



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:20 AM UTC

PDB ID : 2QQP / pdb_00002qqp
Title : Crystal Structure of Authentic Providence Virus
Authors : Speir, J.A.; Taylor, D.J.; Johnson, J.E.
Deposited on : 2007-07-26
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

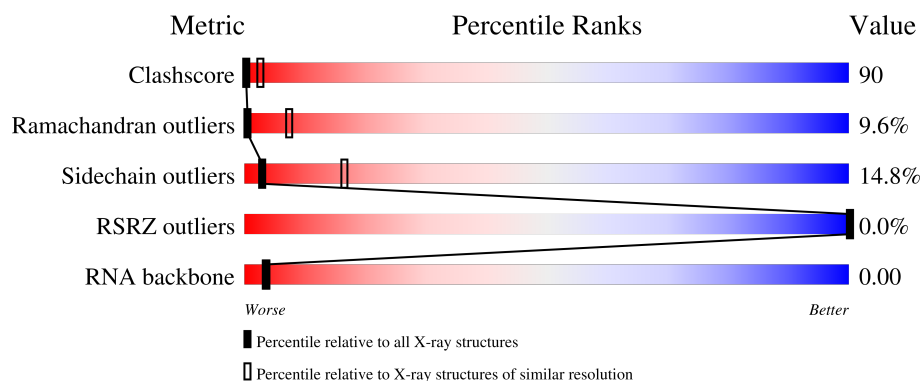
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	
1	C	556	
1	E	556	
1	G	556	
2	B	75	

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Mol	Chain	Length	Quality of chain
2	D	75	9%24%17%•47%
2	F	75	12%59%15%•11%
2	H	75	7%36%7%•49%
3	R	4	25%50%25%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16634 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called p81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3714	2359	604	740	11			
1	C	484	Total	C	N	O	S	0	0	0
			3714	2359	604	740	11			
1	E	517	Total	C	N	O	S	0	0	0
			3948	2505	645	785	13			
1	G	518	Total	C	N	O	S	0	0	0
			3957	2510	646	788	13			

- Molecule 2 is a protein called p81.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	0	0	0
			255	162	44	49			
2	D	40	Total	C	N	O	0	0	0
			263	166	46	51			
2	F	67	Total	C	N	O	0	0	0
			448	282	84	82			
2	H	38	Total	C	N	O	0	0	0
			250	159	43	48			

- Molecule 3 is a RNA chain called RNA (5'-R(*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

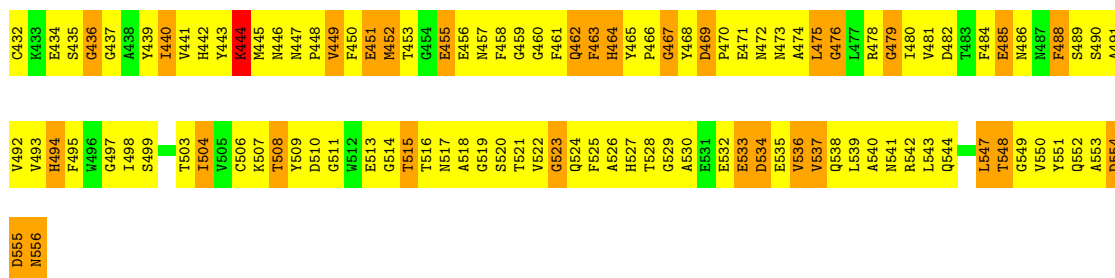
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	C	2	Total 2	O 2	0	0
5	E	2	Total 2	O 2	0	0
5	G	1	Total 1	O 1	0	0

V560 Y561 Q562 A563 D564 D565 N566	S489	Q429	T366	T303	T242	M181	R121	GLY
	S490	F430	V367	V304	L243	M182	P122	THR
	A491	F431	V368	A305	L244	T183	I123	MET
	S492	C432	V369	L306	D245	T184	T124	ASP
	V493	K433	S370		D246	M185	T125	PRO
	H494	F434	V371	T310	C247	V186	I126	PRO
	F495	S435	S372	G311	W248	A187	E127	VAL
	V496	G436	S373	G312	W249	D188	C128	HIS
	G497	G437	S374	T313	V250	L189	G129	GLU
	S499	A438	L375	N314	G251	G190	T130	ILE
Q500 S501 A502 T503 I504 V505 C506 K507 T508 Y509 D510 F511 H512 E513 G514 T515 T516 N517	Q499	V439	T376	N315	A252	T191	V131	CYS
	Q500	I440	G377	T316	H263	G192	S132	ALA
	S501	V441	S378	S317	T254	Q193	E133	THR
	A502	T381		G318	V255	A194	S134	THR
	T503	Y443	T394	K319	V256	A195	D135	Y75
	I504	K444	V382	F320	K257	Q196	L136	D76
	V505	M445	R383	F321	P258	G197	P137	P77
	C506	M446	G384	S322	G259	A198	L138	S78
	K507	M447	V385	V323	S260	P199	D139	E79
	T508	P448	T386	E324	T261	G200	G140	G80
S520 T521 V522 G523 Q524 F525 A526 H527 T528 G529 A530 E531 S532 D533 F534 C535 V536 F537 Q538 L539 N540 H541 R542 L543 Q544 M545 E546 H547 T548 C549	Y509	F449	K387	T325	T262	W201	K141	A81
	D510	V450	G388	T326	L263	Y202	L142	V82
	F511	G451	G327	G327	P264	Y203	W143	G83
	H512	M452	N328	N328	A265	S204	R144	H84
	E513	T453	S392	V329	A266	I205	V145	F85
	G514	G393			E267	Y206	S146	Y86
	T515	E455	T394	V332	R268	Y207	F147	K87
	T516	A456	P395	W333	T269	L208	I148	M89
	N517	M457	V396	T334	S270	P209	S149	D90
	S520	F458	T397	F335	K271	M210	F150	P91
S521 V522 G523 Q524 F525 A526 H527 T528 G529 A530 E531 S532 D533 F534 C535 V536 F537 Q538 L539 N540 H541 R542 L543 Q544 M545 E546 H547 T548 C549	T521	G460	G399	A337	S273	Y212	A152	A92
	V522	F461	I400	P338	M274	A213	F153	G93
	G523	Q462	D401	A339	T275	M214	R154	A94
	Q524	F463	T402	S340	V276	A215	L155	V95
	F525	H464	E403	T341	S277	E216	M156	E96
	A526	Y465	A404	L342	K278	T217	F157	S97
	H527	G466	M405	A343	G218	D219	I158	G98
	T528	G467	M406	E344	S279		A159	K99
	G529	Y468	R407	G345	T282	R220	L160	A100
	A530	D469	G346	G346	F283	T221	A161	L101
E531 S532 D533 F534 C535 V536 F537 Q538 L539 N540 H541 R542 L543 Q544 M545 E546 H547 T548 C549	E531	F470	T410	P347	Q284	M162	G102	G102
	S532	E471	E411	F346	P285	I163	E103	E103
	D533	M472	M412	A349	S286	T225	F104	F104
	F534	H473	P413	E350	N287	G226	N165	S105
	C535	A474	A414	S351	T288	F227	E166	K106
	V536	L475	L415	G352	V289	R228	A167	V107
	F537	G476	T416	S353	A290	K229	L168	P108
	Q538	L477	T417	T354	R291	W230	T169	D109
	L539	R478	E418	S355	T292	Y231	L170	G110
	N540	G479	E419	T356	V293	K232	E171	L111
H541 R542 L543 Q544 M545 E546 H547 T548 C549	H541	T480	V420		G233	T172	R173	R113
	R542	V481	T421	S295	S294	T234	R174	Y114
	L543	D482	T422	N359	T296	T235	N174	L112
	Q544	T483	M423	T360	T297	F236	T175	S115
	M545	F484	V424	T361	P298	E237	F176	V116
	E546	E485	P425	T362	L299	F238	T177	D117
	H547	M486	K426	T363	P300	N239	Q178	A118
	T548	M487	Y427	A364	V301	T179	A119	C120
	C549	F488	F428	P365	L282	T241	T190	

