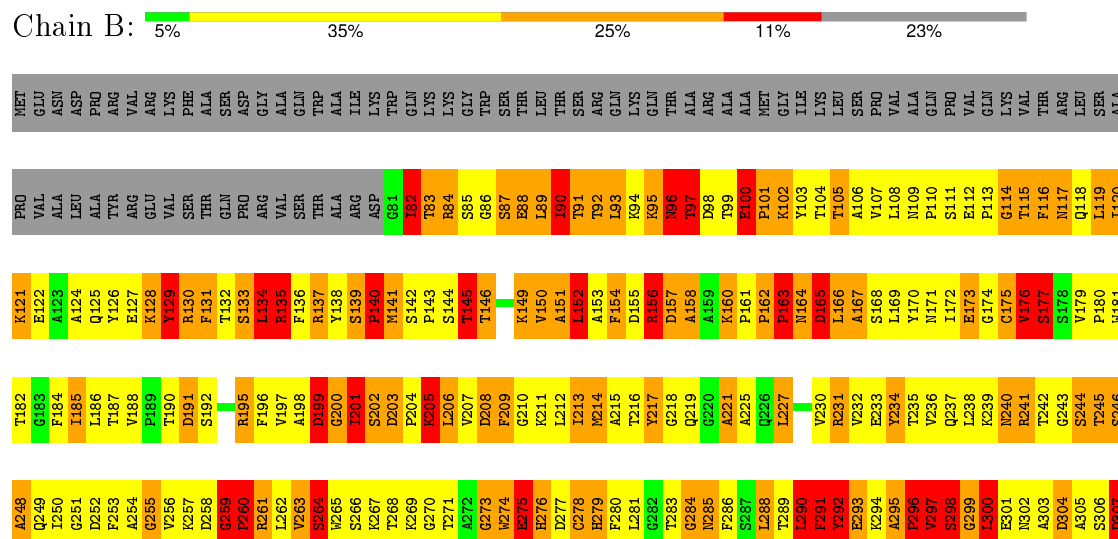
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

• Molecule 1: CAPSID PROTEIN



• Molecule 1: CAPSID PROTEIN



F308
S309
V310
L311
ASP
PRO
ARG
VAL
ARG
LYS
PHE
ALA
SER
ASP
ASP
GLY
ALA
GLN
GLN
TRP
ALA
ALA
ILE
LYS
TRP
E328
R329
LYS
G330
D331
G332
V333
K334
R335
V336
T337
THR
SER
R338
E340
P342
G343
G344
K345
W346
Q347
A348
L349
R350
I351

● Molecule 1: CAPSID PROTEIN



MET	GLU	ASN	ASP	PRO	ARG	VAL	ARG	LYS	PHE	ALA	SER	ASP	GLY	ALA	GLN	GLN	TRP	ALA	ALA	ILE	LYS	TRP	E328	R329	LYS	G330	D331	G332	V333	K334	R335	V336	T337	THR	SER	R338	E340	P342	G343	G344	K345	W346	Q347	A348	L349	R350	I351
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P61	V62	A63	L64	A65	Y66	R67	E68	V69	S70	T71	Q72	P73	R74	V75	S76	T77	A78	R79	D80	G81	I82	T83	R84	S85	G86	S87	E88	L89	I90	T91	T92	L93	K94	K95	N96	T97	D98	T99	E100	P101	K102	Y103	T104	T105	A106	V107	L108	N109	P110	S111	E112	G114	T115	F116	N117	Q118	L119	I120
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K121	E122	A123	I124	Q125	Y126	E127	K128	Y129	R130	F131	T132	S133	L134	R135	F136	R137	Y138	S139	P140	M141	S142	P143	S144	T145	T146	K149	V150	A151	L152	A153	F154	D155	R156	D157	A158	A159	K160	P161	P162	P163	N164	D165	L166	A167	S168	T169	Y170	M171	I172	E173	G174	C175	Y176	S177	S178	V179	P180	W181
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T182	G183	F184	I185	L186	T187	V188	D191	S192	R195	F196	V197	A198	D199	S200	I201	S202	D203	P204	K205	L206	T207	D208	F209	G210	K211	L212	L213	I214	M214	A215	T216	Y217	G218	Q219	G220	A221	A225	Q226	L227	V230	R231	V232	E233	Y234	T235	V236	Q237	L238	K239	N240	R241	T242	G243	S244	T245	S246	A248
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Q249	I250	G251	D252	F253	A254	G255	V256	K257	D258	G259	P260	R261	L262	V263	S264	W265	S266	K267	T268	K269	G270	T271	A272	G273	W274	E275	H276	D277	C278	H279	F280	L281	T283	G284	W285	F286	S287	L288	T289	L290	F291	V292	E293	K294	A295	P296	Y297	S298	G299	I300	E301	N302	A303	D304	A305	S306	D307	F308
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S309	V310	L311	G312	E313	A314	A315	A316	G317	S318	V319	Q320	H321	A322	G323	V324	K325	V326	A327	E328	R329	G330	Q331	G332	V333	K334	R335	V336	T337	T338	E339	E340	Q341	P342	K343	G344	K345	W346	Q347	A348	L349	R350	I351
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE-FLIPPING EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	2.49	42/2070 (2.0%)	2.48	130/2806 (4.6%)
1	B	2.49	42/2070 (2.0%)	2.48	130/2806 (4.6%)
1	C	2.51	56/2285 (2.5%)	2.46	145/3099 (4.7%)
All	All	2.50	140/6425 (2.2%)	2.47	405/8711 (4.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	10
All	All	0	26

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	ILE	C-N	-42.35	0.36	1.34
1	B	201	ILE	C-N	-42.34	0.36	1.34
1	C	201	ILE	C-N	-42.34	0.36	1.34
1	B	93	LEU	N-CA	-41.12	0.64	1.46
1	C	93	LEU	N-CA	-41.10	0.64	1.46
1	A	93	LEU	N-CA	-41.09	0.64	1.46
1	B	259	GLY	C-N	33.08	1.97	1.34
1	A	259	GLY	C-N	33.07	1.97	1.34
1	C	259	GLY	C-N	33.04	1.97	1.34
1	B	133	SER	CB-OG	29.84	1.81	1.42
1	C	133	SER	CB-OG	29.83	1.81	1.42
1	A	133	SER	CB-OG	29.80	1.80	1.42
1	C	82	ILE	C-N	20.46	1.81	1.34
1	A	82	ILE	C-N	20.44	1.81	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	ILE	C-N	20.43	1.81	1.34
1	B	149	LYS	CD-CE	19.48	2.00	1.51
1	C	149	LYS	CD-CE	19.45	1.99	1.51
1	A	149	LYS	CD-CE	19.44	1.99	1.51
1	A	279	HIS	C-N	17.61	1.74	1.34
1	B	279	HIS	C-N	17.59	1.74	1.34
1	C	279	HIS	C-N	17.56	1.74	1.34
1	B	288	LEU	C-N	-17.33	0.94	1.34
1	A	288	LEU	C-N	-17.32	0.94	1.34
1	C	288	LEU	C-N	-17.26	0.94	1.34
1	B	291	PHE	C-N	16.20	1.71	1.34
1	C	291	PHE	C-N	16.18	1.71	1.34
1	A	291	PHE	C-N	16.18	1.71	1.34
1	C	264	SER	C-N	15.12	1.68	1.34
1	A	264	SER	C-N	15.11	1.68	1.34
1	B	264	SER	C-N	15.10	1.68	1.34
1	B	339	GLU	C-N	14.95	1.68	1.34
1	A	339	GLU	C-N	14.94	1.68	1.34
1	C	339	GLU	C-N	14.94	1.68	1.34
1	C	76	SER	N-CA	14.83	1.76	1.46
1	B	297	VAL	C-N	-14.48	1.00	1.34
1	C	297	VAL	C-N	-14.48	1.00	1.34
1	A	297	VAL	C-N	-14.47	1.00	1.34
1	C	53	GLN	C-N	14.34	1.67	1.34
1	B	177	SER	C-N	-12.81	1.04	1.34
1	C	177	SER	C-N	-12.80	1.04	1.34
1	A	177	SER	C-N	-12.79	1.04	1.34
1	A	121	LYS	CE-NZ	12.06	1.79	1.49
1	B	121	LYS	CE-NZ	12.05	1.79	1.49
1	C	121	LYS	CE-NZ	12.05	1.79	1.49
1	B	319	VAL	C-N	12.01	1.61	1.34
1	A	319	VAL	C-N	11.98	1.61	1.34
1	C	319	VAL	C-N	11.98	1.61	1.34
1	B	139	SER	C-N	-11.55	1.12	1.34
1	A	139	SER	C-N	-11.53	1.12	1.34
1	C	139	SER	C-N	-11.53	1.12	1.34
1	C	75	VAL	C-N	11.47	1.60	1.34
1	A	140	PRO	N-CD	-10.96	1.32	1.47
1	C	140	PRO	N-CD	-10.95	1.32	1.47
1	B	140	PRO	N-CD	-10.91	1.32	1.47
1	C	75	VAL	N-CA	10.88	1.68	1.46
1	B	308	PHE	C-N	-9.61	1.11	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	PHE	C-N	-9.61	1.11	1.34
1	C	308	PHE	C-N	-9.60	1.11	1.34
1	A	200	GLY	C-N	-9.39	1.12	1.34
1	B	200	GLY	C-N	-9.38	1.12	1.34
1	C	200	GLY	C-N	-9.37	1.12	1.34
1	B	91	THR	N-CA	9.29	1.65	1.46
1	C	91	THR	N-CA	9.26	1.64	1.46
1	A	91	THR	N-CA	9.26	1.64	1.46
1	B	298	SER	C-N	-9.18	1.16	1.33
1	C	298	SER	C-N	-9.12	1.16	1.33
1	A	298	SER	C-N	-9.11	1.16	1.33
1	B	299	GLY	N-CA	-9.03	1.32	1.46
1	A	299	GLY	N-CA	-9.03	1.32	1.46
1	C	299	GLY	N-CA	-9.01	1.32	1.46
1	C	75	VAL	CA-C	8.91	1.76	1.52
1	C	77	THR	N-CA	8.68	1.63	1.46
1	B	315	ALA	C-N	-8.65	1.14	1.34
1	A	315	ALA	C-N	-8.63	1.14	1.34
1	C	315	ALA	C-N	-8.63	1.14	1.34
1	C	76	SER	CA-C	8.60	1.75	1.52
1	A	299	GLY	CA-C	-8.48	1.38	1.51
1	C	299	GLY	CA-C	-8.48	1.38	1.51
1	B	299	GLY	CA-C	-8.44	1.38	1.51
1	A	260	PRO	C-N	-8.07	1.15	1.34
1	B	260	PRO	C-N	-8.05	1.15	1.34
1	C	260	PRO	C-N	-8.03	1.15	1.34
1	C	74	ARG	C-N	8.00	1.52	1.34
1	C	323	GLY	C-N	-7.71	1.16	1.34
1	B	323	GLY	C-N	-7.70	1.16	1.34
1	A	323	GLY	C-N	-7.67	1.16	1.34
1	C	290	LEU	C-N	7.61	1.51	1.34
1	B	290	LEU	C-N	7.59	1.51	1.34
1	A	290	LEU	C-N	7.58	1.51	1.34
1	C	300	LEU	N-CA	-7.56	1.31	1.46
1	B	300	LEU	N-CA	-7.54	1.31	1.46
1	A	300	LEU	N-CA	-7.53	1.31	1.46
1	B	330	GLY	C-N	7.17	1.50	1.34
1	A	330	GLY	C-N	7.15	1.50	1.34
1	C	330	GLY	C-N	7.09	1.50	1.34
1	B	303	ALA	C-N	7.06	1.50	1.34
1	C	303	ALA	C-N	7.04	1.50	1.34
1	A	303	ALA	C-N	7.04	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	GLY	C-N	-7.00	1.18	1.34
1	A	299	GLY	C-N	-6.99	1.18	1.34
1	C	299	GLY	C-N	-6.95	1.18	1.34
1	C	72	GLN	C-N	6.88	1.47	1.34
1	C	74	ARG	N-CA	6.68	1.59	1.46
1	C	76	SER	C-N	6.65	1.49	1.34
1	C	74	ARG	CA-C	6.48	1.69	1.52
1	B	259	GLY	CA-C	6.44	1.62	1.51
1	C	259	GLY	CA-C	6.44	1.62	1.51
1	A	175	CYS	C-N	-6.37	1.19	1.34
1	C	175	CYS	C-N	-6.36	1.19	1.34
1	A	259	GLY	CA-C	6.35	1.62	1.51
1	B	175	CYS	C-N	-6.34	1.19	1.34
1	A	90	ILE	CA-C	6.26	1.69	1.52
1	B	90	ILE	CA-C	6.26	1.69	1.52
1	C	90	ILE	CA-C	6.25	1.69	1.52
1	A	140	PRO	CA-CB	-6.15	1.41	1.53
1	B	140	PRO	CA-CB	-6.14	1.41	1.53
1	C	140	PRO	CA-CB	-6.11	1.41	1.53
1	B	163	PRO	N-CA	-6.06	1.36	1.47
1	C	163	PRO	N-CA	-6.04	1.36	1.47
1	A	163	PRO	N-CA	-6.04	1.36	1.47
1	A	221	ALA	C-N	5.86	1.47	1.34
1	C	221	ALA	C-N	5.86	1.47	1.34
1	B	221	ALA	C-N	5.85	1.47	1.34
1	B	175	CYS	CA-C	-5.73	1.38	1.52
1	A	175	CYS	CA-C	-5.71	1.38	1.52
1	C	175	CYS	CA-C	-5.71	1.38	1.52
1	C	70	SER	C-N	-5.52	1.21	1.34
1	A	88	GLU	C-N	-5.47	1.21	1.34
1	B	88	GLU	C-N	-5.46	1.21	1.34
1	C	88	GLU	C-N	-5.46	1.21	1.34
1	A	284	GLY	N-CA	5.30	1.54	1.46
1	C	284	GLY	N-CA	5.26	1.53	1.46
1	B	284	GLY	N-CA	5.25	1.53	1.46
1	A	176	VAL	N-CA	-5.25	1.35	1.46
1	B	176	VAL	N-CA	-5.24	1.35	1.46
1	C	176	VAL	N-CA	-5.22	1.35	1.46
1	C	203	ASP	C-N	5.18	1.44	1.34
1	A	203	ASP	C-N	5.18	1.44	1.34
1	B	203	ASP	C-N	5.17	1.44	1.34
1	C	274	TRP	NE1-CE2	-5.03	1.31	1.37

All (405) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ILE	O-C-N	-59.09	28.16	122.70
1	A	201	ILE	O-C-N	-59.06	28.20	122.70
1	C	201	ILE	O-C-N	-59.04	28.24	122.70
1	A	82	ILE	O-C-N	-16.84	95.76	122.70
1	C	82	ILE	O-C-N	-16.83	95.77	122.70
1	B	82	ILE	O-C-N	-16.81	95.80	122.70
1	C	338	THR	O-C-N	15.64	147.72	122.70
1	B	338	THR	O-C-N	15.63	147.70	122.70
1	A	338	THR	O-C-N	15.61	147.68	122.70
1	B	300	LEU	O-C-N	14.54	145.96	122.70
1	A	300	LEU	O-C-N	14.52	145.93	122.70
1	C	300	LEU	O-C-N	14.49	145.89	122.70
1	B	307	ASP	C-N-CA	14.03	156.77	121.70
1	C	307	ASP	C-N-CA	14.02	156.76	121.70
1	A	307	ASP	C-N-CA	14.02	156.75	121.70
1	A	129	TYR	O-C-N	12.93	143.38	122.70
1	C	129	TYR	O-C-N	12.90	143.35	122.70
1	B	129	TYR	O-C-N	12.89	143.32	122.70
1	B	307	ASP	O-C-N	-12.85	102.14	122.70
1	C	307	ASP	O-C-N	-12.85	102.14	122.70
1	A	307	ASP	O-C-N	-12.84	102.16	122.70
1	C	93	LEU	N-CA-C	-12.63	76.89	111.00
1	B	93	LEU	N-CA-C	-12.63	76.89	111.00
1	A	93	LEU	N-CA-C	-12.62	76.93	111.00
1	B	200	GLY	O-C-N	12.49	142.68	122.70
1	C	201	ILE	CA-C-N	12.46	144.62	117.20
1	C	200	GLY	O-C-N	12.46	142.63	122.70
1	B	201	ILE	CA-C-N	12.44	144.57	117.20
1	A	200	GLY	O-C-N	12.44	142.60	122.70
1	A	201	ILE	CA-C-N	12.42	144.52	117.20
1	B	290	LEU	O-C-N	12.41	142.56	122.70
1	A	290	LEU	O-C-N	12.40	142.55	122.70
1	C	264	SER	O-C-N	12.39	142.53	122.70
1	C	290	LEU	O-C-N	12.38	142.51	122.70
1	B	264	SER	O-C-N	12.38	142.50	122.70
1	A	264	SER	O-C-N	12.34	142.45	122.70
1	B	339	GLU	C-N-CA	-12.34	90.86	121.70
1	C	339	GLU	C-N-CA	-12.34	90.86	121.70
1	A	339	GLU	C-N-CA	-12.33	90.88	121.70
1	B	330	GLY	O-C-N	-12.16	103.25	122.70
1	C	330	GLY	O-C-N	-12.11	103.33	122.70
1	A	330	GLY	O-C-N	-12.10	103.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	GLY	O-C-N	11.96	141.83	122.70
1	A	299	GLY	O-C-N	11.95	141.81	122.70
1	B	299	GLY	O-C-N	11.94	141.80	122.70
1	B	297	VAL	C-N-CA	-11.77	92.27	121.70
1	C	297	VAL	C-N-CA	-11.74	92.34	121.70
1	A	297	VAL	C-N-CA	-11.73	92.37	121.70
1	C	338	THR	CA-C-N	-11.54	91.81	117.20
1	A	338	THR	CA-C-N	-11.53	91.84	117.20
1	B	338	THR	CA-C-N	-11.52	91.85	117.20
1	C	264	SER	CA-C-N	-10.45	94.22	117.20
1	B	264	SER	CA-C-N	-10.44	94.23	117.20
1	A	264	SER	CA-C-N	-10.42	94.28	117.20
1	B	300	LEU	CA-C-N	-10.21	94.74	117.20
1	C	300	LEU	CA-C-N	-10.20	94.75	117.20
1	A	300	LEU	CA-C-N	-10.19	94.78	117.20
1	B	200	GLY	CA-C-N	-9.81	95.61	117.20
1	C	200	GLY	CA-C-N	-9.79	95.66	117.20
1	A	200	GLY	CA-C-N	-9.78	95.68	117.20
1	C	313	GLU	O-C-N	9.71	138.23	122.70
1	B	313	GLU	O-C-N	9.70	138.22	122.70
1	A	200	GLY	C-N-CA	9.70	145.94	121.70
1	A	313	GLU	O-C-N	9.69	138.20	122.70
1	C	200	GLY	C-N-CA	9.68	145.91	121.70
1	B	200	GLY	C-N-CA	9.68	145.89	121.70
1	C	279	HIS	O-C-N	-9.60	107.34	122.70
1	B	279	HIS	O-C-N	-9.60	107.34	122.70
1	A	279	HIS	O-C-N	-9.59	107.35	122.70
1	A	129	TYR	CA-C-N	-9.57	96.14	117.20
1	C	129	TYR	CA-C-N	-9.57	96.14	117.20
1	B	129	TYR	CA-C-N	-9.56	96.17	117.20
1	C	140	PRO	N-CD-CG	-9.39	89.12	103.20
1	B	140	PRO	N-CD-CG	-9.38	89.13	103.20
1	A	140	PRO	N-CD-CG	-9.38	89.14	103.20
1	C	299	GLY	CA-C-N	-9.34	96.64	117.20
1	A	100	GLU	O-C-N	-9.34	103.36	121.10
1	C	100	GLU	O-C-N	-9.33	103.36	121.10
1	B	100	GLU	O-C-N	-9.33	103.37	121.10
1	B	299	GLY	CA-C-N	-9.33	96.68	117.20
1	A	299	GLY	CA-C-N	-9.32	96.69	117.20
1	A	335	MET	CA-C-N	-9.31	96.72	117.20
1	C	335	MET	CA-C-N	-9.30	96.73	117.20
1	B	335	MET	CA-C-N	-9.30	96.74	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	PRO	CA-N-CD	9.26	124.66	111.70
1	A	202	SER	CB-CA-C	-9.24	92.53	110.10
1	C	202	SER	CB-CA-C	-9.24	92.54	110.10
1	A	140	PRO	CA-N-CD	9.24	124.63	111.70
1	B	202	SER	CB-CA-C	-9.23	92.56	110.10
1	B	140	PRO	CA-N-CD	9.22	124.61	111.70
1	C	264	SER	C-N-CA	-9.13	98.88	121.70
1	B	264	SER	C-N-CA	-9.12	98.90	121.70
1	A	264	SER	C-N-CA	-9.11	98.94	121.70
1	B	278	CYS	CA-CB-SG	-8.80	98.17	114.00
1	C	278	CYS	CA-CB-SG	-8.77	98.21	114.00
1	A	278	CYS	CA-CB-SG	-8.77	98.22	114.00
1	C	328	GLU	O-C-N	8.68	136.59	122.70
1	A	328	GLU	O-C-N	8.65	136.54	122.70
1	B	328	GLU	O-C-N	8.63	136.51	122.70
1	A	279	HIS	CA-C-N	-8.60	98.27	117.20
1	B	279	HIS	CA-C-N	-8.59	98.31	117.20
1	C	279	HIS	CA-C-N	-8.56	98.36	117.20
1	A	275	GLU	N-CA-C	-8.52	88.01	111.00
1	C	275	GLU	N-CA-C	-8.48	88.10	111.00
1	C	325	LYS	C-N-CA	-8.48	100.50	121.70
1	B	275	GLU	N-CA-C	-8.46	88.16	111.00
1	C	90	ILE	O-C-N	-8.46	109.17	122.70
1	B	325	LYS	C-N-CA	-8.46	100.56	121.70
1	A	325	LYS	C-N-CA	-8.45	100.57	121.70
1	A	90	ILE	O-C-N	-8.44	109.20	122.70
1	B	90	ILE	O-C-N	-8.44	109.20	122.70
1	A	314	ALA	N-CA-C	-8.43	88.23	111.00
1	C	314	ALA	N-CA-C	-8.43	88.25	111.00
1	B	314	ALA	N-CA-C	-8.41	88.29	111.00
1	C	175	CYS	CA-CB-SG	-8.29	99.08	114.00
1	A	175	CYS	CA-CB-SG	-8.28	99.09	114.00
1	C	175	CYS	C-N-CA	-8.28	101.00	121.70
1	B	175	CYS	C-N-CA	-8.28	101.01	121.70
1	A	175	CYS	C-N-CA	-8.27	101.02	121.70
1	B	175	CYS	CA-CB-SG	-8.27	99.11	114.00
1	A	307	ASP	CA-C-N	8.15	135.14	117.20
1	B	307	ASP	CA-C-N	8.15	135.13	117.20
1	C	307	ASP	CA-C-N	8.15	135.12	117.20
1	B	296	PRO	O-C-N	8.14	135.72	122.70
1	A	296	PRO	O-C-N	8.13	135.70	122.70
1	C	163	PRO	O-C-N	8.12	135.69	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	PRO	O-C-N	8.11	135.68	122.70
1	C	296	PRO	O-C-N	8.11	135.68	122.70
1	B	163	PRO	O-C-N	8.11	135.68	122.70
1	C	350	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	A	350	ARG	NE-CZ-NH2	7.98	124.29	120.30
1	C	76	SER	CB-CA-C	-7.98	94.94	110.10
1	B	291	PHE	CB-CG-CD2	-7.97	115.22	120.80
1	C	291	PHE	CB-CG-CD2	-7.97	115.22	120.80
1	B	203	ASP	O-C-N	-7.92	106.05	121.10
1	C	203	ASP	O-C-N	-7.92	106.06	121.10
1	C	291	PHE	N-CA-CB	-7.91	96.36	110.60
1	A	203	ASP	O-C-N	-7.91	106.08	121.10
1	B	291	PHE	N-CA-CB	-7.91	96.36	110.60
1	C	74	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	A	291	PHE	CB-CG-CD2	-7.88	115.29	120.80
1	A	291	PHE	N-CA-CB	-7.87	96.44	110.60
1	B	350	ARG	NE-CZ-NH2	7.87	124.23	120.30
1	B	330	GLY	CA-C-N	7.85	134.47	117.20
1	C	330	GLY	CA-C-N	7.83	134.43	117.20
1	A	330	GLY	CA-C-N	7.82	134.41	117.20
1	C	140	PRO	N-CA-CB	-7.75	94.00	103.30
1	B	273	GLY	O-C-N	7.73	135.07	122.70
1	A	140	PRO	N-CA-CB	-7.72	94.04	103.30
1	C	273	GLY	O-C-N	7.71	135.03	122.70
1	B	140	PRO	N-CA-CB	-7.70	94.06	103.30
1	A	273	GLY	O-C-N	7.70	135.01	122.70
1	A	329	ARG	NE-CZ-NH2	7.57	124.09	120.30
1	A	135	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	B	273	GLY	C-N-CA	-7.53	102.87	121.70
1	C	273	GLY	C-N-CA	-7.52	102.89	121.70
1	A	84	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	A	273	GLY	C-N-CA	-7.51	102.92	121.70
1	C	135	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	C	84	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	195	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	C	57	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	B	135	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	B	84	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	C	63	ALA	O-C-N	7.46	134.63	122.70
1	C	195	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	A	241	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	261	ARG	NE-CZ-NH2	7.43	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	C	241	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	B	261	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	C	261	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	A	130	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	C	130	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	C	329	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	B	130	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	B	156	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	A	156	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	C	156	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	B	241	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	C	79	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	A	290	LEU	CA-C-N	-7.31	101.12	117.20
1	B	290	LEU	CA-C-N	-7.31	101.12	117.20
1	C	290	LEU	CA-C-N	-7.31	101.12	117.20
1	C	57	ARG	O-C-N	7.31	134.39	122.70
1	B	313	GLU	CA-C-N	-7.30	101.14	117.20
1	A	313	GLU	CA-C-N	-7.30	101.15	117.20
1	C	313	GLU	CA-C-N	-7.27	101.21	117.20
1	A	274	TRP	O-C-N	7.26	134.31	122.70
1	C	274	TRP	O-C-N	7.23	134.27	122.70
1	B	274	TRP	O-C-N	7.22	134.26	122.70
1	C	176	VAL	O-C-N	7.20	134.23	122.70
1	B	329	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	176	VAL	O-C-N	7.18	134.19	122.70
1	B	176	VAL	O-C-N	7.15	134.13	122.70
1	B	290	LEU	CB-CA-C	-7.14	96.63	110.20
1	A	290	LEU	CB-CA-C	-7.13	96.66	110.20
1	C	290	LEU	CB-CA-C	-7.12	96.67	110.20
1	B	191	ASP	O-C-N	7.11	134.08	122.70
1	A	191	ASP	O-C-N	7.09	134.04	122.70
1	C	191	ASP	O-C-N	7.08	134.03	122.70
1	C	328	GLU	CA-C-N	-7.01	101.78	117.20
1	A	91	THR	N-CA-CB	7.00	123.59	110.30
1	B	328	GLU	CA-C-N	-6.99	101.82	117.20
1	A	328	GLU	CA-C-N	-6.99	101.82	117.20
1	C	91	THR	N-CA-CB	6.99	123.57	110.30
1	B	91	THR	N-CA-CB	6.98	123.57	110.30
1	B	202	SER	O-C-N	6.95	133.82	122.70
1	A	202	SER	O-C-N	6.94	133.80	122.70
1	C	202	SER	O-C-N	6.93	133.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	O-C-N	6.92	133.78	122.70
1	B	165	ASP	O-C-N	6.91	133.76	122.70
1	C	165	ASP	O-C-N	6.91	133.75	122.70
1	B	341	GLN	O-C-N	-6.90	108.00	121.10
1	A	341	GLN	O-C-N	-6.87	108.04	121.10
1	A	137	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	C	341	GLN	O-C-N	-6.85	108.09	121.10
1	A	338	THR	C-N-CA	6.81	138.74	121.70
1	C	338	THR	C-N-CA	6.80	138.71	121.70
1	B	338	THR	C-N-CA	6.80	138.71	121.70
1	B	137	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	82	ILE	C-N-CA	6.79	138.69	121.70
1	C	69	VAL	O-C-N	-6.78	111.85	122.70
1	C	82	ILE	C-N-CA	6.78	138.65	121.70
1	B	82	ILE	C-N-CA	6.78	138.64	121.70
1	C	137	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	B	273	GLY	CA-C-N	-6.63	102.61	117.20
1	C	273	GLY	CA-C-N	-6.62	102.64	117.20
1	A	273	GLY	CA-C-N	-6.61	102.65	117.20
1	B	274	TRP	C-N-CA	6.58	138.14	121.70
1	C	313	GLU	C-N-CA	6.56	138.09	121.70
1	A	313	GLU	C-N-CA	6.55	138.07	121.70
1	B	313	GLU	C-N-CA	6.55	138.07	121.70
1	C	274	TRP	C-N-CA	6.55	138.07	121.70
1	A	274	TRP	C-N-CA	6.53	138.02	121.70
1	A	202	SER	N-CA-C	6.52	128.59	111.00
1	C	202	SER	N-CA-C	6.52	128.59	111.00
1	B	202	SER	N-CA-C	6.50	128.56	111.00
1	A	102	LYS	CB-CA-C	6.47	123.33	110.40
1	B	102	LYS	CB-CA-C	6.45	123.29	110.40
1	C	102	LYS	CB-CA-C	6.45	123.29	110.40
1	B	199	ASP	O-C-N	6.42	134.12	123.20
1	A	199	ASP	O-C-N	6.42	134.11	123.20
1	C	199	ASP	O-C-N	6.41	134.09	123.20
1	B	329	ARG	O-C-N	6.40	134.08	123.20
1	A	329	ARG	O-C-N	6.39	134.06	123.20
1	C	329	ARG	O-C-N	6.38	134.04	123.20
1	A	175	CYS	CB-CA-C	-6.32	97.76	110.40
1	A	326	VAL	O-C-N	6.31	132.80	122.70
1	C	175	CYS	CB-CA-C	-6.31	97.78	110.40
1	B	175	CYS	CB-CA-C	-6.30	97.80	110.40
1	B	288	LEU	O-C-N	6.29	132.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	VAL	O-C-N	6.28	132.75	122.70
1	C	326	VAL	O-C-N	6.27	132.74	122.70
1	A	288	LEU	O-C-N	6.26	132.72	122.70
1	C	288	LEU	O-C-N	6.25	132.71	122.70
1	C	71	THR	N-CA-CB	-6.17	98.58	110.30
1	A	335	MET	CG-SD-CE	6.15	110.04	100.20
1	C	67	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	B	335	MET	CG-SD-CE	6.14	110.02	100.20
1	C	335	MET	CG-SD-CE	6.13	110.00	100.20
1	A	141	MET	CG-SD-CE	6.08	109.93	100.20
1	B	141	MET	CG-SD-CE	6.08	109.93	100.20
1	C	141	MET	CG-SD-CE	6.07	109.92	100.20
1	C	214	MET	CG-SD-CE	6.05	109.88	100.20
1	B	214	MET	CG-SD-CE	6.03	109.85	100.20
1	A	214	MET	CG-SD-CE	6.03	109.85	100.20
1	A	298	SER	C-N-CA	-6.02	109.66	122.30
1	B	288	LEU	CA-C-N	-6.00	103.99	117.20
1	C	298	SER	C-N-CA	-6.00	109.70	122.30
1	B	298	SER	C-N-CA	-5.99	109.71	122.30
1	C	288	LEU	CA-C-N	-5.98	104.04	117.20
1	A	339	GLU	O-C-N	5.98	132.26	122.70
1	B	339	GLU	O-C-N	5.98	132.26	122.70
1	C	339	GLU	O-C-N	5.98	132.26	122.70
1	A	288	LEU	CA-C-N	-5.96	104.09	117.20
1	C	76	SER	N-CA-C	5.95	127.06	111.00
1	C	53	GLN	O-C-N	-5.94	113.20	122.70
1	C	274	TRP	CA-C-N	-5.93	104.16	117.20
1	A	274	TRP	CA-C-N	-5.91	104.20	117.20
1	A	314	ALA	CB-CA-C	5.88	118.92	110.10
1	B	274	TRP	CA-C-N	-5.88	104.27	117.20
1	C	325	LYS	O-C-N	5.87	132.09	122.70
1	C	317	GLY	O-C-N	-5.86	113.32	122.70
1	A	315	ALA	O-C-N	-5.85	113.34	122.70
1	B	317	GLY	O-C-N	-5.85	113.33	122.70
1	B	202	SER	CA-C-N	-5.85	104.33	117.20
1	A	325	LYS	O-C-N	5.84	132.04	122.70
1	A	162	PRO	O-C-N	-5.84	110.01	121.10
1	B	314	ALA	CB-CA-C	5.84	118.86	110.10
1	C	202	SER	CA-C-N	-5.83	104.38	117.20
1	A	202	SER	CA-C-N	-5.83	104.38	117.20
1	A	317	GLY	O-C-N	-5.83	113.37	122.70
1	B	325	LYS	O-C-N	5.83	132.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	314	ALA	CB-CA-C	5.82	118.82	110.10
1	C	162	PRO	O-C-N	-5.81	110.05	121.10
1	C	315	ALA	O-C-N	-5.81	113.41	122.70
1	B	162	PRO	O-C-N	-5.80	110.07	121.10
1	C	63	ALA	CA-C-N	-5.80	104.44	117.20
1	B	315	ALA	O-C-N	-5.78	113.45	122.70
1	A	130	ARG	CB-CA-C	-5.75	98.91	110.40
1	C	130	ARG	CB-CA-C	-5.73	98.94	110.40
1	B	130	ARG	CB-CA-C	-5.72	98.97	110.40
1	C	231	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	A	231	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	177	SER	CA-C-N	-5.69	104.68	117.20
1	B	231	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	C	177	SER	CA-C-N	-5.69	104.69	117.20
1	B	177	SER	CA-C-N	-5.68	104.70	117.20
1	C	56	THR	CB-CA-C	-5.65	96.34	111.60
1	C	305	ALA	O-C-N	5.60	131.66	122.70
1	A	305	ALA	O-C-N	5.59	131.64	122.70
1	B	305	ALA	O-C-N	5.59	131.64	122.70
1	A	191	ASP	CA-C-N	-5.54	105.00	117.20
1	B	191	ASP	CA-C-N	-5.54	105.02	117.20
1	B	300	LEU	CA-CB-CG	-5.53	102.58	115.30
1	C	300	LEU	CA-CB-CG	-5.53	102.58	115.30
1	C	191	ASP	CA-C-N	-5.53	105.04	117.20
1	A	300	LEU	CA-CB-CG	-5.52	102.60	115.30
1	B	199	ASP	CA-C-N	-5.51	105.18	116.20
1	C	57	ARG	CA-C-N	-5.50	105.09	117.20
1	C	199	ASP	CA-C-N	-5.50	105.20	116.20
1	A	199	ASP	CA-C-N	-5.50	105.21	116.20
1	C	163	PRO	CA-C-N	-5.46	105.18	117.20
1	A	163	PRO	CA-C-N	-5.46	105.19	117.20
1	B	93	LEU	N-CA-CB	-5.46	99.48	110.40
1	C	176	VAL	CA-C-N	-5.46	105.18	117.20
1	A	93	LEU	N-CA-CB	-5.46	99.48	110.40
1	C	93	LEU	N-CA-CB	-5.45	99.49	110.40
1	B	163	PRO	CA-C-N	-5.45	105.21	117.20
1	B	273	GLY	N-CA-C	-5.45	99.48	113.10
1	C	273	GLY	N-CA-C	-5.45	99.48	113.10
1	A	176	VAL	CA-C-N	-5.44	105.23	117.20
1	A	273	GLY	N-CA-C	-5.44	99.50	113.10
1	B	176	VAL	CA-C-N	-5.42	105.29	117.20
1	C	72	GLN	C-N-CD	-5.39	108.73	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ILE	CA-C-N	5.38	129.04	117.20
1	C	90	ILE	CA-C-N	5.38	129.04	117.20
1	B	90	ILE	CA-C-N	5.38	129.03	117.20
1	B	264	SER	CB-CA-C	-5.37	99.90	110.10
1	A	264	SER	CB-CA-C	-5.35	99.94	110.10
1	A	296	PRO	CA-C-N	-5.34	105.45	117.20
1	B	296	PRO	CA-C-N	-5.34	105.46	117.20
1	B	203	ASP	CA-C-N	5.33	132.01	117.10
1	C	203	ASP	CA-C-N	5.33	132.01	117.10
1	C	296	PRO	CA-C-N	-5.32	105.49	117.20
1	A	203	ASP	CA-C-N	5.32	131.99	117.10
1	A	165	ASP	CA-C-N	-5.31	105.51	117.20
1	B	248	ALA	CB-CA-C	-5.31	102.13	110.10
1	C	264	SER	CB-CA-C	-5.31	100.02	110.10
1	C	248	ALA	CB-CA-C	-5.30	102.15	110.10
1	B	165	ASP	CA-C-N	-5.29	105.55	117.20
1	C	165	ASP	CA-C-N	-5.29	105.56	117.20
1	A	248	ALA	CB-CA-C	-5.29	102.17	110.10
1	B	176	VAL	N-CA-CB	-5.29	99.87	111.50
1	C	176	VAL	N-CA-CB	-5.28	99.88	111.50
1	A	176	VAL	N-CA-CB	-5.26	99.93	111.50
1	B	338	THR	CB-CA-C	-5.25	97.44	111.60
1	A	338	THR	CB-CA-C	-5.25	97.44	111.60
1	B	291	PHE	CB-CA-C	5.24	120.88	110.40
1	C	338	THR	CB-CA-C	-5.24	97.45	111.60
1	C	291	PHE	CB-CA-C	5.24	120.87	110.40
1	A	291	PHE	CB-CA-C	5.23	120.87	110.40
1	B	100	GLU	CA-C-N	5.22	131.73	117.10
1	C	100	GLU	CA-C-N	5.22	131.71	117.10
1	A	100	GLU	CA-C-N	5.21	131.69	117.10
1	A	175	CYS	O-C-N	-5.20	114.37	122.70
1	B	175	CYS	O-C-N	-5.20	114.38	122.70
1	B	129	TYR	C-N-CA	5.20	134.69	121.70
1	A	304	ASP	O-C-N	5.19	131.00	122.70
1	B	304	ASP	O-C-N	5.18	130.98	122.70
1	C	129	TYR	C-N-CA	5.18	134.64	121.70
1	A	129	TYR	C-N-CA	5.17	134.62	121.70
1	C	175	CYS	O-C-N	-5.16	114.45	122.70
1	C	304	ASP	O-C-N	5.15	130.94	122.70
1	C	323	GLY	C-N-CA	5.15	134.58	121.70
1	A	323	GLY	C-N-CA	5.15	134.57	121.70
1	C	290	LEU	C-N-CA	5.14	134.56	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	LEU	C-N-CA	5.14	134.55	121.70
1	B	290	LEU	C-N-CA	5.14	134.54	121.70
1	B	176	VAL	CB-CA-C	5.13	121.16	111.40
1	B	323	GLY	C-N-CA	5.13	134.53	121.70
1	A	176	VAL	CB-CA-C	5.13	121.14	111.40
1	A	329	ARG	CA-C-N	-5.13	105.95	116.20
1	C	176	VAL	CB-CA-C	5.12	121.13	111.40
1	C	329	ARG	CA-C-N	-5.11	105.97	116.20
1	B	329	ARG	CA-C-N	-5.11	105.99	116.20
1	A	343	LYS	CB-CA-C	-5.05	100.29	110.40
1	B	343	LYS	CB-CA-C	-5.05	100.29	110.40
1	C	343	LYS	CB-CA-C	-5.05	100.29	110.40
1	C	326	VAL	CA-C-N	-5.05	106.09	117.20
1	C	325	LYS	CA-C-N	-5.05	106.10	117.20
1	A	326	VAL	CA-C-N	-5.04	106.10	117.20
1	A	339	GLU	CA-C-N	-5.04	106.10	117.20
1	B	326	VAL	CA-C-N	-5.04	106.11	117.20
1	A	130	ARG	N-CA-C	5.04	124.60	111.00
1	C	339	GLU	CA-C-N	-5.04	106.12	117.20
1	A	325	LYS	CA-C-N	-5.03	106.13	117.20
1	B	130	ARG	N-CA-C	5.03	124.58	111.00
1	A	290	LEU	N-CA-C	5.03	124.57	111.00
1	B	339	GLU	CA-C-N	-5.02	106.15	117.20
1	C	130	ARG	N-CA-C	5.02	124.56	111.00
1	C	290	LEU	N-CA-C	5.02	124.55	111.00
1	B	290	LEU	N-CA-C	5.01	124.54	111.00
1	B	325	LYS	CA-C-N	-5.01	106.17	117.20

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Mainchain
1	A	177	SER	Mainchain
1	A	201	ILE	Mainchain
1	A	260	PRO	Mainchain
1	A	307	ASP	Mainchain
1	A	330	GLY	Mainchain
1	A	335	MET	Mainchain
1	A	92	THR	Peptide
1	B	100	GLU	Mainchain
1	B	177	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	B	201	ILE	Mainchain
1	B	260	PRO	Mainchain
1	B	307	ASP	Mainchain
1	B	330	GLY	Mainchain
1	B	335	MET	Mainchain
1	B	92	THR	Peptide
1	C	100	GLU	Mainchain
1	C	177	SER	Mainchain
1	C	201	ILE	Mainchain
1	C	260	PRO	Mainchain
1	C	307	ASP	Mainchain
1	C	330	GLY	Mainchain
1	C	335	MET	Mainchain
1	C	59	SER	Mainchain
1	C	69	VAL	Mainchain
1	C	92	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2026	0	1961	1032	0
1	B	2026	0	1962	1050	0
1	C	2238	0	2183	1152	0
All	All	6290	0	6106	3179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 256.