- Molecule 1: p81

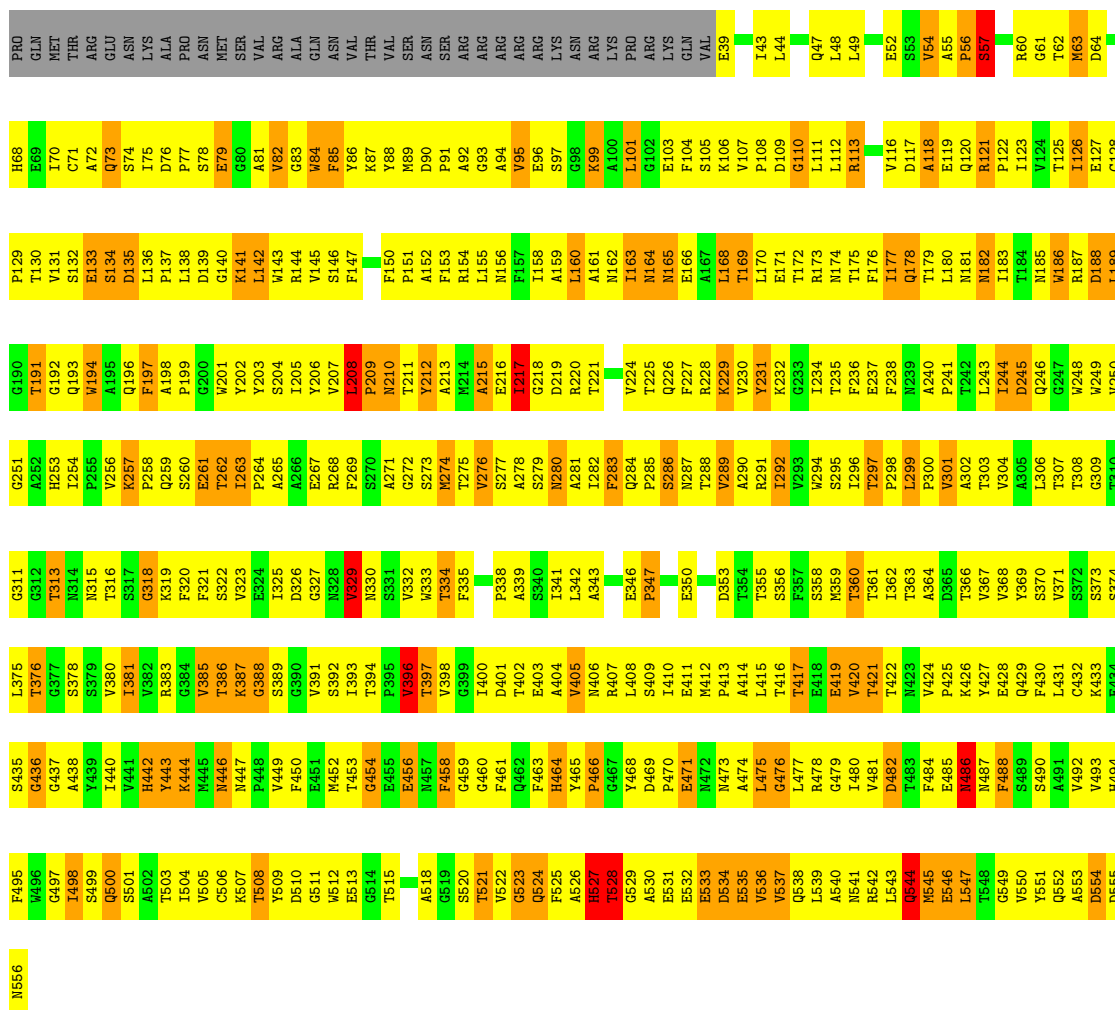
Chain E: 15% 59% 18% 7%

S370	A305	T242	N182	P122	G61
V371	L306	L243	L183	L123	M62
S372	L307	L244	L184	L124	M63
S373	T308	D245	L185	L125	D64
S374	G309	Q246	L186	L126	P65
L375	T310	G247	L187	E127	P66
T376	G311	W248	L188	C128	V67
G377	G312	W249	L189	P129	H68
	T313	V250	G190	T130	E69
V380	N314	G251	L191	V131	I70
L381	N315	A252	G192	S132	C71
V382	T316	H253	Q193	F133	A72
	S317	L254	L194	L134	Q73
V385	G318	P255	A195	D135	
T386	L319	V256	Q196	L136	D76
G387	F320	K257	F197	P137	P77
K388	F321	P258	A198	L138	S78
S389	S322	Q259	P199	D139	E79
G390	V323	S260	G200	G140	G80
V391	E324	E261	L201	K141	A81
	L325	T262	Y202	L142	H82
L393			Y203	L143	Q83
T394	V329	A265	S204	L144	W84
P395	M330	A266	L205	V145	F85
V396	S331	E267	Y206	S146	H86
T397	V332		V207	F147	K87
V398	T333	S270	L208	L148	H88
G399	T334	A271	P209	S149	W89
I400	F335	G272	N210	F150	D90
D401	T336	S273	T211	P151	P91
T402	A337	M274	Y212	A152	A92
E403	P338	T275	M214	F153	G93
		V276	A215	L155	A94
A404	L341	A278	E216	N156	V95
V405	L342		L217	F157	F96
M406	A343		G218	L158	S97
R407	E344	A281	D219	A159	G98
L408		L282	R220	L160	A100
S409	F348	F283	T221	A161	L101
T410	A349	Q284	D222	N162	G102
M412	S350	P285	S223	L163	E103
P413	E351	S286	T224	N164	F104
A414	G352	L287	V225	L165	S105
L415	T353	T288	Q226	E166	K106
T416	F354	V289	Q227	A167	V107
T417	T355	A290	F227	L168	P108
E418	S356	R291	R228	T169	D109
E419	F357	T292	K229	T170	G110
V420	L358	L293	V230	L171	L111
T421	M359	W294	Y231	E171	L112
T422	T360	S295	K232	T172	L113
M423	L415	T296	G233	R173	R114
T424	T361	L362	L234	N174	A114
		T297	T235	T175	S115
V425	T363	P298	T236	F176	V116
K426	A364	L299	E237	T177	D117
T427	T365	P300	V237	L178	P118
V428	T366	V301	T238	Q178	A118
Q429	A367	A302	N239	T179	E119
	V368	T303	A240	L180	Q120
F430	V369	V241	P241	N181	P121