All (3179) 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:C:138:TYR:CB	1:C:184:PHE:CE1	1.75	1.66
1:B:101:PRO:CD	1:B:166:LEU:CD1	1.75	1.65
1:A:138:TYR:CB	1:A:184:PHE:CE1	1.75	1.65
1:A:114:GLY:HA2	1:A:283:THR:CG2	1.25	1.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:HB2	1:A:184:PHE:CZ	1.15	1.63
1:B:138:TYR:CB	1:B:184:PHE:CE1	1.75	1.63
1:C:138:TYR:HB2	1:C:184:PHE:CZ	1.15	1.62
1:C:101:PRO:CD	1:C:166:LEU:HD11	1.22	1.62
1:A:101:PRO:CD	1:A:166:LEU:CD1	1.75	1.60
1:B:138:TYR:HB2	1:B:184:PHE:CZ	1.15	1.60
1:B:101:PRO:CD	1:B:166:LEU:HD11	1.22	1.59
1:B:130:ARG:CD	1:B:237:GLN:CB	1.82	1.58
1:A:130:ARG:CD	1:A:237:GLN:CB	1.81	1.56
1:C:101:PRO:CD	1:C:166:LEU:CD1	1.75	1.56
1:A:101:PRO:CD	1:A:166:LEU:HD11	1.21	1.55
1:C:75:VAL:CA	1:C:75:VAL:C	1.76	1.54
1:C:130:ARG:CD	1:C:237:GLN:CB	1.82	1.53
1:A:278:CYS:H	1:A:334:LYS:CD	1.21	1.52
1:C:278:CYS:H	1:C:334:LYS:CD	1.21	1.52
1:C:75:VAL:CA	1:C:75:VAL:N	1.68	1.52
1:C:101:PRO:HD3	1:C:166:LEU:CD1	1.34	1.50
1:C:76:SER:CA	1:C:76:SER:C	1.75	1.50
1:C:76:SER:N	1:C:76:SER:CA	1.76	1.49
1:B:278:CYS:H	1:B:334:LYS:CD	1.21	1.49
1:A:153:ALA:CB	1:A:174:GLY:HA3	1.43	1.49
1:C:153:ALA:CB	1:C:174:GLY:HA3	1.43	1.48
1:C:185:ILE:HD12	1:C:186:LEU:N	1.18	1.47
1:C:80:ASP:HA	1:C:241:ARG:NH2	1.24	1.47
1:A:114:GLY:CA	1:A:283:THR:HG21	1.00	1.47
1:A:101:PRO:HD3	1:A:166:LEU:CD1	1.34	1.46
1:B:153:ALA:CB	1:B:174:GLY:HA3	1.43	1.46
1:C:107:VAL:CG1	1:C:329:ARG:HE	1.26	1.46
1:A:120:ILE:HG12	1:A:350:ARG:NH2	1.18	1.45
1:C:130:ARG:CD	1:C:237:GLN:HB2	0.98	1.45
1:A:130:ARG:CD	1:A:237:GLN:HB2	0.98	1.45
1:A:114:GLY:N	1:A:283:THR:HB	1.16	1.45
1:B:264:SER:C	1:B:265:TRP:N	1.68	1.45
1:A:121:LYS:NZ	1:A:121:LYS:CE	1.79	1.45
1:B:121:LYS:NZ	1:B:121:LYS:CE	1.79	1.44
1:B:130:ARG:CD	1:B:237:GLN:HB2	0.98	1.44
1:B:296:PRO:CG	1:B:337:THR:HG22	0.96	1.44
1:C:291:PHE:C	1:C:292:TYR:N	1.71	1.44
1:C:339:GLU:C	1:C:340:GLU:N	1.68	1.44
1:C:134:LEU:CA	1:C:233:GLU:O	1.66	1.43
1:B:339:GLU:C	1:B:340:GLU:N	1.68	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLY:N	1:A:283:THR:CB	1.76	1.43
1:B:101:PRO:HD3	1:B:166:LEU:CD1	1.34	1.43
1:C:264:SER:C	1:C:265:TRP:N	1.68	1.43
1:A:264:SER:C	1:A:265:TRP:N	1.68	1.43
1:A:120:ILE:CG1	1:A:350:ARG:NH2	1.81	1.43
1:C:296:PRO:CG	1:C:337:THR:HG22	0.96	1.43
1:A:291:PHE:C	1:A:292:TYR:N	1.71	1.42
1:C:120:ILE:CD1	1:C:350:ARG:HD2	1.48	1.42
1:A:339:GLU:C	1:A:340:GLU:N	1.68	1.42
1:C:121:LYS:NZ	1:C:121:LYS:CE	1.79	1.42
1:C:269:LYS:O	1:C:277:ASP:CB	1.67	1.41
1:C:203:ASP:OD1	1:C:205:LYS:CD	1.68	1.41
1:A:296:PRO:CG	1:A:337:THR:HG22	0.96	1.41
1:A:149:LYS:CE	1:A:149:LYS:CD	1.99	1.41
1:A:185:ILE:HD12	1:A:186:LEU:N	1.18	1.41
1:A:134:LEU:CA	1:A:233:GLU:O	1.66	1.41
1:B:185:ILE:HD12	1:B:186:LEU:N	1.18	1.41
1:A:279:HIS:C	1:A:280:PHE:N	1.74	1.41
1:B:120:ILE:HD13	1:B:284:GLY:CA	1.49	1.41
1:B:185:ILE:CD1	1:B:186:LEU:H	1.32	1.41
1:B:269:LYS:O	1:B:277:ASP:CB	1.67	1.40
1:B:291:PHE:C	1:B:292:TYR:N	1.71	1.40
1:B:120:ILE:CD1	1:B:283:THR:O	1.65	1.40
1:B:246:SER:HB3	1:B:263:VAL:CG1	1.49	1.40
1:B:279:HIS:C	1:B:280:PHE:N	1.74	1.40
1:A:114:GLY:CA	1:A:283:THR:CG2	1.82	1.40
1:A:269:LYS:O	1:A:277:ASP:CB	1.67	1.40
1:B:149:LYS:CD	1:B:149:LYS:CE	2.00	1.40
1:A:203:ASP:OD1	1:A:205:LYS:CD	1.68	1.40
1:B:115:THR:O	1:B:116:PHE:CD1	1.75	1.39
1:B:138:TYR:CB	1:B:184:PHE:CZ	1.96	1.39
1:B:203:ASP:OD1	1:B:205:LYS:CD	1.68	1.39
1:C:279:HIS:C	1:C:280:PHE:N	1.74	1.39
1:C:185:ILE:CD1	1:C:186:LEU:H	1.32	1.39
1:B:134:LEU:CA	1:B:233:GLU:O	1.66	1.38
1:C:149:LYS:CE	1:C:149:LYS:CD	1.99	1.38
1:A:115:THR:O	1:A:116:PHE:CD1	1.76	1.38
1:C:115:THR:O	1:C:116:PHE:CD1	1.76	1.38
1:B:149:LYS:CD	1:B:170:TYR:OH	1.72	1.38
1:A:149:LYS:CD	1:A:170:TYR:OH	1.72	1.38
1:A:113:PRO:HG2	1:A:283:THR:N	1.33	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ARG:O	1:C:351:ILE:CG2	1.71	1.38
1:B:130:ARG:HD3	1:B:237:GLN:CB	1.46	1.37
1:B:248:ALA:HB1	1:B:265:TRP:N	1.34	1.37
1:C:130:ARG:HD2	1:C:237:GLN:CB	1.47	1.37
1:A:130:ARG:HD2	1:A:237:GLN:CB	1.47	1.37
1:A:185:ILE:CD1	1:A:186:LEU:H	1.32	1.37
1:B:296:PRO:HG2	1:B:337:THR:CG2	0.89	1.36
1:A:350:ARG:O	1:A:351:ILE:CG2	1.71	1.36
1:C:138:TYR:CG	1:C:184:PHE:CE1	2.13	1.36
1:C:107:VAL:HG21	1:C:329:ARG:CG	1.54	1.36
1:C:165:ASP:O	1:C:168:SER:HB2	1.26	1.36
1:A:130:ARG:HD3	1:A:237:GLN:CB	1.46	1.36
1:C:149:LYS:CD	1:C:170:TYR:OH	1.72	1.36
1:B:350:ARG:O	1:B:351:ILE:CG2	1.71	1.36
1:B:278:CYS:N	1:B:334:LYS:CD	1.87	1.35
1:A:296:PRO:HG2	1:A:337:THR:CG2	0.89	1.35
1:A:138:TYR:CG	1:A:184:PHE:CE1	2.12	1.35
1:B:138:TYR:CG	1:B:184:PHE:CE1	2.12	1.35
1:C:296:PRO:HG2	1:C:337:THR:CG2	0.89	1.34
1:A:291:PHE:HA	1:A:345:LYS:O	1.22	1.34
1:A:82:ILE:C	1:A:83:THR:N	1.81	1.34
1:B:82:ILE:C	1:B:83:THR:N	1.81	1.34
1:C:153:ALA:HB1	1:C:174:GLY:CA	1.57	1.34
1:C:82:ILE:C	1:C:83:THR:N	1.81	1.34
1:C:278:CYS:N	1:C:334:LYS:CD	1.87	1.34
1:A:133:SER:O	1:A:234:TYR:HA	1.28	1.34
1:A:113:PRO:CG	1:A:283:THR:H	1.39	1.34
1:C:130:ARG:HD3	1:C:237:GLN:CB	1.46	1.34
1:C:138:TYR:CB	1:C:184:PHE:CZ	1.96	1.34
1:A:138:TYR:CD2	1:A:184:PHE:HE1	1.46	1.33
1:C:138:TYR:CD2	1:C:184:PHE:HE1	1.46	1.33
1:B:153:ALA:HB1	1:B:174:GLY:CA	1.57	1.33
1:A:165:ASP:O	1:A:168:SER:HB2	1.26	1.33
1:C:278:CYS:H	1:C:334:LYS:CE	1.41	1.33
1:B:309:SER:O	1:B:322:ALA:HA	1.19	1.33
1:A:248:ALA:CA	1:A:264:SER:O	1.67	1.33
1:C:149:LYS:HG2	1:C:177:SER:OG	1.23	1.33
1:B:138:TYR:CD2	1:B:184:PHE:HE1	1.46	1.33
1:B:130:ARG:HD2	1:B:237:GLN:CB	1.47	1.33
1:C:91:THR:OG1	1:C:325:LYS:CE	1.75	1.33
1:A:153:ALA:HB1	1:A:174:GLY:CA	1.57	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:TRP:CZ3	1:C:348:ALA:O	1.82	1.32
1:A:265:TRP:CZ3	1:A:348:ALA:O	1.82	1.32
1:A:278:CYS:N	1:A:334:LYS:CD	1.87	1.31
1:B:165:ASP:O	1:B:168:SER:HB2	1.26	1.31
1:A:138:TYR:CB	1:A:184:PHE:CZ	1.96	1.31
1:A:278:CYS:H	1:A:334:LYS:CE	1.41	1.31
1:B:278:CYS:H	1:B:334:LYS:CE	1.41	1.31
1:C:71:THR:CG2	1:C:87:SER:OG	1.78	1.31
1:A:198:ALA:HB1	1:A:200:GLY:O	1.17	1.31
1:A:304:ASP:O	1:A:331:GLN:HB3	1.14	1.30
1:C:291:PHE:CA	1:C:345:LYS:O	1.78	1.30
1:C:120:ILE:HD12	1:C:350:ARG:CD	1.62	1.30
1:A:88:GLU:O	1:A:231:ARG:HB2	1.18	1.30
1:B:265:TRP:CZ3	1:B:348:ALA:O	1.82	1.30
1:A:138:TYR:HB3	1:A:184:PHE:CE1	1.51	1.30
1:A:149:LYS:HG2	1:A:177:SER:OG	1.23	1.29
1:A:291:PHE:CA	1:A:345:LYS:O	1.78	1.29
1:B:313:GLU:HG3	1:B:318:SER:CB	1.62	1.29
1:C:107:VAL:CG1	1:C:329:ARG:NE	1.95	1.29
1:B:291:PHE:CA	1:B:345:LYS:O	1.78	1.29
1:C:88:GLU:O	1:C:231:ARG:HB2	1.18	1.29
1:C:309:SER:O	1:C:322:ALA:HA	1.19	1.29
1:B:149:LYS:HG2	1:B:177:SER:OG	1.23	1.29
1:B:291:PHE:HA	1:B:345:LYS:O	1.23	1.29
1:C:154:PHE:CD1	1:C:155:ASP:N	2.01	1.29
1:C:313:GLU:HG3	1:C:318:SER:CB	1.63	1.28
1:C:198:ALA:HB1	1:C:200:GLY:O	1.17	1.28
1:A:119:LEU:CD2	1:A:234:TYR:OH	1.82	1.28
1:B:105:THR:OG1	1:B:211:LYS:CD	1.82	1.28
1:B:327:ALA:HB3	1:B:331:GLN:CD	1.53	1.28
1:B:333:VAL:O	1:B:334:LYS:HD3	1.30	1.28
1:A:105:THR:OG1	1:A:211:LYS:CD	1.82	1.28
1:B:198:ALA:HB1	1:B:200:GLY:O	1.17	1.28
1:B:119:LEU:CD2	1:B:234:TYR:OH	1.82	1.28
1:B:133:SER:CB	1:B:133:SER:OG	1.81	1.27
1:C:105:THR:OG1	1:C:211:LYS:CD	1.82	1.27
1:C:291:PHE:HA	1:C:345:LYS:O	1.23	1.27
1:C:91:THR:HG21	1:C:325:LYS:CE	1.61	1.27
1:C:304:ASP:O	1:C:331:GLN:HB3	1.15	1.27
1:A:309:SER:O	1:A:322:ALA:HA	1.19	1.27
1:A:133:SER:CB	1:A:133:SER:OG	1.81	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLU:HG3	1:A:318:SER:CB	1.63	1.27
1:C:78:ALA:O	1:C:80:ASP:N	1.63	1.27
1:A:154:PHE:CD1	1:A:155:ASP:N	2.01	1.26
1:B:304:ASP:O	1:B:331:GLN:HB3	1.15	1.26
1:C:119:LEU:CD2	1:C:234:TYR:OH	1.82	1.26
1:B:154:PHE:CD1	1:B:155:ASP:N	2.01	1.26
1:B:88:GLU:O	1:B:231:ARG:HB2	1.19	1.26
1:B:246:SER:OG	1:B:265:TRP:CH2	1.81	1.26
1:B:138:TYR:HB3	1:B:184:PHE:CE1	1.51	1.26
1:B:133:SER:O	1:B:234:TYR:HA	1.28	1.26
1:A:327:ALA:HB3	1:A:331:GLN:CD	1.53	1.25
1:C:327:ALA:HB3	1:C:331:GLN:CD	1.53	1.25
1:C:133:SER:O	1:C:234:TYR:HA	1.28	1.25
1:C:80:ASP:CA	1:C:241:ARG:HH22	1.49	1.25
1:A:333:VAL:O	1:A:334:LYS:HD3	1.30	1.25
1:C:133:SER:CB	1:C:133:SER:OG	1.81	1.25
1:C:179:VAL:HG11	1:C:181:TRP:CD1	1.71	1.25
1:C:91:THR:OG1	1:C:325:LYS:NZ	1.68	1.25
1:A:154:PHE:HD1	1:A:155:ASP:N	1.32	1.25
1:B:288:LEU:HD11	1:B:290:LEU:CD2	1.67	1.25
1:B:154:PHE:HD1	1:B:155:ASP:N	1.32	1.24
1:C:138:TYR:HB3	1:C:184:PHE:CE1	1.51	1.24
1:A:179:VAL:HG11	1:A:181:TRP:CD1	1.71	1.24
1:A:156:ARG:O	1:A:210:GLY:HA3	1.36	1.24
1:C:138:TYR:OH	1:C:227:LEU:HB3	1.38	1.24
1:C:333:VAL:O	1:C:334:LYS:HD3	1.30	1.24
1:A:293:GLU:O	1:A:317:GLY:N	1.72	1.23
1:C:156:ARG:O	1:C:210:GLY:HA3	1.36	1.23
1:C:91:THR:CG2	1:C:325:LYS:CE	2.15	1.23
1:C:120:ILE:CD1	1:C:350:ARG:CD	2.14	1.23
1:C:91:THR:CB	1:C:325:LYS:HE3	1.66	1.23
1:A:288:LEU:HD11	1:A:290:LEU:CD2	1.67	1.23
1:B:179:VAL:HG11	1:B:181:TRP:CD1	1.71	1.23
1:B:96:ASN:O	1:B:98:ASP:N	1.70	1.22
1:C:90:ILE:HD11	1:C:232:VAL:CG2	1.69	1.22
1:C:288:LEU:HD11	1:C:290:LEU:CD2	1.66	1.22
1:C:293:GLU:O	1:C:317:GLY:N	1.72	1.22
1:C:201:ILE:HB	1:C:281:LEU:CD2	1.67	1.22
1:A:138:TYR:OH	1:A:227:LEU:HB3	1.38	1.22
1:C:101:PRO:O	1:C:102:LYS:CG	1.88	1.22
1:C:154:PHE:HD1	1:C:155:ASP:N	1.32	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASN:O	1:C:98:ASP:N	1.70	1.22
1:A:96:ASN:O	1:A:98:ASP:N	1.70	1.22
1:B:156:ARG:O	1:B:210:GLY:HA3	1.36	1.22
1:B:293:GLU:O	1:B:317:GLY:N	1.72	1.22
1:C:112:GLU:HG3	1:C:283:THR:O	1.04	1.22
1:B:248:ALA:CB	1:B:265:TRP:N	2.02	1.22
1:B:294:LYS:O	1:B:296:PRO:HD3	1.04	1.22
1:A:327:ALA:CB	1:A:331:GLN:OE1	1.88	1.21
1:B:327:ALA:CB	1:B:331:GLN:OE1	1.88	1.21
1:C:149:LYS:HB3	1:C:217:TYR:CE1	1.75	1.21
1:C:328:GLU:O	1:C:329:ARG:O	1.55	1.21
1:A:101:PRO:O	1:A:102:LYS:CG	1.88	1.21
1:A:328:GLU:O	1:A:329:ARG:O	1.55	1.21
1:A:164:ASN:HD22	1:A:164:ASN:N	1.19	1.21
1:C:327:ALA:CB	1:C:331:GLN:OE1	1.88	1.20
1:A:149:LYS:HB3	1:A:217:TYR:CE1	1.75	1.20
1:A:90:ILE:HD11	1:A:232:VAL:CG2	1.69	1.20
1:B:328:GLU:O	1:B:329:ARG:O	1.55	1.20
1:C:112:GLU:H	1:C:350:ARG:NH2	1.39	1.20
1:B:101:PRO:O	1:B:102:LYS:CG	1.88	1.19
1:B:138:TYR:OH	1:B:227:LEU:HB3	1.38	1.19
1:C:294:LYS:O	1:C:296:PRO:HD3	1.04	1.19
1:B:90:ILE:HD11	1:B:232:VAL:CG2	1.69	1.19
1:B:120:ILE:HD12	1:B:283:THR:C	1.59	1.19
1:A:294:LYS:O	1:A:296:PRO:HD3	1.04	1.19
1:B:149:LYS:HB3	1:B:217:TYR:CE1	1.75	1.19
1:B:106:ALA:HA	1:B:328:GLU:OE1	1.42	1.18
1:C:107:VAL:HB	1:C:283:THR:CB	1.73	1.18
1:C:91:THR:OG1	1:C:325:LYS:HE3	1.30	1.18
1:B:164:ASN:N	1:B:164:ASN:HD22	1.19	1.18
1:C:138:TYR:CG	1:C:184:PHE:HE1	1.56	1.18
1:B:326:VAL:CG1	1:B:327:ALA:H	1.54	1.18
1:B:259:GLY:C	1:B:260:PRO:N	1.97	1.18
1:C:138:TYR:HB3	1:C:184:PHE:CD1	1.78	1.18
1:B:138:TYR:HB3	1:B:184:PHE:CD1	1.78	1.17
1:C:259:GLY:C	1:C:260:PRO:N	1.97	1.17
1:A:101:PRO:C	1:A:102:LYS:HG3	1.57	1.17
1:C:245:THR:OG1	1:C:263:VAL:HG21	1.44	1.17
1:B:295:ALA:N	1:B:316:ALA:HA	1.51	1.17
1:C:107:VAL:CG2	1:C:329:ARG:HG3	1.74	1.17
1:C:91:THR:CB	1:C:325:LYS:CE	2.21	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:HB3	1:A:184:PHE:CD1	1.78	1.17
1:C:295:ALA:N	1:C:316:ALA:HA	1.51	1.17
1:A:259:GLY:C	1:A:260:PRO:N	1.97	1.17
1:A:88:GLU:O	1:A:231:ARG:CB	1.93	1.17
1:C:112:GLU:CG	1:C:283:THR:O	1.92	1.17
1:C:107:VAL:HG13	1:C:329:ARG:NE	1.53	1.16
1:C:120:ILE:HB	1:C:350:ARG:NH1	1.60	1.16
1:A:120:ILE:CG1	1:A:350:ARG:HH22	1.42	1.16
1:B:101:PRO:C	1:B:102:LYS:HG3	1.57	1.16
1:A:116:PHE:O	1:A:120:ILE:HG21	1.46	1.16
1:B:88:GLU:O	1:B:231:ARG:CB	1.93	1.16
1:A:326:VAL:CG1	1:A:327:ALA:H	1.54	1.16
1:B:309:SER:O	1:B:322:ALA:CA	1.94	1.16
1:B:116:PHE:O	1:B:120:ILE:HG21	1.46	1.15
1:B:120:ILE:CD1	1:B:284:GLY:HA3	1.74	1.15
1:C:201:ILE:CB	1:C:281:LEU:CD2	2.24	1.15
1:C:88:GLU:O	1:C:231:ARG:CB	1.93	1.15
1:C:179:VAL:HG11	1:C:181:TRP:NE1	1.61	1.15
1:A:179:VAL:HG11	1:A:181:TRP:NE1	1.61	1.15
1:A:277:ASP:CA	1:A:334:LYS:HD2	1.77	1.15
1:A:249:GLN:NE2	1:A:265:TRP:CE3	2.15	1.15
1:A:138:TYR:CD2	1:A:184:PHE:CE1	2.34	1.14
1:A:326:VAL:HG12	1:A:327:ALA:N	1.60	1.14
1:C:105:THR:OG1	1:C:211:LYS:HD3	0.98	1.14
1:B:297:VAL:CB	1:B:336:VAL:HG13	1.41	1.14
1:B:138:TYR:CD2	1:B:184:PHE:CE1	2.34	1.14
1:A:309:SER:O	1:A:322:ALA:CA	1.94	1.14
1:B:86:GLY:HA2	1:B:234:TYR:CD1	1.83	1.14
1:C:138:TYR:CD2	1:C:184:PHE:CE1	2.34	1.14
1:C:294:LYS:O	1:C:296:PRO:CD	1.96	1.14
1:C:297:VAL:HB	1:C:336:VAL:O	1.47	1.14
1:A:101:PRO:HG3	1:A:217:TYR:CE2	1.83	1.13
1:A:105:THR:OG1	1:A:211:LYS:HD3	0.98	1.13
1:C:116:PHE:O	1:C:120:ILE:HG21	1.46	1.13
1:A:138:TYR:CG	1:A:184:PHE:HE1	1.56	1.13
1:B:179:VAL:HG11	1:B:181:TRP:NE1	1.61	1.13
1:C:277:ASP:CA	1:C:334:LYS:HD2	1.77	1.13
1:C:201:ILE:CB	1:C:281:LEU:HD21	1.76	1.13
1:C:112:GLU:H	1:C:350:ARG:CZ	1.59	1.13
1:A:313:GLU:HG3	1:A:318:SER:HB2	1.29	1.13
1:C:101:PRO:CD	1:C:166:LEU:HD12	1.73	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:O	1:A:296:PRO:CD	1.96	1.13
1:B:149:LYS:HD3	1:B:170:TYR:OH	1.43	1.13
1:A:295:ALA:N	1:A:316:ALA:HA	1.51	1.13
1:C:101:PRO:HG3	1:C:217:TYR:CE2	1.83	1.13
1:A:101:PRO:CD	1:A:166:LEU:HD12	1.73	1.12
1:A:86:GLY:HA2	1:A:234:TYR:CD1	1.83	1.12
1:B:105:THR:OG1	1:B:211:LYS:HD3	0.98	1.12
1:B:297:VAL:HB	1:B:336:VAL:O	1.47	1.13
1:C:107:VAL:HG21	1:C:329:ARG:HG2	1.17	1.12
1:C:86:GLY:HA2	1:C:234:TYR:CD1	1.83	1.12
1:A:297:VAL:HB	1:A:336:VAL:O	1.47	1.12
1:B:107:VAL:HB	1:B:328:GLU:HG3	1.29	1.12
1:C:309:SER:O	1:C:322:ALA:CA	1.94	1.12
1:A:119:LEU:HD22	1:A:234:TYR:CZ	1.85	1.12
1:B:151:ALA:HA	1:B:177:SER:HB2	1.28	1.12
1:C:249:GLN:NE2	1:C:265:TRP:CE3	2.15	1.12
1:B:101:PRO:HG3	1:B:217:TYR:CE2	1.83	1.12
1:A:164:ASN:N	1:A:164:ASN:ND2	1.88	1.12
1:B:277:ASP:CA	1:B:334:LYS:HD2	1.77	1.12
1:C:101:PRO:C	1:C:102:LYS:HG3	1.57	1.12
1:B:126:TYR:CA	1:B:242:THR:HG22	1.80	1.12
1:A:126:TYR:CA	1:A:242:THR:HG22	1.80	1.12
1:C:326:VAL:HG12	1:C:327:ALA:N	1.60	1.12
1:A:101:PRO:HD2	1:A:166:LEU:CD1	1.68	1.12
1:C:164:ASN:ND2	1:C:164:ASN:N	1.88	1.12
1:C:301:GLU:O	1:C:333:VAL:HG13	1.50	1.12
1:C:265:TRP:HZ3	1:C:348:ALA:O	1.20	1.12
1:B:294:LYS:O	1:B:296:PRO:CD	1.96	1.12
1:B:101:PRO:O	1:B:102:LYS:HG3	0.95	1.11
1:B:119:LEU:HD22	1:B:234:TYR:CZ	1.85	1.11
1:B:301:GLU:O	1:B:333:VAL:HG13	1.50	1.11
1:B:265:TRP:HZ3	1:B:348:ALA:O	1.20	1.11
1:B:164:ASN:ND2	1:B:164:ASN:N	1.88	1.11
1:A:301:GLU:O	1:A:333:VAL:HG13	1.50	1.11
1:A:327:ALA:HB3	1:A:331:GLN:OE1	1.48	1.11
1:C:198:ALA:CB	1:C:200:GLY:O	1.97	1.11
1:C:91:THR:CG2	1:C:325:LYS:HE2	1.72	1.11
1:B:198:ALA:CB	1:B:200:GLY:O	1.97	1.11
1:C:101:PRO:O	1:C:102:LYS:HG3	0.95	1.11
1:C:295:ALA:H	1:C:316:ALA:CA	1.63	1.11
1:A:120:ILE:HG12	1:A:350:ARG:CZ	1.79	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:CA	1:C:242:THR:HG22	1.80	1.11
1:C:313:GLU:HG3	1:C:318:SER:HB2	1.28	1.10
1:A:101:PRO:O	1:A:102:LYS:HG3	0.95	1.10
1:A:295:ALA:H	1:A:316:ALA:CA	1.63	1.10
1:B:138:TYR:CG	1:B:184:PHE:HE1	1.56	1.10
1:B:313:GLU:HG3	1:B:318:SER:HB2	1.28	1.10
1:B:326:VAL:HG12	1:B:327:ALA:N	1.60	1.10
1:C:151:ALA:HA	1:C:177:SER:HB2	1.28	1.10
1:C:164:ASN:N	1:C:164:ASN:HD22	1.19	1.10
1:C:119:LEU:HD22	1:C:234:TYR:CZ	1.85	1.10
1:C:326:VAL:CG1	1:C:327:ALA:H	1.54	1.10
1:A:198:ALA:CB	1:A:200:GLY:O	1.97	1.10
1:C:201:ILE:CA	1:C:281:LEU:CD2	2.28	1.10
1:A:315:ALA:CB	1:A:318:SER:HB3	1.82	1.10
1:C:116:PHE:O	1:C:120:ILE:CG2	2.00	1.10
1:C:315:ALA:CB	1:C:318:SER:HB3	1.82	1.10
1:C:80:ASP:CA	1:C:241:ARG:NH2	2.10	1.10
1:B:295:ALA:H	1:B:316:ALA:CA	1.63	1.09
1:A:86:GLY:CA	1:A:234:TYR:CD1	2.34	1.09
1:C:101:PRO:HD2	1:C:166:LEU:CD1	1.68	1.09
1:C:86:GLY:CA	1:C:234:TYR:CD1	2.34	1.09
1:A:265:TRP:HZ3	1:A:348:ALA:O	1.20	1.09
1:C:69:VAL:HG12	1:C:70:SER:H	1.09	1.09
1:C:249:GLN:HB3	1:C:265:TRP:HZ3	1.17	1.09
1:B:149:LYS:HD2	1:B:170:TYR:OH	1.44	1.09
1:B:86:GLY:CA	1:B:234:TYR:CD1	2.34	1.09
1:A:149:LYS:CG	1:A:177:SER:OG	2.01	1.09
1:B:149:LYS:CG	1:B:177:SER:OG	2.01	1.09
1:C:179:VAL:CG2	1:C:180:PRO:HD2	1.83	1.09
1:A:315:ALA:HB1	1:A:318:SER:H	1.16	1.09
1:B:278:CYS:HB3	1:B:333:VAL:O	1.52	1.09
1:C:160:LYS:HG3	1:C:161:PRO:HD2	1.11	1.09
1:C:107:VAL:HG13	1:C:329:ARG:HE	0.92	1.09
1:B:297:VAL:HB	1:B:336:VAL:HG13	1.26	1.09
1:C:149:LYS:HD2	1:C:170:TYR:OH	1.44	1.08
1:B:116:PHE:O	1:B:120:ILE:CG2	2.00	1.08
1:B:315:ALA:CB	1:B:318:SER:HB3	1.82	1.08
1:C:134:LEU:HD21	1:C:188:VAL:HG21	1.08	1.08
1:C:71:THR:HG21	1:C:87:SER:OG	0.92	1.08
1:B:288:LEU:HD11	1:B:290:LEU:CG	1.84	1.08
1:C:107:VAL:CG2	1:C:283:THR:OG1	2.01	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ALA:HB1	1:C:318:SER:N	1.67	1.08
1:C:297:VAL:HB	1:C:336:VAL:HG13	1.27	1.08
1:A:288:LEU:HD11	1:A:290:LEU:CG	1.84	1.08
1:C:130:ARG:HD3	1:C:237:GLN:CA	1.83	1.08
1:A:315:ALA:HB1	1:A:318:SER:N	1.67	1.08
1:C:113:PRO:CB	1:C:351:ILE:O	2.01	1.08
1:A:315:ALA:HB2	1:A:318:SER:HB3	1.36	1.08
1:C:244:SER:O	1:C:245:THR:HG22	1.54	1.08
1:C:160:LYS:O	1:C:328:GLU:OE2	1.72	1.08
1:B:248:ALA:HA	1:B:265:TRP:CG	1.64	1.08
1:B:249:GLN:HB3	1:B:265:TRP:HZ3	1.17	1.08
1:B:255:GLY:HA2	1:B:342:PRO:HB3	1.33	1.08
1:A:151:ALA:HA	1:A:177:SER:HB2	1.28	1.07
1:B:101:PRO:CD	1:B:166:LEU:HD12	1.73	1.07
1:C:327:ALA:N	1:C:331:GLN:OE1	1.87	1.07
1:A:149:LYS:HD2	1:A:170:TYR:OH	1.44	1.07
1:A:179:VAL:CG2	1:A:180:PRO:HD2	1.83	1.07
1:A:130:ARG:HD3	1:A:237:GLN:CA	1.84	1.07
1:C:149:LYS:CG	1:C:177:SER:OG	2.01	1.07
1:A:297:VAL:HB	1:A:336:VAL:HG13	1.26	1.07
1:A:116:PHE:O	1:A:120:ILE:CG2	2.00	1.07
1:B:179:VAL:CG2	1:B:180:PRO:HD2	1.83	1.07
1:C:172:ILE:O	1:C:173:GLU:O	1.72	1.07
1:A:127:GLU:OE2	1:C:155:ASP:OD1	1.71	1.07
1:B:315:ALA:HB1	1:B:318:SER:N	1.67	1.07
1:B:327:ALA:N	1:B:331:GLN:OE1	1.87	1.07
1:C:130:ARG:HB2	1:C:237:GLN:HB3	1.07	1.07
1:B:156:ARG:O	1:B:210:GLY:CA	2.03	1.07
1:A:156:ARG:O	1:A:210:GLY:CA	2.03	1.07
1:A:244:SER:O	1:A:245:THR:HG22	1.54	1.07
1:C:296:PRO:CG	1:C:337:THR:CG2	1.76	1.07
1:A:86:GLY:HA2	1:A:234:TYR:CE1	1.90	1.07
1:C:69:VAL:HG12	1:C:70:SER:N	1.66	1.07
1:B:125:GLN:HA	1:B:243:GLY:HA2	1.37	1.06
1:B:86:GLY:HA2	1:B:234:TYR:CE1	1.90	1.06
1:C:152:LEU:HD22	1:C:186:LEU:CD1	1.85	1.06
1:A:172:ILE:O	1:A:173:GLU:O	1.72	1.06
1:A:125:GLN:HA	1:A:243:GLY:HA2	1.36	1.06
1:A:278:CYS:HB3	1:A:333:VAL:O	1.53	1.06
1:B:244:SER:O	1:B:245:THR:HG22	1.54	1.06
1:C:288:LEU:HD11	1:C:290:LEU:CG	1.84	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:HD3	1:B:237:GLN:CA	1.84	1.06
1:B:166:LEU:O	1:B:169:LEU:N	1.88	1.06
1:C:278:CYS:HB3	1:C:333:VAL:O	1.53	1.06
1:A:166:LEU:O	1:A:169:LEU:N	1.88	1.06
1:A:252:ASP:OD2	1:A:345:LYS:HE2	1.55	1.06
1:B:101:PRO:HD2	1:B:166:LEU:CD1	1.68	1.06
1:C:107:VAL:CB	1:C:283:THR:HB	1.85	1.06
1:B:248:ALA:CA	1:B:265:TRP:N	2.19	1.06
1:A:114:GLY:N	1:A:283:THR:CG2	2.10	1.06
1:A:160:LYS:HG3	1:A:161:PRO:HD2	1.11	1.06
1:A:134:LEU:HD21	1:A:188:VAL:HG21	1.08	1.06
1:A:327:ALA:N	1:A:331:GLN:OE1	1.87	1.06
1:B:315:ALA:HB1	1:B:318:SER:H	1.16	1.06
1:B:86:GLY:CA	1:B:234:TYR:HD1	1.68	1.06
1:C:248:ALA:O	1:C:262:LEU:O	1.73	1.06
1:B:152:LEU:HD22	1:B:186:LEU:CD1	1.85	1.06
1:C:278:CYS:N	1:C:334:LYS:HD2	1.68	1.06
1:B:160:LYS:HG3	1:B:161:PRO:HD2	1.11	1.06
1:B:172:ILE:O	1:B:173:GLU:O	1.72	1.06
1:A:304:ASP:O	1:A:331:GLN:CB	2.03	1.06
1:C:107:VAL:CG2	1:C:329:ARG:CG	2.31	1.06
1:C:288:LEU:HD11	1:C:290:LEU:HD21	1.31	1.06
1:A:114:GLY:H	1:A:283:THR:CB	1.50	1.05
1:B:315:ALA:HB2	1:B:318:SER:HB3	1.36	1.05
1:C:86:GLY:HA2	1:C:234:TYR:CE1	1.90	1.05
1:B:339:GLU:C	1:B:340:GLU:CA	2.24	1.05
1:A:120:ILE:CD1	1:A:350:ARG:NH2	2.17	1.05
1:B:291:PHE:CB	1:B:345:LYS:O	2.03	1.05
1:C:156:ARG:O	1:C:210:GLY:CA	2.03	1.05
1:C:277:ASP:HA	1:C:334:LYS:HD2	1.35	1.05
1:C:166:LEU:O	1:C:169:LEU:N	1.88	1.05
1:C:201:ILE:CA	1:C:281:LEU:HD21	1.85	1.05
1:C:255:GLY:HA2	1:C:342:PRO:HB3	1.33	1.05
1:A:249:GLN:HB3	1:A:265:TRP:HZ3	1.17	1.05
1:C:96:ASN:OD1	1:C:216:THR:O	1.74	1.05
1:A:339:GLU:C	1:A:340:GLU:CA	2.24	1.05
1:B:304:ASP:O	1:B:331:GLN:CB	2.04	1.05
1:C:327:ALA:HB3	1:C:331:GLN:OE1	1.48	1.05
1:C:291:PHE:CB	1:C:345:LYS:O	2.03	1.05
1:C:339:GLU:C	1:C:340:GLU:CA	2.24	1.05
1:A:288:LEU:HD11	1:A:290:LEU:HD21	1.31	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PHE:CB	1:A:345:LYS:O	2.04	1.05
1:A:152:LEU:HD22	1:A:186:LEU:CD1	1.85	1.04
1:A:114:GLY:HA3	1:A:283:THR:HG21	1.35	1.04
1:A:86:GLY:CA	1:A:234:TYR:HD1	1.68	1.04
1:C:113:PRO:HB2	1:C:351:ILE:O	1.56	1.04
1:A:113:PRO:C	1:A:283:THR:HB	1.77	1.04
1:A:255:GLY:HA2	1:A:342:PRO:HB3	1.33	1.04
1:B:277:ASP:HA	1:B:334:LYS:HD2	1.34	1.04
1:A:130:ARG:HB2	1:A:237:GLN:HB3	1.07	1.04
1:B:179:VAL:CG1	1:B:181:TRP:CD1	2.40	1.04
1:C:315:ALA:HB2	1:C:318:SER:HB3	1.36	1.04
1:C:107:VAL:HG21	1:C:283:THR:OG1	1.57	1.04
1:C:252:ASP:OD2	1:C:345:LYS:HE2	1.55	1.04
1:A:149:LYS:HD3	1:A:170:TYR:OH	1.43	1.04
1:A:179:VAL:CG1	1:A:181:TRP:CD1	2.40	1.04
1:B:278:CYS:N	1:B:334:LYS:HD2	1.68	1.04
1:C:304:ASP:O	1:C:331:GLN:CB	2.04	1.04
1:A:96:ASN:OD1	1:A:216:THR:O	1.74	1.03
1:C:107:VAL:HG21	1:C:329:ARG:HG3	1.34	1.03
1:B:130:ARG:HB2	1:B:237:GLN:HB3	1.07	1.03
1:C:130:ARG:HB2	1:C:237:GLN:CB	1.88	1.03
1:B:297:VAL:HB	1:B:336:VAL:C	1.78	1.03
1:B:89:LEU:HD23	1:B:89:LEU:C	1.78	1.03
1:C:179:VAL:CG1	1:C:181:TRP:CD1	2.40	1.03
1:C:315:ALA:HB1	1:C:318:SER:H	1.16	1.03
1:B:134:LEU:HD21	1:B:188:VAL:HG21	1.08	1.03
1:B:286:PHE:HA	1:B:351:ILE:CG2	1.89	1.03
1:B:288:LEU:HD11	1:B:290:LEU:HD21	1.31	1.03
1:C:297:VAL:HB	1:C:336:VAL:C	1.78	1.03
1:A:308:PHE:CE2	1:A:310:VAL:CG2	2.42	1.03
1:A:89:LEU:C	1:A:89:LEU:HD23	1.78	1.03
1:B:252:ASP:OD2	1:B:345:LYS:HE2	1.55	1.03
1:A:278:CYS:N	1:A:334:LYS:HD2	1.68	1.03
1:B:96:ASN:OD1	1:B:216:THR:O	1.74	1.03
1:C:201:ILE:HA	1:C:281:LEU:CD2	1.87	1.03
1:A:157:ASP:CB	1:B:127:GLU:OE1	2.06	1.03
1:C:290:LEU:HD22	1:C:346:TRP:HB2	1.41	1.03
1:A:286:PHE:HA	1:A:351:ILE:CG2	1.89	1.03
1:C:107:VAL:HG11	1:C:329:ARG:NE	1.69	1.03
1:B:119:LEU:HD22	1:B:234:TYR:OH	0.86	1.02
1:C:119:LEU:HD22	1:C:234:TYR:OH	0.86	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:HD23	1:C:89:LEU:C	1.78	1.02
1:B:308:PHE:CE2	1:B:310:VAL:CG2	2.42	1.02
1:C:254:ALA:O	1:C:256:VAL:N	1.91	1.02
1:A:119:LEU:HD22	1:A:234:TYR:OH	0.86	1.02
1:A:149:LYS:HD3	1:A:170:TYR:HH	0.91	1.02
1:B:327:ALA:HB3	1:B:331:GLN:OE1	1.48	1.02
1:B:120:ILE:HG13	1:B:350:ARG:HE	1.23	1.02
1:C:86:GLY:CA	1:C:234:TYR:HD1	1.68	1.02
1:C:107:VAL:H	1:C:283:THR:CG2	1.72	1.02
1:B:246:SER:HB3	1:B:263:VAL:HG11	1.07	1.02
1:B:246:SER:CB	1:B:263:VAL:HG11	1.90	1.02
1:B:296:PRO:CG	1:B:337:THR:CG2	1.76	1.02
1:A:297:VAL:HB	1:A:336:VAL:C	1.78	1.02
1:B:254:ALA:O	1:B:256:VAL:N	1.91	1.02
1:C:149:LYS:HD3	1:C:170:TYR:HH	0.88	1.02
1:C:308:PHE:CE2	1:C:310:VAL:CG2	2.42	1.02
1:A:254:ALA:O	1:A:256:VAL:N	1.91	1.02
1:C:149:LYS:CD	1:C:170:TYR:HH	1.59	1.02
1:A:130:ARG:HB2	1:A:237:GLN:CB	1.88	1.02
1:B:326:VAL:HG12	1:B:327:ALA:H	1.18	1.02
1:C:326:VAL:HG12	1:C:327:ALA:H	1.18	1.02
1:A:278:CYS:N	1:A:334:LYS:HD3	1.72	1.01
1:C:286:PHE:HA	1:C:351:ILE:CG2	1.89	1.01
1:B:278:CYS:N	1:B:334:LYS:HD3	1.71	1.01
1:C:338:THR:OG1	1:C:339:GLU:HB2	1.60	1.01
1:B:290:LEU:HD22	1:B:346:TRP:HB2	1.41	1.01
1:A:134:LEU:CD2	1:A:188:VAL:HG21	1.91	1.01
1:A:86:GLY:N	1:A:234:TYR:CD1	2.29	1.01
1:C:85:SER:HA	1:C:234:TYR:O	1.60	1.01
1:B:86:GLY:N	1:B:234:TYR:CD1	2.29	1.01
1:C:68:GLU:OE2	1:C:137:ARG:NH2	1.94	1.01
1:C:165:ASP:O	1:C:168:SER:CB	2.07	1.01
1:B:165:ASP:O	1:B:168:SER:CB	2.07	1.01
1:C:135:ARG:HG3	1:C:233:GLU:HB3	1.43	1.01
1:B:134:LEU:HD21	1:B:188:VAL:CG2	1.91	1.01
1:C:86:GLY:N	1:C:234:TYR:CD1	2.29	1.01
1:A:277:ASP:HA	1:A:334:LYS:HD2	1.35	1.01
1:A:165:ASP:O	1:A:168:SER:CB	2.07	1.01
1:B:130:ARG:HB2	1:B:237:GLN:CB	1.88	1.00
1:C:278:CYS:N	1:C:334:LYS:HD3	1.71	1.00
1:A:326:VAL:HG12	1:A:327:ALA:H	1.18	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:CD2	1:B:188:VAL:HG21	1.91	1.00
1:B:269:LYS:C	1:B:277:ASP:HB3	1.82	1.00
1:A:133:SER:O	1:A:234:TYR:CA	2.09	1.00
1:C:253:PHE:HA	1:C:258:ASP:HA	1.44	1.00
1:A:338:THR:OG1	1:A:339:GLU:HB2	1.60	1.00
1:B:120:ILE:CD1	1:B:283:THR:C	2.21	1.00
1:C:133:SER:O	1:C:234:TYR:CA	2.09	1.00
1:C:278:CYS:H	1:C:334:LYS:HE2	1.27	1.00
1:A:249:GLN:HB3	1:A:265:TRP:CZ3	1.97	1.00
1:A:203:ASP:CG	1:A:205:LYS:HD3	1.81	1.00
1:A:134:LEU:HD21	1:A:188:VAL:CG2	1.91	1.00
1:B:246:SER:HB3	1:B:263:VAL:HG12	1.44	1.00
1:C:125:GLN:HA	1:C:243:GLY:HA2	1.37	1.00
1:B:338:THR:OG1	1:B:339:GLU:HB2	1.60	1.00
1:A:185:ILE:CD1	1:A:186:LEU:N	2.05	1.00
1:B:278:CYS:N	1:B:334:LYS:CE	2.20	1.00
1:A:253:PHE:HA	1:A:258:ASP:HA	1.44	0.99
1:B:133:SER:O	1:B:234:TYR:CA	2.09	0.99
1:B:253:PHE:HA	1:B:258:ASP:HA	1.44	0.99
1:B:120:ILE:CG1	1:B:350:ARG:HE	1.74	0.99
1:B:249:GLN:HB3	1:B:265:TRP:CZ3	1.97	0.99
1:A:101:PRO:HG3	1:A:217:TYR:HE2	1.28	0.99
1:A:308:PHE:CE2	1:A:310:VAL:HG23	1.97	0.99
1:B:308:PHE:CE2	1:B:310:VAL:HG23	1.97	0.99
1:C:308:PHE:CE2	1:C:310:VAL:HG23	1.97	0.99
1:C:79:ARG:O	1:C:80:ASP:HB2	1.61	0.99
1:B:101:PRO:HG3	1:B:217:TYR:HE2	1.28	0.99
1:B:85:SER:HA	1:B:234:TYR:O	1.60	0.99
1:B:278:CYS:N	1:B:334:LYS:HE2	1.78	0.99
1:C:297:VAL:CB	1:C:336:VAL:HG13	1.41	0.99
1:B:203:ASP:CG	1:B:205:LYS:HD3	1.81	0.99
1:C:152:LEU:HD22	1:C:186:LEU:HD13	1.45	0.99
1:C:134:LEU:CD2	1:C:188:VAL:HG21	1.91	0.99
1:A:297:VAL:CB	1:A:336:VAL:HG13	1.41	0.99
1:A:152:LEU:HD22	1:A:186:LEU:HD13	1.45	0.98
1:A:252:ASP:CG	1:A:345:LYS:HG2	1.84	0.98
1:A:269:LYS:HG2	1:A:270:GLY:N	1.75	0.98
1:B:152:LEU:HD22	1:B:186:LEU:HD13	1.45	0.98
1:A:85:SER:HA	1:A:234:TYR:O	1.60	0.98
1:B:278:CYS:H	1:B:334:LYS:HD3	1.25	0.98
1:B:278:CYS:H	1:B:334:LYS:HE2	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLN:HB3	1:C:265:TRP:CZ3	1.97	0.98
1:A:174:GLY:C	1:A:175:CYS:SG	2.42	0.98
1:B:174:GLY:C	1:B:175:CYS:SG	2.42	0.98
1:C:134:LEU:HD21	1:C:188:VAL:CG2	1.91	0.98
1:B:160:LYS:HG3	1:B:161:PRO:CD	1.93	0.98
1:A:269:LYS:C	1:A:277:ASP:HB3	1.82	0.98
1:B:252:ASP:CG	1:B:345:LYS:HG2	1.84	0.98
1:A:277:ASP:C	1:A:334:LYS:HD2	1.84	0.98
1:B:277:ASP:C	1:B:334:LYS:HD2	1.84	0.98
1:A:290:LEU:HD22	1:A:346:TRP:HB2	1.41	0.98
1:C:160:LYS:HG3	1:C:161:PRO:CD	1.93	0.98
1:A:135:ARG:HG3	1:A:233:GLU:HB3	1.43	0.98
1:A:296:PRO:CG	1:A:337:THR:CG2	1.76	0.98
1:B:179:VAL:HG23	1:B:180:PRO:HD2	1.46	0.98
1:C:269:LYS:C	1:C:277:ASP:HB3	1.82	0.98
1:A:160:LYS:HG3	1:A:161:PRO:CD	1.93	0.98
1:A:278:CYS:H	1:A:334:LYS:HE2	1.26	0.98
1:C:185:ILE:CD1	1:C:186:LEU:N	2.05	0.98
1:C:277:ASP:C	1:C:334:LYS:HD2	1.84	0.98
1:C:278:CYS:CB	1:C:333:VAL:O	2.12	0.98
1:B:119:LEU:HD22	1:B:234:TYR:HH	1.15	0.97
1:C:252:ASP:CG	1:C:345:LYS:HG2	1.84	0.97
1:A:278:CYS:N	1:A:334:LYS:HE2	1.78	0.97
1:B:112:GLU:OE1	1:B:283:THR:OG1	1.81	0.97
1:C:143:PRO:O	1:C:146:THR:CG2	2.13	0.97
1:C:269:LYS:HG2	1:C:270:GLY:N	1.75	0.97
1:C:278:CYS:N	1:C:334:LYS:HE2	1.78	0.97
1:C:203:ASP:CG	1:C:205:LYS:HD3	1.81	0.97
1:C:290:LEU:CD2	1:C:346:TRP:HB2	1.94	0.97
1:C:77:THR:HG22	1:C:78:ALA:N	1.78	0.97
1:B:248:ALA:C	1:B:265:TRP:N	2.16	0.97
1:B:315:ALA:O	1:B:316:ALA:C	2.00	0.97
1:B:269:LYS:HG2	1:B:270:GLY:N	1.75	0.97
1:C:174:GLY:C	1:C:175:CYS:SG	2.42	0.97
1:B:135:ARG:HG3	1:B:233:GLU:HB3	1.43	0.97
1:B:105:THR:HG1	1:B:211:LYS:CD	1.69	0.97
1:B:278:CYS:CB	1:B:333:VAL:O	2.12	0.97
1:C:149:LYS:HD3	1:C:170:TYR:OH	1.43	0.97
1:A:248:ALA:CB	1:A:263:VAL:O	2.07	0.97
1:A:290:LEU:CD2	1:A:346:TRP:HB2	1.94	0.97
1:C:101:PRO:HD2	1:C:166:LEU:HD12	1.38	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LYS:NZ	1:C:221:ALA:HA	1.80	0.97
1:A:143:PRO:O	1:A:146:THR:CG2	2.13	0.96
1:A:154:PHE:CE1	1:A:155:ASP:C	2.39	0.96
1:B:143:PRO:O	1:B:146:THR:CG2	2.13	0.96
1:C:154:PHE:CE1	1:C:155:ASP:C	2.39	0.96
1:C:274:TRP:NE1	1:C:339:GLU:O	1.98	0.96
1:B:155:ASP:HB2	1:B:172:ILE:HD11	1.47	0.96
1:B:149:LYS:HD3	1:B:170:TYR:HH	1.13	0.96
1:A:155:ASP:HB2	1:A:172:ILE:HD11	1.47	0.96
1:A:326:VAL:HG12	1:A:327:ALA:O	1.65	0.96
1:C:278:CYS:H	1:C:334:LYS:HD3	1.25	0.96
1:B:274:TRP:NE1	1:B:339:GLU:O	1.98	0.96
1:A:206:LEU:O	1:A:206:LEU:HD12	1.66	0.96
1:B:291:PHE:HB2	1:B:346:TRP:HB3	1.48	0.96
1:C:150:VAL:HG12	1:C:150:VAL:O	1.65	0.96
1:A:113:PRO:O	1:A:115:THR:N	1.99	0.96
1:B:106:ALA:CA	1:B:328:GLU:OE1	2.13	0.96
1:A:179:VAL:HG23	1:A:180:PRO:HD2	1.46	0.96
1:A:350:ARG:C	1:A:351:ILE:HG22	1.86	0.96
1:B:154:PHE:CE1	1:B:155:ASP:C	2.39	0.96
1:C:113:PRO:O	1:C:115:THR:N	1.99	0.96
1:B:296:PRO:HG2	1:B:337:THR:CB	1.95	0.96
1:A:285:ASN:O	1:A:351:ILE:HG23	1.66	0.96
1:A:150:VAL:HG12	1:A:150:VAL:O	1.65	0.96
1:A:296:PRO:HG2	1:A:337:THR:CB	1.95	0.96
1:C:107:VAL:HG13	1:C:329:ARG:CZ	1.96	0.96
1:C:112:GLU:N	1:C:350:ARG:CZ	2.29	0.96
1:C:296:PRO:HG2	1:C:337:THR:CB	1.95	0.96
1:B:290:LEU:CD2	1:B:346:TRP:HB2	1.94	0.95
1:C:138:TYR:HB2	1:C:184:PHE:CE2	1.99	0.95
1:C:315:ALA:O	1:C:316:ALA:C	2.00	0.95
1:C:326:VAL:HG12	1:C:327:ALA:O	1.65	0.95
1:C:285:ASN:O	1:C:351:ILE:HG23	1.66	0.95
1:B:150:VAL:HG12	1:B:150:VAL:O	1.65	0.95
1:B:149:LYS:CB	1:B:217:TYR:HE1	1.79	0.95
1:A:149:LYS:CB	1:A:217:TYR:HE1	1.79	0.95
1:A:350:ARG:O	1:A:351:ILE:HG22	0.78	0.95
1:B:116:PHE:O	1:B:284:GLY:HA2	1.65	0.95
1:A:274:TRP:NE1	1:A:339:GLU:O	1.98	0.95
1:A:278:CYS:N	1:A:334:LYS:CE	2.20	0.95
1:A:278:CYS:CB	1:A:333:VAL:O	2.12	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:NH1	1:B:236:VAL:O	2.00	0.95
1:C:206:LEU:HD12	1:C:206:LEU:O	1.66	0.95
1:B:113:PRO:O	1:B:115:THR:N	1.99	0.95
1:C:130:ARG:CB	1:C:237:GLN:HB3	1.96	0.95
1:B:206:LEU:O	1:B:206:LEU:HD12	1.66	0.95
1:C:149:LYS:CB	1:C:217:TYR:HE1	1.79	0.95
1:C:201:ILE:CA	1:C:281:LEU:HD23	1.94	0.95
1:A:130:ARG:CB	1:A:237:GLN:HB3	1.96	0.95
1:B:285:ASN:O	1:B:351:ILE:HG23	1.66	0.95
1:C:350:ARG:O	1:C:351:ILE:HG22	0.78	0.95
1:B:246:SER:CB	1:B:263:VAL:CG1	2.44	0.95
1:B:107:VAL:H	1:B:328:GLU:CG	1.79	0.95
1:B:121:LYS:HD3	1:B:351:ILE:C	1.85	0.95
1:B:326:VAL:HG12	1:B:327:ALA:O	1.65	0.95
1:C:291:PHE:HB2	1:C:346:TRP:HB3	1.48	0.95
1:B:350:ARG:O	1:B:351:ILE:HG22	0.78	0.95
1:B:95:LYS:NZ	1:B:221:ALA:HA	1.80	0.95
1:A:86:GLY:N	1:A:234:TYR:HD1	1.62	0.95
1:A:277:ASP:OD1	1:A:334:LYS:HE2	1.67	0.95
1:C:179:VAL:HG23	1:C:180:PRO:HD2	1.46	0.95
1:A:138:TYR:HB2	1:A:184:PHE:CE2	1.99	0.94
1:A:291:PHE:HB2	1:A:346:TRP:HB3	1.48	0.94
1:B:350:ARG:C	1:B:351:ILE:HG22	1.86	0.94
1:C:107:VAL:H	1:C:283:THR:HG21	1.31	0.94
1:C:155:ASP:HB2	1:C:172:ILE:HD11	1.47	0.94
1:A:130:ARG:NH1	1:A:236:VAL:O	2.00	0.94
1:A:269:LYS:O	1:A:277:ASP:HB3	0.76	0.94
1:B:138:TYR:HB2	1:B:184:PHE:CE2	2.00	0.94
1:B:149:LYS:HB3	1:B:217:TYR:HE1	1.11	0.94
1:A:101:PRO:CG	1:A:166:LEU:CD1	2.45	0.94
1:A:95:LYS:NZ	1:A:221:ALA:HA	1.80	0.94
1:B:277:ASP:OD1	1:B:334:LYS:HE2	1.67	0.94
1:C:101:PRO:HG3	1:C:217:TYR:HE2	1.28	0.94
1:C:91:THR:CG2	1:C:325:LYS:NZ	2.28	0.94
1:B:185:ILE:CD1	1:B:186:LEU:N	2.05	0.94
1:B:141:MET:HG3	1:B:141:MET:O	1.66	0.94
1:B:269:LYS:O	1:B:277:ASP:HB3	0.76	0.94
1:B:130:ARG:CB	1:B:237:GLN:HB3	1.96	0.94
1:C:350:ARG:C	1:C:351:ILE:HG22	1.86	0.94
1:B:101:PRO:CG	1:B:166:LEU:CD1	2.45	0.94
1:C:130:ARG:NH1	1:C:236:VAL:O	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:VAL:CG1	1:B:327:ALA:N	2.19	0.94
1:B:338:THR:OG1	1:B:339:GLU:N	1.94	0.94
1:A:199:ASP:OD2	1:C:157:ASP:OD2	1.85	0.94
1:B:315:ALA:CB	1:B:318:SER:CB	2.46	0.94
1:C:277:ASP:OD1	1:C:334:LYS:HE2	1.67	0.94
1:A:248:ALA:HB3	1:A:263:VAL:O	1.10	0.94
1:B:95:LYS:HZ3	1:B:225:ALA:H	1.17	0.93
1:B:89:LEU:CD2	1:B:89:LEU:C	2.37	0.93
1:A:105:THR:HG1	1:A:211:LYS:CD	1.70	0.93
1:C:269:LYS:O	1:C:277:ASP:HB3	0.76	0.93
1:C:120:ILE:CB	1:C:350:ARG:NH1	2.32	0.93
1:C:89:LEU:CD2	1:C:89:LEU:C	2.37	0.93
1:B:163:PRO:CA	1:B:164:ASN:HD22	1.82	0.93
1:A:149:LYS:HB3	1:A:217:TYR:HE1	1.11	0.93
1:C:101:PRO:CG	1:C:166:LEU:CD1	2.46	0.93
1:A:124:ALA:HB1	1:A:245:THR:HG22	1.51	0.93
1:B:124:ALA:HB1	1:B:245:THR:HG22	1.51	0.93
1:B:289:THR:HG23	1:B:321:TRP:CE3	2.03	0.93
1:B:82:ILE:HD11	1:B:122:GLU:OE2	1.69	0.93
1:B:154:PHE:HB2	1:B:212:LEU:CD1	1.99	0.93
1:C:265:TRP:O	1:C:281:LEU:N	2.02	0.93
1:C:141:MET:HG3	1:C:141:MET:O	1.66	0.93
1:A:160:LYS:CD	1:B:199:ASP:HB2	1.98	0.93
1:C:289:THR:HG23	1:C:321:TRP:CE3	2.03	0.93
1:B:246:SER:OG	1:B:265:TRP:CZ2	2.04	0.93
1:B:265:TRP:O	1:B:281:LEU:N	2.02	0.93
1:A:141:MET:HG3	1:A:141:MET:O	1.66	0.93
1:C:154:PHE:HB2	1:C:212:LEU:CD1	1.99	0.93
1:A:315:ALA:CB	1:A:318:SER:CB	2.46	0.92
1:A:82:ILE:HD11	1:A:122:GLU:OE2	1.69	0.92
1:B:86:GLY:N	1:B:234:TYR:HD1	1.63	0.92
1:A:265:TRP:O	1:A:281:LEU:N	2.02	0.92
1:A:157:ASP:HB2	1:B:127:GLU:OE1	1.67	0.92
1:A:119:LEU:HD22	1:A:234:TYR:HH	1.11	0.92
1:C:333:VAL:O	1:C:334:LYS:CD	2.18	0.92
1:C:86:GLY:N	1:C:234:TYR:HD1	1.63	0.92
1:A:154:PHE:HB2	1:A:212:LEU:CD1	1.99	0.92
1:C:82:ILE:HD11	1:C:122:GLU:OE2	1.69	0.92
1:A:338:THR:OG1	1:A:339:GLU:N	1.94	0.92
1:B:333:VAL:O	1:B:334:LYS:CD	2.18	0.92
1:C:107:VAL:CB	1:C:283:THR:CB	2.45	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ALA:CB	1:C:318:SER:CB	2.46	0.92
1:A:278:CYS:H	1:A:334:LYS:HD3	1.25	0.92
1:A:285:ASN:O	1:A:351:ILE:CG2	2.18	0.92
1:B:163:PRO:C	1:B:164:ASN:HD22	1.73	0.92
1:C:107:VAL:HB	1:C:283:THR:HB	0.93	0.92
1:B:296:PRO:CB	1:B:337:THR:HG22	2.00	0.92
1:C:294:LYS:C	1:C:296:PRO:HD3	1.90	0.92
1:C:342:PRO:O	1:C:343:LYS:HD3	1.70	0.92
1:C:149:LYS:HB3	1:C:217:TYR:HE1	1.11	0.92
1:C:120:ILE:HB	1:C:350:ARG:HH11	1.34	0.92
1:A:163:PRO:C	1:A:164:ASN:HD22	1.73	0.91
1:A:289:THR:HG23	1:A:321:TRP:CE3	2.03	0.91
1:A:89:LEU:C	1:A:89:LEU:CD2	2.37	0.91
1:B:285:ASN:O	1:B:351:ILE:CG2	2.17	0.91
1:C:120:ILE:HD13	1:C:350:ARG:HD3	1.50	0.91
1:C:126:TYR:HA	1:C:242:THR:HG22	1.50	0.91
1:A:163:PRO:CA	1:A:164:ASN:HD22	1.82	0.91
1:A:315:ALA:O	1:A:316:ALA:C	2.00	0.91
1:B:150:VAL:O	1:B:150:VAL:CG1	2.18	0.91
1:B:294:LYS:C	1:B:296:PRO:HD3	1.90	0.91
1:A:157:ASP:HB3	1:B:127:GLU:OE1	1.69	0.91
1:C:163:PRO:CA	1:C:164:ASN:HD22	1.82	0.91
1:C:296:PRO:CB	1:C:337:THR:HG22	2.00	0.91
1:A:286:PHE:HA	1:A:351:ILE:HG22	1.52	0.91
1:C:83:THR:HG22	1:C:84:ARG:H	1.34	0.91
1:A:126:TYR:HA	1:A:242:THR:HG22	1.50	0.91
1:A:130:ARG:HD3	1:A:237:GLN:N	1.84	0.91
1:C:163:PRO:C	1:C:164:ASN:HD22	1.73	0.91
1:C:338:THR:OG1	1:C:339:GLU:N	1.94	0.91
1:A:294:LYS:C	1:A:296:PRO:HD3	1.90	0.91
1:A:313:GLU:CG	1:A:318:SER:CB	2.49	0.91
1:C:124:ALA:HB1	1:C:245:THR:HG22	1.51	0.91
1:C:143:PRO:O	1:C:146:THR:HG23	1.71	0.91
1:C:112:GLU:N	1:C:350:ARG:NH2	2.17	0.91
1:B:130:ARG:HD3	1:B:237:GLN:N	1.84	0.91
1:C:313:GLU:CG	1:C:318:SER:CB	2.49	0.91
1:A:126:TYR:N	1:A:242:THR:HG22	1.86	0.91
1:A:83:THR:HG22	1:A:84:ARG:H	1.34	0.91
1:C:113:PRO:C	1:C:115:THR:H	1.74	0.91
1:C:134:LEU:HA	1:C:233:GLU:O	0.73	0.91
1:C:285:ASN:O	1:C:351:ILE:CG2	2.17	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:PRO:O	1:A:343:LYS:HD3	1.70	0.91
1:B:313:GLU:CG	1:B:318:SER:CB	2.49	0.91
1:A:333:VAL:O	1:A:334:LYS:CD	2.18	0.90
1:B:277:ASP:HA	1:B:334:LYS:CD	2.02	0.90
1:C:119:LEU:HD22	1:C:234:TYR:HH	1.29	0.90
1:C:130:ARG:HD3	1:C:237:GLN:N	1.84	0.90
1:A:143:PRO:O	1:A:146:THR:HG23	1.71	0.90
1:B:120:ILE:HD12	1:B:283:THR:O	0.73	0.90
1:B:164:ASN:ND2	1:B:164:ASN:H	1.47	0.90