• Molecule 1: p81

Chain G: 17% 56% 19% 7%



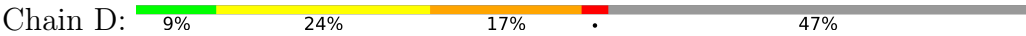
• Molecule 2: p81

Chain B: 13% 28% 9% 48%



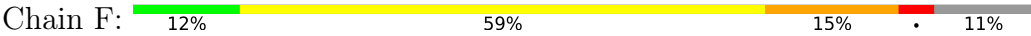
LYS
ALA
ARG
ARG
ALA
ALA
ARG
ARG
ALA
ALA
ARG
ARG
LYS

• Molecule 2: p81



ILE
LYS
ALA
ARG
ARG
ALA
ALA
ARG
ARG
ALA
ALA
LYS

• Molecule 2: p81



• Molecule 2: p81



SER
ILE
LYS
ALA
ARG
ARG
ALA
ALA
ARG
ARG
ALA
LYS

• Molecule 3: RNA (5'-R(*UP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	659.79Å 434.07Å 415.85Å 90.00° 126.13° 90.00°	Depositor
Resolution (Å)	49.42 – 3.80 49.42 – 3.80	Depositor EDS
% Data completeness (in resolution range)	28.6 (49.42-3.80) 24.7 (49.42-3.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.285 , (Not available) 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.059 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.12	EDS
Total number of atoms	16634	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	2/3807 (0.1%)	1.14	31/5203 (0.6%)
1	C	0.68	1/3807 (0.0%)	1.15	32/5203 (0.6%)
1	E	0.70	3/4047 (0.1%)	1.17	51/5532 (0.9%)
1	G	0.67	1/4056 (0.0%)	1.15	32/5544 (0.6%)
2	B	0.68	0/256	1.05	2/346 (0.6%)
2	D	0.79	0/264	1.52	8/357 (2.2%)
2	F	0.81	0/450	1.30	5/606 (0.8%)
2	H	0.70	0/251	1.06	3/339 (0.9%)
3	R	1.03	0/84	0.93	1/128 (0.8%)
All	All	0.69	7/17022 (0.0%)	1.16	165/23258 (0.7%)

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	1
1	C	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	527	HIS	ND1-CE1	5.23	1.37	1.32
1	E	494	HIS	ND1-CE1	5.22	1.37	1.32
1	A	464	HIS	ND1-CE1	5.14	1.37	1.32
1	E	464	HIS	ND1-CE1	5.12	1.37	1.32
1	C	527	HIS	ND1-CE1	5.10	1.37	1.32
1	G	442	HIS	ND1-CE1	5.07	1.37	1.32
1	A	527	HIS	ND1-CE1	5.03	1.37	1.32

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	415	LEU	N-CA-C	-10.58	102.56	114.62
1	C	220	ARG	N-CA-C	-9.48	101.71	113.28
1	E	555	ASP	N-CA-C	-9.31	101.62	113.72
1	G	374	SER	N-CA-C	-9.07	102.35	113.15
1	A	133	GLU	N-CA-C	-8.56	102.96	113.41
2	D	569	LEU	N-CA-C	-8.38	102.14	111.28
1	A	317	SER	N-CA-C	-8.17	101.94	112.23
2	F	610	VAL	N-CA-C	-8.07	101.83	110.23
2	D	580	SER	N-CA-C	-8.01	102.49	111.14
1	C	113	ARG	N-CA-C	-7.99	102.51	111.14
1	C	455	GLU	N-CA-C	-7.96	103.36	113.23
1	A	447	ASN	CA-C-N	7.83	129.63	119.84
1	A	447	ASN	C-N-CA	7.83	129.63	119.84
1	G	212	TYR	N-CA-C	-7.71	102.88	111.28
1	E	262	THR	N-CA-C	7.34	120.33	110.35
1	A	267	GLU	N-CA-C	7.33	119.78	108.12
1	G	54	VAL	N-CA-C	7.31	118.35	108.11
1	G	113	ARG	N-CA-C	-7.17	102.65	111.40
1	E	284	GLN	CA-C-N	7.08	128.68	119.84
1	E	284	GLN	C-N-CA	7.08	128.68	119.84
2	F	601	GLU	N-CA-C	7.02	117.30	108.45
2	F	617	SER	N-CA-C	6.99	118.69	111.14
1	E	527	HIS	CB-CG-CD2	-6.96	122.16	131.20
1	E	494	HIS	CB-CG-CD2	-6.84	122.31	131.20
1	E	197	PHE	N-CA-C	-6.79	106.88	114.62
1	G	442	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	C	527	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	E	464	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	E	156	ASN	CA-CB-CG	6.59	119.19	112.60
1	C	140	GLY	N-CA-C	-6.55	105.83	115.72
1	E	208	LEU	CA-C-N	6.55	128.03	119.84
1	E	208	LEU	C-N-CA	6.55	128.03	119.84
1	A	464	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	G	262	THR	N-CA-C	6.50	120.63	110.17
1	A	527	HIS	CB-CG-CD2	-6.46	122.80	131.20
2	D	560	THR	N-CA-C	-6.43	103.55	111.40
1	A	262	THR	N-CA-C	6.43	120.36	110.20
2	D	590	VAL	N-CA-C	-6.41	104.66	113.00
2	B	594	GLN	N-CA-C	6.41	119.52	110.23
1	G	260	SER	N-CA-C	6.37	119.90	110.48
1	A	140	GLY	N-CA-C	-6.36	103.93	114.48
1	A	113	ARG	N-CA-C	-6.35	104.46	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	208	LEU	CA-C-N	6.25	127.65	119.84
1	G	208	LEU	C-N-CA	6.25	127.65	119.84
1	C	284	GLN	CA-C-N	6.25	127.65	119.84
1	C	284	GLN	C-N-CA	6.25	127.65	119.84
1	E	372	SER	N-CA-C	6.21	119.25	108.76
1	C	170	LEU	N-CA-C	-6.19	104.45	111.07
1	A	542	ARG	N-CA-C	-6.18	103.86	111.40
1	E	488	PHE	N-CA-C	6.09	118.57	110.53
1	E	504	ILE	N-CA-C	6.07	116.60	107.80
1	E	321	PHE	N-CA-C	6.04	118.49	109.25
1	E	363	THR	N-CA-C	-5.98	102.63	110.53
1	E	479	GLY	N-CA-C	-5.96	103.20	112.45
1	A	190	GLY	N-CA-C	-5.95	105.35	113.27
1	G	479	GLY	N-CA-C	-5.94	105.14	112.33
1	E	527	HIS	CB-CG-ND1	5.93	131.60	122.70
1	G	381	ILE	N-CA-C	5.92	115.26	106.85
1	E	494	HIS	CB-CG-ND1	5.92	131.58	122.70
1	G	389	SER	N-CA-C	5.89	118.06	108.76
1	G	534	ASP	N-CA-C	-5.89	105.20	112.38
1	E	220	ARG	N-CA-C	5.87	120.49	112.68
2	F	569	LEU	N-CA-C	-5.85	104.91	111.28
1	E	317	SER	N-CA-C	-5.85	105.03	114.09
1	G	263	ILE	CA-C-N	5.84	125.85	119.90
1	G	263	ILE	C-N-CA	5.84	125.85	119.90
1	A	107	VAL	CA-C-N	5.82	127.11	119.84
1	A	107	VAL	C-N-CA	5.82	127.11	119.84
1	C	262	THR	N-CA-C	5.80	119.36	110.20
1	E	416	THR	N-CA-C	5.79	118.10	109.59
2	D	593	VAL	N-CA-C	5.79	115.97	107.75
2	H	593	VAL	N-CA-C	5.77	115.56	107.37
1	G	490	SER	N-CA-C	-5.77	101.48	110.42
1	E	554	ASP	N-CA-C	-5.76	106.23	113.72
1	C	141	LYS	N-CA-C	-5.75	102.25	110.59
1	E	116	VAL	N-CA-C	-5.75	101.52	109.46
1	C	527	HIS	CB-CG-ND1	5.75	131.32	122.70
1	C	257	LYS	CA-C-N	5.75	127.02	119.84
1	C	257	LYS	C-N-CA	5.75	127.02	119.84
1	C	321	PHE	N-CA-C	5.73	118.07	108.96
1	C	344	GLU	N-CA-C	-5.69	104.05	111.74
1	G	488	PHE	N-CA-C	5.67	118.87	110.48
1	G	442	HIS	CB-CG-ND1	5.65	131.18	122.70
1	C	360	THR	N-CA-C	-5.64	105.14	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	520	SER	N-CA-C	-5.62	106.09	114.64
1	C	104	PHE	N-CA-C	5.59	119.72	113.01
1	A	299	LEU	CA-C-N	5.59	125.59	119.89
1	A	299	LEU	C-N-CA	5.59	125.59	119.89
1	C	481	VAL	N-CA-C	5.59	115.70	107.15
1	A	464	HIS	CB-CG-ND1	5.58	131.06	122.70
1	A	527	HIS	CB-CG-ND1	5.57	131.05	122.70
1	E	464	HIS	CB-CG-ND1	5.56	131.04	122.70
1	A	389	SER	N-CA-C	5.55	118.15	107.44
2	D	579	PRO	N-CA-C	-5.54	106.93	113.86
1	A	529	GLY	N-CA-C	-5.54	104.88	111.36
1	C	421	THR	N-CA-C	5.53	118.06	111.71
1	E	402	THR	N-CA-C	5.52	118.78	107.69
1	C	407	ARG	N-CA-C	-5.51	101.55	110.32
2	D	563	ALA	N-CA-C	-5.51	105.17	111.07
1	G	101	LEU	N-CA-C	5.50	118.79	109.76
2	D	595	ALA	N-CA-C	5.49	117.62	110.43
2	B	592	ALA	N-CA-C	5.47	117.38	108.63
1	E	212	TYR	N-CA-C	-5.45	105.50	111.82
1	E	325	ILE	N-CA-C	5.45	115.54	108.35
1	E	54	VAL	N-CA-C	5.45	115.99	110.05
1	A	364	ALA	N-CA-C	-5.44	105.27	112.34
1	E	128	CYS	CA-C-N	5.43	126.63	119.84
1	E	128	CYS	C-N-CA	5.43	126.63	119.84
1	E	284	GLN	N-CA-C	5.42	117.86	110.01
1	A	257	LYS	N-CA-C	-5.41	103.36	110.39
1	E	299	LEU	CA-C-N	5.40	125.33	119.76
1	E	299	LEU	C-N-CA	5.40	125.33	119.76
1	E	309	GLY	N-CA-C	5.39	120.88	112.31
1	E	47	GLN	N-CA-C	-5.38	105.58	111.82
1	A	410	ILE	N-CA-C	5.38	115.61	107.75
1	G	215	ALA	N-CA-C	5.38	117.82	110.24
1	E	469	ASP	CA-C-N	5.36	125.05	119.64
1	E	469	ASP	C-N-CA	5.36	125.05	119.64
1	A	141	LYS	N-CA-C	-5.34	101.41	109.85
1	E	137	PRO	N-CA-C	-5.34	107.06	114.27
1	G	554	ASP	N-CA-C	-5.33	104.41	112.99
1	C	465	TYR	CA-C-N	-5.33	114.47	119.85
1	C	465	TYR	C-N-CA	-5.33	114.47	119.85
1	G	521	THR	N-CA-C	-5.33	106.96	112.93
1	E	303	THR	N-CA-C	5.33	118.29	110.30
1	G	535	GLU	N-CA-C	-5.27	105.00	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	ASN	N-CA-C	5.27	117.83	109.24
1	C	505	VAL	N-CA-C	-5.26	101.95	108.89
1	G	347	PRO	N-CA-C	-5.25	102.86	110.80
1	C	317	SER	N-CA-C	-5.25	107.42	113.88
1	C	388	GLY	N-CA-C	-5.24	108.45	114.69
1	E	164	ASN	N-CA-C	-5.23	102.00	110.32
2	H	593	VAL	CB-CA-C	-5.23	106.26	111.80
1	E	172	THR	N-CA-C	-5.23	105.27	110.97
1	E	344	GLU	N-CA-C	-5.22	104.19	111.39
3	R	2	U	N1-C1'-C2'	5.20	119.80	112.00
1	C	212	TYR	N-CA-C	-5.19	105.62	111.28
1	E	96	GLU	N-CA-C	-5.18	106.79	113.01
1	E	65	PRO	CA-C-N	5.17	126.31	119.84
1	E	65	PRO	C-N-CA	5.17	126.31	119.84
2	H	591	GLY	N-CA-C	5.17	120.41	112.51
1	A	421	THR	N-CA-C	-5.15	105.31	111.03
1	C	547	LEU	N-CA-C	5.15	117.95	110.17
1	G	471	GLU	N-CA-C	-5.14	105.30	112.45
1	E	181	ASN	N-CA-C	-5.14	106.17	112.90
1	G	299	LEU	CA-C-N	5.13	124.89	119.76
1	G	299	LEU	C-N-CA	5.13	124.89	119.76
1	E	45	LYS	CA-C-N	5.12	125.56	120.14
1	E	45	LYS	C-N-CA	5.12	125.56	120.14
1	A	206	TYR	CA-CB-CG	-5.12	104.69	113.90
1	C	263	ILE	N-CA-C	-5.10	102.61	107.76
1	C	183	ILE	CB-CA-C	-5.09	106.14	112.45
1	A	161	ALA	N-CA-C	5.08	117.10	109.23
1	A	308	THR	N-CA-C	5.08	116.32	107.49
1	A	327	GLY	N-CA-C	5.07	118.39	110.88
1	C	491	ALA	N-CA-C	5.07	117.59	110.14
1	G	128	CYS	N-CA-C	-5.06	103.10	110.08
1	E	463	PHE	N-CA-C	5.06	117.80	109.76
1	G	396	VAL	N-CA-C	5.04	114.97	108.82
1	A	263	ILE	CA-C-N	5.04	126.14	119.84
1	A	263	ILE	C-N-CA	5.04	126.14	119.84
1	E	394	THR	N-CA-C	5.03	116.80	109.30
2	F	560	THR	N-CA-C	-5.03	105.93	111.71
1	G	283	PHE	N-CA-C	-5.03	106.73	112.86
1	G	261	GLU	N-CA-C	-5.00	101.72	109.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	TYR	Sidechain
1	C	206	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3714	0	3548	692	0
1	C	3714	0	3548	716	0
1	E	3948	0	3786	784	0
1	G	3957	0	3792	742	0
2	B	255	0	275	45	0
2	D	263	0	281	69	0
2	F	448	0	491	93	0
2	H	250	0	270	51	0
3	R	77	0	42	4	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	1	0
5	G	1	0	0	0	0
All	All	16634	0	16033	2923	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 90.