1:C:201:ILE:HA	1:C:281:LEU:HD21	1.49	0.90
1:B:296:PRO:CD	1:B:337:THR:HG22	2.01	0.90
1:B:342:PRO:O	1:B:343:LYS:HD3	1.70	0.90
1:B:126:TYR:HA	1:B:242:THR:HG22	1.50	0.90
1:C:130:ARG:HH11	1:C:237:GLN:HA	1.36	0.90
1:A:134:LEU:HA	1:A:233:GLU:O	0.73	0.90
1:A:134:LEU:CD2	1:A:188:VAL:CG2	2.49	0.90
1:A:308:PHE:HE2	1:A:310:VAL:HG21	1.34	0.90
1:A:296:PRO:CB	1:A:337:THR:HG22	2.00	0.90
1:A:277:ASP:HA	1:A:334:LYS:CD	2.02	0.90
1:B:300:LEU:HG	1:B:308:PHE:CZ	2.06	0.90
1:C:264:SER:C	1:C:265:TRP:CA	2.40	0.90
1:A:296:PRO:CD	1:A:337:THR:HG22	2.01	0.90
1:B:83:THR:HG22	1:B:84:ARG:H	1.34	0.90
1:B:134:LEU:HA	1:B:233:GLU:O	0.73	0.90
1:C:134:LEU:CD2	1:C:188:VAL:CG2	2.49	0.90
1:A:95:LYS:NZ	1:A:221:ALA:CA	2.35	0.90
1:B:113:PRO:C	1:B:115:THR:H	1.74	0.90
1:C:164:ASN:ND2	1:C:164:ASN:H	1.47	0.90
1:C:126:TYR:N	1:C:242:THR:HG22	1.86	0.90
1:C:245:THR:CB	1:C:263:VAL:HG21	2.01	0.90
1:C:300:LEU:HG	1:C:308:PHE:CZ	2.06	0.90
1:C:308:PHE:HE2	1:C:310:VAL:HG21	1.34	0.90
1:C:113:PRO:HB3	1:C:351:ILE:O	1.70	0.90
1:A:296:PRO:HG2	1:A:337:THR:HG21	1.51	0.90
1:B:115:THR:O	1:B:116:PHE:HD1	1.48	0.89
1:C:274:TRP:CD1	1:C:339:GLU:O	2.25	0.89
1:B:89:LEU:CD2	1:B:89:LEU:O	2.20	0.89
1:A:186:LEU:HD23	1:A:187:THR:N	1.87	0.89
1:A:304:ASP:OD2	1:A:331:GLN:HA	1.73	0.89
1:B:186:LEU:HD23	1:B:187:THR:N	1.87	0.89
1:C:150:VAL:CG1	1:C:150:VAL:O	2.18	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:CB	1:B:265:TRP:CZ3	2.56	0.89
1:B:203:ASP:OD1	1:B:205:LYS:HD3	0.71	0.89
1:A:249:GLN:CB	1:A:265:TRP:CZ3	2.56	0.89
1:A:130:ARG:HH11	1:A:237:GLN:HA	1.36	0.89
1:A:164:ASN:ND2	1:A:164:ASN:H	1.47	0.89
1:B:130:ARG:HH11	1:B:237:GLN:HA	1.36	0.89
1:C:304:ASP:OD2	1:C:331:GLN:HA	1.72	0.89
1:C:277:ASP:HA	1:C:334:LYS:CD	2.02	0.89
1:C:89:LEU:O	1:C:89:LEU:CD2	2.20	0.89
1:A:264:SER:C	1:A:265:TRP:CA	2.40	0.89
1:C:203:ASP:OD1	1:C:205:LYS:HD3	0.71	0.89
1:A:203:ASP:OD1	1:A:205:LYS:HD3	0.71	0.89
1:A:89:LEU:CD2	1:A:89:LEU:O	2.20	0.89
1:B:126:TYR:N	1:B:242:THR:HG22	1.86	0.89
1:C:201:ILE:CG1	1:C:281:LEU:HD21	2.02	0.89
1:C:286:PHE:HA	1:C:351:ILE:HG22	1.52	0.89
1:A:150:VAL:O	1:A:150:VAL:CG1	2.18	0.89
1:C:95:LYS:NZ	1:C:221:ALA:CA	2.35	0.89
1:B:248:ALA:HB1	1:B:265:TRP:H	1.00	0.89
1:C:130:ARG:HD3	1:C:237:GLN:HB2	0.97	0.89
1:C:107:VAL:HG22	1:C:329:ARG:HG3	1.55	0.89
1:C:244:SER:O	1:C:245:THR:CG2	2.21	0.89
1:C:201:ILE:HB	1:C:281:LEU:HD22	1.54	0.88
1:B:274:TRP:CD1	1:B:339:GLU:O	2.26	0.88
1:B:154:PHE:HB2	1:B:212:LEU:HD12	1.56	0.88
1:A:90:ILE:HD11	1:A:232:VAL:HG23	1.53	0.88
1:C:249:GLN:CB	1:C:265:TRP:CZ3	2.56	0.88
1:C:120:ILE:HD13	1:C:350:ARG:CD	2.02	0.88
1:C:296:PRO:CD	1:C:337:THR:HG22	2.01	0.88
1:A:300:LEU:HG	1:A:308:PHE:CZ	2.07	0.88
1:A:154:PHE:HB2	1:A:212:LEU:HD12	1.56	0.88
1:B:308:PHE:HE2	1:B:310:VAL:HG21	1.34	0.88
1:C:91:THR:HG1	1:C:325:LYS:HE3	1.39	0.88
1:B:264:SER:C	1:B:265:TRP:CA	2.40	0.88
1:A:244:SER:O	1:A:245:THR:CG2	2.21	0.88
1:B:143:PRO:O	1:B:146:THR:HG23	1.71	0.88
1:A:274:TRP:CD1	1:A:339:GLU:O	2.26	0.88
1:A:115:THR:O	1:A:116:PHE:HD1	1.48	0.88
1:C:186:LEU:HD23	1:C:187:THR:N	1.87	0.88
1:B:95:LYS:NZ	1:B:221:ALA:CA	2.35	0.88
1:B:130:ARG:HD3	1:B:237:GLN:HB2	0.97	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HG3	1:B:232:VAL:N	1.87	0.88
1:B:244:SER:O	1:B:245:THR:CG2	2.21	0.88
1:C:245:THR:HA	1:C:263:VAL:CG2	2.04	0.88
1:C:296:PRO:HG2	1:C:337:THR:HG21	1.51	0.88
1:B:90:ILE:HD11	1:B:232:VAL:HG23	1.53	0.87
1:C:71:THR:HG21	1:C:87:SER:CB	2.04	0.87
1:B:109:ASN:OD1	1:B:110:PRO:HD2	1.74	0.87
1:C:152:LEU:O	1:C:186:LEU:HD12	1.74	0.87
1:C:154:PHE:HB2	1:C:212:LEU:HD12	1.56	0.87
1:C:107:VAL:HG11	1:C:329:ARG:HE	1.31	0.87
1:C:231:ARG:HG3	1:C:232:VAL:N	1.87	0.87
1:C:308:PHE:CE2	1:C:310:VAL:HG21	2.07	0.87
1:A:130:ARG:HD3	1:A:237:GLN:HB2	0.97	0.87
1:B:308:PHE:CE2	1:B:310:VAL:HG21	2.07	0.87
1:B:304:ASP:OD2	1:B:331:GLN:HA	1.73	0.87
1:C:90:ILE:HD11	1:C:232:VAL:HG23	1.53	0.87
1:B:134:LEU:CD2	1:B:188:VAL:CG2	2.49	0.87
1:C:115:THR:O	1:C:116:PHE:HD1	1.48	0.87
1:A:109:ASN:OD1	1:A:110:PRO:HD2	1.74	0.87
1:C:251:GLY:O	1:C:346:TRP:CD2	2.28	0.87
1:A:308:PHE:CE2	1:A:310:VAL:HG21	2.07	0.87
1:C:130:ARG:HH11	1:C:237:GLN:CA	1.88	0.87
1:A:248:ALA:HA	1:A:264:SER:O	0.97	0.87
1:A:130:ARG:HH11	1:A:237:GLN:CA	1.88	0.87
1:A:318:SER:OG	1:A:319:VAL:N	2.07	0.87
1:B:149:LYS:HG2	1:B:177:SER:HG	1.36	0.87
1:B:286:PHE:HA	1:B:351:ILE:HG22	1.52	0.87
1:C:76:SER:CB	1:C:76:SER:C	2.43	0.87
1:A:248:ALA:HB1	1:A:265:TRP:N	1.87	0.87
1:C:278:CYS:N	1:C:334:LYS:CE	2.20	0.87
1:C:68:GLU:HG2	1:C:137:ARG:HH22	1.38	0.87
1:B:264:SER:CA	1:B:265:TRP:N	2.38	0.87
1:B:251:GLY:O	1:B:346:TRP:CD2	2.28	0.86
1:B:318:SER:OG	1:B:319:VAL:N	2.07	0.86
1:A:231:ARG:HG3	1:A:232:VAL:N	1.87	0.86
1:A:95:LYS:HZ2	1:A:221:ALA:HA	1.40	0.86
1:B:134:LEU:HA	1:B:233:GLU:C	1.95	0.86
1:C:109:ASN:OD1	1:C:110:PRO:HD2	1.74	0.86
1:C:264:SER:CA	1:C:265:TRP:N	2.38	0.86
1:C:56:THR:HG23	1:C:57:ARG:N	1.89	0.86
1:B:82:ILE:HG21	1:B:238:LEU:HB2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:HA	1:C:233:GLU:C	1.94	0.86
1:A:251:GLY:O	1:A:346:TRP:CD2	2.28	0.86
1:C:130:ARG:NE	1:C:237:GLN:HB2	1.90	0.86
1:A:152:LEU:O	1:A:186:LEU:HD12	1.74	0.86
1:A:95:LYS:HZ3	1:A:225:ALA:H	1.22	0.86
1:B:101:PRO:CG	1:B:166:LEU:HD11	2.05	0.86
1:C:288:LEU:CD1	1:C:290:LEU:CD2	2.53	0.86
1:C:120:ILE:CD1	1:C:350:ARG:HD3	2.03	0.86
1:A:264:SER:CA	1:A:265:TRP:N	2.38	0.86
1:B:288:LEU:CD1	1:B:290:LEU:CD2	2.53	0.86
1:C:154:PHE:HE1	1:C:155:ASP:O	1.59	0.86
1:A:130:ARG:NE	1:A:237:GLN:HB2	1.90	0.86
1:A:82:ILE:HG21	1:A:238:LEU:HB2	1.56	0.86
1:C:318:SER:OG	1:C:319:VAL:N	2.07	0.86
1:A:125:GLN:HA	1:A:243:GLY:CA	2.06	0.86
1:A:288:LEU:HD11	1:A:290:LEU:HG	1.57	0.86
1:A:288:LEU:CD1	1:A:290:LEU:CD2	2.53	0.86
1:A:89:LEU:HD22	1:A:89:LEU:O	1.75	0.86
1:B:130:ARG:HH11	1:B:237:GLN:CA	1.88	0.86
1:C:198:ALA:C	1:C:200:GLY:H	1.77	0.86
1:C:125:GLN:HA	1:C:243:GLY:CA	2.06	0.86
1:A:154:PHE:HE1	1:A:155:ASP:O	1.59	0.85
1:C:59:SER:O	1:C:61:PRO:HD3	1.74	0.85
1:C:72:GLN:HE21	1:C:72:GLN:HA	1.38	0.85
1:C:89:LEU:HD22	1:C:89:LEU:O	1.75	0.85
1:A:113:PRO:C	1:A:115:THR:H	1.74	0.85
1:A:136:PHE:CE1	1:A:232:VAL:HG22	2.12	0.85
1:B:152:LEU:O	1:B:186:LEU:HD12	1.74	0.85
1:C:101:PRO:CG	1:C:166:LEU:HD11	2.06	0.85
1:B:130:ARG:NE	1:B:237:GLN:HB2	1.90	0.85
1:C:136:PHE:CE1	1:C:232:VAL:HG22	2.12	0.85
1:C:277:ASP:OD1	1:C:279:HIS:ND1	2.10	0.85
1:C:69:VAL:CG1	1:C:70:SER:H	1.81	0.85
1:C:90:ILE:HD11	1:C:232:VAL:HG21	1.58	0.85
1:A:138:TYR:HH	1:A:227:LEU:HB3	1.41	0.85
1:A:277:ASP:OD1	1:A:279:HIS:ND1	2.10	0.85
1:A:90:ILE:HD11	1:A:232:VAL:HG21	1.58	0.85
1:B:119:LEU:CD2	1:B:234:TYR:CE2	2.60	0.85
1:A:296:PRO:CG	1:A:337:THR:CB	2.52	0.85
1:A:315:ALA:HB1	1:A:318:SER:CB	2.07	0.85
1:B:154:PHE:HE1	1:B:155:ASP:O	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:HZ2	1:B:221:ALA:HA	1.40	0.85
1:B:277:ASP:OD1	1:B:279:HIS:ND1	2.10	0.85
1:C:179:VAL:HG22	1:C:180:PRO:HD2	1.58	0.85
1:C:107:VAL:HG23	1:C:283:THR:HG21	1.56	0.85
1:A:119:LEU:CD2	1:A:234:TYR:CE2	2.60	0.84
1:B:328:GLU:C	1:B:329:ARG:O	2.14	0.84
1:C:82:ILE:HG21	1:C:238:LEU:HB2	1.56	0.84
1:C:80:ASP:HA	1:C:241:ARG:CZ	2.07	0.84
1:B:296:PRO:CG	1:B:337:THR:CB	2.52	0.84
1:B:121:LYS:HD3	1:B:351:ILE:OXT	1.76	0.84
1:B:125:GLN:HA	1:B:243:GLY:CA	2.06	0.84
1:A:269:LYS:HG2	1:A:270:GLY:H	1.42	0.84
1:A:149:LYS:HG2	1:A:177:SER:HG	1.38	0.84
1:B:107:VAL:H	1:B:328:GLU:CD	1.79	0.84
1:C:288:LEU:HD11	1:C:290:LEU:HG	1.57	0.84
1:A:114:GLY:HA2	1:A:283:THR:HG22	1.57	0.84
1:A:198:ALA:C	1:A:200:GLY:H	1.77	0.84
1:A:130:ARG:HD2	1:A:237:GLN:HB2	0.85	0.84
1:C:107:VAL:N	1:C:283:THR:HG21	1.92	0.84
1:A:179:VAL:HG22	1:A:180:PRO:HD2	1.58	0.84
1:B:315:ALA:HB1	1:B:318:SER:CB	2.07	0.84
1:B:89:LEU:O	1:B:89:LEU:HD22	1.75	0.84
1:B:198:ALA:C	1:B:200:GLY:H	1.77	0.84
1:C:119:LEU:CD2	1:C:234:TYR:CE2	2.60	0.84
1:C:77:THR:HG22	1:C:78:ALA:H	1.37	0.84
1:A:105:THR:O	1:A:328:GLU:OE2	1.96	0.84
1:C:149:LYS:HD3	1:C:217:TYR:OH	1.78	0.84
1:C:133:SER:C	1:C:234:TYR:HA	1.99	0.84
1:C:130:ARG:HD2	1:C:237:GLN:HB2	0.85	0.84
1:C:245:THR:CA	1:C:263:VAL:HG21	2.07	0.84
1:A:315:ALA:HB1	1:A:318:SER:CA	2.08	0.84
1:A:327:ALA:CB	1:A:331:GLN:CD	2.39	0.84
1:B:179:VAL:HG22	1:B:180:PRO:HD2	1.58	0.84
1:B:149:LYS:HD3	1:B:217:TYR:OH	1.78	0.84
1:B:130:ARG:HD2	1:B:237:GLN:HB2	0.85	0.84
1:B:288:LEU:CD1	1:B:290:LEU:HD21	2.08	0.84
1:B:90:ILE:HD11	1:B:232:VAL:HG21	1.58	0.84
1:C:315:ALA:HB1	1:C:318:SER:CA	2.08	0.84
1:C:327:ALA:CA	1:C:331:GLN:OE1	2.26	0.84
1:A:130:ARG:CD	1:A:237:GLN:HB3	2.02	0.83
1:A:291:PHE:O	1:A:292:TYR:HB3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:PHE:CE1	1:B:232:VAL:HG22	2.12	0.83
1:B:288:LEU:HD21	1:B:290:LEU:HD11	1.60	0.83
1:C:288:LEU:CD1	1:C:290:LEU:HD21	2.08	0.83
1:C:328:GLU:C	1:C:329:ARG:O	2.14	0.83
1:C:296:PRO:CG	1:C:337:THR:CB	2.52	0.83
1:A:288:LEU:HD21	1:A:290:LEU:HD11	1.60	0.83
1:B:107:VAL:N	1:B:328:GLU:CD	2.29	0.83
1:C:338:THR:HG1	1:C:339:GLU:HB2	1.43	0.83
1:A:160:LYS:HD3	1:B:199:ASP:HB2	1.56	0.83
1:B:291:PHE:O	1:B:292:TYR:HB3	1.78	0.83
1:B:315:ALA:HB1	1:B:318:SER:CA	2.08	0.83
1:B:246:SER:HG	1:B:265:TRP:HH2	1.17	0.83
1:C:295:ALA:HB1	1:C:315:ALA:N	1.93	0.83
1:C:315:ALA:HB1	1:C:318:SER:CB	2.08	0.83
1:A:101:PRO:CG	1:A:166:LEU:HD11	2.06	0.83
1:A:120:ILE:CB	1:A:350:ARG:HH22	1.92	0.83
1:B:107:VAL:CB	1:B:328:GLU:HG3	1.99	0.83
1:C:95:LYS:HZ2	1:C:221:ALA:HA	1.41	0.83
1:A:327:ALA:CA	1:A:331:GLN:OE1	2.26	0.83
1:C:251:GLY:O	1:C:346:TRP:CE3	2.31	0.83
1:C:120:ILE:CB	1:C:350:ARG:HH11	1.88	0.83
1:C:288:LEU:HG	1:C:289:THR:N	1.94	0.83
1:A:119:LEU:CD2	1:A:234:TYR:CZ	2.54	0.83
1:A:251:GLY:O	1:A:346:TRP:CE3	2.31	0.83
1:A:296:PRO:CG	1:A:337:THR:HG21	2.06	0.83
1:A:300:LEU:HD11	1:A:333:VAL:CG1	2.09	0.83
1:A:277:ASP:OD1	1:A:334:LYS:CE	2.27	0.83
1:B:327:ALA:CA	1:B:331:GLN:OE1	2.26	0.83
1:B:120:ILE:HG13	1:B:350:ARG:NE	1.93	0.83
1:C:249:GLN:HE22	1:C:265:TRP:N	1.77	0.83
1:C:291:PHE:O	1:C:292:TYR:HB3	1.78	0.83
1:B:296:PRO:CG	1:B:337:THR:HG21	2.06	0.83
1:A:133:SER:C	1:A:234:TYR:HA	1.99	0.82
1:A:153:ALA:CB	1:A:174:GLY:CA	2.35	0.82
1:A:295:ALA:HB1	1:A:315:ALA:N	1.93	0.82
1:B:288:LEU:HD11	1:B:290:LEU:HG	1.58	0.82
1:B:288:LEU:HG	1:B:289:THR:N	1.94	0.82
1:C:79:ARG:O	1:C:80:ASP:CB	2.27	0.82
1:C:55:VAL:HG22	1:C:56:THR:N	1.93	0.82
1:A:170:TYR:CE1	1:A:217:TYR:OH	2.32	0.82
1:B:251:GLY:O	1:B:346:TRP:CE3	2.31	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:HG2	1:C:177:SER:HG	1.41	0.82
1:C:78:ALA:C	1:C:80:ASP:H	1.82	0.82
1:A:249:GLN:HE22	1:A:265:TRP:N	1.77	0.82
1:A:340:GLU:O	1:A:342:PRO:HD2	1.79	0.82
1:A:288:LEU:CD1	1:A:290:LEU:HD21	2.08	0.82
1:B:153:ALA:CB	1:B:174:GLY:CA	2.35	0.82
1:C:91:THR:HG21	1:C:325:LYS:HE2	0.87	0.82
1:A:149:LYS:HD3	1:A:217:TYR:OH	1.78	0.82
1:B:120:ILE:HD13	1:B:284:GLY:N	1.95	0.82
1:C:277:ASP:OD1	1:C:334:LYS:CE	2.27	0.82
1:A:249:GLN:NE2	1:A:265:TRP:HE3	1.77	0.82
1:C:66:TYR:CE2	1:C:183:GLY:HA3	2.14	0.82
1:A:152:LEU:HD22	1:A:186:LEU:HD12	1.61	0.82
1:C:249:GLN:NE2	1:C:265:TRP:HE3	1.78	0.82
1:B:277:ASP:OD1	1:B:334:LYS:CE	2.27	0.82
1:A:134:LEU:HA	1:A:233:GLU:C	1.95	0.82
1:A:95:LYS:NZ	1:A:225:ALA:N	2.28	0.82
1:B:248:ALA:CA	1:B:265:TRP:CG	2.45	0.82
1:B:169:LEU:O	1:B:172:ILE:HG22	1.80	0.82
1:B:95:LYS:NZ	1:B:225:ALA:N	2.28	0.82
1:C:288:LEU:HD21	1:C:290:LEU:HD11	1.60	0.82
1:C:300:LEU:HD11	1:C:333:VAL:CG1	2.09	0.82
1:A:90:ILE:O	1:A:90:ILE:HG22	1.78	0.81
1:B:152:LEU:HD22	1:B:186:LEU:HD12	1.61	0.81
1:C:269:LYS:HG2	1:C:270:GLY:H	1.42	0.81
1:A:285:ASN:ND2	1:A:324:VAL:O	2.13	0.81
1:A:288:LEU:HG	1:A:289:THR:N	1.94	0.81
1:B:295:ALA:HB1	1:B:315:ALA:N	1.93	0.81
1:B:300:LEU:HD11	1:B:333:VAL:CG1	2.09	0.81
1:A:126:TYR:N	1:A:242:THR:CG2	2.43	0.81
1:B:126:TYR:N	1:B:242:THR:CG2	2.43	0.81
1:B:170:TYR:CE1	1:B:217:TYR:OH	2.32	0.81
1:B:285:ASN:ND2	1:B:324:VAL:O	2.13	0.81
1:C:170:TYR:CE1	1:C:217:TYR:OH	2.32	0.81
1:A:120:ILE:CG2	1:A:350:ARG:NH2	2.43	0.81
1:A:328:GLU:C	1:A:329:ARG:O	2.14	0.81
1:B:90:ILE:O	1:B:90:ILE:HG22	1.78	0.81
1:C:296:PRO:CG	1:C:337:THR:HG21	2.06	0.81
1:A:296:PRO:HG3	1:A:337:THR:CG2	2.07	0.81
1:B:133:SER:C	1:B:234:TYR:HA	1.99	0.81
1:B:251:GLY:O	1:B:346:TRP:CE2	2.34	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:O	1:C:172:ILE:HG22	1.80	0.81
1:C:90:ILE:O	1:C:90:ILE:HG22	1.78	0.81
1:A:286:PHE:HA	1:A:351:ILE:HG21	1.61	0.81
1:B:138:TYR:C	1:B:139:SER:O	2.16	0.81
1:A:107:VAL:O	1:A:115:THR:HG21	1.81	0.81
1:A:156:ARG:NE	1:B:240:ASN:CG	2.34	0.81
1:C:249:GLN:HE22	1:C:265:TRP:H	1.29	0.81
1:C:285:ASN:ND2	1:C:324:VAL:O	2.13	0.81
1:A:169:LEU:O	1:A:172:ILE:HG22	1.80	0.81
1:B:101:PRO:CG	1:B:166:LEU:HD12	2.10	0.81
1:B:107:VAL:O	1:B:115:THR:HG21	1.81	0.81
1:B:164:ASN:H	1:B:164:ASN:HD22	0.82	0.81
1:B:128:LYS:HA	1:B:195:ARG:O	1.80	0.81
1:C:101:PRO:CG	1:C:166:LEU:HD12	2.10	0.81
1:C:152:LEU:HD22	1:C:186:LEU:HD12	1.61	0.81
1:B:96:ASN:HD21	1:B:102:LYS:HD3	1.45	0.81
1:B:90:ILE:CD1	1:B:232:VAL:CG2	2.58	0.81
1:C:128:LYS:HA	1:C:195:ARG:O	1.80	0.81
1:C:130:ARG:CD	1:C:237:GLN:HB3	2.02	0.81
1:C:130:ARG:HD2	1:C:237:GLN:HE21	1.46	0.81
1:B:340:GLU:O	1:B:342:PRO:HD2	1.80	0.81
1:B:107:VAL:H	1:B:328:GLU:CB	1.93	0.80
1:C:340:GLU:O	1:C:342:PRO:HD2	1.80	0.80
1:A:112:GLU:O	1:A:115:THR:HG22	1.81	0.80
1:C:300:LEU:HD11	1:C:333:VAL:HG12	1.63	0.80
1:C:251:GLY:O	1:C:346:TRP:CE2	2.34	0.80
1:A:101:PRO:HG3	1:A:217:TYR:CD2	2.17	0.80
1:C:107:VAL:O	1:C:115:THR:HG21	1.81	0.80
1:C:315:ALA:CB	1:C:318:SER:H	1.94	0.80
1:A:128:LYS:HA	1:A:195:ARG:O	1.80	0.80
1:A:251:GLY:O	1:A:346:TRP:CE2	2.34	0.80
1:B:174:GLY:C	1:B:175:CYS:HG	1.83	0.80
1:B:130:ARG:HD2	1:B:237:GLN:HE21	1.46	0.80
1:A:227:LEU:HD12	1:A:227:LEU:H	1.47	0.80
1:C:95:LYS:NZ	1:C:225:ALA:N	2.28	0.80
1:A:96:ASN:HD21	1:A:102:LYS:HD3	1.45	0.80
1:B:269:LYS:HG2	1:B:270:GLY:H	1.42	0.80
1:B:286:PHE:HA	1:B:351:ILE:HG21	1.61	0.80
1:C:153:ALA:CB	1:C:174:GLY:CA	2.35	0.80
1:A:248:ALA:CB	1:A:249:GLN:NE2	2.45	0.80
1:A:164:ASN:HD22	1:A:164:ASN:H	0.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:NZ	1:B:225:ALA:H	1.80	0.80
1:B:326:VAL:HG12	1:B:327:ALA:C	2.02	0.80
1:C:96:ASN:HD21	1:C:102:LYS:HD3	1.45	0.80
1:C:119:LEU:CD2	1:C:234:TYR:CZ	2.54	0.80
1:B:300:LEU:HD11	1:B:333:VAL:HG12	1.63	0.80
1:C:107:VAL:CG2	1:C:283:THR:CB	2.59	0.80
1:C:126:TYR:N	1:C:242:THR:CG2	2.43	0.80
1:A:90:ILE:CD1	1:A:232:VAL:CG2	2.58	0.80
1:B:112:GLU:O	1:B:115:THR:HG22	1.81	0.80
1:C:227:LEU:H	1:C:227:LEU:HD12	1.47	0.80
1:A:95:LYS:NZ	1:A:225:ALA:H	1.80	0.80
1:B:291:PHE:HB2	1:B:345:LYS:O	1.82	0.79
1:C:120:ILE:HB	1:C:350:ARG:HH12	1.46	0.79
1:C:296:PRO:HG3	1:C:337:THR:CG2	2.07	0.79
1:A:293:GLU:O	1:A:317:GLY:CA	2.31	0.79
1:A:300:LEU:HD11	1:A:333:VAL:HG12	1.63	0.79
1:C:112:GLU:O	1:C:115:THR:HG22	1.81	0.79
1:C:101:PRO:HG3	1:C:217:TYR:CD2	2.17	0.79
1:C:249:GLN:HB3	1:C:348:ALA:O	1.83	0.79
1:C:164:ASN:H	1:C:164:ASN:HD22	0.82	0.79
1:A:130:ARG:HD2	1:A:237:GLN:HE21	1.46	0.79
1:B:119:LEU:CD2	1:B:234:TYR:CZ	2.54	0.79
1:A:138:TYR:C	1:A:139:SER:O	2.16	0.79
1:B:101:PRO:HG3	1:B:217:TYR:CD2	2.17	0.79
1:B:293:GLU:O	1:B:317:GLY:CA	2.31	0.79
1:C:138:TYR:C	1:C:139:SER:O	2.16	0.79
1:A:300:LEU:CD1	1:A:333:VAL:HG12	2.13	0.79
1:C:293:GLU:O	1:C:317:GLY:CA	2.31	0.79
1:C:300:LEU:CD1	1:C:333:VAL:HG12	2.13	0.79
1:B:227:LEU:H	1:B:227:LEU:HD12	1.47	0.79
1:B:289:THR:O	1:B:290:LEU:HB3	1.83	0.79
1:C:326:VAL:HG12	1:C:327:ALA:C	2.02	0.79
1:A:315:ALA:CB	1:A:318:SER:H	1.94	0.79
1:B:175:CYS:HB2	1:B:176:VAL:HB	1.65	0.79
1:A:249:GLN:HB3	1:A:348:ALA:O	1.83	0.79
1:B:101:PRO:HD2	1:B:166:LEU:HD12	1.38	0.78
1:C:133:SER:HB3	1:C:235:THR:HG22	1.64	0.78
1:C:291:PHE:HB2	1:C:345:LYS:O	1.82	0.78
1:C:95:LYS:NZ	1:C:225:ALA:H	1.80	0.78
1:C:296:PRO:CD	1:C:337:THR:CG2	2.60	0.78
1:B:133:SER:HB3	1:B:235:THR:HG22	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HG12	1:A:238:LEU:HD12	1.66	0.78
1:C:133:SER:N	1:C:235:THR:HG22	1.99	0.78
1:A:101:PRO:HD2	1:A:166:LEU:HD12	1.38	0.78
1:A:169:LEU:C	1:A:169:LEU:HD23	2.04	0.78
1:B:114:GLY:HA2	1:B:326:VAL:C	1.68	0.78
1:B:169:LEU:HD23	1:B:169:LEU:C	2.04	0.78
1:B:120:ILE:HG21	1:B:284:GLY:CA	2.12	0.78
1:B:300:LEU:CD1	1:B:333:VAL:HG12	2.13	0.78
1:B:296:PRO:CD	1:B:337:THR:CG2	2.60	0.78
1:A:338:THR:HG1	1:A:339:GLU:HB2	1.46	0.78
1:A:133:SER:HB3	1:A:235:THR:HG22	1.64	0.78
1:A:326:VAL:HG12	1:A:327:ALA:C	2.02	0.78
1:B:236:VAL:HG12	1:B:238:LEU:HD12	1.66	0.78
1:C:179:VAL:HG11	1:C:181:TRP:HE1	1.49	0.78
1:C:286:PHE:HA	1:C:351:ILE:HG21	1.61	0.78
1:C:71:THR:HG21	1:C:87:SER:HG	0.95	0.78
1:C:289:THR:O	1:C:290:LEU:HB3	1.83	0.78
1:C:249:GLN:O	1:C:348:ALA:N	2.17	0.78
1:B:249:GLN:HB3	1:B:348:ALA:O	1.83	0.78
1:A:339:GLU:C	1:A:340:GLU:HA	2.04	0.78
1:B:249:GLN:O	1:B:348:ALA:N	2.17	0.78
1:C:339:GLU:C	1:C:340:GLU:HA	2.04	0.78
1:A:175:CYS:HB2	1:A:176:VAL:HB	1.65	0.78
1:B:117:ASN:O	1:B:117:ASN:ND2	2.17	0.78
1:C:105:THR:HG21	1:C:328:GLU:HB3	1.64	0.78
1:A:249:GLN:HE22	1:A:265:TRP:H	1.29	0.78
1:A:296:PRO:CD	1:A:337:THR:CG2	2.60	0.78
1:A:163:PRO:CA	1:A:164:ASN:ND2	2.47	0.78
1:A:120:ILE:HD13	1:A:350:ARG:NH2	1.97	0.78
1:B:120:ILE:HD13	1:B:284:GLY:HA3	0.81	0.78
1:C:90:ILE:CD1	1:C:232:VAL:CG2	2.58	0.78
1:C:107:VAL:CG1	1:C:329:ARG:CZ	2.60	0.78
1:C:179:VAL:CG2	1:C:180:PRO:CD	2.62	0.78
1:C:97:THR:HA	1:C:219:GLN:CA	2.14	0.78
1:A:117:ASN:ND2	1:A:117:ASN:O	2.17	0.78
1:A:199:ASP:HB2	1:C:160:LYS:HD3	1.65	0.77
1:B:135:ARG:HB2	1:B:185:ILE:HD11	1.67	0.77
1:A:134:LEU:O	1:A:134:LEU:HG	1.83	0.77
1:A:135:ARG:HB2	1:A:185:ILE:HD11	1.67	0.77
1:A:291:PHE:HB2	1:A:345:LYS:O	1.82	0.77
1:C:95:LYS:HZ3	1:C:225:ALA:H	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:O	1:B:134:LEU:HG	1.83	0.77
1:C:124:ALA:O	1:C:244:SER:N	2.18	0.77
1:B:133:SER:N	1:B:235:THR:HG22	1.99	0.77
1:B:204:PRO:C	1:B:205:LYS:HD2	2.05	0.77
1:A:156:ARG:O	1:A:158:ALA:N	2.18	0.77
1:A:249:GLN:O	1:A:348:ALA:N	2.17	0.77
1:B:163:PRO:CA	1:B:164:ASN:ND2	2.47	0.77
1:B:276:HIS:CG	1:B:277:ASP:H	2.03	0.77
1:B:339:GLU:C	1:B:340:GLU:HA	2.04	0.77
1:C:204:PRO:C	1:C:205:LYS:HD2	2.04	0.77
1:A:97:THR:HA	1:A:219:GLN:CA	2.14	0.77
1:C:160:LYS:N	1:C:328:GLU:OE2	2.18	0.77
1:C:327:ALA:CB	1:C:331:GLN:CD	2.39	0.77
1:A:204:PRO:C	1:A:205:LYS:HD2	2.05	0.77
1:C:163:PRO:CA	1:C:164:ASN:ND2	2.47	0.77
1:C:236:VAL:HG12	1:C:238:LEU:HD12	1.66	0.77
1:C:95:LYS:HZ1	1:C:225:ALA:N	1.82	0.77
1:A:160:LYS:HE2	1:B:199:ASP:OD2	1.84	0.77
1:A:251:GLY:O	1:A:346:TRP:CZ3	2.38	0.77
1:A:313:GLU:HB2	1:A:315:ALA:N	2.00	0.77
1:B:156:ARG:O	1:B:158:ALA:N	2.18	0.77
1:B:120:ILE:CD1	1:B:284:GLY:CA	2.44	0.77
1:C:97:THR:HA	1:C:218:GLY:O	1.85	0.77
1:A:105:THR:O	1:A:328:GLU:CD	2.23	0.76
1:A:101:PRO:CG	1:A:166:LEU:HD12	2.10	0.76
1:C:169:LEU:C	1:C:169:LEU:HD23	2.04	0.76
1:C:251:GLY:O	1:C:346:TRP:CZ3	2.38	0.76
1:B:315:ALA:CB	1:B:318:SER:H	1.94	0.76
1:C:117:ASN:O	1:C:117:ASN:ND2	2.17	0.76
1:C:86:GLY:CA	1:C:234:TYR:CE1	2.66	0.76
1:B:117:ASN:HA	1:B:285:ASN:N	2.01	0.76
1:B:313:GLU:HB2	1:B:315:ALA:N	2.00	0.76
1:B:315:ALA:O	1:B:317:GLY:N	2.18	0.76
1:C:313:GLU:HB2	1:C:315:ALA:N	2.00	0.76
1:A:97:THR:HA	1:A:218:GLY:O	1.85	0.76
1:A:276:HIS:CG	1:A:277:ASP:H	2.03	0.76
1:B:185:ILE:HD12	1:B:186:LEU:CA	2.16	0.76
1:B:300:LEU:CD1	1:B:333:VAL:CG1	2.64	0.76
1:C:134:LEU:HG	1:C:134:LEU:O	1.83	0.76
1:A:149:LYS:HE2	1:A:151:ALA:HA	1.66	0.76
1:A:289:THR:O	1:A:290:LEU:HB3	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:CD1	1:A:333:VAL:CG1	2.64	0.76
1:A:314:ALA:O	1:A:315:ALA:CB	2.34	0.76
1:B:114:GLY:CA	1:B:326:VAL:HG12	2.14	0.76
1:C:144:SER:C	1:C:146:THR:H	1.89	0.76
1:C:175:CYS:HB2	1:C:176:VAL:HB	1.65	0.76
1:A:133:SER:N	1:A:235:THR:HG22	1.99	0.76
1:B:109:ASN:ND2	1:B:329:ARG:NH2	2.33	0.76
1:C:156:ARG:O	1:C:158:ALA:N	2.18	0.76
1:C:109:ASN:HD21	1:C:197:VAL:HG23	1.50	0.76
1:B:97:THR:HA	1:B:219:GLN:CA	2.14	0.76
1:A:149:LYS:CB	1:A:217:TYR:CE1	2.60	0.76
1:C:135:ARG:HB2	1:C:185:ILE:HD11	1.67	0.76
1:C:105:THR:HG1	1:C:211:LYS:HD3	0.93	0.76
1:A:114:GLY:CA	1:A:283:THR:CB	2.40	0.76
1:A:315:ALA:O	1:A:317:GLY:N	2.18	0.76
1:B:310:VAL:HA	1:B:321:TRP:O	1.86	0.76
1:C:314:ALA:O	1:C:315:ALA:CB	2.34	0.76
1:A:149:LYS:HB3	1:A:217:TYR:CD1	2.20	0.75
1:B:251:GLY:O	1:B:346:TRP:CZ3	2.38	0.75
1:C:276:HIS:CG	1:C:277:ASP:H	2.03	0.75
1:C:83:THR:HG22	1:C:84:ARG:N	2.01	0.75
1:A:109:ASN:HD21	1:A:197:VAL:HG23	1.50	0.75
1:A:185:ILE:HD12	1:A:186:LEU:CA	2.16	0.75
1:A:120:ILE:HG23	1:A:350:ARG:NH2	2.01	0.75
1:C:149:LYS:HE2	1:C:151:ALA:HA	1.66	0.75
1:C:59:SER:C	1:C:61:PRO:HD3	2.06	0.75
1:A:138:TYR:O	1:A:139:SER:C	2.24	0.75
1:B:109:ASN:HD21	1:B:197:VAL:HG23	1.50	0.75
1:B:279:HIS:CA	1:B:280:PHE:N	2.50	0.75
1:C:149:LYS:HB3	1:C:217:TYR:CD1	2.20	0.75
1:C:279:HIS:CA	1:C:280:PHE:N	2.50	0.75
1:C:301:GLU:O	1:C:333:VAL:CG1	2.34	0.75
1:C:91:THR:CB	1:C:325:LYS:NZ	2.47	0.75
1:A:149:LYS:CD	1:A:170:TYR:HH	1.64	0.75
1:B:149:LYS:HE2	1:B:151:ALA:HA	1.66	0.75
1:B:314:ALA:O	1:B:315:ALA:CB	2.33	0.75
1:C:115:THR:O	1:C:116:PHE:CG	2.40	0.75
1:C:306:SER:HB3	1:C:325:LYS:HB3	1.69	0.75
1:A:179:VAL:HG11	1:A:181:TRP:HE1	1.49	0.75
1:B:138:TYR:CG	1:B:184:PHE:CZ	2.62	0.75
1:C:136:PHE:CZ	1:C:212:LEU:HD22	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PRO:HG3	1:B:337:THR:CG2	2.07	0.75
1:A:271:THR:HG21	1:A:275:GLU:OE2	1.87	0.75
1:B:97:THR:HA	1:B:218:GLY:O	1.85	0.75
1:A:144:SER:C	1:A:146:THR:H	1.89	0.75
1:A:292:TYR:HB2	1:A:318:SER:O	1.86	0.75
1:C:154:PHE:HD1	1:C:155:ASP:H	0.75	0.75
1:C:300:LEU:CD1	1:C:333:VAL:CG1	2.64	0.75
1:A:156:ARG:HD3	1:B:240:ASN:HB3	1.67	0.75
1:C:288:LEU:CD1	1:C:290:LEU:HG	2.17	0.75
1:C:277:ASP:OD1	1:C:334:LYS:NZ	2.20	0.75
1:A:130:ARG:HD2	1:A:237:GLN:HB3	1.64	0.75
1:A:310:VAL:HA	1:A:321:TRP:O	1.86	0.75
1:C:315:ALA:O	1:C:317:GLY:N	2.18	0.75
1:C:68:GLU:HG2	1:C:137:ARG:NH2	2.02	0.75
1:B:306:SER:HB3	1:B:325:LYS:HB3	1.69	0.75
1:A:127:GLU:OE1	1:C:157:ASP:CB	2.34	0.74
1:A:279:HIS:CA	1:A:280:PHE:N	2.50	0.74
1:A:289:THR:O	1:A:290:LEU:CB	2.35	0.74
1:B:277:ASP:OD1	1:B:334:LYS:NZ	2.20	0.74
1:A:115:THR:O	1:A:116:PHE:CG	2.40	0.74
1:A:174:GLY:O	1:A:175:CYS:SG	2.45	0.74
1:B:144:SER:C	1:B:146:THR:H	1.89	0.74
1:B:126:TYR:CA	1:B:242:THR:CG2	2.64	0.74
1:C:107:VAL:HG13	1:C:329:ARG:NH2	2.02	0.74
1:A:306:SER:HB3	1:A:325:LYS:HB3	1.69	0.74
1:A:83:THR:HG22	1:A:84:ARG:N	2.01	0.74
1:B:130:ARG:HD2	1:B:237:GLN:HB3	1.64	0.74
1:B:149:LYS:CB	1:B:217:TYR:CE1	2.60	0.74
1:B:241:ARG:HD2	1:B:241:ARG:N	2.03	0.74
1:C:310:VAL:HA	1:C:321:TRP:O	1.86	0.74
1:C:112:GLU:C	1:C:350:ARG:NH2	2.39	0.74
1:A:136:PHE:CD1	1:A:232:VAL:HG22	2.23	0.74
1:A:157:ASP:OD2	1:B:199:ASP:OD2	2.05	0.74
1:B:83:THR:HG22	1:B:84:ARG:N	2.01	0.74
1:C:136:PHE:CD1	1:C:232:VAL:HG22	2.23	0.74
1:C:271:THR:HG21	1:C:275:GLU:OE2	1.87	0.74
1:A:241:ARG:N	1:A:241:ARG:HD2	2.03	0.74
1:A:326:VAL:CG1	1:A:331:GLN:HG3	2.17	0.74
1:B:149:LYS:HB3	1:B:217:TYR:CD1	2.20	0.74
1:B:292:TYR:HB2	1:B:318:SER:O	1.87	0.74
1:A:179:VAL:CG2	1:A:180:PRO:CD	2.62	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:CB	1:A:235:THR:HG22	2.18	0.74
1:B:115:THR:O	1:B:116:PHE:CG	2.40	0.74
1:B:179:VAL:HG11	1:B:181:TRP:HE1	1.49	0.74
1:B:248:ALA:HA	1:B:265:TRP:CD1	2.20	0.74
1:B:174:GLY:O	1:B:175:CYS:SG	2.45	0.74
1:B:179:VAL:CG2	1:B:180:PRO:CD	2.62	0.74
1:B:310:VAL:C	1:B:311:LEU:HD12	2.08	0.74
1:C:292:TYR:HB2	1:C:318:SER:O	1.86	0.74
1:C:75:VAL:CB	1:C:75:VAL:N	2.51	0.74
1:A:101:PRO:C	1:A:102:LYS:CG	2.42	0.74
1:C:109:ASN:HA	1:C:129:TYR:OH	1.88	0.74
1:B:136:PHE:CZ	1:B:212:LEU:HD22	2.22	0.74
1:C:185:ILE:HD12	1:C:186:LEU:CA	2.16	0.74
1:C:85:SER:CA	1:C:234:TYR:O	2.36	0.74
1:B:136:PHE:CD1	1:B:232:VAL:HG22	2.23	0.74
1:B:326:VAL:CG1	1:B:331:GLN:HG3	2.17	0.74
1:C:78:ALA:C	1:C:80:ASP:N	2.32	0.74
1:A:120:ILE:HG12	1:A:350:ARG:NH1	2.03	0.73
1:B:133:SER:CB	1:B:235:THR:HG22	2.17	0.73
1:B:301:GLU:O	1:B:333:VAL:CG1	2.34	0.73
1:C:71:THR:OG1	1:C:87:SER:HB2	1.87	0.73
1:C:241:ARG:HD2	1:C:241:ARG:N	2.03	0.73
1:B:271:THR:HG21	1:B:275:GLU:OE2	1.87	0.73
1:A:135:ARG:HB3	1:A:186:LEU:O	1.88	0.73
1:B:154:PHE:CD1	1:B:154:PHE:C	2.62	0.73
1:B:149:LYS:HD3	1:B:217:TYR:CE1	2.24	0.73
1:C:76:SER:OG	1:C:76:SER:C	2.26	0.73
1:A:149:LYS:HD3	1:A:217:TYR:CE1	2.24	0.73
1:C:154:PHE:CE1	1:C:155:ASP:O	2.41	0.73
1:C:174:GLY:O	1:C:175:CYS:SG	2.45	0.73
1:C:200:GLY:HA2	1:C:264:SER:HB3	1.70	0.73
1:C:326:VAL:CG1	1:C:331:GLN:HG3	2.17	0.73
1:C:94:LYS:O	1:C:95:LYS:O	2.07	0.73
1:A:136:PHE:CZ	1:A:212:LEU:HD22	2.22	0.73
1:A:288:LEU:CD1	1:A:290:LEU:HG	2.17	0.73
1:A:283:THR:OG1	1:A:329:ARG:HG2	1.89	0.73
1:A:120:ILE:HD13	1:A:350:ARG:HH21	1.52	0.73
1:A:86:GLY:CA	1:A:234:TYR:CE1	2.66	0.73
1:C:201:ILE:N	1:C:281:LEU:HD23	2.02	0.73
1:C:283:THR:OG1	1:C:329:ARG:HG2	1.89	0.73
1:A:114:GLY:H	1:A:283:THR:HB	0.94	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:OD1	1:A:334:LYS:NZ	2.20	0.73
1:B:289:THR:O	1:B:290:LEU:CB	2.35	0.73
1:C:297:VAL:O	1:C:298:SER:OG	2.07	0.73
1:A:297:VAL:O	1:A:298:SER:OG	2.07	0.73
1:A:149:LYS:HE2	1:A:151:ALA:CA	2.19	0.73
1:B:241:ARG:H	1:B:241:ARG:HD2	1.54	0.73
1:C:149:LYS:HE2	1:C:151:ALA:CA	2.19	0.73
1:B:135:ARG:HB3	1:B:186:LEU:O	1.88	0.73
1:C:310:VAL:C	1:C:311:LEU:HD12	2.08	0.73
1:B:120:ILE:CD1	1:B:284:GLY:N	2.50	0.73
1:B:253:PHE:CD2	1:B:346:TRP:HZ3	2.07	0.73
1:B:94:LYS:O	1:B:95:LYS:O	2.06	0.73
1:C:133:SER:CB	1:C:235:THR:HG22	2.17	0.73
1:C:149:LYS:CB	1:C:217:TYR:CE1	2.60	0.73
1:C:90:ILE:CD1	1:C:232:VAL:HG23	2.19	0.73
1:B:338:THR:OG1	1:B:339:GLU:CB	2.37	0.73
1:A:310:VAL:C	1:A:311:LEU:HD12	2.08	0.73
1:B:288:LEU:CD1	1:B:290:LEU:HG	2.17	0.73
1:A:241:ARG:H	1:A:241:ARG:HD2	1.54	0.73
1:A:301:GLU:O	1:A:333:VAL:CG1	2.34	0.72
1:B:154:PHE:HD1	1:B:155:ASP:H	0.75	0.72
1:A:253:PHE:CD2	1:A:346:TRP:HZ3	2.07	0.72
1:A:326:VAL:HG13	1:A:331:GLN:CG	2.20	0.72
1:B:116:PHE:O	1:B:120:ILE:HG22	1.90	0.72
1:C:313:GLU:HG3	1:C:318:SER:HB3	1.69	0.72
1:C:241:ARG:HD2	1:C:241:ARG:H	1.54	0.72
1:C:69:VAL:CG1	1:C:70:SER:N	2.38	0.72
1:A:127:GLU:OE1	1:C:157:ASP:HB2	1.90	0.72
1:A:132:THR:HG22	1:A:235:THR:O	1.89	0.72
1:A:94:LYS:O	1:A:95:LYS:O	2.06	0.72
1:B:132:THR:HG22	1:B:235:THR:O	1.89	0.72
1:C:149:LYS:HD3	1:C:217:TYR:CE1	2.24	0.72
1:A:116:PHE:O	1:A:120:ILE:HG22	1.90	0.72
1:B:276:HIS:ND1	1:B:277:ASP:N	2.38	0.72
1:C:135:ARG:HB3	1:C:186:LEU:O	1.88	0.72
1:A:276:HIS:ND1	1:A:277:ASP:N	2.38	0.72
1:B:85:SER:CA	1:B:234:TYR:O	2.36	0.72
1:B:288:LEU:CG	1:B:289:THR:N	2.50	0.72
1:C:91:THR:HB	1:C:325:LYS:HE3	1.71	0.72
1:C:72:GLN:NE2	1:C:72:GLN:HA	2.04	0.72
1:A:109:ASN:HA	1:A:129:TYR:OH	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:CA	1:C:242:THR:CG2	2.64	0.72
1:C:107:VAL:HG23	1:C:283:THR:CG2	2.19	0.72
1:B:179:VAL:HG22	1:B:180:PRO:CD	2.19	0.72
1:C:339:GLU:CA	1:C:340:GLU:N	2.53	0.72
1:B:313:GLU:HG3	1:B:318:SER:HB3	1.69	0.72
1:C:253:PHE:CD2	1:C:346:TRP:HZ3	2.07	0.72
1:B:246:SER:CB	1:B:265:TRP:CZ2	2.56	0.72
1:B:339:GLU:CA	1:B:340:GLU:N	2.53	0.72
1:A:267:LYS:O	1:A:279:HIS:HB2	1.90	0.72
1:A:308:PHE:CD2	1:A:310:VAL:HG23	2.25	0.72
1:B:124:ALA:O	1:B:244:SER:N	2.18	0.72
1:C:288:LEU:CG	1:C:289:THR:N	2.50	0.72
1:C:295:ALA:CB	1:C:315:ALA:N	2.53	0.72
1:C:326:VAL:HG13	1:C:331:GLN:CG	2.20	0.72
1:A:154:PHE:HD1	1:A:155:ASP:H	0.75	0.71
1:A:169:LEU:O	1:A:169:LEU:HD23	1.90	0.71
1:A:290:LEU:HD22	1:A:346:TRP:CB	2.20	0.71
1:B:127:GLU:O	1:B:128:LYS:HB2	1.89	0.71
1:B:90:ILE:CD1	1:B:232:VAL:HG23	2.19	0.71
1:C:154:PHE:CD1	1:C:154:PHE:C	2.62	0.71
1:C:308:PHE:CD2	1:C:310:VAL:HG23	2.25	0.71
1:A:236:VAL:HG12	1:A:237:GLN:N	2.05	0.71
1:B:238:LEU:HD12	1:B:238:LEU:N	2.05	0.71
1:B:308:PHE:CD2	1:B:310:VAL:HG23	2.25	0.71
1:C:132:THR:HG22	1:C:235:THR:O	1.89	0.71
1:C:245:THR:OG1	1:C:263:VAL:CG2	2.32	0.71
1:C:290:LEU:HD22	1:C:346:TRP:CB	2.20	0.71
1:C:117:ASN:CG	1:C:351:ILE:OXT	2.29	0.71
1:A:124:ALA:HB1	1:A:245:THR:CG2	2.20	0.71
1:A:154:PHE:C	1:A:154:PHE:CD1	2.62	0.71
1:A:124:ALA:O	1:A:244:SER:N	2.18	0.71
1:A:149:LYS:NZ	1:A:170:TYR:CE1	2.52	0.71
1:B:109:ASN:HA	1:B:129:TYR:OH	1.88	0.71
1:B:236:VAL:HG12	1:B:237:GLN:N	2.05	0.71
1:B:86:GLY:CA	1:B:234:TYR:CE1	2.66	0.71
1:C:267:LYS:O	1:C:279:HIS:HB2	1.90	0.71
1:A:127:GLU:O	1:A:128:LYS:HB2	1.89	0.71
1:A:179:VAL:HG22	1:A:180:PRO:CD	2.19	0.71
1:A:85:SER:CA	1:A:234:TYR:O	2.36	0.71
1:A:238:LEU:HD12	1:A:238:LEU:N	2.05	0.71
1:A:313:GLU:HG3	1:A:318:SER:HB3	1.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:THR:HG23	1:B:243:GLY:H	1.56	0.71
1:C:55:VAL:CG2	1:C:56:THR:H	2.03	0.71
1:B:149:LYS:HE2	1:B:151:ALA:CA	2.19	0.71
1:C:127:GLU:O	1:C:128:LYS:HB2	1.89	0.71
1:C:252:ASP:OD2	1:C:345:LYS:CE	2.37	0.71
1:C:91:THR:HG23	1:C:325:LYS:HZ3	1.55	0.71
1:A:295:ALA:CB	1:A:315:ALA:N	2.53	0.71
1:A:90:ILE:CD1	1:A:232:VAL:HG23	2.19	0.71
1:B:124:ALA:HB1	1:B:245:THR:CG2	2.20	0.71
1:B:117:ASN:HA	1:B:284:GLY:HA2	1.71	0.71
1:B:326:VAL:HG13	1:B:331:GLN:CG	2.20	0.71
1:C:169:LEU:HD23	1:C:169:LEU:O	1.90	0.71
1:C:276:HIS:ND1	1:C:277:ASP:N	2.38	0.71
1:B:297:VAL:O	1:B:298:SER:OG	2.07	0.71
1:A:138:TYR:CG	1:A:184:PHE:CZ	2.62	0.71
1:B:179:VAL:HG21	1:B:181:TRP:HD1	1.56	0.71
1:C:179:VAL:CG2	1:C:181:TRP:HD1	2.03	0.71
1:C:238:LEU:N	1:C:238:LEU:HD12	2.05	0.71
1:C:242:THR:HG23	1:C:243:GLY:N	2.05	0.71
1:C:201:ILE:HG13	1:C:281:LEU:HD21	1.73	0.71
1:C:286:PHE:HA	1:C:350:ARG:O	1.91	0.71
1:C:56:THR:HG23	1:C:57:ARG:H	1.56	0.71
1:C:236:VAL:HG12	1:C:237:GLN:N	2.05	0.71
1:A:113:PRO:CA	1:A:283:THR:HB	2.21	0.71
1:A:130:ARG:HD2	1:A:237:GLN:NE2	2.06	0.71
1:B:179:VAL:CG2	1:B:181:TRP:HD1	2.03	0.71
1:B:242:THR:HG23	1:B:243:GLY:N	2.05	0.71
1:B:295:ALA:CB	1:B:315:ALA:N	2.53	0.71
1:B:169:LEU:HD23	1:B:169:LEU:O	1.90	0.70
1:C:179:VAL:HG22	1:C:180:PRO:CD	2.19	0.70
1:C:130:ARG:HD2	1:C:237:GLN:NE2	2.06	0.70
1:A:242:THR:HG23	1:A:243:GLY:H	1.56	0.70
1:B:290:LEU:HD22	1:B:346:TRP:CB	2.20	0.70
1:B:109:ASN:HD22	1:B:329:ARG:NH2	1.87	0.70
1:A:154:PHE:CE1	1:A:155:ASP:O	2.41	0.70
1:A:179:VAL:CG2	1:A:181:TRP:HD1	2.03	0.70
1:B:130:ARG:HD2	1:B:237:GLN:NE2	2.06	0.70
1:B:154:PHE:CE1	1:B:155:ASP:O	2.41	0.70
1:C:242:THR:HG23	1:C:243:GLY:H	1.56	0.70
1:B:138:TYR:O	1:B:139:SER:C	2.24	0.70
1:B:286:PHE:HA	1:B:350:ARG:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PRO:CG	1:A:217:TYR:CD2	2.75	0.70
1:A:242:THR:HG23	1:A:243:GLY:N	2.05	0.70
1:B:109:ASN:HD22	1:B:329:ARG:HH21	1.37	0.70
1:C:137:ARG:O	1:C:230:VAL:HG13	1.91	0.70
1:A:286:PHE:HA	1:A:350:ARG:O	1.91	0.70
1:B:267:LYS:O	1:B:279:HIS:HB2	1.90	0.70
1:C:156:ARG:O	1:C:210:GLY:N	2.25	0.70
1:C:55:VAL:CG2	1:C:56:THR:N	2.53	0.70
1:A:167:ALA:O	1:A:171:ASN:CG	2.30	0.70
1:A:137:ARG:O	1:A:230:VAL:HG13	1.91	0.70
1:A:252:ASP:OD1	1:A:253:PHE:N	2.24	0.70
1:B:101:PRO:CG	1:B:217:TYR:CD2	2.75	0.70
1:C:105:THR:HG21	1:C:328:GLU:CB	2.21	0.70
1:A:339:GLU:CA	1:A:340:GLU:N	2.53	0.70
1:A:129:TYR:HA	1:A:237:GLN:O	1.92	0.70
1:A:156:ARG:O	1:A:210:GLY:N	2.25	0.70
1:A:313:GLU:CG	1:A:318:SER:OG	2.40	0.70
1:B:101:PRO:C	1:B:102:LYS:CG	2.42	0.70
1:C:101:PRO:CG	1:C:217:TYR:CD2	2.75	0.70
1:C:313:GLU:CG	1:C:318:SER:OG	2.40	0.70
1:C:80:ASP:HA	1:C:241:ARG:HH22	0.70	0.70
1:A:288:LEU:CG	1:A:289:THR:N	2.50	0.70
1:C:116:PHE:O	1:C:120:ILE:HG22	1.90	0.70
1:B:167:ALA:O	1:B:171:ASN:CG	2.30	0.70
1:B:313:GLU:CG	1:B:318:SER:OG	2.40	0.70
1:C:179:VAL:HG21	1:C:181:TRP:HD1	1.56	0.70
1:A:338:THR:OG1	1:A:339:GLU:CB	2.37	0.70
1:A:297:VAL:HB	1:A:336:VAL:CG1	1.98	0.70
1:A:170:TYR:CZ	1:A:217:TYR:OH	2.45	0.69
1:B:137:ARG:O	1:B:230:VAL:HG13	1.92	0.69
1:B:252:ASP:OD1	1:B:253:PHE:N	2.24	0.69
1:C:167:ALA:O	1:C:171:ASN:CG	2.30	0.69
1:B:129:TYR:HA	1:B:237:GLN:O	1.92	0.69
1:B:326:VAL:HG13	1:B:331:GLN:HG3	1.74	0.69
1:C:124:ALA:HB1	1:C:245:THR:CG2	2.20	0.69
1:C:66:TYR:CZ	1:C:183:GLY:HA3	2.27	0.69
1:A:185:ILE:HD12	1:A:186:LEU:H	0.65	0.69
1:B:122:GLU:O	1:B:122:GLU:HG2	1.93	0.69
1:C:149:LYS:NZ	1:C:170:TYR:CE1	2.52	0.69
1:C:91:THR:CG2	1:C:325:LYS:HZ3	2.02	0.69
1:A:252:ASP:OD2	1:A:345:LYS:CE	2.37	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:HZ1	1:A:225:ALA:N	1.89	0.69
1:B:156:ARG:O	1:B:210:GLY:N	2.25	0.69
1:C:138:TYR:CG	1:C:184:PHE:CZ	2.62	0.69
1:C:138:TYR:O	1:C:139:SER:C	2.24	0.69
1:C:173:GLU:HG3	1:C:174:GLY:N	2.08	0.69
1:C:244:SER:O	1:C:245:THR:CB	2.41	0.69
1:C:252:ASP:OD1	1:C:253:PHE:N	2.24	0.69
1:C:326:VAL:HG13	1:C:331:GLN:HG3	1.74	0.69
1:B:117:ASN:HA	1:B:284:GLY:CA	2.22	0.69
1:C:326:VAL:HG13	1:C:327:ALA:H	1.54	0.69
1:C:333:VAL:C	1:C:334:LYS:HD3	2.12	0.69
1:A:122:GLU:HG2	1:A:122:GLU:O	1.93	0.69
1:A:169:LEU:HD22	1:A:170:TYR:HD1	1.58	0.69
1:B:169:LEU:HD22	1:B:170:TYR:HD1	1.58	0.69
1:B:170:TYR:CZ	1:B:217:TYR:OH	2.45	0.69
1:B:295:ALA:H	1:B:316:ALA:HA	0.69	0.69
1:A:143:PRO:O	1:A:146:THR:HG22	1.92	0.69
1:A:103:TYR:HE1	1:A:169:LEU:HD12	1.56	0.69
1:A:179:VAL:HG21	1:A:181:TRP:HD1	1.56	0.69
1:A:278:CYS:CA	1:A:333:VAL:O	2.41	0.69
1:B:327:ALA:HB3	1:B:331:GLN:NE2	2.07	0.69
1:C:103:TYR:HE1	1:C:169:LEU:HD12	1.56	0.69
1:B:155:ASP:CB	1:B:172:ILE:HD11	2.23	0.69
1:B:170:TYR:OH	1:B:217:TYR:OH	2.11	0.69
1:B:173:GLU:HG3	1:B:174:GLY:N	2.08	0.69
1:B:283:THR:OG1	1:B:329:ARG:HG2	1.89	0.69
1:C:327:ALA:HB3	1:C:331:GLN:NE2	2.07	0.69
1:C:278:CYS:CA	1:C:333:VAL:O	2.41	0.69
1:C:338:THR:OG1	1:C:339:GLU:CB	2.37	0.69
1:A:295:ALA:H	1:A:316:ALA:HA	0.69	0.69
1:B:103:TYR:HE1	1:B:169:LEU:HD12	1.56	0.69
1:C:289:THR:O	1:C:290:LEU:CB	2.35	0.69
1:C:75:VAL:C	1:C:75:VAL:CB	2.59	0.69
1:A:124:ALA:O	1:A:243:GLY:HA2	1.93	0.69
1:B:143:PRO:O	1:B:146:THR:HG22	1.92	0.69
1:B:120:ILE:HG12	1:B:350:ARG:HE	1.56	0.69
1:C:101:PRO:C	1:C:102:LYS:CG	2.42	0.69
1:A:126:TYR:CA	1:A:242:THR:CG2	2.64	0.68
1:A:290:LEU:O	1:A:290:LEU:HD12	1.93	0.68
1:C:155:ASP:CB	1:C:172:ILE:HD11	2.23	0.68
1:C:129:TYR:HA	1:C:237:GLN:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ALA:O	1:B:243:GLY:HA2	1.93	0.68
1:B:244:SER:O	1:B:245:THR:CB	2.41	0.68
1:B:327:ALA:CB	1:B:331:GLN:CD	2.39	0.68
1:A:160:LYS:NZ	1:B:199:ASP:HB3	2.08	0.68
1:B:278:CYS:CA	1:B:333:VAL:O	2.41	0.68
1:C:170:TYR:OH	1:C:217:TYR:OH	2.11	0.68
1:C:230:VAL:HG12	1:C:231:ARG:N	2.09	0.68
1:A:248:ALA:O	1:A:263:VAL:HA	1.93	0.68
1:B:258:ASP:CG	1:B:259:GLY:H	1.95	0.68
1:C:122:GLU:O	1:C:122:GLU:HG2	1.93	0.68
1:C:120:ILE:HD11	1:C:350:ARG:HB3	1.73	0.68
1:A:173:GLU:HG3	1:A:174:GLY:N	2.08	0.68
1:A:327:ALA:HB3	1:A:331:GLN:NE2	2.07	0.68
1:C:251:GLY:O	1:C:346:TRP:CH2	2.47	0.68
1:C:95:LYS:HZ2	1:C:221:ALA:CA	2.02	0.68
1:A:269:LYS:HE2	1:A:270:GLY:O	1.94	0.68
1:C:143:PRO:O	1:C:146:THR:HG22	1.92	0.68
1:C:124:ALA:O	1:C:243:GLY:HA2	1.93	0.68
1:B:269:LYS:HE2	1:B:270:GLY:O	1.94	0.68
1:B:289:THR:C	1:B:290:LEU:HG	2.14	0.68
1:B:251:GLY:O	1:B:346:TRP:CH2	2.47	0.68
1:C:127:GLU:O	1:C:128:LYS:CB	2.42	0.68
1:C:83:THR:O	1:C:84:ARG:HG2	1.94	0.68
1:A:244:SER:O	1:A:245:THR:CB	2.41	0.68
1:B:290:LEU:HD12	1:B:290:LEU:O	1.93	0.68
1:C:149:LYS:HD3	1:C:217:TYR:CZ	2.29	0.68
1:C:185:ILE:HD13	1:C:186:LEU:H	1.53	0.68
1:B:254:ALA:N	1:B:257:LYS:O	2.27	0.68
1:B:149:LYS:NZ	1:B:170:TYR:CE1	2.52	0.68
1:C:105:THR:CG2	1:C:328:GLU:CB	2.72	0.68
1:C:295:ALA:H	1:C:316:ALA:HA	0.69	0.68
1:A:254:ALA:N	1:A:257:LYS:O	2.27	0.68
1:A:136:PHE:HE1	1:A:232:VAL:HG22	1.59	0.67
1:A:258:ASP:CG	1:A:259:GLY:H	1.95	0.67
1:B:286:PHE:CA	1:B:351:ILE:HG21	2.25	0.67
1:C:290:LEU:O	1:C:290:LEU:HD12	1.93	0.67
1:A:149:LYS:HD3	1:A:217:TYR:CZ	2.29	0.67
1:A:251:GLY:O	1:A:346:TRP:CH2	2.47	0.67
1:B:149:LYS:HD3	1:B:217:TYR:CZ	2.29	0.67
1:B:120:ILE:CA	1:B:350:ARG:HH21	2.06	0.67
1:C:258:ASP:CG	1:C:259:GLY:H	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:GLY:O	1:C:346:TRP:CZ2	2.47	0.67
1:A:104:THR:O	1:A:105:THR:C	2.33	0.67
1:A:127:GLU:O	1:A:128:LYS:CB	2.42	0.67
1:A:289:THR:C	1:A:290:LEU:HG	2.14	0.67
1:B:104:THR:O	1:B:105:THR:C	2.33	0.67
1:A:230:VAL:HG12	1:A:231:ARG:N	2.09	0.67
1:A:251:GLY:O	1:A:346:TRP:CZ2	2.47	0.67
1:A:83:THR:O	1:A:84:ARG:HG2	1.94	0.67
1:B:230:VAL:HG12	1:B:231:ARG:N	2.09	0.67
1:B:251:GLY:O	1:B:346:TRP:CZ2	2.48	0.67
1:C:104:THR:O	1:C:105:THR:C	2.33	0.67
1:C:340:GLU:O	1:C:342:PRO:CD	2.43	0.67
1:C:169:LEU:HD22	1:C:170:TYR:HD1	1.58	0.67
1:C:95:LYS:O	1:C:96:ASN:HB2	1.95	0.67
1:C:269:LYS:HE2	1:C:270:GLY:O	1.94	0.67
1:B:127:GLU:O	1:B:128:LYS:CB	2.42	0.67
1:A:96:ASN:ND2	1:A:102:LYS:HD3	2.10	0.67
1:A:163:PRO:HA	1:A:164:ASN:ND2	2.10	0.67
1:B:163:PRO:HA	1:B:164:ASN:ND2	2.10	0.67
1:C:113:PRO:C	1:C:115:THR:N	2.43	0.67
1:C:130:ARG:HD2	1:C:237:GLN:HB3	1.64	0.67
1:A:156:ARG:CD	1:B:240:ASN:OD1	2.43	0.66
1:C:163:PRO:HA	1:C:164:ASN:ND2	2.10	0.66
1:C:253:PHE:CE2	1:C:346:TRP:CZ3	2.83	0.66
1:A:300:LEU:CG	1:A:308:PHE:CZ	2.78	0.66
1:A:326:VAL:HG13	1:A:331:GLN:HG3	1.74	0.66
1:B:326:VAL:HG13	1:B:327:ALA:H	1.54	0.66
1:A:172:ILE:HA	1:B:242:THR:O	1.95	0.66
1:A:333:VAL:C	1:A:334:LYS:HD3	2.12	0.66
1:B:96:ASN:ND2	1:B:102:LYS:HD3	2.10	0.66
1:B:136:PHE:CE1	1:B:212:LEU:HD22	2.31	0.66
1:C:135:ARG:HG3	1:C:233:GLU:CB	2.23	0.66
1:C:254:ALA:N	1:C:257:LYS:O	2.27	0.66
1:A:126:TYR:O	1:A:242:THR:HG21	1.95	0.66
1:A:95:LYS:O	1:A:96:ASN:HB2	1.95	0.66
1:B:113:PRO:C	1:B:115:THR:N	2.43	0.66
1:B:236:VAL:HG12	1:B:238:LEU:CD1	2.26	0.66
1:A:95:LYS:HZ2	1:A:221:ALA:CA	2.05	0.66
1:B:109:ASN:HB2	1:B:208:ASP:HB3	1.77	0.66
1:C:136:PHE:CE1	1:C:212:LEU:HD22	2.31	0.66
1:C:208:ASP:OD1	1:C:329:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:HD12	1:C:65:ALA:H	1.60	0.66
1:A:308:PHE:HE2	1:A:310:VAL:CG2	1.92	0.66
1:B:253:PHE:CE2	1:B:346:TRP:CZ3	2.83	0.66
1:B:333:VAL:C	1:B:334:LYS:HD3	2.12	0.66
1:C:107:VAL:HG23	1:C:283:THR:OG1	1.95	0.66
1:C:286:PHE:CA	1:C:351:ILE:HG21	2.25	0.66
1:C:308:PHE:HE2	1:C:310:VAL:CG2	1.92	0.66
1:C:91:THR:HG23	1:C:325:LYS:NZ	2.07	0.66
1:B:340:GLU:O	1:B:342:PRO:CD	2.43	0.66
1:C:261:ARG:O	1:C:261:ARG:HG3	1.94	0.66
1:A:170:TYR:OH	1:A:217:TYR:OH	2.11	0.66
1:A:82:ILE:O	1:A:83:THR:N	2.29	0.66
1:B:252:ASP:OD2	1:B:345:LYS:CE	2.37	0.66
1:B:83:THR:O	1:B:84:ARG:HG2	1.94	0.66
1:C:126:TYR:O	1:C:242:THR:HG21	1.95	0.66
1:C:289:THR:C	1:C:290:LEU:HG	2.14	0.66
1:B:306:SER:O	1:B:307:ASP:O	2.14	0.66
1:A:268:THR:O	1:A:268:THR:HG23	1.96	0.66
1:A:286:PHE:CA	1:A:351:ILE:HG21	2.25	0.66
1:B:130:ARG:NH1	1:B:237:GLN:HA	2.10	0.66
1:C:236:VAL:HG12	1:C:238:LEU:CD1	2.26	0.66
1:A:253:PHE:CE2	1:A:346:TRP:CZ3	2.83	0.66
1:B:117:ASN:HA	1:B:285:ASN:H	1.61	0.66
1:C:124:ALA:CB	1:C:245:THR:CG2	2.74	0.66
1:A:306:SER:O	1:A:307:ASP:O	2.14	0.66
1:A:261:ARG:HG3	1:A:261:ARG:O	1.94	0.66
1:A:120:ILE:HG12	1:A:350:ARG:HH22	0.81	0.66
1:C:120:ILE:HD12	1:C:350:ARG:HH11	1.61	0.66
1:C:268:THR:HG23	1:C:268:THR:O	1.96	0.66
1:B:297:VAL:CB	1:B:336:VAL:O	2.36	0.66
1:A:249:GLN:HB2	1:A:265:TRP:CZ3	2.30	0.66
1:A:185:ILE:HD13	1:A:186:LEU:H	1.53	0.65
1:B:120:ILE:HG21	1:B:284:GLY:HA2	1.76	0.65
1:B:261:ARG:HG3	1:B:261:ARG:O	1.94	0.65
1:B:124:ALA:CB	1:B:245:THR:CG2	2.74	0.65
1:C:96:ASN:ND2	1:C:102:LYS:HD3	2.10	0.65
1:C:297:VAL:CB	1:C:336:VAL:O	2.36	0.65
1:B:312:GLY:HA3	1:B:320:GLN:HG2	1.78	0.65
1:A:136:PHE:CE1	1:A:212:LEU:HD22	2.31	0.65
1:A:326:VAL:HG13	1:A:327:ALA:H	1.54	0.65
1:B:126:TYR:O	1:B:242:THR:HG21	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:GLN:O	1:C:119:LEU:HB2	1.97	0.65
1:A:340:GLU:O	1:A:342:PRO:CD	2.43	0.65
1:C:66:TYR:OH	1:C:183:GLY:HA3	1.97	0.65
1:C:68:GLU:CG	1:C:137:ARG:NH2	2.59	0.65
1:C:245:THR:HA	1:C:263:VAL:HG23	1.79	0.65
1:C:326:VAL:HG12	1:C:327:ALA:CA	2.27	0.65
1:B:246:SER:CB	1:B:263:VAL:HG12	2.21	0.65
1:A:120:ILE:CG2	1:A:350:ARG:HH22	2.08	0.65
1:A:155:ASP:CB	1:A:172:ILE:HD11	2.23	0.65
1:A:153:ALA:HA	1:A:186:LEU:HD11	1.78	0.65
1:B:119:LEU:CD2	1:B:234:TYR:HE2	2.10	0.65
1:C:153:ALA:HA	1:C:186:LEU:HD11	1.78	0.65
1:C:138:TYR:HH	1:C:227:LEU:HB3	1.61	0.65
1:B:156:ARG:HD3	1:C:240:ASN:OD1	1.97	0.65
1:A:236:VAL:HG12	1:A:238:LEU:CD1	2.26	0.65
1:B:268:THR:HG23	1:B:268:THR:O	1.96	0.65
1:B:95:LYS:O	1:B:96:ASN:HB2	1.95	0.65
1:B:249:GLN:HB2	1:B:265:TRP:CZ3	2.31	0.65
1:A:109:ASN:HB2	1:A:208:ASP:HB3	1.77	0.65
1:B:326:VAL:HG12	1:B:327:ALA:CA	2.27	0.65
1:C:306:SER:O	1:C:307:ASP:O	2.14	0.65
1:A:205:LYS:HD2	1:A:205:LYS:N	2.12	0.65
1:A:166:LEU:O	1:A:167:ALA:C	2.36	0.65
1:C:109:ASN:HB2	1:C:208:ASP:HB3	1.77	0.65
1:B:306:SER:HB3	1:B:325:LYS:CB	2.27	0.65
1:A:124:ALA:CB	1:A:245:THR:CG2	2.74	0.65
1:B:196:PHE:O	1:B:207:VAL:HG23	1.97	0.65
1:B:300:LEU:CG	1:B:308:PHE:CZ	2.78	0.65
1:B:82:ILE:O	1:B:83:THR:N	2.29	0.65
1:C:170:TYR:CZ	1:C:217:TYR:OH	2.45	0.65
1:C:309:SER:O	1:C:321:TRP:O	2.15	0.65
1:B:205:LYS:HD2	1:B:205:LYS:N	2.12	0.65
1:A:196:PHE:O	1:A:207:VAL:HG23	1.97	0.65
1:B:95:LYS:HZ1	1:B:221:ALA:CA	2.09	0.65
1:C:107:VAL:H	1:C:283:THR:HG22	1.61	0.65
1:C:105:THR:HG23	1:C:328:GLU:N	2.12	0.65
1:A:160:LYS:CE	1:B:199:ASP:CB	2.76	0.64
1:A:172:ILE:O	1:A:173:GLU:C	2.36	0.64
1:B:166:LEU:O	1:B:167:ALA:C	2.36	0.64
1:B:172:ILE:O	1:B:173:GLU:C	2.36	0.64
1:C:207:VAL:HG13	1:C:208:ASP:CG	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:C	1:C:308:PHE:HZ	2.00	0.64
1:A:127:GLU:OE1	1:C:157:ASP:HB3	1.98	0.64
1:A:151:ALA:CA	1:A:177:SER:HB2	2.17	0.64
1:A:300:LEU:C	1:A:308:PHE:HZ	2.00	0.64
1:B:185:ILE:HD13	1:B:186:LEU:H	1.53	0.64
1:C:300:LEU:CG	1:C:308:PHE:CZ	2.78	0.64
1:C:306:SER:HB3	1:C:325:LYS:CB	2.27	0.64
1:B:246:SER:OG	1:B:265:TRP:HH2	1.67	0.64
1:A:118:GLN:O	1:A:119:LEU:HB2	1.97	0.64
1:A:199:ASP:HB2	1:C:160:LYS:CD	2.27	0.64
1:B:120:ILE:HG21	1:B:284:GLY:HA3	1.78	0.64
1:B:309:SER:O	1:B:321:TRP:O	2.15	0.64
1:C:136:PHE:HE1	1:C:232:VAL:HG22	1.59	0.64
1:A:125:GLN:C	1:A:242:THR:CG2	2.66	0.64
1:B:130:ARG:HD2	1:B:237:GLN:CG	2.27	0.64
1:B:136:PHE:HE1	1:B:232:VAL:HG22	1.59	0.64
1:B:253:PHE:CD2	1:B:346:TRP:CZ3	2.85	0.64
1:C:152:LEU:CD2	1:C:186:LEU:HD13	2.25	0.64
1:A:269:LYS:CG	1:A:270:GLY:N	2.58	0.64
1:B:118:GLN:O	1:B:119:LEU:HB2	1.96	0.64
1:B:125:GLN:C	1:B:242:THR:CG2	2.66	0.64
1:B:153:ALA:HA	1:B:186:LEU:HD11	1.78	0.64
1:C:125:GLN:C	1:C:242:THR:CG2	2.66	0.64
1:C:166:LEU:O	1:C:167:ALA:C	2.36	0.64
1:B:207:VAL:HG13	1:B:208:ASP:CG	2.18	0.64
1:C:68:GLU:OE2	1:C:139:SER:OG	2.14	0.64
1:B:296:PRO:HG3	1:B:337:THR:CB	2.27	0.64
1:A:207:VAL:HG13	1:A:208:ASP:CG	2.18	0.64
1:A:309:SER:O	1:A:322:ALA:CB	2.46	0.64
1:B:274:TRP:NE1	1:B:340:GLU:OE1	2.31	0.64
1:B:117:ASN:CA	1:B:285:ASN:N	2.61	0.64
1:C:196:PHE:O	1:C:207:VAL:HG23	1.97	0.64
1:C:309:SER:O	1:C:322:ALA:CB	2.46	0.64
1:C:76:SER:HA	1:C:76:SER:N	2.01	0.64
1:B:300:LEU:C	1:B:308:PHE:HZ	2.00	0.64
1:C:120:ILE:HD12	1:C:350:ARG:HD2	0.70	0.64
1:C:327:ALA:HB2	1:C:331:GLN:OE1	1.96	0.64
1:C:253:PHE:CD2	1:C:346:TRP:CZ3	2.85	0.64
1:A:154:PHE:CZ	1:A:156:ARG:HA	2.33	0.64
1:C:138:TYR:O	1:C:139:SER:O	2.15	0.64
1:C:163:PRO:HG3	1:C:168:SER:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:CD2	1:C:234:TYR:HE2	2.10	0.64
1:C:249:GLN:O	1:C:347:GLN:HA	1.98	0.64
1:A:249:GLN:O	1:A:347:GLN:HA	1.98	0.64
1:A:297:VAL:CB	1:A:336:VAL:O	2.36	0.64
1:A:312:GLY:HA3	1:A:320:GLN:HG2	1.78	0.64
1:A:154:PHE:CE1	1:A:156:ARG:N	2.66	0.63
1:A:163:PRO:HG3	1:A:168:SER:HB3	1.80	0.63
1:A:86:GLY:N	1:A:234:TYR:O	2.31	0.63
1:C:154:PHE:CZ	1:C:156:ARG:HA	2.33	0.63
1:C:172:ILE:O	1:C:173:GLU:C	2.36	0.63
1:C:249:GLN:HB2	1:C:265:TRP:CZ3	2.30	0.63
1:A:313:GLU:CG	1:A:318:SER:HB2	2.19	0.63
1:A:326:VAL:HG12	1:A:327:ALA:CA	2.27	0.63
1:B:154:PHE:CE1	1:B:156:ARG:N	2.66	0.63
1:B:152:LEU:CD2	1:B:186:LEU:HD13	2.25	0.63
1:B:156:ARG:O	1:B:209:PHE:C	2.37	0.63
1:A:306:SER:HB3	1:A:325:LYS:CB	2.27	0.63
1:A:231:ARG:HG3	1:A:232:VAL:H	1.63	0.63
1:A:125:GLN:C	1:A:242:THR:HG22	2.19	0.63
1:C:61:PRO:HD2	1:C:181:TRP:CZ3	2.33	0.63
1:C:107:VAL:HG13	1:C:329:ARG:HH21	1.64	0.63
1:B:206:LEU:CD1	1:B:206:LEU:O	2.45	0.63
1:C:312:GLY:HA3	1:C:320:GLN:HG2	1.78	0.63
1:A:156:ARG:O	1:A:209:PHE:C	2.37	0.63
1:A:253:PHE:CD2	1:A:346:TRP:CZ3	2.85	0.63
1:C:154:PHE:CE1	1:C:156:ARG:N	2.66	0.63
1:C:205:LYS:HD2	1:C:205:LYS:N	2.12	0.63
1:A:130:ARG:HD2	1:A:237:GLN:CG	2.27	0.63
1:A:292:TYR:CB	1:A:318:SER:O	2.47	0.63
1:A:309:SER:O	1:A:321:TRP:O	2.15	0.63
1:B:155:ASP:O	1:B:156:ARG:C	2.36	0.63
1:B:163:PRO:HG3	1:B:168:SER:HB3	1.80	0.63
1:B:86:GLY:N	1:B:234:TYR:O	2.31	0.63
1:A:166:LEU:O	1:A:168:SER:N	2.32	0.63
1:A:130:ARG:NH1	1:A:237:GLN:HA	2.10	0.63
1:B:292:TYR:CB	1:B:318:SER:O	2.47	0.63
1:B:309:SER:O	1:B:322:ALA:CB	2.46	0.63
1:C:156:ARG:O	1:C:209:PHE:C	2.37	0.63
1:B:138:TYR:O	1:B:139:SER:O	2.15	0.63
1:B:95:LYS:HZ1	1:B:221:ALA:HB1	1.61	0.63
1:B:95:LYS:HZ1	1:B:225:ALA:N	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLU:CD	1:C:137:ARG:NH2	2.51	0.63
1:B:249:GLN:O	1:B:347:GLN:HA	1.98	0.63
1:C:206:LEU:CD1	1:C:206:LEU:O	2.45	0.63
1:C:125:GLN:C	1:C:242:THR:HG22	2.19	0.63
1:C:135:ARG:CB	1:C:186:LEU:O	2.47	0.63
1:C:170:TYR:C	1:C:171:ASN:HD22	2.02	0.63
1:A:155:ASP:O	1:A:156:ARG:C	2.36	0.63
1:A:95:LYS:HZ1	1:A:221:ALA:CA	2.12	0.63
1:B:135:ARG:CB	1:B:186:LEU:O	2.47	0.63
1:C:160:LYS:C	1:C:328:GLU:OE2	2.36	0.63
1:C:231:ARG:HG3	1:C:232:VAL:H	1.63	0.63
1:A:274:TRP:NE1	1:A:340:GLU:OE1	2.31	0.63
1:B:154:PHE:CZ	1:B:156:ARG:HA	2.33	0.62
1:B:166:LEU:O	1:B:168:SER:N	2.32	0.62
1:B:109:ASN:ND2	1:B:197:VAL:HG23	2.14	0.62
1:B:107:VAL:N	1:B:328:GLU:CG	2.59	0.62
1:B:83:THR:HG23	1:B:236:VAL:O	2.00	0.62
1:C:68:GLU:CG	1:C:137:ARG:HH22	2.12	0.62
1:C:105:THR:OG1	1:C:328:GLU:HB2	1.97	0.62
1:C:83:THR:CG2	1:C:84:ARG:H	2.08	0.62
1:C:86:GLY:N	1:C:234:TYR:O	2.31	0.62
1:A:206:LEU:O	1:A:206:LEU:CD1	2.45	0.62
1:A:83:THR:HG23	1:A:236:VAL:O	2.00	0.62
1:B:83:THR:CG2	1:B:84:ARG:H	2.08	0.62
1:A:135:ARG:CB	1:A:186:LEU:O	2.47	0.62
1:A:188:VAL:O	1:A:188:VAL:HG23	1.99	0.62
1:A:236:VAL:CG1	1:A:237:GLN:N	2.62	0.62
1:C:166:LEU:O	1:C:168:SER:N	2.32	0.62
1:C:82:ILE:HG23	1:C:83:THR:N	2.15	0.62
1:C:296:PRO:HG3	1:C:337:THR:HB	1.81	0.62
1:B:213:ILE:O	1:B:214:MET:HG3	2.00	0.62
1:C:120:ILE:CD1	1:C:350:ARG:HH11	2.12	0.62
1:A:136:PHE:CE2	1:A:212:LEU:HD11	2.35	0.62
1:A:137:ARG:O	1:A:230:VAL:HG22	1.98	0.62
1:A:138:TYR:O	1:A:139:SER:O	2.15	0.62
1:B:109:ASN:HB3	1:B:329:ARG:HH21	1.64	0.62
1:B:137:ARG:O	1:B:230:VAL:HG22	1.98	0.62
1:C:137:ARG:O	1:C:230:VAL:HG22	1.98	0.62
1:C:292:TYR:CB	1:C:318:SER:O	2.47	0.62
1:B:236:VAL:CG1	1:B:237:GLN:N	2.62	0.62
1:B:327:ALA:HB2	1:B:331:GLN:OE1	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ARG:NH1	1:C:237:GLN:HA	2.10	0.62
1:A:213:ILE:O	1:A:214:MET:HG3	2.00	0.62
1:B:107:VAL:H	1:B:328:GLU:HB2	1.64	0.62
1:A:296:PRO:HG3	1:A:337:THR:HB	1.81	0.62
1:A:157:ASP:OD1	1:A:157:ASP:O	2.18	0.62
1:A:124:ALA:HB1	1:A:244:SER:O	2.00	0.62
1:B:188:VAL:HG23	1:B:188:VAL:O	1.99	0.62
1:B:136:PHE:CE2	1:B:212:LEU:HD11	2.35	0.62
1:B:82:ILE:HG23	1:B:83:THR:N	2.15	0.62
1:C:112:GLU:O	1:C:114:GLY:N	2.33	0.62
1:C:157:ASP:OD1	1:C:157:ASP:O	2.18	0.62
1:C:82:ILE:O	1:C:83:THR:N	2.29	0.62
1:A:83:THR:CG2	1:A:84:ARG:H	2.08	0.62
1:C:136:PHE:CE2	1:C:212:LEU:HD11	2.35	0.62
1:C:155:ASP:O	1:C:156:ARG:C	2.36	0.62
1:C:186:LEU:C	1:C:186:LEU:HD23	2.20	0.62
1:C:109:ASN:ND2	1:C:197:VAL:HG23	2.14	0.62
1:C:124:ALA:HB1	1:C:244:SER:O	2.00	0.62
1:B:124:ALA:HB1	1:B:244:SER:O	2.00	0.62
1:C:105:THR:CG2	1:C:328:GLU:HB2	2.29	0.62
1:C:83:THR:HG23	1:C:236:VAL:O	2.00	0.62
1:B:291:PHE:C	1:B:292:TYR:CA	2.67	0.61
1:B:313:GLU:CG	1:B:318:SER:HB2	2.19	0.61
1:B:114:GLY:HA2	1:B:326:VAL:HG12	1.81	0.61
1:C:201:ILE:HB	1:C:281:LEU:HD23	1.74	0.61
1:C:98:ASP:OD1	1:C:99:THR:N	2.33	0.61
1:C:55:VAL:HG22	1:C:56:THR:H	1.60	0.61
1:B:237:GLN:C	1:B:238:LEU:HD12	2.21	0.61
1:B:125:GLN:C	1:B:242:THR:HG22	2.19	0.61
1:A:156:ARG:CZ	1:B:240:ASN:CB	2.78	0.61
1:B:130:ARG:HB3	1:B:237:GLN:H	1.66	0.61
1:B:130:ARG:CB	1:B:237:GLN:CB	2.68	0.61
1:B:117:ASN:CA	1:B:285:ASN:H	2.11	0.61
1:C:236:VAL:CG1	1:C:237:GLN:N	2.62	0.61
1:B:157:ASP:O	1:B:157:ASP:OD1	2.18	0.61
1:A:119:LEU:CD2	1:A:234:TYR:HE2	2.10	0.61
1:A:286:PHE:CD2	1:A:350:ARG:HA	2.35	0.61
1:B:314:ALA:O	1:B:315:ALA:HB2	2.00	0.61
1:C:136:PHE:CE2	1:C:212:LEU:CD1	2.84	0.61
1:A:170:TYR:C	1:A:171:ASN:HD22	2.02	0.61
1:B:300:LEU:C	1:B:308:PHE:CZ	2.74	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HB3	1:A:237:GLN:H	1.66	0.61
1:A:152:LEU:CD2	1:A:186:LEU:HD13	2.25	0.61
1:A:300:LEU:C	1:A:308:PHE:CZ	2.74	0.61
1:A:314:ALA:O	1:A:315:ALA:HB2	2.01	0.61
1:B:144:SER:C	1:B:146:THR:N	2.54	0.61
1:B:124:ALA:HB2	1:B:245:THR:HG21	1.82	0.61
1:C:300:LEU:C	1:C:308:PHE:CZ	2.74	0.61
1:C:213:ILE:O	1:C:214:MET:HG3	2.00	0.61
1:A:144:SER:C	1:A:146:THR:N	2.54	0.61
1:A:156:ARG:HD3	1:B:240:ASN:CB	2.30	0.61
1:A:327:ALA:HB2	1:A:331:GLN:OE1	1.96	0.61
1:B:169:LEU:HD22	1:B:170:TYR:CD1	2.36	0.61
1:C:130:ARG:HD2	1:C:237:GLN:CG	2.27	0.61
1:A:135:ARG:HG3	1:A:233:GLU:CB	2.23	0.61
1:A:83:THR:HG23	1:A:130:ARG:NH1	2.15	0.61
1:B:135:ARG:HG3	1:B:233:GLU:CB	2.23	0.61
1:B:313:GLU:HG3	1:B:318:SER:OG	2.01	0.61
1:C:188:VAL:O	1:C:188:VAL:HG23	1.99	0.61
1:B:296:PRO:HG3	1:B:337:THR:HB	1.81	0.61
1:A:112:GLU:O	1:A:114:GLY:N	2.33	0.61
1:A:237:GLN:C	1:A:238:LEU:HD12	2.21	0.61
1:A:82:ILE:HG23	1:A:83:THR:N	2.15	0.61
1:A:98:ASP:OD1	1:A:99:THR:N	2.33	0.61
1:B:156:ARG:NH1	1:B:173:GLU:OE1	2.34	0.61
1:B:186:LEU:C	1:B:186:LEU:HD23	2.20	0.61
1:B:134:LEU:HD23	1:B:188:VAL:CG2	2.31	0.61
1:B:308:PHE:HE2	1:B:310:VAL:CG2	1.92	0.61
1:C:85:SER:C	1:C:234:TYR:CE1	2.74	0.61
1:C:264:SER:C	1:C:265:TRP:HA	2.21	0.61
1:A:124:ALA:HB2	1:A:245:THR:HG21	1.82	0.61
1:B:83:THR:HG23	1:B:130:ARG:NH1	2.15	0.61
1:C:95:LYS:NZ	1:C:221:ALA:CB	2.64	0.61
1:C:286:PHE:CD2	1:C:350:ARG:HA	2.35	0.61
1:C:274:TRP:NE1	1:C:340:GLU:OE1	2.31	0.61
1:B:112:GLU:HB2	1:B:329:ARG:HE	1.66	0.60
1:C:306:SER:O	1:C:307:ASP:C	2.40	0.60
1:C:77:THR:CG2	1:C:78:ALA:H	2.03	0.60
1:A:113:PRO:C	1:A:115:THR:N	2.43	0.60
1:A:129:TYR:CB	1:A:237:GLN:O	2.49	0.60
1:A:136:PHE:CD2	1:A:212:LEU:HD21	2.36	0.60
1:A:136:PHE:CE2	1:A:212:LEU:CD1	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:CE	1:B:199:ASP:HB2	2.30	0.60
1:A:156:ARG:NH1	1:A:173:GLU:OE1	2.34	0.60
1:B:98:ASP:OD1	1:B:99:THR:N	2.33	0.60
1:C:134:LEU:HD23	1:C:188:VAL:CG2	2.31	0.60
1:A:264:SER:C	1:A:265:TRP:HA	2.22	0.60
1:A:290:LEU:CD1	1:A:290:LEU:C	2.70	0.60
1:B:129:TYR:CB	1:B:237:GLN:O	2.49	0.60
1:B:136:PHE:CD2	1:B:212:LEU:HD21	2.37	0.60
1:B:286:PHE:CD2	1:B:350:ARG:HA	2.35	0.60
1:C:237:GLN:C	1:C:238:LEU:HD12	2.21	0.60
1:C:291:PHE:C	1:C:292:TYR:CA	2.67	0.60
1:C:311:LEU:N	1:C:311:LEU:HD12	2.16	0.60
1:C:151:ALA:CA	1:C:177:SER:HB2	2.17	0.60
1:C:314:ALA:O	1:C:315:ALA:HB2	2.01	0.60
1:A:306:SER:O	1:A:307:ASP:C	2.40	0.60
1:A:95:LYS:NZ	1:A:221:ALA:CB	2.64	0.60
1:B:170:TYR:C	1:B:171:ASN:HD22	2.02	0.60
1:C:290:LEU:CD1	1:C:290:LEU:C	2.69	0.60
1:A:120:ILE:O	1:A:120:ILE:CG1	2.50	0.60
1:A:186:LEU:HD23	1:A:186:LEU:C	2.20	0.60
1:B:300:LEU:HB3	1:B:310:VAL:HG21	1.84	0.60
1:C:83:THR:HG23	1:C:130:ARG:NH1	2.15	0.60
1:C:156:ARG:NH1	1:C:173:GLU:OE1	2.34	0.60
1:C:200:GLY:HA3	1:C:201:ILE:HG22	1.84	0.60
1:C:112:GLU:C	1:C:350:ARG:HH21	2.04	0.60
1:C:117:ASN:ND2	1:C:351:ILE:OXT	2.35	0.60
1:A:85:SER:C	1:A:234:TYR:CE1	2.74	0.60
1:A:311:LEU:HD12	1:A:311:LEU:N	2.16	0.60
1:B:231:ARG:HG3	1:B:232:VAL:H	1.63	0.60
1:B:290:LEU:C	1:B:290:LEU:CD1	2.70	0.60
1:B:85:SER:C	1:B:234:TYR:CE1	2.74	0.60
1:C:124:ALA:HB2	1:C:245:THR:HG21	1.82	0.60
1:C:144:SER:C	1:C:146:THR:N	2.54	0.60
1:B:120:ILE:O	1:B:120:ILE:CG1	2.50	0.60
1:B:136:PHE:CE2	1:B:212:LEU:CD1	2.84	0.60
1:C:245:THR:HA	1:C:263:VAL:HG21	1.69	0.60
1:A:134:LEU:HD23	1:A:188:VAL:CG2	2.31	0.60
1:A:200:GLY:HA3	1:A:201:ILE:HG22	1.84	0.60
1:A:296:PRO:HG3	1:A:337:THR:CB	2.27	0.60
1:B:95:LYS:NZ	1:B:221:ALA:CB	2.64	0.60
1:C:120:ILE:CG2	1:C:350:ARG:NH1	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PRO:HB2	1:C:165:ASP:H	1.66	0.60
1:A:169:LEU:C	1:A:169:LEU:CD2	2.70	0.59
1:B:163:PRO:HB2	1:B:165:ASP:H	1.66	0.59
1:B:179:VAL:HG21	1:B:181:TRP:CD1	2.37	0.59
1:B:311:LEU:N	1:B:311:LEU:HD12	2.16	0.59
1:C:169:LEU:HD22	1:C:170:TYR:CD1	2.35	0.59
1:C:136:PHE:CD2	1:C:212:LEU:HD21	2.37	0.59
1:B:264:SER:C	1:B:265:TRP:HA	2.22	0.59
1:B:306:SER:O	1:B:307:ASP:C	2.40	0.59
1:B:163:PRO:CB	1:B:164:ASN:HD22	2.15	0.59
1:A:156:ARG:CZ	1:B:240:ASN:HA	2.32	0.59
1:C:129:TYR:CB	1:C:237:GLN:O	2.49	0.59
1:C:277:ASP:HA	1:C:334:LYS:CE	2.32	0.59
1:B:149:LYS:CD	1:B:177:SER:OG	2.50	0.59
1:A:163:PRO:CB	1:A:164:ASN:HD22	2.15	0.59
1:A:277:ASP:HA	1:A:334:LYS:CE	2.32	0.59
1:B:169:LEU:C	1:B:169:LEU:CD2	2.70	0.59
1:B:217:TYR:CD1	1:B:217:TYR:N	2.69	0.59
1:C:169:LEU:CD2	1:C:169:LEU:C	2.70	0.59
1:C:96:ASN:C	1:C:98:ASP:N	2.55	0.59
1:A:342:PRO:C	1:A:343:LYS:HD3	2.23	0.59
1:A:97:THR:CA	1:A:218:GLY:O	2.50	0.59
1:C:203:ASP:O	1:C:205:LYS:N	2.34	0.59
1:B:203:ASP:O	1:B:205:LYS:N	2.34	0.59
1:A:300:LEU:HB3	1:A:310:VAL:HG21	1.84	0.59
1:C:97:THR:CA	1:C:218:GLY:O	2.50	0.59
1:B:307:ASP:O	1:B:323:GLY:O	2.21	0.59
1:C:230:VAL:HG12	1:C:231:ARG:H	1.68	0.59
1:B:342:PRO:C	1:B:343:LYS:HD3	2.23	0.59
1:A:248:ALA:HB1	1:A:249:GLN:NE2	2.16	0.59
1:B:207:VAL:HG13	1:B:208:ASP:OD2	2.03	0.59
1:C:120:ILE:CG1	1:C:120:ILE:O	2.50	0.59
1:A:203:ASP:O	1:A:205:LYS:N	2.34	0.59
1:A:169:LEU:HD22	1:A:170:TYR:CD1	2.36	0.59
1:B:277:ASP:HA	1:B:334:LYS:CE	2.32	0.59
1:C:163:PRO:CB	1:C:164:ASN:HD22	2.15	0.59
1:C:130:ARG:HB3	1:C:237:GLN:H	1.66	0.59
1:C:245:THR:OG1	1:C:263:VAL:HG11	2.03	0.59
1:A:105:THR:O	1:A:328:GLU:OE1	2.20	0.59
1:A:109:ASN:ND2	1:A:197:VAL:HG23	2.14	0.59
1:A:112:GLU:O	1:A:113:PRO:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG21	1:A:181:TRP:CD1	2.37	0.59
1:A:207:VAL:HG13	1:A:208:ASP:OD2	2.03	0.59
1:A:130:ARG:CB	1:A:237:GLN:CB	2.68	0.59
1:B:179:VAL:HG13	1:B:181:TRP:CD1	2.38	0.59
1:C:130:ARG:CB	1:C:237:GLN:CB	2.68	0.59
1:B:97:THR:CA	1:B:218:GLY:O	2.50	0.59
1:A:217:TYR:CD1	1:A:217:TYR:N	2.69	0.58
1:A:280:PHE:HD2	1:A:331:GLN:O	1.86	0.58
1:C:307:ASP:O	1:C:323:GLY:O	2.21	0.58
1:A:307:ASP:O	1:A:323:GLY:O	2.21	0.58
1:A:291:PHE:C	1:A:292:TYR:CA	2.67	0.58
1:C:207:VAL:HG13	1:C:208:ASP:OD2	2.03	0.58
1:B:138:TYR:HH	1:B:227:LEU:HB3	1.61	0.58
1:B:315:ALA:HA	1:B:318:SER:HB2	1.84	0.58
1:B:340:GLU:OE1	1:B:340:GLU:HA	2.04	0.58
1:A:163:PRO:HB2	1:A:165:ASP:H	1.66	0.58
1:A:138:TYR:HD2	1:A:184:PHE:CE1	2.16	0.58
1:A:83:THR:HA	1:A:236:VAL:O	2.04	0.58
1:B:109:ASN:ND2	1:B:329:ARG:HH21	1.98	0.58
1:B:336:VAL:HG13	1:B:336:VAL:O	2.03	0.58
1:B:172:ILE:HG23	1:B:172:ILE:O	2.03	0.58
1:B:200:GLY:HA3	1:B:201:ILE:HG22	1.84	0.58
1:A:340:GLU:OE1	1:A:340:GLU:HA	2.04	0.58
1:C:213:ILE:C	1:C:214:MET:HG3	2.24	0.58
1:A:300:LEU:HD11	1:A:333:VAL:HG11	1.85	0.58
1:B:227:LEU:H	1:B:227:LEU:CD1	2.17	0.58
1:A:173:GLU:HB3	1:B:241:ARG:HB2	1.86	0.58
1:B:291:PHE:HB2	1:B:346:TRP:CB	2.29	0.58
1:C:172:ILE:HG23	1:C:172:ILE:O	2.03	0.58
1:C:291:PHE:HB2	1:C:346:TRP:CB	2.29	0.58
1:C:300:LEU:HB3	1:C:310:VAL:HG21	1.84	0.58
1:A:138:TYR:HE2	1:A:180:PRO:HA	1.68	0.58
1:B:83:THR:HA	1:B:236:VAL:O	2.03	0.58
1:C:95:LYS:HZ1	1:C:221:ALA:CA	2.15	0.58
1:C:296:PRO:HG3	1:C:337:THR:CB	2.27	0.58
1:A:336:VAL:O	1:A:336:VAL:HG13	2.03	0.58
1:A:172:ILE:O	1:A:172:ILE:HG23	2.03	0.58
1:B:280:PHE:HD2	1:B:331:GLN:O	1.86	0.58
1:C:138:TYR:HE2	1:C:180:PRO:HA	1.68	0.58
1:B:95:LYS:HZ3	1:B:225:ALA:N	1.88	0.58
1:C:179:VAL:HG21	1:C:181:TRP:CD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ALA:HA	1:A:318:SER:HB2	1.84	0.58
1:A:302:ASN:CB	1:A:333:VAL:HG22	2.34	0.58
1:B:179:VAL:CG1	1:B:181:TRP:HD1	2.14	0.58
1:B:138:TYR:HD2	1:B:184:PHE:CE1	2.16	0.58
1:B:326:VAL:CG1	1:B:327:ALA:O	2.48	0.58
1:C:105:THR:HG1	1:C:211:LYS:CD	1.86	0.58
1:C:315:ALA:HA	1:C:318:SER:HB2	1.84	0.58
1:C:342:PRO:C	1:C:343:LYS:HD3	2.23	0.58
1:A:105:THR:HG1	1:A:211:LYS:HD3	0.75	0.57
1:B:138:TYR:HE2	1:B:180:PRO:HA	1.68	0.57
1:B:95:LYS:HZ1	1:B:221:ALA:CB	2.17	0.57
1:C:160:LYS:O	1:C:328:GLU:CD	2.41	0.57
1:C:340:GLU:OE1	1:C:340:GLU:HA	2.04	0.57
1:A:227:LEU:CD1	1:A:227:LEU:H	2.17	0.57
1:B:302:ASN:CB	1:B:333:VAL:HG22	2.34	0.57
1:C:302:ASN:CB	1:C:333:VAL:HG22	2.34	0.57
1:B:338:THR:HG1	1:B:339:GLU:HB2	1.69	0.57
1:C:336:VAL:O	1:C:336:VAL:HG13	2.03	0.57
1:A:170:TYR:HE1	1:A:217:TYR:OH	1.87	0.57
1:B:151:ALA:CA	1:B:177:SER:HB2	2.17	0.57
1:B:238:LEU:CD1	1:B:238:LEU:N	2.67	0.57
1:C:112:GLU:O	1:C:113:PRO:C	2.41	0.57
1:C:217:TYR:CD1	1:C:217:TYR:N	2.69	0.57
1:A:95:LYS:HZ1	1:A:221:ALA:HB1	1.67	0.57
1:C:185:ILE:HD12	1:C:186:LEU:H	0.65	0.57
1:A:213:ILE:C	1:A:214:MET:HG3	2.24	0.57
1:B:136:PHE:HB3	1:B:230:VAL:HG11	1.87	0.57
1:C:163:PRO:C	1:C:164:ASN:ND2	2.44	0.57
1:C:238:LEU:N	1:C:238:LEU:CD1	2.67	0.57
1:A:230:VAL:HG12	1:A:231:ARG:H	1.68	0.57
1:A:238:LEU:CD1	1:A:238:LEU:N	2.67	0.57
1:C:136:PHE:HB3	1:C:230:VAL:HG11	1.87	0.57
1:B:248:ALA:N	1:B:265:TRP:CH2	2.65	0.57
1:A:136:PHE:HB3	1:A:230:VAL:HG11	1.87	0.57
1:A:179:VAL:CG1	1:A:181:TRP:HD1	2.14	0.57
1:B:163:PRO:C	1:B:164:ASN:ND2	2.44	0.57
1:C:280:PHE:HD2	1:C:331:GLN:O	1.86	0.57
1:A:154:PHE:CD1	1:A:155:ASP:C	2.78	0.57
1:A:258:ASP:CG	1:A:259:GLY:N	2.58	0.57
1:C:83:THR:HA	1:C:236:VAL:O	2.03	0.57
1:C:250:ILE:HA	1:C:347:GLN:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PHE:HB2	1:A:346:TRP:CB	2.29	0.57
1:B:124:ALA:CB	1:B:245:THR:HG21	2.35	0.57
1:C:198:ALA:HB1	1:C:200:GLY:C	2.14	0.57
1:C:61:PRO:HD2	1:C:181:TRP:HZ3	1.67	0.57
1:C:78:ALA:O	1:C:80:ASP:CA	2.52	0.57
1:A:250:ILE:HA	1:A:347:GLN:HA	1.87	0.57
1:A:160:LYS:NZ	1:B:199:ASP:CB	2.68	0.57
1:B:149:LYS:CE	1:B:151:ALA:HA	2.35	0.57
1:B:300:LEU:HD11	1:B:333:VAL:HG11	1.85	0.57
1:C:152:LEU:CD1	1:C:184:PHE:HE2	2.18	0.57
1:A:124:ALA:CB	1:A:245:THR:HG21	2.35	0.56
1:B:152:LEU:HD12	1:B:184:PHE:HE2	1.70	0.56
1:C:154:PHE:CD1	1:C:155:ASP:C	2.78	0.56
1:C:138:TYR:HA	1:C:230:VAL:HG22	1.86	0.56
1:C:302:ASN:HB2	1:C:333:VAL:HG22	1.87	0.56
1:A:326:VAL:CG1	1:A:327:ALA:O	2.48	0.56
1:B:105:THR:HG1	1:B:211:LYS:HD3	0.74	0.56
1:B:258:ASP:CG	1:B:259:GLY:N	2.58	0.56
1:B:86:GLY:N	1:B:234:TYR:CE1	2.74	0.56
1:C:111:SER:HA	1:C:350:ARG:HH12	1.69	0.56
1:C:179:VAL:CG1	1:C:181:TRP:HD1	2.14	0.56
1:C:265:TRP:CH2	1:C:348:ALA:O	2.52	0.56
1:A:138:TYR:HA	1:A:230:VAL:HG22	1.86	0.56
1:B:152:LEU:CD1	1:B:184:PHE:HE2	2.18	0.56
1:A:152:LEU:CD1	1:A:184:PHE:HE2	2.18	0.56
1:B:250:ILE:HA	1:B:347:GLN:HA	1.87	0.56
1:B:213:ILE:C	1:B:214:MET:HG3	2.24	0.56
1:A:120:ILE:CD1	1:A:350:ARG:CZ	2.83	0.56
1:A:120:ILE:O	1:A:120:ILE:HG13	2.05	0.56
1:B:290:LEU:HD12	1:B:290:LEU:C	2.26	0.56
1:C:198:ALA:CA	1:C:200:GLY:O	2.54	0.56
1:A:198:ALA:HB1	1:A:200:GLY:C	2.14	0.56
1:B:154:PHE:CD1	1:B:155:ASP:C	2.78	0.56
1:B:162:PRO:C	1:B:163:PRO:O	2.42	0.56
1:A:156:ARG:NH1	1:B:240:ASN:HB3	2.20	0.56
1:C:285:ASN:HD22	1:C:286:PHE:N	2.04	0.56
1:B:138:TYR:HA	1:B:230:VAL:HG22	1.86	0.56
1:B:198:ALA:HB1	1:B:200:GLY:C	2.14	0.56
1:B:285:ASN:HD22	1:B:286:PHE:N	2.03	0.56
1:C:82:ILE:CG2	1:C:238:LEU:HB2	2.32	0.56
1:A:300:LEU:HD12	1:A:333:VAL:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:O	1:B:120:ILE:HG13	2.05	0.56
1:B:170:TYR:HE1	1:B:217:TYR:OH	1.86	0.56
1:A:240:ASN:CG	1:C:156:ARG:CZ	2.74	0.56
1:C:112:GLU:O	1:C:283:THR:O	2.23	0.56
1:C:124:ALA:CB	1:C:245:THR:HG21	2.35	0.56
1:C:201:ILE:HA	1:C:281:LEU:HD23	1.67	0.56
1:A:145:THR:O	1:A:145:THR:CG2	2.54	0.56
1:A:116:PHE:HE2	1:A:234:TYR:CE2	2.24	0.56
1:A:152:LEU:HD12	1:A:184:PHE:HE2	1.71	0.56
1:B:230:VAL:HG12	1:B:231:ARG:H	1.68	0.56
1:C:152:LEU:HD12	1:C:184:PHE:HE2	1.70	0.56
1:C:153:ALA:HB1	1:C:174:GLY:HA3	0.62	0.56
1:A:163:PRO:C	1:A:164:ASN:ND2	2.44	0.56
1:A:198:ALA:CA	1:A:200:GLY:O	2.54	0.56
1:A:290:LEU:C	1:A:290:LEU:HD12	2.26	0.56
1:B:104:THR:O	1:B:105:THR:O	2.24	0.56
1:B:117:ASN:HA	1:B:284:GLY:C	2.27	0.56
1:C:149:LYS:CE	1:C:151:ALA:HA	2.35	0.56
1:A:104:THR:O	1:A:105:THR:O	2.24	0.55
1:B:121:LYS:CD	1:B:351:ILE:OXT	2.51	0.55
1:B:198:ALA:CA	1:B:200:GLY:O	2.54	0.55
1:B:112:GLU:CB	1:B:329:ARG:HE	2.19	0.55
1:B:302:ASN:HB2	1:B:333:VAL:HG22	1.87	0.55
1:C:277:ASP:HA	1:C:334:LYS:NZ	2.21	0.55
1:C:289:THR:HG23	1:C:321:TRP:CZ3	2.41	0.55
1:C:277:ASP:HA	1:C:334:LYS:HZ2	1.71	0.55
1:B:145:THR:O	1:B:145:THR:CG2	2.54	0.55
1:C:145:THR:CG2	1:C:145:THR:O	2.54	0.55
1:A:156:ARG:CD	1:B:240:ASN:HB3	2.36	0.55
1:A:156:ARG:HG2	1:B:240:ASN:OD1	2.05	0.55
1:A:149:LYS:CD	1:A:177:SER:OG	2.50	0.55
1:A:277:ASP:HA	1:A:334:LYS:HZ2	1.71	0.55
1:C:300:LEU:HD11	1:C:333:VAL:HG11	1.85	0.55
1:A:302:ASN:HB2	1:A:333:VAL:HG22	1.88	0.55
1:A:120:ILE:CB	1:A:350:ARG:NH2	2.58	0.55
1:C:111:SER:HA	1:C:350:ARG:NH1	2.21	0.55
1:C:300:LEU:CA	1:C:308:PHE:HZ	2.19	0.55
1:A:277:ASP:HA	1:A:334:LYS:NZ	2.21	0.55
1:B:277:ASP:HA	1:B:334:LYS:NZ	2.21	0.55
1:C:104:THR:O	1:C:105:THR:O	2.24	0.55
1:C:120:ILE:HG13	1:C:120:ILE:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:LEU:H	1:C:227:LEU:CD1	2.17	0.55
1:C:258:ASP:CG	1:C:259:GLY:N	2.58	0.55
1:A:291:PHE:CE1	1:A:335:MET:CE	2.90	0.55
1:A:300:LEU:CA	1:A:308:PHE:HZ	2.19	0.55
1:C:77:THR:CG2	1:C:78:ALA:N	2.49	0.55
1:A:274:TRP:CD1	1:A:339:GLU:C	2.80	0.55
1:B:109:ASN:HB3	1:B:329:ARG:NH2	2.22	0.55
1:B:295:ALA:N	1:B:316:ALA:CA	2.40	0.55
1:B:300:LEU:CA	1:B:308:PHE:HZ	2.19	0.55
1:C:162:PRO:C	1:C:163:PRO:O	2.42	0.55
1:C:274:TRP:CD1	1:C:339:GLU:C	2.80	0.55
1:A:153:ALA:HB1	1:A:174:GLY:HA3	0.62	0.55
1:B:126:TYR:C	1:B:242:THR:CG2	2.76	0.55
1:B:300:LEU:CB	1:B:308:PHE:HZ	2.20	0.55
1:C:116:PHE:HE2	1:C:234:TYR:CE2	2.24	0.55
1:C:291:PHE:CE1	1:C:335:MET:CE	2.90	0.55
1:C:297:VAL:HB	1:C:336:VAL:CG1	1.98	0.55
1:B:185:ILE:HD12	1:B:186:LEU:H	0.65	0.55
1:B:300:LEU:HD12	1:B:333:VAL:CG1	2.36	0.55
1:C:300:LEU:CB	1:C:308:PHE:HZ	2.20	0.55
1:C:326:VAL:CG1	1:C:327:ALA:O	2.48	0.55
1:B:341:GLN:O	1:B:343:LYS:HG2	2.07	0.55
1:A:97:THR:O	1:A:97:THR:OG1	2.25	0.55
1:A:126:TYR:C	1:A:242:THR:CG2	2.75	0.55
1:B:133:SER:HB3	1:B:235:THR:CG2	2.35	0.55
1:C:290:LEU:C	1:C:290:LEU:HD12	2.26	0.55
1:A:285:ASN:HD22	1:A:286:PHE:N	2.03	0.54
1:B:113:PRO:HB2	1:B:326:VAL:HB	1.89	0.54
1:B:95:LYS:HZ2	1:B:221:ALA:CA	2.07	0.54
1:B:291:PHE:CE1	1:B:335:MET:CE	2.90	0.54
1:C:116:PHE:HB2	1:C:350:ARG:NH2	2.22	0.54
1:A:136:PHE:CZ	1:A:212:LEU:CD2	2.91	0.54
1:B:116:PHE:HE2	1:B:234:TYR:CE2	2.24	0.54
1:B:289:THR:HG23	1:B:321:TRP:CZ3	2.42	0.54
1:C:100:GLU:O	1:C:101:PRO:O	2.25	0.54
1:C:197:VAL:HG22	1:C:198:ALA:H	1.72	0.54
1:C:248:ALA:HA	1:C:265:TRP:CH2	2.43	0.54
1:A:86:GLY:N	1:A:234:TYR:CE1	2.74	0.54
1:B:107:VAL:CB	1:B:328:GLU:CG	2.76	0.54
1:B:197:VAL:HG22	1:B:198:ALA:N	2.23	0.54
1:C:197:VAL:HG22	1:C:198:ALA:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ARG:O	1:C:209:PHE:O	2.26	0.54
1:C:95:LYS:HZ2	1:C:221:ALA:CB	2.20	0.54
1:C:86:GLY:N	1:C:234:TYR:CE1	2.74	0.54
1:B:274:TRP:CD1	1:B:339:GLU:C	2.80	0.54
1:C:274:TRP:CD1	1:C:339:GLU:HA	2.42	0.54
1:A:156:ARG:O	1:A:209:PHE:O	2.26	0.54
1:B:277:ASP:HA	1:B:334:LYS:HZ2	1.72	0.54
1:C:107:VAL:CG2	1:C:329:ARG:HE	2.21	0.54
1:A:304:ASP:CG	1:A:332:GLY:H	2.11	0.54
1:B:136:PHE:CZ	1:B:212:LEU:CD2	2.91	0.54
1:B:154:PHE:CD1	1:B:155:ASP:CA	2.90	0.54
1:B:153:ALA:HB1	1:B:174:GLY:HA3	0.62	0.54
1:B:82:ILE:CG2	1:B:238:LEU:HB2	2.32	0.54
1:A:156:ARG:CD	1:B:240:ASN:CG	2.75	0.54
1:B:107:VAL:N	1:B:328:GLU:OE1	2.40	0.54
1:C:306:SER:HB2	1:C:325:LYS:H	1.72	0.54
1:C:304:ASP:CG	1:C:332:GLY:H	2.11	0.54
1:A:306:SER:HB2	1:A:325:LYS:H	1.72	0.54
1:A:109:ASN:CA	1:A:129:TYR:OH	2.55	0.54
1:B:130:ARG:O	1:B:131:PHE:HB2	2.08	0.54
1:B:191:ASP:OD1	1:B:209:PHE:CZ	2.61	0.54
1:C:191:ASP:OD1	1:C:209:PHE:CZ	2.61	0.54
1:C:126:TYR:C	1:C:242:THR:CG2	2.75	0.54
1:B:306:SER:HB2	1:B:325:LYS:H	1.72	0.54
1:A:130:ARG:O	1:A:131:PHE:HB2	2.08	0.54
1:A:149:LYS:CE	1:A:151:ALA:HA	2.35	0.54
1:A:197:VAL:HG22	1:A:198:ALA:N	2.23	0.54
1:A:300:LEU:O	1:A:308:PHE:CZ	2.61	0.54
1:B:265:TRP:CH2	1:B:348:ALA:O	2.52	0.54
1:A:120:ILE:CG1	1:A:350:ARG:CZ	2.60	0.54
1:C:95:LYS:NZ	1:C:221:ALA:HB1	2.22	0.54
1:C:300:LEU:HD12	1:C:333:VAL:CG1	2.36	0.54
1:B:274:TRP:CD1	1:B:339:GLU:HA	2.42	0.54
1:C:213:ILE:O	1:C:214:MET:CG	2.56	0.54
1:A:276:HIS:CG	1:A:277:ASP:N	2.74	0.54
1:A:300:LEU:CB	1:A:308:PHE:HZ	2.20	0.54
1:C:133:SER:HB3	1:C:235:THR:CG2	2.35	0.54
1:C:138:TYR:HD2	1:C:184:PHE:CE1	2.16	0.54
1:C:90:ILE:CG2	1:C:90:ILE:O	2.54	0.54
1:A:341:GLN:O	1:A:343:LYS:HG2	2.07	0.54
1:C:97:THR:OG1	1:C:97:THR:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASP:OD1	1:A:209:PHE:CZ	2.61	0.54
1:A:289:THR:HG23	1:A:321:TRP:CZ3	2.41	0.54
1:B:156:ARG:O	1:B:209:PHE:O	2.26	0.54
1:B:276:HIS:CG	1:B:277:ASP:N	2.74	0.54
1:C:173:GLU:HG3	1:C:174:GLY:H	1.73	0.54
1:C:339:GLU:O	1:C:340:GLU:HA	2.08	0.54
1:A:100:GLU:O	1:A:101:PRO:O	2.25	0.53
1:A:179:VAL:HG22	1:A:180:PRO:N	2.23	0.53
1:A:197:VAL:HG22	1:A:198:ALA:H	1.72	0.53
1:A:85:SER:C	1:A:234:TYR:CD1	2.82	0.53
1:B:179:VAL:HG22	1:B:180:PRO:N	2.23	0.53
1:C:170:TYR:HE1	1:C:217:TYR:OH	1.86	0.53
1:C:326:VAL:CG1	1:C:327:ALA:N	2.19	0.53
1:C:85:SER:C	1:C:234:TYR:CD1	2.82	0.53
1:C:199:ASP:N	1:C:199:ASP:OD1	2.40	0.53
1:A:133:SER:HB3	1:A:235:THR:CG2	2.35	0.53
1:B:244:SER:O	1:B:245:THR:HB	2.08	0.53
1:B:95:LYS:NZ	1:B:221:ALA:HB1	2.22	0.53
1:C:313:GLU:HB2	1:C:314:ALA:C	2.29	0.53
1:A:265:TRP:CH2	1:A:348:ALA:O	2.52	0.53
1:A:274:TRP:CD1	1:A:339:GLU:HA	2.42	0.53
1:A:293:GLU:HA	1:A:317:GLY:HA2	1.91	0.53
1:B:293:GLU:HA	1:B:317:GLY:HA2	1.90	0.53
1:B:304:ASP:CG	1:B:332:GLY:H	2.11	0.53
1:B:300:LEU:O	1:B:308:PHE:CZ	2.61	0.53
1:C:341:GLN:O	1:C:343:LYS:HG2	2.08	0.53
1:A:339:GLU:O	1:A:340:GLU:HA	2.08	0.53
1:A:199:ASP:OD1	1:A:199:ASP:N	2.40	0.53
1:B:113:PRO:HG3	1:B:120:ILE:CD1	2.39	0.53
1:B:85:SER:C	1:B:234:TYR:CD1	2.82	0.53
1:C:276:HIS:CG	1:C:277:ASP:N	2.74	0.53
1:B:213:ILE:O	1:B:214:MET:CG	2.56	0.53
1:A:120:ILE:CG2	1:A:350:ARG:HH21	2.20	0.53
1:A:156:ARG:CZ	1:B:240:ASN:CG	2.77	0.53
1:A:82:ILE:CG2	1:A:238:LEU:HB2	2.32	0.53
1:A:244:SER:O	1:A:245:THR:HB	2.08	0.53
1:B:100:GLU:O	1:B:101:PRO:O	2.25	0.53
1:C:269:LYS:HB3	1:C:277:ASP:OD2	2.09	0.53
1:B:271:THR:CG2	1:B:275:GLU:OE2	2.56	0.53
1:B:149:LYS:HE2	1:B:151:ALA:CB	2.39	0.53
1:B:179:VAL:HG13	1:B:182:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:SER:HB3	1:B:227:LEU:O	2.09	0.53
1:B:269:LYS:HB3	1:B:277:ASP:OD2	2.09	0.53
1:C:300:LEU:O	1:C:308:PHE:CZ	2.61	0.53
1:A:271:THR:CG2	1:A:275:GLU:OE2	2.56	0.53
1:B:197:VAL:HG22	1:B:198:ALA:H	1.72	0.53
1:C:113:PRO:HG2	1:C:350:ARG:CA	2.16	0.53
1:C:130:ARG:O	1:C:131:PHE:HB2	2.08	0.53
1:C:179:VAL:HG22	1:C:180:PRO:N	2.23	0.53
1:C:179:VAL:HG13	1:C:181:TRP:CD1	2.38	0.53
1:C:269:LYS:CG	1:C:270:GLY:N	2.58	0.53
1:B:339:GLU:O	1:B:340:GLU:OE1	2.27	0.53
1:B:339:GLU:O	1:B:340:GLU:HA	2.08	0.53
1:C:271:THR:CG2	1:C:275:GLU:OE2	2.56	0.53
1:A:149:LYS:HE2	1:A:151:ALA:CB	2.39	0.53
1:A:269:LYS:HB3	1:A:277:ASP:OD2	2.09	0.53
1:A:313:GLU:HB2	1:A:314:ALA:C	2.29	0.53
1:B:120:ILE:CA	1:B:350:ARG:NH2	2.66	0.53
1:C:142:SER:HB3	1:C:227:LEU:O	2.09	0.53
1:C:82:ILE:HG12	1:C:83:THR:N	2.24	0.53
1:A:119:LEU:HD23	1:A:234:TYR:CE2	2.43	0.53
1:A:162:PRO:C	1:A:163:PRO:O	2.42	0.53
1:A:101:PRO:CG	1:A:217:TYR:CE2	2.74	0.53
1:A:95:LYS:NZ	1:A:221:ALA:HB1	2.22	0.53
1:B:315:ALA:HB1	1:B:318:SER:HB3	1.72	0.53
1:C:136:PHE:CZ	1:C:212:LEU:CD2	2.91	0.53
1:B:112:GLU:HB3	1:B:115:THR:CG2	2.40	0.52
1:B:173:GLU:HG3	1:B:174:GLY:H	1.73	0.52
1:B:199:ASP:N	1:B:199:ASP:OD1	2.40	0.52
1:B:300:LEU:CG	1:B:308:PHE:HZ	2.20	0.52
1:B:82:ILE:HD12	1:B:126:TYR:CE2	2.44	0.52
1:C:109:ASN:CA	1:C:129:TYR:OH	2.55	0.52
1:C:179:VAL:CG1	1:C:182:THR:HG22	2.39	0.52
1:A:142:SER:HB3	1:A:227:LEU:O	2.09	0.52
1:B:101:PRO:CG	1:B:217:TYR:CE2	2.74	0.52
1:B:129:TYR:CA	1:B:237:GLN:O	2.57	0.52
1:B:295:ALA:HB1	1:B:314:ALA:C	2.30	0.52
1:B:350:ARG:O	1:B:351:ILE:CB	2.53	0.52
1:C:112:GLU:HB3	1:C:115:THR:CG2	2.39	0.52
1:A:113:PRO:HG3	1:A:120:ILE:CD1	2.39	0.52
1:A:112:GLU:HB3	1:A:115:THR:CG2	2.39	0.52
1:B:109:ASN:CA	1:B:129:TYR:OH	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:CB	1:B:185:ILE:HD11	2.38	0.52
1:B:152:LEU:HD12	1:B:184:PHE:CE2	2.45	0.52
1:C:135:ARG:CB	1:C:185:ILE:HD11	2.38	0.52
1:A:248:ALA:O	1:A:263:VAL:CA	2.52	0.52
1:A:82:ILE:HG12	1:A:83:THR:N	2.24	0.52
1:A:94:LYS:O	1:A:95:LYS:C	2.48	0.52
1:B:84:ARG:HG3	1:B:119:LEU:HD11	1.91	0.52
1:B:185:ILE:CD1	1:B:186:LEU:O	2.58	0.52
1:B:236:VAL:CG1	1:B:237:GLN:H	2.23	0.52
1:B:285:ASN:HD22	1:B:286:PHE:H	1.58	0.52
1:C:293:GLU:HA	1:C:317:GLY:HA2	1.91	0.52
1:C:78:ALA:O	1:C:81:GLY:N	2.42	0.52
1:C:339:GLU:O	1:C:340:GLU:OE1	2.27	0.52
1:A:213:ILE:O	1:A:214:MET:CG	2.56	0.52
1:A:113:PRO:HG2	1:A:283:THR:H	0.49	0.52
1:A:300:LEU:CG	1:A:308:PHE:HZ	2.20	0.52
1:A:304:ASP:OD2	1:A:332:GLY:N	2.43	0.52
1:A:82:ILE:HD12	1:A:126:TYR:CE2	2.44	0.52
1:C:128:LYS:O	1:C:129:TYR:HB3	2.10	0.52
1:C:149:LYS:CD	1:C:177:SER:OG	2.50	0.52
1:C:152:LEU:HD12	1:C:184:PHE:CE2	2.45	0.52
1:C:154:PHE:CB	1:C:212:LEU:HD12	2.35	0.52
1:C:71:THR:CG2	1:C:87:SER:CB	2.77	0.52
1:C:94:LYS:O	1:C:95:LYS:C	2.48	0.52
1:A:179:VAL:HG13	1:A:182:THR:HG22	1.90	0.52
1:B:94:LYS:O	1:B:95:LYS:C	2.48	0.52
1:C:126:TYR:C	1:C:242:THR:HG22	2.30	0.52
1:C:350:ARG:O	1:C:351:ILE:CB	2.53	0.52
1:A:160:LYS:HD3	1:B:199:ASP:CB	2.36	0.52
1:A:185:ILE:CD1	1:A:186:LEU:O	2.58	0.52
1:A:129:TYR:CA	1:A:237:GLN:O	2.57	0.52
1:A:239:LYS:O	1:A:240:ASN:O	2.28	0.52
1:C:239:LYS:O	1:C:240:ASN:O	2.28	0.52
1:C:54:LYS:O	1:C:55:VAL:HB	2.08	0.52
1:A:285:ASN:HD22	1:A:286:PHE:H	1.58	0.52
1:B:239:LYS:O	1:B:240:ASN:O	2.28	0.52
1:B:313:GLU:HB2	1:B:314:ALA:C	2.29	0.52
1:C:113:PRO:HG3	1:C:120:ILE:CD1	2.39	0.52
1:C:82:ILE:HD12	1:C:126:TYR:CE2	2.44	0.52
1:C:304:ASP:OD2	1:C:332:GLY:N	2.43	0.52
1:A:248:ALA:HB2	1:A:265:TRP:CE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PRO:HG2	1:A:283:THR:CA	2.35	0.52
1:A:152:LEU:HD12	1:A:184:PHE:CE2	2.45	0.52
1:B:119:LEU:HD23	1:B:234:TYR:CE2	2.43	0.52