All (2923) 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:475:LEU:HD11	1:E:267:GLU:CG	1.36	1.52
1:C:297:THR:HG23	1:C:476:GLY:CA	1.55	1.35
1:C:120:GLN:NE2	1:C:208:LEU:HB3	1.45	1.29
1:E:297:THR:HG22	1:E:298:PRO:CD	1.64	1.27
1:C:475:LEU:HD11	1:E:267:GLU:CB	1.68	1.21
1:E:220:ARG:NH1	1:G:215:ALA:HB1	1.56	1.21
1:C:297:THR:CG2	1:C:476:GLY:HA3	1.70	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:THR:CG2	1:E:298:PRO:HD3	1.71	1.20
1:G:416:THR:HB	1:G:419:GLU:HB2	1.23	1.14
1:A:475:LEU:HD22	1:C:267:GLU:HG2	1.28	1.14
1:A:383:ARG:HH11	1:A:383:ARG:HB2	1.04	1.13
1:E:220:ARG:HH11	1:G:215:ALA:CB	1.62	1.13
1:E:198:ALA:HB3	1:E:201:TRP:HB2	1.27	1.11
1:A:234:ILE:HG12	1:A:508:THR:HG23	1.30	1.11
1:C:297:THR:CG2	1:C:476:GLY:CA	2.26	1.10
1:A:383:ARG:HB2	1:A:383:ARG:NH1	1.64	1.10
1:E:220:ARG:HD2	1:G:215:ALA:HB2	1.22	1.09
1:A:549:GLY:HA2	1:C:113:ARG:HH21	1.16	1.09
1:A:262:THR:HA	1:A:406:ASN:HB3	1.35	1.08
1:C:475:LEU:CD1	1:E:267:GLU:CG	2.31	1.08
1:E:255:PRO:HB3	1:E:445:MET:HG2	1.30	1.08
1:G:168:LEU:HD22	1:G:173:ARG:HG3	1.34	1.08
1:C:273:SER:HB3	1:C:475:LEU:HD12	1.28	1.08
1:G:297:THR:CG2	1:G:476:GLY:HA3	1.83	1.08
1:C:475:LEU:CD1	1:E:267:GLU:HB2	1.84	1.07
1:G:297:THR:HG21	1:G:476:GLY:HA3	1.10	1.07
1:G:47:GLN:NE2	1:G:63:MET:HA	1.70	1.06
1:E:416:THR:HB	1:E:419:GLU:HB2	1.08	1.05
1:C:475:LEU:HD11	1:E:267:GLU:HG2	1.32	1.05
1:A:225:THR:HG23	1:A:517:ASN:HB2	1.40	1.03
1:C:105:SER:HB2	1:C:117:ASP:HB2	1.40	1.02
1:C:475:LEU:HD11	1:E:267:GLU:CD	1.83	1.02
1:A:107:VAL:HG23	1:A:230:VAL:HG22	1.38	1.02
1:A:129:PRO:HG2	1:A:163:ILE:HG23	1.41	1.02
1:A:413:PRO:HA	1:C:517:ASN:OD1	1.59	1.02
1:C:184:THR:HG21	1:C:295:SER:HB2	1.41	1.01
1:C:363:THR:HG23	1:C:365:ASP:H	1.23	1.00
1:C:405:VAL:HG11	1:C:477:LEU:HD13	1.41	1.00
1:C:87:LYS:HD3	1:C:91:PRO:HA	1.39	1.00
1:G:297:THR:HG21	1:G:476:GLY:CA	1.91	0.99
1:A:404:ALA:HB3	1:E:261:GLU:OE2	1.60	0.99
1:C:475:LEU:CD1	1:E:267:GLU:CB	2.40	0.99
1:A:400:ILE:HG12	1:A:401:ASP:H	1.22	0.99
1:A:404:ALA:HB1	1:E:261:GLU:HB3	1.44	0.99
2:F:599:ILE:O	2:F:600:LEU:HG	1.61	0.99
1:C:275:THR:HG23	1:C:478:ARG:HH22	1.25	0.98
1:A:538:GLN:HG2	2:B:582:ILE:HD13	1.43	0.98
1:E:237:GLU:HG3	1:E:507:LYS:HE2	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:ALA:HB3	1:G:284:GLN:HG3	1.39	0.98
1:G:132:SER:C	1:G:134:SER:H	1.69	0.98
2:F:564:LEU:O	2:F:567:ILE:HG23	1.64	0.97
1:C:275:THR:HG23	1:C:478:ARG:NH2	1.79	0.97
1:A:363:THR:HG22	1:A:365:ASP:H	1.30	0.97
2:H:578:THR:HG22	2:H:581:VAL:H	1.27	0.97
1:A:73:GLN:HE22	2:F:578:THR:HG21	1.28	0.96
1:G:198:ALA:HB3	1:G:201:TRP:HB2	1.44	0.96
1:E:385:VAL:HG12	1:E:392:SER:HB3	1.48	0.96
1:C:302:ALA:HB2	1:C:338:PRO:HG3	1.48	0.96
1:A:549:GLY:CA	1:C:113:ARG:HH21	1.79	0.95
1:E:69:GLU:HA	1:E:78:SER:HA	1.47	0.95
1:G:189:LEU:H	1:G:189:LEU:HD23	1.27	0.95
1:E:297:THR:HG23	1:E:476:GLY:HA3	1.45	0.95
1:G:274:MET:HE2	1:G:296:ILE:HD11	1.48	0.95
1:A:262:THR:HA	1:A:406:ASN:CB	1.96	0.94
1:E:273:SER:H	1:E:297:THR:HB	1.31	0.94
1:C:272:GLY:HA3	1:C:298:PRO:HD3	1.50	0.94
1:G:274:MET:HB3	1:G:296:ILE:HG13	1.49	0.94
1:A:127:GLU:HA	1:A:503:THR:HG22	1.50	0.94
1:E:253:HIS:CD2	1:E:549:GLY:HA3	2.01	0.94
1:E:266:ALA:HB3	1:E:402:THR:HB	1.50	0.94
1:C:246:GLN:HG3	1:G:241:PRO:HB3	1.50	0.93
1:A:531:GLU:HG3	2:F:583:LYS:HE3	1.48	0.93
1:A:255:PRO:O	1:C:225:THR:HG21	1.67	0.93
1:G:544:GLN:O	1:G:547:LEU:HD23	1.66	0.93
1:A:516:THR:HB	1:E:423:ASN:HB3	1.50	0.93
1:A:285:PRO:HB2	1:A:288:THR:HB	1.49	0.93
1:C:120:GLN:NE2	1:C:208:LEU:CB	2.31	0.93
1:G:106:LYS:HG3	1:G:117:ASP:HB3	1.50	0.92
1:A:480:ILE:H	1:A:480:ILE:HD12	1.30	0.92
1:A:276:VAL:HG21	1:A:369:TYR:HE1	1.33	0.92
1:E:416:THR:CB	1:E:419:GLU:HB2	1.99	0.92
1:A:198:ALA:HB3	1:A:201:TRP:HB2	1.52	0.91
2:D:581:VAL:O	2:D:585:ILE:HD12	1.70	0.91
1:G:225:THR:HG22	1:G:226:GLN:HG3	1.52	0.91
1:G:329:VAL:HG22	1:G:362:ILE:HG12	1.53	0.91
1:E:174:ASN:HA	1:E:177:ILE:HD12	1.53	0.91
1:C:234:ILE:HD11	1:C:236:PHE:CZ	2.06	0.90
1:A:171:GLU:H	1:A:171:GLU:CD	1.79	0.90