1:B:300:LEU:O	1:B:308:PHE:CE2	2.63	0.52
1:B:304:ASP:OD2	1:B:332:GLY:N	2.43	0.52
1:C:149:LYS:HE2	1:C:151:ALA:CB	2.39	0.52
1:C:125:GLN:C	1:C:242:THR:HG23	2.30	0.52
1:A:126:TYR:C	1:A:242:THR:HG22	2.30	0.52
1:A:295:ALA:N	1:A:316:ALA:CA	2.40	0.52
1:B:136:PHE:HB3	1:B:230:VAL:CG1	2.40	0.52
1:B:221:ALA:O	1:B:225:ALA:HB2	2.10	0.52
1:A:84:ARG:HG3	1:A:119:LEU:HD11	1.91	0.51
1:A:125:GLN:C	1:A:242:THR:HG23	2.30	0.51
1:B:179:VAL:CG1	1:B:182:THR:HG22	2.39	0.51
1:B:125:GLN:C	1:B:242:THR:HG23	2.30	0.51
1:C:166:LEU:C	1:C:168:SER:N	2.61	0.51
1:C:179:VAL:HG13	1:C:182:THR:HG22	1.90	0.51
1:C:300:LEU:O	1:C:308:PHE:CE2	2.63	0.51
1:C:84:ARG:HG3	1:C:119:LEU:HD11	1.91	0.51
1:A:136:PHE:HB3	1:A:230:VAL:CG1	2.40	0.51
1:B:100:GLU:O	1:B:101:PRO:C	2.48	0.51
1:C:185:ILE:CD1	1:C:186:LEU:O	2.58	0.51
1:C:236:VAL:CG1	1:C:237:GLN:H	2.23	0.51
1:C:244:SER:O	1:C:245:THR:HB	2.08	0.51
1:C:285:ASN:HD22	1:C:286:PHE:H	1.58	0.51
1:A:339:GLU:O	1:A:340:GLU:OE1	2.27	0.51
1:A:179:VAL:HG13	1:A:181:TRP:CD1	2.38	0.51
1:A:128:LYS:HG3	1:A:196:PHE:CD2	2.46	0.51
1:A:243:GLY:O	1:A:244:SER:HB2	2.11	0.51
1:A:113:PRO:CB	1:A:283:THR:HB	2.41	0.51
1:A:82:ILE:O	1:A:83:THR:OG1	2.18	0.51
1:B:144:SER:O	1:B:146:THR:N	2.44	0.51
1:B:103:TYR:CE1	1:B:169:LEU:HD12	2.43	0.51
1:C:138:TYR:CZ	1:C:150:VAL:HG21	2.45	0.51
1:C:83:THR:CB	1:C:130:ARG:HH12	2.24	0.51
1:C:56:THR:CG2	1:C:57:ARG:N	2.58	0.51
1:A:144:SER:O	1:A:146:THR:N	2.44	0.51
1:A:173:GLU:HG3	1:A:174:GLY:H	1.73	0.51
1:A:221:ALA:O	1:A:225:ALA:HB2	2.10	0.51
1:B:128:LYS:HG3	1:B:196:PHE:CD2	2.46	0.51
1:B:154:PHE:CB	1:B:212:LEU:HD12	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:H	1:B:241:ARG:CD	2.22	0.51
1:B:243:GLY:O	1:B:244:SER:HB2	2.11	0.51
1:B:93:LEU:HD12	1:B:138:TYR:HE1	1.75	0.51
1:C:154:PHE:CD1	1:C:155:ASP:CA	2.90	0.51
1:C:90:ILE:HD11	1:C:232:VAL:HG22	1.83	0.51
1:A:128:LYS:O	1:A:129:TYR:HB3	2.10	0.51
1:A:149:LYS:HD3	1:A:217:TYR:HE1	1.73	0.51
1:A:153:ALA:CA	1:A:174:GLY:HA3	2.33	0.51
1:A:103:TYR:CD1	1:A:215:ALA:HB2	2.46	0.51
1:A:236:VAL:CG1	1:A:237:GLN:H	2.23	0.51
1:A:93:LEU:HD12	1:A:138:TYR:HE1	1.75	0.51
1:C:136:PHE:HB3	1:C:230:VAL:CG1	2.40	0.51
1:C:295:ALA:HB1	1:C:314:ALA:C	2.30	0.51
1:A:179:VAL:CG1	1:A:182:THR:HG22	2.39	0.51
1:A:154:PHE:CB	1:A:212:LEU:HD12	2.35	0.51
1:A:95:LYS:HZ1	1:A:221:ALA:CB	2.22	0.51
1:A:160:LYS:HZ3	1:B:199:ASP:HB3	1.74	0.51
1:B:82:ILE:HG12	1:B:83:THR:N	2.24	0.51
1:C:230:VAL:CG1	1:C:231:ARG:N	2.74	0.51
1:A:103:TYR:CE1	1:A:169:LEU:HD12	2.43	0.51
1:C:188:VAL:O	1:C:188:VAL:CG2	2.59	0.51
1:C:149:LYS:HD3	1:C:217:TYR:HE1	1.73	0.51
1:C:221:ALA:O	1:C:225:ALA:HB2	2.10	0.51
1:C:313:GLU:CG	1:C:318:SER:HB2	2.19	0.51
1:B:337:THR:OG1	1:B:343:LYS:NZ	2.42	0.51
1:C:241:ARG:H	1:C:241:ARG:CD	2.22	0.51
1:A:241:ARG:H	1:A:241:ARG:CD	2.22	0.51
1:A:130:ARG:CB	1:A:237:GLN:N	2.74	0.51
1:A:151:ALA:HA	1:A:177:SER:CB	2.21	0.51
1:B:117:ASN:CB	1:B:285:ASN:N	2.67	0.51
1:B:101:PRO:CB	1:B:217:TYR:CD2	2.94	0.51
1:C:162:PRO:HD3	1:C:328:GLU:OE1	2.11	0.51
1:C:235:THR:O	1:C:235:THR:HG23	2.09	0.51
1:C:93:LEU:HD12	1:C:138:TYR:HE1	1.75	0.51
1:A:138:TYR:CZ	1:A:150:VAL:HG21	2.45	0.51
1:A:101:PRO:CB	1:A:217:TYR:CD2	2.94	0.51
1:A:96:ASN:C	1:A:98:ASP:N	2.55	0.51
1:B:83:THR:CB	1:B:130:ARG:HH12	2.24	0.51
1:C:243:GLY:O	1:C:244:SER:HB2	2.11	0.51
1:C:295:ALA:HB2	1:C:315:ALA:CB	2.37	0.51
1:A:300:LEU:O	1:A:308:PHE:CE2	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ALA:HB1	1:A:314:ALA:C	2.30	0.50
1:B:103:TYR:CD1	1:B:215:ALA:HB2	2.46	0.50
1:B:86:GLY:HA2	1:B:234:TYR:HE1	1.68	0.50
1:C:128:LYS:HG3	1:C:196:PHE:CD2	2.46	0.50
1:C:103:TYR:CD1	1:C:215:ALA:HB2	2.46	0.50
1:C:95:LYS:HZ1	1:C:221:ALA:HB1	1.75	0.50
1:A:116:PHE:CE2	1:A:234:TYR:CE2	3.00	0.50
1:B:128:LYS:O	1:B:129:TYR:HB3	2.10	0.50
1:B:279:HIS:HB3	1:B:280:PHE:N	2.27	0.50
1:C:85:SER:O	1:C:234:TYR:CE1	2.65	0.50
1:C:125:GLN:CA	1:C:243:GLY:HA2	2.27	0.50
1:A:107:VAL:HA	1:A:211:LYS:HA	1.93	0.50
1:A:90:ILE:CG2	1:A:90:ILE:O	2.54	0.50
1:B:138:TYR:CZ	1:B:150:VAL:HG21	2.45	0.50
1:C:314:ALA:O	1:C:315:ALA:HB3	2.11	0.50
1:B:153:ALA:CA	1:B:174:GLY:HA3	2.33	0.50
1:C:129:TYR:CA	1:C:237:GLN:O	2.57	0.50
1:C:279:HIS:HB3	1:C:280:PHE:N	2.26	0.50
1:C:300:LEU:CG	1:C:308:PHE:HZ	2.20	0.50
1:C:120:ILE:CG1	1:C:350:ARG:HH11	2.24	0.50
1:A:83:THR:CB	1:A:130:ARG:HH12	2.24	0.50
1:A:85:SER:O	1:A:234:TYR:CE1	2.65	0.50
1:B:116:PHE:CE2	1:B:234:TYR:CE2	3.00	0.50
1:B:156:ARG:HD3	1:C:240:ASN:CG	2.31	0.50
1:B:85:SER:O	1:B:234:TYR:CE1	2.65	0.50
1:C:144:SER:O	1:C:146:THR:N	2.44	0.50
1:A:248:ALA:HB2	1:A:249:GLN:NE2	2.25	0.50
1:A:157:ASP:OD1	1:A:157:ASP:C	2.50	0.50
1:A:130:ARG:CB	1:A:237:GLN:H	2.25	0.50
1:C:158:ALA:C	1:C:211:LYS:H	1.93	0.50
1:C:112:GLU:CA	1:C:350:ARG:NH2	2.74	0.50
1:A:154:PHE:CD1	1:A:155:ASP:CA	2.90	0.50
1:A:300:LEU:CB	1:A:308:PHE:CZ	2.95	0.50
1:B:130:ARG:CB	1:B:237:GLN:N	2.74	0.50
1:B:293:GLU:O	1:B:317:GLY:HA2	2.09	0.50
1:B:107:VAL:HA	1:B:211:LYS:HA	1.93	0.50
1:B:114:GLY:O	1:B:327:ALA:HA	2.08	0.50
1:B:130:ARG:CB	1:B:237:GLN:H	2.25	0.50
1:A:156:ARG:CG	1:B:240:ASN:OD1	2.60	0.50
1:C:101:PRO:CB	1:C:217:TYR:CD2	2.94	0.50
1:C:130:ARG:CB	1:C:237:GLN:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ALA:N	1:B:263:VAL:HG12	2.27	0.50
1:A:166:LEU:C	1:A:168:SER:N	2.61	0.50
1:B:136:PHE:HD1	1:B:231:ARG:O	1.95	0.50
1:B:235:THR:HG23	1:B:235:THR:O	2.09	0.50
1:B:288:LEU:C	1:B:289:THR:OG1	2.49	0.50
1:B:278:CYS:CA	1:B:334:LYS:HD3	2.42	0.50
1:B:291:PHE:CG	1:B:345:LYS:O	2.64	0.50
1:A:240:ASN:OD1	1:C:156:ARG:CD	2.60	0.49
1:A:295:ALA:HB2	1:A:315:ALA:CB	2.37	0.49
1:C:167:ALA:O	1:C:171:ASN:ND2	2.45	0.49
1:C:293:GLU:O	1:C:317:GLY:HA2	2.09	0.49
1:A:296:PRO:CD	1:A:337:THR:HG21	2.38	0.49
1:A:167:ALA:O	1:A:171:ASN:ND2	2.45	0.49
1:B:133:SER:O	1:B:234:TYR:CB	2.60	0.49
1:C:86:GLY:HA2	1:C:234:TYR:HE1	1.68	0.49
1:A:264:SER:OG	1:A:265:TRP:N	2.45	0.49
1:B:157:ASP:C	1:B:157:ASP:OD1	2.50	0.49
1:A:279:HIS:HB3	1:A:280:PHE:N	2.27	0.49
1:B:173:GLU:CG	1:B:174:GLY:N	2.72	0.49
1:B:188:VAL:CG2	1:B:188:VAL:O	2.59	0.49
1:B:277:ASP:CG	1:B:334:LYS:HZ3	2.16	0.49
1:C:153:ALA:CA	1:C:174:GLY:HA3	2.33	0.49
1:C:66:TYR:HE2	1:C:183:GLY:HA3	1.73	0.49
1:A:188:VAL:O	1:A:188:VAL:CG2	2.59	0.49
1:A:293:GLU:O	1:A:317:GLY:HA2	2.09	0.49
1:B:133:SER:N	1:B:235:THR:CG2	2.74	0.49
1:B:151:ALA:HA	1:B:177:SER:CB	2.21	0.49
1:C:150:VAL:CG2	1:C:227:LEU:HD23	2.43	0.49
1:A:150:VAL:CG2	1:A:227:LEU:HD23	2.43	0.49
1:A:156:ARG:NH1	1:B:240:ASN:CA	2.76	0.49
1:B:120:ILE:HG13	1:B:350:ARG:CZ	2.43	0.49
1:B:88:GLU:O	1:B:231:ARG:HB3	2.05	0.49
1:C:107:VAL:HA	1:C:211:LYS:HA	1.93	0.49
1:C:130:ARG:CB	1:C:237:GLN:H	2.25	0.49
1:C:151:ALA:HA	1:C:177:SER:CB	2.21	0.49
1:C:71:THR:OG1	1:C:87:SER:CB	2.59	0.49
1:A:133:SER:N	1:A:235:THR:CG2	2.74	0.49
1:A:136:PHE:HD1	1:A:231:ARG:O	1.95	0.49
1:A:235:THR:O	1:A:235:THR:HG23	2.09	0.49
1:C:112:GLU:CD	1:C:283:THR:O	2.49	0.49
1:C:290:LEU:HD23	1:C:346:TRP:HB2	1.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:O	1:B:347:GLN:CA	2.61	0.49
1:B:264:SER:OG	1:B:265:TRP:N	2.45	0.49
1:A:150:VAL:HG23	1:A:227:LEU:HD23	1.94	0.49
1:A:173:GLU:CG	1:A:174:GLY:N	2.72	0.49
1:A:230:VAL:CG1	1:A:231:ARG:N	2.74	0.49
1:A:288:LEU:C	1:A:289:THR:OG1	2.49	0.49
1:B:109:ASN:CB	1:B:329:ARG:NH2	2.76	0.49
1:B:150:VAL:CG2	1:B:227:LEU:HD23	2.43	0.49
1:B:167:ALA:O	1:B:171:ASN:ND2	2.45	0.49
1:B:244:SER:C	1:B:245:THR:HG22	2.31	0.49
1:B:300:LEU:CB	1:B:308:PHE:CZ	2.95	0.49
1:C:150:VAL:HG23	1:C:227:LEU:HD23	1.94	0.49
1:C:291:PHE:CG	1:C:345:LYS:O	2.64	0.49
1:C:85:SER:O	1:C:234:TYR:HE1	1.96	0.49
1:A:101:PRO:CG	1:A:217:TYR:HD2	2.26	0.49
1:B:150:VAL:HG23	1:B:227:LEU:HD23	1.94	0.49
1:B:85:SER:O	1:B:234:TYR:HE1	1.96	0.49
1:A:240:ASN:HB3	1:C:156:ARG:NH1	2.28	0.49
1:A:163:PRO:HB2	1:A:165:ASP:N	2.28	0.49
1:A:291:PHE:C	1:A:292:TYR:HB3	2.33	0.49
1:B:107:VAL:O	1:B:115:THR:CG2	2.56	0.49
1:B:152:LEU:O	1:B:186:LEU:CD1	2.55	0.49
1:C:157:ASP:OD1	1:C:157:ASP:C	2.50	0.49
1:C:116:PHE:CE2	1:C:234:TYR:CE2	3.00	0.49
1:C:100:GLU:O	1:C:101:PRO:C	2.48	0.49
1:C:133:SER:O	1:C:234:TYR:CB	2.60	0.49
1:C:241:ARG:CD	1:C:241:ARG:N	2.75	0.49
1:B:163:PRO:HB2	1:B:165:ASP:N	2.28	0.48
1:B:242:THR:CG2	1:B:243:GLY:H	2.22	0.48
1:B:290:LEU:HD23	1:B:346:TRP:HB2	1.90	0.48
1:C:107:VAL:CG1	1:C:329:ARG:NH2	2.72	0.48
1:C:109:ASN:O	1:C:110:PRO:C	2.51	0.48
1:C:119:LEU:HD23	1:C:234:TYR:CE2	2.43	0.48
1:C:278:CYS:CA	1:C:334:LYS:HD3	2.42	0.48
1:B:244:SER:OG	1:B:245:THR:N	2.46	0.48
1:B:92:THR:HG23	1:B:93:LEU:O	2.14	0.48
1:C:264:SER:OG	1:C:265:TRP:N	2.45	0.48
1:C:249:GLN:NE2	1:C:265:TRP:N	2.54	0.48
1:C:291:PHE:C	1:C:292:TYR:HB3	2.33	0.48
1:A:249:GLN:O	1:A:347:GLN:CA	2.61	0.48
1:A:105:THR:HG23	1:A:105:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HH11	1:A:236:VAL:C	2.16	0.48
1:A:244:SER:OG	1:A:245:THR:N	2.46	0.48
1:A:92:THR:HG23	1:A:93:LEU:O	2.14	0.48
1:B:333:VAL:C	1:B:334:LYS:CD	2.78	0.48
1:B:248:ALA:N	1:B:265:TRP:CZ3	2.82	0.48
1:C:336:VAL:O	1:C:337:THR:CG2	2.62	0.48
1:A:248:ALA:HB2	1:A:265:TRP:CD2	2.48	0.48
1:B:150:VAL:O	1:B:151:ALA:C	2.52	0.48
1:B:166:LEU:C	1:B:168:SER:N	2.61	0.48
1:B:126:TYR:C	1:B:242:THR:HG22	2.30	0.48
1:C:300:LEU:CB	1:C:308:PHE:CZ	2.95	0.48
1:C:339:GLU:O	1:C:340:GLU:CA	2.60	0.48
1:A:135:ARG:CB	1:A:185:ILE:HD11	2.38	0.48
1:A:85:SER:O	1:A:234:TYR:HE1	1.96	0.48
1:B:106:ALA:HA	1:B:328:GLU:HB3	1.96	0.48
1:B:130:ARG:HH11	1:B:236:VAL:C	2.16	0.48
1:C:107:VAL:O	1:C:115:THR:CG2	2.56	0.48
1:C:103:TYR:CE1	1:C:169:LEU:HD12	2.43	0.48
1:C:101:PRO:CG	1:C:217:TYR:CE2	2.74	0.48
1:C:83:THR:HG23	1:C:130:ARG:CZ	2.44	0.48
1:C:84:ARG:HD2	1:C:119:LEU:HD13	1.94	0.48
1:C:336:VAL:O	1:C:337:THR:HG23	2.14	0.48
1:C:204:PRO:N	1:C:205:LYS:HD2	2.28	0.48
1:A:150:VAL:O	1:A:151:ALA:C	2.52	0.48
1:A:179:VAL:CG2	1:A:181:TRP:CD1	2.93	0.48
1:B:105:THR:HG23	1:B:105:THR:O	2.14	0.48
1:B:84:ARG:HD2	1:B:119:LEU:HD13	1.94	0.48
1:C:163:PRO:CG	1:C:168:SER:CB	2.92	0.48
1:B:204:PRO:N	1:B:205:LYS:HD2	2.28	0.48
1:B:141:MET:CG	1:B:141:MET:O	2.46	0.48
1:A:83:THR:HG23	1:A:130:ARG:CZ	2.44	0.48
1:A:291:PHE:CG	1:A:345:LYS:O	2.64	0.48
1:B:88:GLU:OE2	1:B:118:GLN:HB3	2.13	0.48
1:B:291:PHE:C	1:B:292:TYR:HB3	2.33	0.48
1:B:83:THR:HG23	1:B:130:ARG:CZ	2.44	0.48
1:C:150:VAL:O	1:C:151:ALA:C	2.52	0.48
1:C:136:PHE:HD1	1:C:231:ARG:O	1.95	0.48
1:C:120:ILE:CD1	1:C:350:ARG:HB3	2.42	0.48
1:C:111:SER:HB3	1:C:197:VAL:CG2	2.44	0.48
1:C:163:PRO:HB2	1:C:165:ASP:N	2.28	0.48
1:C:88:GLU:OE2	1:C:118:GLN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:SER:HB3	1:A:197:VAL:CG2	2.44	0.48
1:A:290:LEU:HB2	1:A:346:TRP:HA	1.96	0.48
1:C:107:VAL:CG2	1:C:283:THR:HG21	2.37	0.48
1:B:336:VAL:O	1:B:337:THR:CG2	2.62	0.48
1:A:120:ILE:HG23	1:A:350:ARG:HH22	1.73	0.48
1:A:84:ARG:HD2	1:A:119:LEU:HD13	1.94	0.48
1:A:88:GLU:OE2	1:A:118:GLN:HB3	2.14	0.48
1:B:144:SER:HA	1:B:181:TRP:HB3	1.96	0.48
1:B:230:VAL:CG1	1:B:231:ARG:N	2.74	0.48
1:A:156:ARG:NH1	1:B:240:ASN:HA	2.29	0.48
1:B:296:PRO:CD	1:B:337:THR:HG21	2.39	0.48
1:A:336:VAL:O	1:A:337:THR:CG2	2.62	0.48
1:A:203:ASP:OD1	1:A:205:LYS:CG	2.56	0.48
1:B:163:PRO:CG	1:B:168:SER:HB3	2.44	0.47
1:B:90:ILE:O	1:B:90:ILE:CG2	2.54	0.47
1:C:244:SER:OG	1:C:245:THR:N	2.46	0.47
1:C:89:LEU:HD23	1:C:90:ILE:N	2.28	0.47
1:C:92:THR:HG23	1:C:93:LEU:O	2.14	0.47
1:B:336:VAL:O	1:B:337:THR:HG23	2.14	0.47
1:A:133:SER:O	1:A:234:TYR:CB	2.60	0.47
1:A:158:ALA:C	1:A:211:LYS:H	1.93	0.47
1:B:314:ALA:O	1:B:315:ALA:HB3	2.11	0.47
1:C:130:ARG:HB3	1:C:237:GLN:N	2.30	0.47
1:C:269:LYS:HG2	1:C:270:GLY:O	2.14	0.47
1:A:339:GLU:O	1:A:340:GLU:CA	2.60	0.47
1:A:156:ARG:HD3	1:B:240:ASN:OD1	2.13	0.47
1:A:269:LYS:HG2	1:A:270:GLY:O	2.14	0.47
1:B:111:SER:HB3	1:B:197:VAL:CG2	2.44	0.47
1:B:163:PRO:CG	1:B:168:SER:CB	2.92	0.47
1:A:240:ASN:OD1	1:C:156:ARG:HD3	2.14	0.47
1:A:240:ASN:OD1	1:C:156:ARG:NE	2.47	0.47
1:C:101:PRO:CG	1:C:217:TYR:HD2	2.26	0.47
1:C:295:ALA:N	1:C:316:ALA:CA	2.40	0.47
1:C:343:LYS:HB2	1:C:344:GLY:H	1.13	0.47
1:A:204:PRO:N	1:A:205:LYS:HD2	2.28	0.47
1:A:206:LEU:HD22	1:C:206:LEU:HB2	1.96	0.47
1:A:152:LEU:O	1:A:186:LEU:CD1	2.55	0.47
1:A:289:THR:O	1:A:290:LEU:HG	2.14	0.47
1:B:185:ILE:HD11	1:B:186:LEU:O	2.15	0.47
1:B:269:LYS:HG2	1:B:270:GLY:O	2.14	0.47
1:C:185:ILE:HD11	1:C:186:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLN:O	1:C:347:GLN:CA	2.61	0.47
1:A:336:VAL:O	1:A:337:THR:HG23	2.14	0.47
1:A:144:SER:HA	1:A:181:TRP:HB3	1.96	0.47
1:A:185:ILE:HD11	1:A:186:LEU:O	2.15	0.47
1:B:290:LEU:HB2	1:B:346:TRP:HA	1.96	0.47
1:C:278:CYS:N	1:C:333:VAL:O	2.48	0.47
1:B:203:ASP:OD1	1:B:205:LYS:CG	2.56	0.47
1:A:109:ASN:OD1	1:A:129:TYR:OH	2.32	0.47
1:A:150:VAL:O	1:A:151:ALA:O	2.32	0.47
1:A:163:PRO:CG	1:A:168:SER:CB	2.92	0.47
1:A:114:GLY:HA2	1:A:283:THR:HG21	0.47	0.47
1:B:109:ASN:OD1	1:B:129:TYR:OH	2.32	0.47
1:B:136:PHE:CE2	1:B:212:LEU:CD2	2.98	0.47
1:B:150:VAL:O	1:B:151:ALA:O	2.32	0.47
1:B:82:ILE:O	1:B:83:THR:OG1	2.18	0.47
1:C:105:THR:O	1:C:105:THR:HG23	2.14	0.47
1:C:136:PHE:CE2	1:C:212:LEU:CD2	2.98	0.47
1:B:338:THR:OG1	1:B:339:GLU:CA	2.63	0.47
1:C:134:LEU:CD2	1:C:188:VAL:HG22	2.41	0.47
1:C:150:VAL:O	1:C:151:ALA:O	2.32	0.47
1:A:109:ASN:O	1:A:110:PRO:C	2.51	0.47
1:A:89:LEU:HD23	1:A:90:ILE:N	2.28	0.47
1:B:279:HIS:CB	1:B:280:PHE:N	2.78	0.47
1:C:130:ARG:HH11	1:C:236:VAL:C	2.16	0.47
1:A:338:THR:OG1	1:A:339:GLU:CA	2.63	0.47
1:A:136:PHE:CE2	1:A:212:LEU:CD2	2.98	0.47
1:A:163:PRO:CG	1:A:168:SER:HB3	2.44	0.47
1:C:313:GLU:HG3	1:C:315:ALA:HA	1.97	0.47
1:B:254:ALA:O	1:B:257:LYS:N	2.38	0.47
1:A:279:HIS:CB	1:A:280:PHE:N	2.78	0.47
1:A:313:GLU:HG3	1:A:315:ALA:HA	1.97	0.47
1:A:278:CYS:N	1:A:333:VAL:O	2.48	0.47
1:B:295:ALA:HB2	1:B:315:ALA:CB	2.37	0.47
1:C:144:SER:HA	1:C:181:TRP:HB3	1.96	0.47
1:C:107:VAL:HG22	1:C:211:LYS:HB3	1.97	0.47
1:C:291:PHE:CD1	1:C:292:TYR:N	2.83	0.47
1:C:277:ASP:CG	1:C:334:LYS:HZ3	2.17	0.47
1:C:296:PRO:CD	1:C:337:THR:HG21	2.39	0.47
1:A:113:PRO:CG	1:A:283:THR:N	2.23	0.47
1:A:291:PHE:CD1	1:A:292:TYR:N	2.83	0.47
1:A:333:VAL:C	1:A:334:LYS:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:CG	1:A:334:LYS:HZ3	2.18	0.47
1:B:162:PRO:O	1:B:163:PRO:O	2.33	0.47
1:B:291:PHE:CD1	1:B:292:TYR:N	2.83	0.47
1:C:162:PRO:O	1:C:163:PRO:O	2.33	0.47
1:C:179:VAL:CG2	1:C:181:TRP:CD1	2.93	0.47
1:C:107:VAL:CB	1:C:329:ARG:HE	2.14	0.47
1:C:338:THR:OG1	1:C:339:GLU:CA	2.63	0.47
1:A:314:ALA:O	1:A:315:ALA:HB3	2.11	0.46
1:B:101:PRO:HG2	1:B:166:LEU:HD12	1.94	0.46
1:C:152:LEU:O	1:C:186:LEU:CD1	2.55	0.46
1:A:185:ILE:HD12	1:A:186:LEU:C	2.36	0.46
1:B:100:GLU:C	1:B:101:PRO:O	2.54	0.46
1:B:149:LYS:HE2	1:B:151:ALA:HB2	1.96	0.46
1:B:230:VAL:CG1	1:B:231:ARG:H	2.28	0.46
1:B:278:CYS:N	1:B:333:VAL:O	2.48	0.46
1:C:149:LYS:O	1:C:216:THR:HA	2.15	0.46
1:C:174:GLY:O	1:C:175:CYS:CB	2.64	0.46
1:C:185:ILE:HD12	1:C:186:LEU:C	2.36	0.46
1:C:234:TYR:CD2	1:C:236:VAL:HG23	2.50	0.46
1:C:71:THR:HG23	1:C:71:THR:O	2.16	0.46
1:A:100:GLU:O	1:A:101:PRO:C	2.48	0.46
1:A:107:VAL:O	1:A:115:THR:CG2	2.56	0.46
1:A:101:PRO:HG2	1:A:166:LEU:HD12	1.94	0.46
1:A:269:LYS:CE	1:A:270:GLY:O	2.63	0.46
1:C:290:LEU:HB2	1:C:346:TRP:HA	1.96	0.46
1:C:273:GLY:O	1:C:274:TRP:C	2.53	0.46
1:A:141:MET:CG	1:A:141:MET:O	2.46	0.46
1:A:162:PRO:O	1:A:163:PRO:O	2.33	0.46
1:C:162:PRO:O	1:C:163:PRO:C	2.51	0.46
1:C:174:GLY:C	1:C:175:CYS:HG	2.11	0.46
1:A:112:GLU:O	1:A:112:GLU:HG3	2.16	0.46
1:B:289:THR:O	1:B:290:LEU:HG	2.14	0.46
1:C:289:THR:O	1:C:290:LEU:HG	2.14	0.46
1:B:273:GLY:O	1:B:274:TRP:C	2.53	0.46
1:B:174:GLY:O	1:B:175:CYS:CB	2.64	0.46
1:B:179:VAL:CG1	1:B:181:TRP:NE1	2.54	0.46
1:A:156:ARG:CZ	1:B:240:ASN:CA	2.93	0.46
1:C:133:SER:N	1:C:235:THR:CG2	2.74	0.46
1:C:149:LYS:HE2	1:C:151:ALA:HB2	1.96	0.46
1:C:249:GLN:CG	1:C:263:VAL:O	2.64	0.46
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:C	1:A:101:PRO:O	2.54	0.46
1:A:149:LYS:HE2	1:A:151:ALA:HB2	1.96	0.46
1:A:291:PHE:HD2	1:A:346:TRP:HE3	1.63	0.46
1:A:95:LYS:HZ2	1:A:221:ALA:CB	2.27	0.46
1:B:185:ILE:HD12	1:B:186:LEU:C	2.36	0.46
1:B:149:LYS:O	1:B:216:THR:HA	2.15	0.46
1:B:101:PRO:CG	1:B:217:TYR:HD2	2.26	0.46
1:B:269:LYS:O	1:B:277:ASP:CA	2.57	0.46
1:C:136:PHE:CE2	1:C:212:LEU:HD21	2.51	0.46
1:C:172:ILE:C	1:C:173:GLU:O	2.51	0.46
1:B:249:GLN:CG	1:B:263:VAL:O	2.64	0.46
1:A:234:TYR:CD2	1:A:236:VAL:HG23	2.50	0.46
1:A:278:CYS:CA	1:A:334:LYS:HD3	2.42	0.46
1:B:112:GLU:O	1:B:112:GLU:HG3	2.16	0.46
1:B:124:ALA:HB2	1:B:350:ARG:HH12	1.81	0.46
1:B:89:LEU:HD23	1:B:90:ILE:N	2.28	0.46
1:C:163:PRO:CG	1:C:168:SER:HB3	2.44	0.46
1:C:230:VAL:CG1	1:C:231:ARG:H	2.28	0.46
1:C:107:VAL:N	1:C:283:THR:CG2	2.53	0.46
1:C:333:VAL:C	1:C:334:LYS:CD	2.78	0.46
1:A:249:GLN:CG	1:A:263:VAL:O	2.64	0.46
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.71	0.46
1:A:181:TRP:O	1:A:181:TRP:CE3	2.69	0.46
1:A:199:ASP:OD2	1:C:160:LYS:HE2	2.15	0.46
1:B:313:GLU:HG3	1:B:315:ALA:HA	1.97	0.46
1:C:244:SER:C	1:C:245:THR:HG22	2.31	0.46
1:B:297:VAL:HB	1:B:336:VAL:CG1	1.98	0.46
1:A:297:VAL:HG12	1:A:336:VAL:HG11	0.98	0.46
1:A:127:GLU:O	1:A:128:LYS:CG	2.64	0.46
1:A:125:GLN:CA	1:A:243:GLY:HA2	2.27	0.46
1:B:109:ASN:O	1:B:110:PRO:C	2.51	0.46
1:B:134:LEU:CD2	1:B:188:VAL:HG22	2.41	0.46
1:C:95:LYS:HZ1	1:C:221:ALA:C	2.18	0.46
1:C:74:ARG:C	1:C:75:VAL:HG23	2.37	0.46
1:A:149:LYS:O	1:A:216:THR:HA	2.15	0.45
1:B:234:TYR:CD2	1:B:236:VAL:HG23	2.50	0.45
1:C:127:GLU:O	1:C:128:LYS:CG	2.64	0.45
1:C:181:TRP:O	1:C:181:TRP:CE3	2.69	0.45
1:C:133:SER:CA	1:C:235:THR:HG22	2.47	0.45
1:C:126:TYR:C	1:C:242:THR:HG21	2.37	0.45
1:C:279:HIS:CB	1:C:280:PHE:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:THR:HG23	1:C:275:GLU:HG2	1.97	0.45
1:A:174:GLY:O	1:A:175:CYS:CB	2.64	0.45
1:B:181:TRP:CE3	1:B:181:TRP:O	2.69	0.45
1:C:100:GLU:C	1:C:101:PRO:O	2.54	0.45
1:A:134:LEU:CD2	1:A:188:VAL:HG22	2.41	0.45
1:A:136:PHE:CE2	1:A:212:LEU:HD21	2.51	0.45
1:A:230:VAL:CG1	1:A:231:ARG:H	2.28	0.45
1:A:252:ASP:OD2	1:A:345:LYS:HG2	2.16	0.45
1:A:290:LEU:HD23	1:A:346:TRP:HB2	1.90	0.45
1:A:350:ARG:O	1:A:351:ILE:CB	2.53	0.45
1:B:84:ARG:CD	1:B:119:LEU:HD13	2.47	0.45
1:C:89:LEU:HA	1:C:230:VAL:O	2.17	0.45
1:B:271:THR:HG23	1:B:275:GLU:HG2	1.97	0.45
1:A:271:THR:HG23	1:A:275:GLU:HG2	1.97	0.45
1:A:171:ASN:O	1:B:242:THR:O	2.35	0.45
1:A:350:ARG:C	1:A:351:ILE:CG2	2.58	0.45
1:B:120:ILE:CG1	1:B:350:ARG:NE	2.57	0.45
1:B:280:PHE:HZ	1:B:324:VAL:HG21	1.81	0.45
1:C:280:PHE:HZ	1:C:324:VAL:HG21	1.81	0.45
1:C:89:LEU:HD23	1:C:89:LEU:O	2.00	0.45
1:A:153:ALA:HB2	1:A:175:CYS:N	2.32	0.45
1:A:236:VAL:CG1	1:A:238:LEU:CD1	2.94	0.45
1:A:280:PHE:HZ	1:A:324:VAL:HG21	1.81	0.45
1:B:269:LYS:CE	1:B:270:GLY:O	2.63	0.45
1:B:326:VAL:HG13	1:B:331:GLN:OE1	2.17	0.45
1:C:109:ASN:OD1	1:C:129:TYR:OH	2.32	0.45
1:C:84:ARG:CD	1:C:119:LEU:HD13	2.46	0.45
1:C:236:VAL:CG1	1:C:238:LEU:CD1	2.94	0.45
1:C:288:LEU:C	1:C:289:THR:OG1	2.49	0.45
1:A:273:GLY:O	1:A:274:TRP:C	2.53	0.45
1:A:156:ARG:NE	1:B:240:ASN:OD1	2.50	0.45
1:A:107:VAL:HG22	1:A:211:LYS:HB3	1.98	0.45
1:B:120:ILE:CG2	1:B:284:GLY:HA3	2.45	0.45
1:B:295:ALA:HB2	1:B:315:ALA:HB3	1.99	0.45
1:B:107:VAL:N	1:B:328:GLU:HB2	2.31	0.45
1:A:249:GLN:NE2	1:A:265:TRP:N	2.54	0.45
1:B:315:ALA:O	1:B:318:SER:N	2.50	0.45
1:C:118:GLN:O	1:C:118:GLN:HG2	2.17	0.45
1:C:198:ALA:C	1:C:200:GLY:N	2.55	0.45
1:C:291:PHE:HD2	1:C:346:TRP:HE3	1.63	0.45
1:C:337:THR:HG1	1:C:343:LYS:HZ2	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:O	1:A:118:GLN:HG2	2.17	0.45
1:A:290:LEU:HD13	1:A:291:PHE:HB3	1.98	0.45
1:B:116:PHE:O	1:B:284:GLY:CA	2.51	0.45
1:B:118:GLN:HG2	1:B:118:GLN:O	2.17	0.45
1:B:136:PHE:CE2	1:B:212:LEU:HD21	2.51	0.45
1:C:153:ALA:HB2	1:C:175:CYS:N	2.32	0.45
1:C:288:LEU:CD1	1:C:290:LEU:CG	2.70	0.45
1:C:290:LEU:HD13	1:C:291:PHE:HB3	1.98	0.45
1:C:315:ALA:O	1:C:318:SER:N	2.50	0.45
1:A:109:ASN:O	1:A:111:SER:N	2.50	0.45
1:A:179:VAL:CG1	1:A:181:TRP:NE1	2.54	0.45
1:A:84:ARG:CD	1:A:119:LEU:HD13	2.46	0.45
1:A:88:GLU:O	1:A:231:ARG:HB3	2.05	0.45
1:B:107:VAL:HG22	1:B:211:LYS:HB3	1.97	0.45
1:B:291:PHE:HD2	1:B:346:TRP:HE3	1.63	0.45
1:B:106:ALA:C	1:B:328:GLU:OE1	2.55	0.45
1:C:101:PRO:CD	1:C:217:TYR:HD2	2.30	0.45
1:A:271:THR:CG2	1:A:275:GLU:HG2	2.47	0.45
1:A:156:ARG:NH1	1:B:240:ASN:CB	2.78	0.45
1:A:101:PRO:HD3	1:A:166:LEU:HD11	0.47	0.45
1:A:295:ALA:HB2	1:A:315:ALA:HB3	1.99	0.45
1:B:115:THR:C	1:B:116:PHE:CD1	2.78	0.45
1:B:101:PRO:HD3	1:B:166:LEU:HD11	0.47	0.45
1:B:97:THR:OG1	1:B:97:THR:O	2.25	0.45
1:A:172:ILE:C	1:A:173:GLU:O	2.51	0.44
1:A:130:ARG:HB3	1:A:237:GLN:N	2.30	0.44
1:A:242:THR:CG2	1:A:243:GLY:H	2.22	0.44
1:B:290:LEU:HD13	1:B:291:PHE:HB3	1.98	0.44
1:C:112:GLU:O	1:C:112:GLU:HG3	2.16	0.44
1:A:89:LEU:HA	1:A:230:VAL:O	2.17	0.44
1:A:315:ALA:O	1:A:318:SER:N	2.50	0.44
1:B:172:ILE:C	1:B:173:GLU:O	2.51	0.44
1:C:105:THR:HA	1:C:212:LEU:O	2.18	0.44
1:C:253:PHE:HZ	1:C:268:THR:HG21	1.82	0.44
1:A:126:TYR:C	1:A:242:THR:HG21	2.37	0.44
1:A:300:LEU:HA	1:A:300:LEU:HD12	1.27	0.44
1:A:104:THR:O	1:A:328:GLU:OE1	2.34	0.44
1:B:242:THR:CG2	1:B:243:GLY:N	2.73	0.44
1:C:268:THR:CG2	1:C:268:THR:O	2.66	0.44
1:C:326:VAL:HG13	1:C:331:GLN:OE1	2.17	0.44
1:C:95:LYS:HZ1	1:C:221:ALA:CB	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:VAL:HG12	1:B:336:VAL:HG11	0.97	0.44
1:C:213:ILE:HG23	1:C:214:MET:N	2.32	0.44
1:B:269:LYS:CG	1:B:270:GLY:H	2.23	0.44
1:C:109:ASN:O	1:C:111:SER:N	2.50	0.44
1:B:213:ILE:HG23	1:B:214:MET:N	2.32	0.44
1:A:101:PRO:HB3	1:A:217:TYR:CD2	2.53	0.44
1:A:326:VAL:HG13	1:A:331:GLN:OE1	2.17	0.44
1:B:101:PRO:HB3	1:B:217:TYR:CD2	2.53	0.44
1:B:153:ALA:HB2	1:B:175:CYS:N	2.32	0.44
1:B:133:SER:CA	1:B:235:THR:HG22	2.47	0.44
1:B:126:TYR:C	1:B:242:THR:HG21	2.37	0.44
1:A:101:PRO:CD	1:A:217:TYR:HD2	2.30	0.44
1:A:95:LYS:HZ1	1:A:221:ALA:C	2.20	0.44
1:B:127:GLU:O	1:B:128:LYS:CG	2.64	0.44
1:B:101:PRO:CD	1:B:217:TYR:HD2	2.30	0.44
1:B:149:LYS:CG	1:B:217:TYR:HE1	2.29	0.44
1:B:253:PHE:HZ	1:B:268:THR:HG21	1.82	0.44
1:B:291:PHE:C	1:B:292:TYR:CB	2.86	0.44
1:C:163:PRO:HG3	1:C:168:SER:CB	2.47	0.44
1:C:101:PRO:HD3	1:C:166:LEU:HD11	0.47	0.44
1:C:295:ALA:HB2	1:C:315:ALA:HB3	1.98	0.44
1:B:336:VAL:C	1:B:337:THR:HG23	2.37	0.44
1:A:253:PHE:HZ	1:A:268:THR:HG21	1.81	0.44
1:B:109:ASN:O	1:B:111:SER:N	2.51	0.44
1:B:89:LEU:HA	1:B:230:VAL:O	2.17	0.44
1:C:137:ARG:N	1:C:230:VAL:HG13	2.33	0.44
1:A:336:VAL:C	1:A:337:THR:HG23	2.37	0.44
1:A:105:THR:HA	1:A:212:LEU:O	2.18	0.44
1:A:244:SER:C	1:A:245:THR:HG22	2.31	0.44
1:B:163:PRO:HG3	1:B:168:SER:CB	2.47	0.44
1:B:105:THR:HA	1:B:212:LEU:O	2.18	0.44
1:B:84:ARG:NE	1:B:119:LEU:CD1	2.81	0.44
1:C:291:PHE:C	1:C:292:TYR:CB	2.86	0.44
1:B:158:ALA:C	1:B:211:LYS:H	1.93	0.44
1:A:242:THR:O	1:C:171:ASN:O	2.35	0.44
1:C:262:LEU:HA	1:C:262:LEU:HD23	1.71	0.44
1:B:271:THR:CG2	1:B:275:GLU:HG2	2.47	0.44
1:C:336:VAL:C	1:C:337:THR:HG23	2.37	0.44
1:A:149:LYS:CG	1:A:217:TYR:HE1	2.29	0.43
1:A:133:SER:CA	1:A:235:THR:HG22	2.47	0.43
1:A:113:PRO:C	1:A:283:THR:CG2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LYS:HD3	1:C:328:GLU:HB2	1.55	0.43
1:C:84:ARG:NE	1:C:119:LEU:CD1	2.81	0.43
1:C:271:THR:CG2	1:C:275:GLU:HG2	2.47	0.43
1:C:72:GLN:HE21	1:C:73:PRO:HD2	1.83	0.43
1:A:325:LYS:O	1:A:325:LYS:HG2	2.18	0.43
1:B:105:THR:OG1	1:B:211:LYS:HD2	2.03	0.43
1:C:101:PRO:HB3	1:C:217:TYR:CD2	2.53	0.43
1:C:105:THR:CG2	1:C:328:GLU:N	2.78	0.43
1:B:306:SER:HB2	1:B:325:LYS:N	2.33	0.43
1:C:107:VAL:HG23	1:C:283:THR:CB	2.34	0.43
1:C:154:PHE:CZ	1:C:156:ARG:CA	3.01	0.43
1:A:121:LYS:O	1:A:121:LYS:HG3	2.19	0.43
1:C:56:THR:HG23	1:C:57:ARG:HB3	1.99	0.43
1:A:315:ALA:CA	1:A:318:SER:HB2	2.49	0.43
1:B:126:TYR:O	1:B:242:THR:CG2	2.66	0.43
1:B:149:LYS:HD3	1:B:217:TYR:HE1	1.73	0.43
1:A:336:VAL:O	1:A:336:VAL:CG1	2.66	0.43
1:A:213:ILE:HG23	1:A:214:MET:N	2.32	0.43
1:B:121:LYS:O	1:B:121:LYS:HG3	2.19	0.43
1:B:137:ARG:N	1:B:230:VAL:HG13	2.33	0.43
1:B:278:CYS:O	1:B:333:VAL:O	2.37	0.43
1:B:82:ILE:HD13	1:B:82:ILE:HG21	1.78	0.43
1:C:149:LYS:CG	1:C:217:TYR:HE1	2.29	0.43
1:C:243:GLY:O	1:C:244:SER:CB	2.67	0.43
1:C:293:GLU:O	1:C:316:ALA:C	2.52	0.43
1:B:325:LYS:O	1:B:325:LYS:HG2	2.18	0.43
1:A:291:PHE:C	1:A:292:TYR:CB	2.86	0.43
1:A:326:VAL:CG1	1:A:327:ALA:N	2.19	0.43
1:A:96:ASN:O	1:A:96:ASN:ND2	2.51	0.43
1:B:186:LEU:C	1:B:186:LEU:CD2	2.87	0.43
1:B:291:PHE:CE1	1:B:335:MET:HE1	2.53	0.43
1:B:96:ASN:ND2	1:B:96:ASN:O	2.51	0.43
1:C:76:SER:OG	1:C:77:THR:N	2.50	0.43
1:A:120:ILE:HG12	1:A:350:ARG:HH12	1.81	0.43
1:A:137:ARG:N	1:A:230:VAL:HG13	2.33	0.43
1:A:84:ARG:NE	1:A:119:LEU:CD1	2.81	0.43
1:B:125:GLN:CA	1:B:243:GLY:HA2	2.27	0.43
1:C:246:SER:H	1:C:263:VAL:HG21	1.83	0.43
1:C:121:LYS:HG3	1:C:121:LYS:O	2.19	0.43
1:C:254:ALA:O	1:C:257:LYS:N	2.38	0.43
1:A:254:ALA:O	1:A:257:LYS:N	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLY:O	1:A:244:SER:CB	2.67	0.43
1:B:120:ILE:HA	1:B:350:ARG:HH21	1.82	0.43
1:C:126:TYR:O	1:C:242:THR:CG2	2.66	0.43
1:A:246:SER:HB2	1:A:263:VAL:HG21	1.27	0.43
1:A:130:ARG:CG	1:A:131:PHE:N	2.79	0.43
1:A:130:ARG:NH1	1:A:236:VAL:C	2.70	0.43
1:C:125:GLN:HA	1:C:243:GLY:N	2.34	0.43
1:C:87:SER:HA	1:C:231:ARG:HD2	2.01	0.43
1:C:91:THR:CB	1:C:325:LYS:HZ1	2.13	0.43
1:A:113:PRO:CG	1:A:283:THR:CA	2.97	0.43
1:B:311:LEU:N	1:B:311:LEU:CD1	2.82	0.43
1:C:154:PHE:CE1	1:C:156:ARG:CA	3.02	0.43
1:C:216:THR:OG1	1:C:227:LEU:HD21	2.18	0.43
1:C:242:THR:CG2	1:C:243:GLY:N	2.73	0.43
1:C:325:LYS:O	1:C:325:LYS:HG2	2.18	0.43
1:A:126:TYR:O	1:A:242:THR:CG2	2.66	0.42
1:B:236:VAL:CG1	1:B:238:LEU:CD1	2.94	0.42
1:B:243:GLY:O	1:B:244:SER:CB	2.67	0.42
1:B:95:LYS:HZ1	1:B:221:ALA:C	2.22	0.42
1:C:130:ARG:NH1	1:C:236:VAL:C	2.70	0.42
1:C:169:LEU:C	1:C:171:ASN:H	2.22	0.42
1:C:236:VAL:CG1	1:C:238:LEU:HD11	2.49	0.42
1:A:306:SER:HB2	1:A:325:LYS:N	2.33	0.42
1:A:125:GLN:HA	1:A:243:GLY:N	2.34	0.42
1:A:154:PHE:CE1	1:A:156:ARG:CA	3.02	0.42
1:A:169:LEU:C	1:A:171:ASN:H	2.23	0.42
1:A:266:SER:HA	1:A:280:PHE:HA	2.02	0.42
1:A:315:ALA:CA	1:A:318:SER:CB	2.97	0.42
1:B:111:SER:HB3	1:B:197:VAL:HG21	2.01	0.42
1:C:137:ARG:O	1:C:230:VAL:HA	2.19	0.42
1:C:266:SER:HA	1:C:280:PHE:HA	2.02	0.42
1:C:309:SER:C	1:C:322:ALA:HA	2.20	0.42
1:C:95:LYS:HB3	1:C:96:ASN:H	1.60	0.42
1:B:336:VAL:CG1	1:B:336:VAL:O	2.66	0.42
1:A:162:PRO:O	1:A:163:PRO:C	2.51	0.42
1:A:216:THR:OG1	1:A:227:LEU:HD21	2.18	0.42
1:A:119:LEU:CD2	1:A:234:TYR:HH	1.98	0.42
1:B:216:THR:OG1	1:B:227:LEU:HD21	2.18	0.42
1:B:258:ASP:OD1	1:B:259:GLY:N	2.52	0.42
1:C:111:SER:HB3	1:C:197:VAL:HG21	2.02	0.42
1:C:96:ASN:O	1:C:96:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:O	1:A:230:VAL:HA	2.19	0.42
1:B:105:THR:O	1:B:328:GLU:OE1	2.37	0.42
1:B:289:THR:CG2	1:B:321:TRP:CZ3	3.03	0.42
1:B:90:ILE:HD11	1:B:232:VAL:HG22	1.83	0.42
1:C:302:ASN:HB3	1:C:308:PHE:CE1	2.55	0.42
1:C:304:ASP:OD2	1:C:331:GLN:CA	2.57	0.42
1:C:273:GLY:O	1:C:275:GLU:HB3	2.19	0.42
1:C:341:GLN:O	1:C:342:PRO:C	2.58	0.42
1:A:111:SER:HB3	1:A:197:VAL:HG21	2.02	0.42
1:A:82:ILE:HG21	1:A:82:ILE:HD13	1.78	0.42
1:B:137:ARG:O	1:B:230:VAL:HA	2.19	0.42
1:B:114:GLY:CA	1:B:326:VAL:C	2.62	0.42
1:C:112:GLU:H	1:C:350:ARG:NH1	2.12	0.42
1:C:113:PRO:HG2	1:C:350:ARG:C	2.40	0.42
1:C:293:GLU:CA	1:C:317:GLY:HA2	2.50	0.42
1:C:60:ALA:HA	1:C:61:PRO:HD2	1.81	0.42
1:A:341:GLN:HB2	1:A:341:GLN:HE21	1.72	0.42
1:A:302:ASN:HB3	1:A:308:PHE:CE1	2.55	0.42
1:B:154:PHE:CE1	1:B:156:ARG:CA	3.02	0.42
1:C:315:ALA:CA	1:C:318:SER:HB2	2.49	0.42
1:C:289:THR:CG2	1:C:321:TRP:CZ3	3.03	0.42
1:C:291:PHE:CE1	1:C:335:MET:HE3	2.54	0.42
1:B:269:LYS:CG	1:B:270:GLY:N	2.58	0.42
1:B:293:GLU:CA	1:B:317:GLY:HA2	2.50	0.42
1:B:302:ASN:HB3	1:B:308:PHE:CE1	2.55	0.42
1:C:258:ASP:OD1	1:C:259:GLY:N	2.52	0.42
1:C:269:LYS:CG	1:C:270:GLY:H	2.23	0.42
1:C:107:VAL:CG1	1:C:329:ARG:HH21	2.30	0.42
1:B:313:GLU:HB2	1:B:315:ALA:CA	2.50	0.42
1:B:309:SER:C	1:B:322:ALA:HA	2.20	0.42
1:A:240:ASN:CG	1:C:156:ARG:NE	2.73	0.42
1:C:163:PRO:CG	1:C:168:SER:HB2	2.50	0.42
1:C:75:VAL:HG12	1:C:76:SER:N	2.35	0.42
1:B:294:LYS:O	1:B:296:PRO:CG	2.65	0.42
1:B:339:GLU:O	1:B:340:GLU:CA	2.60	0.42
1:A:156:ARG:CZ	1:B:240:ASN:HB3	2.47	0.42
1:A:186:LEU:C	1:A:186:LEU:CD2	2.87	0.42
1:A:236:VAL:CG1	1:A:238:LEU:HD11	2.49	0.42
1:A:292:TYR:CD1	1:A:292:TYR:C	2.94	0.42
1:A:87:SER:HA	1:A:231:ARG:HD2	2.01	0.42
1:B:169:LEU:C	1:B:171:ASN:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASP:OD2	1:B:345:LYS:HG2	2.16	0.42
1:C:208:ASP:HB2	1:C:329:ARG:HH22	1.85	0.42
1:A:115:THR:C	1:A:116:PHE:CD1	2.78	0.42
1:A:258:ASP:OD1	1:A:259:GLY:N	2.52	0.42
1:A:291:PHE:CD2	1:A:345:LYS:O	2.73	0.42
1:B:185:ILE:HD12	1:B:186:LEU:O	2.20	0.42
1:B:93:LEU:HD12	1:B:138:TYR:CE1	2.54	0.42
1:C:292:TYR:C	1:C:292:TYR:CD1	2.93	0.42
1:B:273:GLY:O	1:B:275:GLU:HB3	2.19	0.42
1:C:336:VAL:O	1:C:336:VAL:CG1	2.66	0.42
1:A:93:LEU:HD12	1:A:138:TYR:CE1	2.54	0.41
1:B:125:GLN:HA	1:B:243:GLY:N	2.34	0.41
1:B:130:ARG:CG	1:B:131:PHE:N	2.79	0.41
1:B:149:LYS:CD	1:B:217:TYR:HE1	2.33	0.41
1:B:134:LEU:N	1:B:233:GLU:O	2.44	0.41
1:B:266:SER:HA	1:B:280:PHE:HA	2.02	0.41
1:C:186:LEU:C	1:C:186:LEU:CD2	2.87	0.41
1:C:269:LYS:C	1:C:277:ASP:CB	2.63	0.41
1:B:236:VAL:CG1	1:B:238:LEU:HD11	2.50	0.41
1:C:264:SER:OG	1:C:265:TRP:CA	2.69	0.41
1:C:269:LYS:CE	1:C:270:GLY:O	2.63	0.41
1:A:172:ILE:HG21	1:A:172:ILE:HD13	1.88	0.41
1:C:93:LEU:CD1	1:C:138:TYR:HE1	2.33	0.41
1:C:245:THR:CB	1:C:263:VAL:CG2	2.88	0.41
1:B:264:SER:OG	1:B:265:TRP:CA	2.68	0.41
1:A:273:GLY:O	1:A:275:GLU:HB3	2.19	0.41
1:A:128:LYS:O	1:A:238:LEU:HA	2.20	0.41
1:A:149:LYS:CD	1:A:217:TYR:HE1	2.33	0.41
1:A:289:THR:CG2	1:A:321:TRP:CZ3	3.03	0.41
1:A:278:CYS:O	1:A:333:VAL:O	2.37	0.41
1:B:136:PHE:CE2	1:B:212:LEU:HD13	2.56	0.41
1:B:124:ALA:HB2	1:B:350:ARG:NH1	2.36	0.41
1:C:231:ARG:CG	1:C:232:VAL:H	2.27	0.41
1:A:185:ILE:HD12	1:A:186:LEU:O	2.20	0.41
1:A:82:ILE:HG22	1:A:82:ILE:H	1.62	0.41
1:A:86:GLY:HA2	1:A:234:TYR:HE1	1.68	0.41
1:B:154:PHE:CZ	1:B:156:ARG:CA	3.02	0.41
1:B:170:TYR:C	1:B:171:ASN:ND2	2.72	0.41
1:B:278:CYS:HB3	1:B:333:VAL:C	2.35	0.41
1:B:279:HIS:O	1:B:280:PHE:N	2.42	0.41
1:B:87:SER:HA	1:B:231:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:N	1:C:233:GLU:O	2.54	0.41
1:C:278:CYS:O	1:C:333:VAL:O	2.37	0.41
1:C:55:VAL:O	1:C:57:ARG:N	2.52	0.41
1:C:66:TYR:HE2	1:C:183:GLY:CA	2.32	0.41
1:A:163:PRO:CG	1:A:168:SER:HB2	2.50	0.41
1:A:191:ASP:HB2	1:A:192:SER:H	1.41	0.41
1:A:197:VAL:CG2	1:A:198:ALA:H	2.34	0.41
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.98	0.41
1:B:130:ARG:HB3	1:B:237:GLN:N	2.30	0.41
1:B:315:ALA:CA	1:B:318:SER:CB	2.97	0.41
1:B:109:ASN:CB	1:B:329:ARG:HH21	2.30	0.41
1:C:71:THR:CG2	1:C:87:SER:HG	1.90	0.41
1:A:249:GLN:HG3	1:A:263:VAL:O	2.21	0.41
1:A:248:ALA:CB	1:A:265:TRP:N	2.71	0.41
1:A:93:LEU:CD1	1:A:138:TYR:CE1	3.03	0.41
1:A:93:LEU:CD1	1:A:138:TYR:HE1	2.33	0.41
1:A:136:PHE:CG	1:A:212:LEU:HD21	2.56	0.41
1:A:308:PHE:HE1	1:A:333:VAL:CG1	2.34	0.41
1:A:293:GLU:CA	1:A:317:GLY:HA2	2.50	0.41
1:B:162:PRO:O	1:B:163:PRO:C	2.50	0.41
1:B:163:PRO:CG	1:B:168:SER:HB2	2.50	0.41
1:C:128:LYS:O	1:C:238:LEU:HA	2.21	0.41
1:C:269:LYS:O	1:C:277:ASP:CA	2.57	0.41
1:C:315:ALA:CA	1:C:318:SER:CB	2.97	0.41
1:B:249:GLN:HG3	1:B:263:VAL:O	2.21	0.41
1:A:264:SER:OG	1:A:265:TRP:CA	2.69	0.41
1:A:136:PHE:CE2	1:A:212:LEU:HD13	2.56	0.41
1:B:93:LEU:CD1	1:B:138:TYR:CE1	3.03	0.41
1:B:197:VAL:CG2	1:B:198:ALA:H	2.33	0.41
1:B:292:TYR:C	1:B:292:TYR:CD1	2.94	0.41
1:C:249:GLN:HG3	1:C:263:VAL:O	2.21	0.41
1:C:289:THR:O	1:C:290:LEU:CG	2.69	0.41
1:A:255:GLY:HA2	1:A:342:PRO:CB	2.25	0.41
1:A:170:TYR:HH	1:A:217:TYR:HH	1.49	0.41
1:A:293:GLU:O	1:A:316:ALA:C	2.52	0.41
1:B:300:LEU:HD12	1:B:300:LEU:HA	1.27	0.41
1:B:291:PHE:CD2	1:B:345:LYS:O	2.73	0.41
1:C:136:PHE:CG	1:C:212:LEU:HD21	2.56	0.41
1:C:93:LEU:CD1	1:C:138:TYR:CE1	3.03	0.41
1:C:101:PRO:HG2	1:C:166:LEU:HD12	1.94	0.41
1:C:185:ILE:HD12	1:C:186:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:PHE:CZ	1:C:268:THR:HG21	2.56	0.41
1:C:308:PHE:HE1	1:C:333:VAL:CG1	2.34	0.41
1:C:252:ASP:OD1	1:C:345:LYS:HG2	2.20	0.41
1:C:252:ASP:OD2	1:C:345:LYS:HG2	2.16	0.41
1:A:253:PHE:CZ	1:A:268:THR:HG21	2.56	0.41
1:A:302:ASN:HB3	1:A:308:PHE:CD1	2.56	0.41
1:B:93:LEU:CD1	1:B:138:TYR:HE1	2.33	0.41
1:B:278:CYS:O	1:B:333:VAL:N	2.34	0.41
1:B:304:ASP:OD2	1:B:331:GLN:CA	2.57	0.41
1:C:130:ARG:HB2	1:C:237:GLN:CA	2.49	0.41
1:C:291:PHE:CD2	1:C:345:LYS:O	2.73	0.41
1:C:313:GLU:HB2	1:C:315:ALA:CA	2.50	0.41
1:A:294:LYS:O	1:A:296:PRO:CG	2.65	0.41
1:A:231:ARG:CG	1:A:232:VAL:H	2.27	0.41
1:B:308:PHE:HE1	1:B:333:VAL:CG1	2.34	0.41
1:C:86:GLY:O	1:C:87:SER:CB	2.69	0.41
1:C:88:GLU:O	1:C:231:ARG:HB3	2.05	0.41
1:C:91:THR:HG23	1:C:92:THR:N	2.36	0.41
1:A:139:SER:HA	1:A:140:PRO:HD3	1.13	0.40
1:A:252:ASP:OD1	1:A:345:LYS:HG2	2.20	0.40
1:B:133:SER:CB	1:B:235:THR:CG2	2.94	0.40
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.98	0.40
1:A:156:ARG:NH2	1:B:240:ASN:HA	2.36	0.40
1:B:299:GLY:HA2	1:B:335:MET:HG2	2.03	0.40
1:C:149:LYS:CD	1:C:217:TYR:HE1	2.33	0.40
1:C:114:GLY:HA2	1:C:285:ASN:H	1.57	0.40
1:B:343:LYS:HB2	1:B:344:GLY:H	1.13	0.40
1:A:313:GLU:HB2	1:A:315:ALA:CA	2.50	0.40
1:A:309:SER:C	1:A:322:ALA:HA	2.20	0.40
1:B:139:SER:HA	1:B:140:PRO:HD3	1.13	0.40
1:B:253:PHE:CZ	1:B:268:THR:HG21	2.56	0.40
1:B:302:ASN:HB3	1:B:308:PHE:CD1	2.56	0.40
1:C:120:ILE:HD13	1:C:120:ILE:HG21	1.87	0.40
1:C:296:PRO:HD2	1:C:337:THR:CG2	2.49	0.40
1:A:149:LYS:HG2	1:A:150:VAL:H	1.87	0.40
1:A:156:ARG:HD3	1:B:240:ASN:CG	2.38	0.40
1:A:86:GLY:O	1:A:87:SER:CB	2.69	0.40
1:B:149:LYS:HG2	1:B:150:VAL:H	1.87	0.40
1:B:128:LYS:O	1:B:238:LEU:HA	2.21	0.40
1:B:95:LYS:HB3	1:B:96:ASN:H	1.60	0.40
1:C:130:ARG:HB3	1:C:131:PHE:H	1.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:VAL:O	1:C:176:VAL:CG1	2.69	0.40
1:C:278:CYS:HB3	1:C:333:VAL:C	2.35	0.40
1:C:302:ASN:HB3	1:C:308:PHE:CD1	2.56	0.40
1:C:313:GLU:HG2	1:C:313:GLU:H	1.62	0.40
1:C:82:ILE:HD13	1:C:238:LEU:HD22	2.03	0.40
1:C:75:VAL:CG2	1:C:75:VAL:N	2.84	0.40
1:B:341:GLN:O	1:B:342:PRO:C	2.58	0.40
1:C:341:GLN:HE21	1:C:341:GLN:HB2	1.72	0.40
1:A:135:ARG:N	1:A:233:GLU:O	2.54	0.40
1:A:82:ILE:HD13	1:A:238:LEU:HD22	2.03	0.40
1:B:136:PHE:CG	1:B:212:LEU:HD21	2.56	0.40
1:C:297:VAL:HG12	1:C:336:VAL:HG11	0.98	0.40
1:A:341:GLN:O	1:A:342:PRO:C	2.58	0.40
1:B:190:THR:HG22	1:B:191:ASP:O	2.22	0.40
1:C:245:THR:CA	1:C:263:VAL:CG2	2.73	0.40
1:C:93:LEU:HD12	1:C:138:TYR:CE1	2.54	0.40
1:B:248:ALA:HA	1:B:265:TRP:CA	2.52	0.40
1:B:255:GLY:HA2	1:B:342:PRO:CB	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	263/347 (76%)	144 (55%)	60 (23%)	59 (22%)	0	2
1	B	263/347 (76%)	144 (55%)	60 (23%)	59 (22%)	0	2
1	C	291/347 (84%)	161 (55%)	64 (22%)	66 (23%)	0	2
All	All	817/1041 (78%)	449 (55%)	184 (22%)	184 (22%)	0	2