1:C:425:PRO:HB2	1:E:62:THR:HG21	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:581:VAL:HG12	2:D:585:ILE:HD11	1.51	0.90
1:E:309:GLY:HA3	1:E:331:SER:HA	1.52	0.90
1:E:163:ILE:H	1:E:163:ILE:HD12	1.37	0.90
1:G:405:VAL:HG21	1:G:477:LEU:HD22	1.53	0.90
1:A:375:LEU:HB3	1:A:378:SER:HB3	1.51	0.90
1:C:396:VAL:HG12	1:C:397:THR:H	1.36	0.90
1:E:250:VAL:HG22	1:E:429:GLN:HG3	1.54	0.90
1:G:234:ILE:HG12	1:G:508:THR:HB	1.54	0.89
1:A:198:ALA:HB1	1:A:199:PRO:HD2	1.53	0.89
1:E:416:THR:HB	1:E:419:GLU:CB	2.01	0.89
1:A:394:THR:O	1:A:396:VAL:HG23	1.72	0.89
1:C:371:VAL:HG23	1:C:381:ILE:HB	1.53	0.89
1:C:154:ARG:HB3	1:C:211:THR:HG22	1.52	0.89
1:C:293:VAL:HG22	1:C:324:GLU:HG3	1.55	0.89
1:G:248:TRP:HE1	1:G:429:GLN:HG2	1.34	0.89
1:E:220:ARG:HD2	1:G:215:ALA:CB	2.03	0.88
1:A:242:THR:HA	1:A:245:ASP:HB2	1.55	0.88
1:C:103:GLU:HG3	1:C:117:ASP:OD1	1.74	0.88
1:A:446:ASN:HB2	1:A:487:ASN:HA	1.55	0.88
1:C:275:THR:HB	1:C:391:VAL:HG11	1.54	0.88
1:E:309:GLY:CA	1:E:331:SER:HA	2.03	0.88
1:A:385:VAL:HG22	1:A:392:SER:HB2	1.55	0.88
1:C:275:THR:HG21	1:C:478:ARG:NH1	1.88	0.88
1:E:187:ARG:HH12	1:E:215:ALA:HA	1.37	0.88
1:C:405:VAL:CG1	1:C:477:LEU:HD13	2.04	0.88
1:A:380:VAL:HG12	1:A:381:ILE:H	1.36	0.88
1:A:405:VAL:HG11	1:A:477:LEU:HD22	1.53	0.87
1:A:447:ASN:CB	1:C:451:GLU:HG3	2.03	0.87
1:A:297:THR:CG2	1:A:478:ARG:HE	1.86	0.87
1:C:164:ASN:OD1	1:C:166:GLU:HB3	1.74	0.87
1:G:47:GLN:HE22	1:G:63:MET:HA	1.31	0.87
1:C:120:GLN:HE22	1:C:208:LEU:HB3	1.39	0.87
1:G:122:PRO:HG2	1:G:508:THR:HG23	1.57	0.86
1:E:169:THR:HB	1:E:172:THR:OG1	1.75	0.86
1:A:371:VAL:HG22	1:A:381:ILE:HG21	1.56	0.86
1:C:215:ALA:HB3	1:C:218:GLY:HA2	1.54	0.86
1:A:154:ARG:HB3	1:A:211:THR:HG22	1.56	0.86
1:G:411:GLU:HA	1:G:464:HIS:HB3	1.55	0.86
1:E:297:THR:HG22	1:E:298:PRO:HD3	0.90	0.86
2:B:588:GLN:HG3	2:B:593:VAL:HA	1.57	0.86
1:C:457:ASN:O	1:C:457:ASN:ND2	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:481:VAL:O	1:G:482:ASP:HB2	1.75	0.86
1:E:274:MET:HE2	1:E:294:TRP:HE1	1.38	0.86
1:E:465:TYR:CG	1:E:466:PRO:HD2	2.11	0.86
1:G:183:ILE:O	1:G:478:ARG:HB2	1.75	0.86
1:E:73:GLN:HB3	2:F:574:LYS:HA	1.57	0.86
1:E:220:ARG:HH11	1:G:215:ALA:HB1	0.72	0.86
1:E:198:ALA:HB1	1:E:199:PRO:HD2	1.56	0.86
1:G:278:ALA:HB3	1:G:387:LYS:HA	1.56	0.86
1:C:313:THR:HA	1:C:325:ILE:HG22	1.55	0.85
1:G:207:VAL:CG1	1:G:212:TYR:HB2	2.05	0.85
1:G:362:ILE:HG22	1:G:367:VAL:HG13	1.58	0.85
1:G:127:GLU:HG2	1:G:503:THR:HG21	1.58	0.85
1:E:55:ALA:HB1	1:E:56:PRO:HD2	1.56	0.85
1:G:111:LEU:HG	1:G:112:LEU:HD12	1.59	0.85
1:A:395:PRO:HB3	1:C:267:GLU:HB3	1.59	0.85
1:C:297:THR:HG23	1:C:476:GLY:HA3	0.85	0.85
1:A:461:PHE:HE1	1:A:480:ILE:HB	1.40	0.84
1:A:281:ALA:HB2	1:A:291:ARG:HB2	1.59	0.84
1:C:120:GLN:HE21	1:C:208:LEU:HB3	1.40	0.84
1:A:549:GLY:HA2	1:C:113:ARG:NH2	1.93	0.84
1:A:107:VAL:HG11	1:A:450:PHE:HD1	1.40	0.84
1:C:396:VAL:HG12	1:C:397:THR:N	1.90	0.84
1:G:131:VAL:O	1:G:282:ILE:HG23	1.78	0.83
1:G:154:ARG:HG2	1:G:211:THR:HG22	1.60	0.83
1:A:252:ALA:HB2	1:A:427:TYR:HB2	1.60	0.83
1:E:284:GLN:CB	1:E:289:VAL:HG11	2.07	0.83
1:E:457:ASN:HD21	1:E:486:ASN:HB3	1.43	0.83
1:C:332:VAL:HG22	1:C:358:SER:HB2	1.61	0.83
1:G:307:THR:HB	1:G:332:VAL:HG12	1.60	0.83
1:C:421:THR:HG21	1:G:123:ILE:HD12	1.60	0.83
1:C:405:VAL:HG11	1:C:477:LEU:CD1	2.09	0.83
1:A:366:THR:O	1:A:367:VAL:HG23	1.79	0.83
1:A:371:VAL:H	1:A:381:ILE:HG22	1.42	0.83
1:A:443:TYR:HE2	1:A:445:MET:HE3	1.44	0.83
1:C:475:LEU:CD2	1:E:267:GLU:HB2	2.09	0.82
1:G:207:VAL:HG11	1:G:212:TYR:HB2	1.62	0.82
1:E:214:MET:HE2	1:G:521:THR:HB	1.62	0.82
1:G:241:PRO:CG	1:G:244:ILE:HB	2.09	0.82
1:G:292:ILE:HD11	1:G:325:ILE:HG13	1.61	0.82
1:C:184:THR:HG21	1:C:295:SER:CB	2.09	0.82
1:E:220:ARG:CD	1:G:215:ALA:HB2	2.06	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:SER:H	1:C:297:THR:HB	1.44	0.82
1:E:265:ALA:HB2	1:E:404:ALA:HB2	1.61	0.82
1:A:342:LEU:HD22	1:A:347:PRO:HA	1.60	0.82
1:C:363:THR:CG2	1:C:366:THR:H	1.92	0.82
1:C:339:ALA:HB3	1:C:400:ILE:HD11	1.62	0.82
1:E:229:LYS:HB2	1:E:485:GLU:HG2	1.61	0.82
1:G:447:ASN:ND2	1:G:449:VAL:HG12	1.95	0.82