All (184) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	87	SER
1	A	90	ILE
1	A	95	LYS
1	A	96	ASN
1	A	97	THR
1	A	119	LEU
1	A	128	LYS
1	A	140	PRO
1	A	157	ASP
1	A	160	LYS
1	A	166	LEU
1	A	173	GLU
1	A	202	SER
1	A	209	PHE
1	A	227	LEU
1	A	240	ASN
1	A	244	SER
1	A	245	THR
1	A	246	SER
1	A	255	GLY
1	A	290	LEU
1	A	293	GLU
1	A	295	ALA
1	A	307	ASP
1	A	316	ALA
1	A	329	ARG
1	A	339	GLU
1	A	341	GLN
1	B	83	THR
1	B	87	SER
1	B	90	ILE
1	B	95	LYS
1	B	96	ASN
1	B	97	THR
1	B	119	LEU
1	B	128	LYS
1	B	140	PRO
1	B	157	ASP
1	B	160	LYS
1	B	166	LEU
1	B	173	GLU
1	B	202	SER

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Mol	Chain	Res	Type
1	B	209	PHE
1	B	227	LEU
1	B	240	ASN
1	B	244	SER
1	B	245	THR
1	B	246	SER
1	B	255	GLY
1	B	290	LEU
1	B	293	GLU
1	B	295	ALA
1	B	307	ASP
1	B	316	ALA
1	B	329	ARG
1	B	339	GLU
1	B	341	GLN
1	C	55	VAL
1	C	56	THR
1	C	77	THR
1	C	79	ARG
1	C	80	ASP
1	C	83	THR
1	C	87	SER
1	C	90	ILE
1	C	95	LYS
1	C	96	ASN
1	C	97	THR
1	C	119	LEU
1	C	128	LYS
1	C	140	PRO
1	C	157	ASP
1	C	160	LYS
1	C	166	LEU
1	C	173	GLU
1	C	202	SER
1	C	209	PHE
1	C	227	LEU
1	C	240	ASN
1	C	244	SER
1	C	245	THR
1	C	246	SER
1	C	255	GLY
1	C	290	LEU

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Mol	Chain	Res	Type
1	C	293	GLU
1	C	295	ALA
1	C	307	ASP
1	C	316	ALA
1	C	329	ARG
1	C	339	GLU
1	C	341	GLN
1	A	101	PRO
1	A	105	THR
1	A	114	GLY
1	A	115	THR
1	A	116	PHE
1	A	151	ALA
1	A	156	ARG
1	A	158	ALA
1	A	167	ALA
1	A	291	PHE
1	A	292	TYR
1	A	296	PRO
1	A	315	ALA
1	B	101	PRO
1	B	105	THR
1	B	114	GLY
1	B	115	THR
1	B	116	PHE
1	B	151	ALA
1	B	156	ARG
1	B	158	ALA
1	B	167	ALA
1	B	291	PHE
1	B	292	TYR
1	B	296	PRO
1	B	315	ALA
1	C	69	VAL
1	C	101	PRO
1	C	105	THR
1	C	114	GLY
1	C	115	THR
1	C	116	PHE
1	C	151	ALA
1	C	156	ARG
1	C	158	ALA

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Mol	Chain	Res	Type
1	C	167	ALA
1	C	291	PHE
1	C	292	TYR
1	C	296	PRO
1	C	315	ALA
1	A	145	THR
1	A	152	LEU
1	A	263	VAL
1	B	145	THR
1	B	152	LEU
1	B	263	VAL
1	C	145	THR
1	C	152	LEU
1	C	263	VAL
1	A	131	PHE
1	A	205	LYS
1	A	298	SER
1	A	343	LYS
1	B	131	PHE
1	B	205	LYS
1	B	298	SER
1	B	343	LYS
1	C	131	PHE
1	C	205	LYS
1	C	298	SER
1	C	343	LYS
1	A	134	LEU
1	A	163	PRO
1	A	201	ILE
1	A	260	PRO
1	A	300	LEU
1	A	314	ALA
1	B	82	ILE
1	B	134	LEU
1	B	163	PRO
1	B	201	ILE
1	B	260	PRO
1	B	300	LEU
1	B	314	ALA
1	C	134	LEU
1	C	163	PRO
1	C	201	ILE