1:E:284:GLN:HB2	1:E:289:VAL:HG11	1.60	0.81
1:G:534:ASP:HA	1:G:537:VAL:HB	1.61	0.81
2:H:578:THR:HG22	2:H:581:VAL:N	1.93	0.81
1:E:185:ASN:CG	1:E:318:GLY:HA3	2.05	0.81
2:D:578:THR:HG22	2:D:580:SER:H	1.44	0.81
1:G:408:LEU:HB2	1:G:461:PHE:HB3	1.61	0.81
1:G:248:TRP:HE1	1:G:429:GLN:CG	1.94	0.81
1:E:122:PRO:O	1:E:508:THR:HG23	1.81	0.81
1:E:148:ILE:HG12	1:E:412:MET:HE1	1.63	0.81
1:C:229:LYS:H	1:C:485:GLU:HG3	1.45	0.81
1:E:90:ASP:HB2	2:F:561:VAL:HB	1.62	0.81
1:A:405:VAL:HG11	1:A:477:LEU:CD2	2.10	0.81
1:A:383:ARG:HH11	1:A:383:ARG:CB	1.90	0.80
1:C:87:LYS:CE	1:C:95:VAL:HG23	2.11	0.80
1:C:306:LEU:HD13	1:C:311:GLY:HA2	1.63	0.80
1:G:363:THR:HG22	1:G:364:ALA:H	1.45	0.80
1:A:244:ILE:HD11	1:A:501:SER:HB2	1.64	0.80
1:A:313:THR:HG1	1:A:333:TRP:CD1	1.99	0.80
1:A:414:ALA:HB2	1:C:517:ASN:O	1.81	0.80
1:E:299:LEU:HD12	1:E:300:PRO:HD2	1.62	0.80
1:G:258:PRO:HB3	1:G:410:ILE:HG12	1.63	0.80
1:C:302:ALA:HB2	1:C:338:PRO:CG	2.12	0.80
1:G:130:THR:HB	1:G:282:ILE:HD13	1.62	0.80
1:G:132:SER:C	1:G:134:SER:N	2.33	0.80
1:E:435:SER:O	1:E:437:GLY:N	2.14	0.80
1:G:447:ASN:HD21	1:G:449:VAL:HG12	1.47	0.80
1:C:87:LYS:C	1:C:89:MET:H	1.88	0.80
1:C:274:MET:HE2	1:C:394:THR:HB	1.64	0.80
1:C:475:LEU:CD1	1:E:267:GLU:HG2	2.03	0.79
1:G:444:LYS:HB3	1:G:450:PHE:CE2	2.16	0.79
1:A:249:TRP:O	1:A:429:GLN:HG2	1.82	0.79
1:E:43:ILE:HB	1:E:67:VAL:HB	1.61	0.79
1:A:447:ASN:HB3	1:C:451:GLU:HG3	1.65	0.79
1:G:241:PRO:HG3	1:G:244:ILE:HB	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:ILE:O	1:G:217:ILE:HD13	1.83	0.79
1:A:455:GLU:HG3	1:E:259:GLN:HB2	1.62	0.79
1:A:370:SER:HB2	1:A:381:ILE:O	1.83	0.79
1:E:107:VAL:O	1:E:530:ALA:HB3	1.82	0.79
1:E:469:ASP:CG	1:E:471:GLU:HG2	2.08	0.79
1:C:435:SER:O	1:C:437:GLY:N	2.14	0.79
1:E:116:VAL:HG21	1:E:522:VAL:CG1	2.13	0.79
1:G:93:GLY:O	1:G:97:SER:HB3	1.82	0.79
1:A:435:SER:O	1:A:437:GLY:N	2.14	0.78
1:A:151:PRO:HB2	1:A:485:GLU:HB3	1.66	0.78
1:A:279:SER:HA	1:A:387:LYS:CG	2.14	0.78
1:C:143:TRP:HE1	1:C:498:ILE:HG22	1.48	0.78
1:G:396:VAL:HG12	1:G:397:THR:H	1.45	0.78
1:A:259:GLN:HB2	1:C:455:GLU:HG3	1.65	0.78
1:A:279:SER:HA	1:A:387:LYS:HG3	1.64	0.78
1:C:439:TYR:CE2	1:C:556:ASN:HA	2.19	0.78
1:C:475:LEU:CD1	1:E:267:GLU:CD	2.54	0.78
1:E:107:VAL:HB	1:E:228:ARG:HH11	1.48	0.78
1:A:448:PRO:HD3	1:C:111:LEU:HD22	1.65	0.78
1:C:267:GLU:HA	1:C:267:GLU:OE1	1.83	0.78
1:G:189:LEU:HD23	1:G:189:LEU:N	1.99	0.78
1:C:154:ARG:HG2	1:C:482:ASP:OD1	1.83	0.78
1:E:237:GLU:HG3	1:E:507:LYS:CE	2.13	0.78
1:A:329:VAL:HG23	1:A:362:ILE:HG13	1.65	0.77
1:G:77:PRO:HA	1:G:533:GLU:OE2	1.82	0.77
1:C:398:VAL:HB	1:C:400:ILE:HD13	1.66	0.77
1:E:284:GLN:HB3	1:E:285:PRO:HD2	1.65	0.77
1:E:457:ASN:ND2	1:E:486:ASN:HB3	1.98	0.77
1:A:262:THR:CA	1:A:406:ASN:HB3	2.13	0.77
1:A:297:THR:OG1	1:A:298:PRO:HD3	1.85	0.77
1:E:278:ALA:HB2	1:E:385:VAL:HG21	1.67	0.77
1:A:517:ASN:O	1:E:414:ALA:HB2	1.85	0.77
1:G:168:LEU:HD23	1:G:172:THR:HB	1.65	0.77
1:G:174:ASN:ND2	1:G:468:TYR:HA	1.98	0.77
1:C:542:ARG:O	1:C:546:GLU:HB2	1.84	0.77
1:E:56:PRO:HB2	1:G:554:ASP:HA	1.67	0.77
1:A:453:THR:HG21	1:A:484:PHE:O	1.84	0.77
1:C:168:LEU:HD13	1:C:201:TRP:CZ3	2.19	0.77
1:A:400:ILE:HG12	1:A:401:ASP:N	2.00	0.77
1:C:87:LYS:O	1:C:91:PRO:HD3	1.84	0.77
1:A:341:ILE:O	1:A:342:LEU:HD23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LYS:HD3	1:A:450:PHE:CD2	2.20	0.76
1:C:297:THR:CG2	1:C:476:GLY:HA2	2.13	0.76
1:A:105:SER:O	1:A:230:VAL:HG21	1.84	0.76
1:C:290:ALA:N	1:C:362:ILE:HD11	1.99	0.76
1:E:173:ARG:O	1:E:176:PHE:HB3	1.84	0.76
1:G:416:THR:HB	1:G:419:GLU:CB	2.09	0.76
1:A:371:VAL:H	1:A:381:ILE:CG2	1.97	0.76
1:C:164:ASN:ND2	1:C:200:GLY:HA3	2.00	0.76
1:E:278:ALA:HA	1:E:292:ILE:HG22	1.66	0.76
1:A:517:ASN:OD1	1:E:413:PRO:HA	1.86	0.76
1:C:143:TRP:NE1	1:C:498:ILE:HG22	2.00	0.76
1:E:418:GLU:HA	1:E:421:THR:HG23	1.65	0.76
1:E:435:SER:C	1:E:437:GLY:H	1.90	0.76
1:G:191:THR:HG23	1:G:193:GLN:HG2	1.68	0.76
1:G:248:TRP:HD1	1:G:431:LEU:HD23	1.50	0.76
1:A:113:ARG:HG3	1:E:443:TYR:CE2	2.21	0.76
1:A:189:LEU:N	1:A:189:LEU:HD12	2.00	0.76
1:A:371:VAL:HG22	1:A:381:ILE:CG2	2.14	0.76