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Mol	Chain	Res	Type
1	C	260	PRO
1	C	300	LEU
1	C	314	ALA
1	A	82	ILE
1	A	313	GLU
1	B	313	GLU
1	C	71	THR
1	C	82	ILE
1	C	313	GLU
1	A	297	VAL
1	B	297	VAL
1	C	297	VAL
1	B	259	GLY
1	C	259	GLY
1	A	259	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	215/282 (76%)	178 (83%)	37 (17%)	2	17
1	B	215/282 (76%)	179 (83%)	36 (17%)	3	19
1	C	238/282 (84%)	200 (84%)	38 (16%)	3	21
All	All	668/846 (79%)	557 (83%)	111 (17%)	6	19

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	91	THR
1	A	96	ASN
1	A	97	THR
1	A	108	LEU
1	A	117	ASN
1	A	120	ILE

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Mol	Chain	Res	Type
1	A	129	TYR
1	A	134	LEU
1	A	135	ARG
1	A	145	THR
1	A	146	THR
1	A	150	VAL
1	A	152	LEU
1	A	154	PHE
1	A	164	ASN
1	A	165	ASP
1	A	176	VAL
1	A	185	ILE
1	A	192	SER
1	A	199	ASP
1	A	205	LYS
1	A	206	LEU
1	A	208	ASP
1	A	213	ILE
1	A	217	TYR
1	A	234	TYR
1	A	260	PRO
1	A	264	SER
1	A	275	GLU
1	A	276	HIS
1	A	285	ASN
1	A	290	LEU
1	A	292	TYR
1	A	300	LEU
1	A	313	GLU
1	A	339	GLU
1	B	89	LEU
1	B	91	THR
1	B	96	ASN
1	B	97	THR
1	B	108	LEU
1	B	117	ASN
1	B	120	ILE
1	B	129	TYR
1	B	134	LEU
1	B	135	ARG
1	B	145	THR
1	B	146	THR

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Mol	Chain	Res	Type
1	B	150	VAL
1	B	152	LEU
1	B	154	PHE
1	B	164	ASN
1	B	165	ASP
1	B	176	VAL
1	B	185	ILE
1	B	192	SER
1	B	199	ASP
1	B	205	LYS
1	B	206	LEU
1	B	208	ASP
1	B	213	ILE
1	B	217	TYR
1	B	234	TYR
1	B	264	SER
1	B	275	GLU
1	B	276	HIS
1	B	285	ASN
1	B	290	LEU
1	B	292	TYR
1	B	300	LEU
1	B	313	GLU
1	B	339	GLU
1	C	58	LEU
1	C	79	ARG
1	C	89	LEU
1	C	91	THR
1	C	96	ASN
1	C	97	THR
1	C	108	LEU
1	C	117	ASN
1	C	120	ILE
1	C	129	TYR
1	C	134	LEU
1	C	135	ARG
1	C	145	THR
1	C	146	THR
1	C	150	VAL
1	C	152	LEU
1	C	154	PHE
1	C	164	ASN

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Mol	Chain	Res	Type
1	C	165	ASP
1	C	176	VAL
1	C	185	ILE
1	C	192	SER
1	C	199	ASP
1	C	205	LYS
1	C	206	LEU
1	C	208	ASP
1	C	213	ILE
1	C	217	TYR
1	C	234	TYR
1	C	264	SER
1	C	275	GLU
1	C	276	HIS
1	C	285	ASN
1	C	290	LEU
1	C	292	TYR
1	C	300	LEU
1	C	313	GLU
1	C	339	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	117	ASN
1	A	118	GLN
1	A	125	GLN
1	A	164	ASN
1	A	171	ASN
1	A	226	GLN
1	A	237	GLN
1	A	249	GLN
1	A	285	ASN
1	A	341	GLN
1	B	96	ASN
1	B	109	ASN
1	B	118	GLN
1	B	125	GLN
1	B	164	ASN
1	B	171	ASN
1	B	226	GLN

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Mol	Chain	Res	Type
1	B	237	GLN
1	B	285	ASN
1	B	341	GLN
1	C	72	GLN
1	C	96	ASN
1	C	117	ASN
1	C	118	GLN
1	C	125	GLN
1	C	164	ASN
1	C	171	ASN
1	C	226	GLN
1	C	237	GLN
1	C	249	GLN
1	C	285	ASN
1	C	341	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.