1:C:154:ARG:HB3	1:C:211:THR:CG2	2.16	0.76
1:A:103:GLU:HG3	1:A:117:ASP:OD2	1.85	0.76
1:A:297:THR:HG23	1:A:478:ARG:HE	1.50	0.76
1:A:485:GLU:HG3	1:A:488:PHE:H	1.50	0.76
1:E:418:GLU:HA	1:E:421:THR:CG2	2.16	0.76
1:C:304:VAL:HG12	1:C:305:ALA:H	1.50	0.76
1:A:461:PHE:CE1	1:A:480:ILE:HB	2.21	0.76
1:G:188:ASP:OD1	1:G:316:THR:HG22	1.86	0.76
1:C:458:PHE:HB2	1:C:483:THR:HG23	1.68	0.75
1:C:545:MET:HE2	1:C:546:GLU:HA	1.67	0.75
1:G:412:MET:SD	1:G:413:PRO:HD2	2.27	0.75
1:C:105:SER:CB	1:C:117:ASP:HB2	2.16	0.75
1:E:228:ARG:HB3	1:E:452:MET:CE	2.16	0.75
1:G:306:LEU:HD22	1:G:311:GLY:HA2	1.67	0.75
1:G:329:VAL:HG13	1:G:362:ILE:HG23	1.68	0.75
1:C:297:THR:HB	1:C:298:PRO:HD3	1.68	0.75
1:C:407:ARG:HH21	1:C:478:ARG:HB2	1.52	0.75
1:E:412:MET:SD	1:E:413:PRO:HD2	2.27	0.75
1:G:248:TRP:CD1	1:G:431:LEU:HD23	2.20	0.75
1:A:239:ASN:HB3	1:A:503:THR:O	1.86	0.75
1:C:407:ARG:HD2	1:C:462:GLN:CB	2.16	0.75
1:E:452:MET:HE2	1:E:452:MET:HA	1.68	0.75
1:A:178:GLN:NE2	1:A:390:GLY:HA2	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:PRO:HG2	1:G:57:SER:H	1.52	0.75
1:G:142:LEU:HA	1:G:500:GLN:H	1.52	0.75
1:A:423:ASN:HA	1:C:523:GLY:HA3	1.69	0.75
1:A:276:VAL:HG21	1:A:369:TYR:CE1	2.19	0.74
1:A:447:ASN:HB2	1:C:451:GLU:HA	1.68	0.74
1:A:475:LEU:HD22	1:C:267:GLU:CG	2.15	0.74
1:C:304:VAL:HG12	1:C:305:ALA:N	2.00	0.74
1:G:142:LEU:HD12	1:G:497:GLY:HA2	1.67	0.74
1:E:98:GLY:C	1:G:63:MET:HE1	2.12	0.74
1:E:210:ASN:ND2	1:G:524:GLN:HG3	2.01	0.74
1:C:139:ASP:CG	1:C:141:LYS:HG3	2.12	0.74
1:G:92:ALA:O	1:G:95:VAL:HG13	1.87	0.74
1:G:199:PRO:HD3	1:G:388:GLY:HA3	1.69	0.74
1:A:108:PRO:HB2	1:A:533:GLU:HB2	1.67	0.74
1:E:73:GLN:OE1	2:F:574:LYS:HB2	1.87	0.74
1:G:460:GLY:HA2	1:G:481:VAL:HA	1.67	0.74
1:G:465:TYR:CG	1:G:466:PRO:HD2	2.22	0.74
2:D:583:LYS:O	2:D:587:GLN:HG3	1.86	0.74
1:C:235:THR:HG22	1:C:439:TYR:CD1	2.22	0.74
1:C:180:LEU:HA	1:C:183:ILE:HD11	1.70	0.74
1:A:263:ILE:HB	1:A:405:VAL:O	1.87	0.74
1:C:375:LEU:HB3	1:C:378:SER:HB3	1.70	0.74
1:E:107:VAL:HB	1:E:228:ARG:NH1	2.03	0.74
1:E:262:THR:HA	1:E:406:ASN:HA	1.68	0.74
1:E:274:MET:HE2	1:E:294:TRP:NE1	2.03	0.74
1:G:542:ARG:O	1:G:546:GLU:HG2	1.88	0.74
3:R:1:U:H2'	3:R:2:U:C6	2.22	0.74
1:E:63:MET:HE1	1:G:101:LEU:HD23	1.70	0.74
1:G:122:PRO:HG2	1:G:508:THR:CG2	2.18	0.74
1:G:405:VAL:CG2	1:G:477:LEU:HD22	2.18	0.74
1:G:444:LYS:HB3	1:G:450:PHE:HE2	1.50	0.74
1:A:447:ASN:HB2	1:C:451:GLU:HG3	1.68	0.74
1:E:139:ASP:O	1:E:141:LYS:N	2.19	0.74
1:G:205:ILE:HD13	1:G:480:ILE:HD11	1.70	0.73
1:A:342:LEU:CD2	1:A:347:PRO:HA	2.17	0.73
1:E:79:GLU:HB3	1:E:101:LEU:HD12	1.68	0.73
1:E:416:THR:HG22	1:E:418:GLU:H	1.53	0.73
1:G:287:ASN:HA	1:G:364:ALA:HB2	1.68	0.73
1:A:276:VAL:HG13	1:A:294:TRP:HB2	1.70	0.73
1:A:380:VAL:HG12	1:A:381:ILE:N	2.03	0.73
1:A:124:VAL:HG23	1:A:506:CYS:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:SER:HB3	1:E:206:TYR:OH	1.88	0.73
1:E:533:GLU:HA	1:E:533:GLU:OE2	1.87	0.73
1:G:306:LEU:HD21	1:G:309:GLY:O	1.87	0.73
1:G:346:GLU:OE1	1:G:347:PRO:HD2	1.88	0.73
1:A:124:VAL:HG11	1:A:206:TYR:CD2	2.24	0.73
2:D:579:PRO:HG2	1:E:535:GLU:OE1	1.89	0.73
1:E:248:TRP:HA	1:E:431:LEU:HA	1.71	0.73
1:E:314:ASN:O	1:E:324:GLU:HB3	1.89	0.73
1:E:445:MET:HB2	1:E:489:SER:HB2	1.71	0.73
1:E:252:ALA:HB2	1:E:427:TYR:HB2	1.71	0.73
2:F:596:ASN:HB2	2:F:597:PRO:CD	2.19	0.73
1:C:475:LEU:CD1	1:E:267:GLU:OE2	2.37	0.73
1:C:363:THR:HG22	1:C:366:THR:O	1.89	0.73
1:C:407:ARG:HD3	1:C:460:GLY:O	1.87	0.73
1:G:251:GLY:C	1:G:550:VAL:HG21	2.14	0.73
1:A:449:VAL:HG12	1:E:448:PRO:HG2	1.71	0.72
1:A:480:ILE:HD12	1:A:480:ILE:N	2.02	0.72
1:C:277:SER:HB3	1:C:391:VAL:HG22	1.71	0.72
1:C:400:ILE:N	1:C:400:ILE:HD12	2.04	0.72
1:G:132:SER:O	1:G:134:SER:N	2.21	0.72
1:G:176:PHE:O	1:G:179:THR:HB	1.89	0.72
1:C:181:ASN:O	1:C:407:ARG:NH2	2.22	0.72
1:G:405:VAL:HG21	1:G:477:LEU:CD2	2.19	0.72
1:G:546:GLU:HA	1:G:546:GLU:OE2	1.88	0.72
1:E:252:ALA:HB1	1:E:424:VAL:HG11	1.71	0.72
1:A:229:LYS:HD3	1:A:512:TRP:HB3	1.69	0.72
1:E:359:MET:SD	1:E:362:ILE:HD11	2.28	0.72
1:C:107:VAL:HG22	1:C:230:VAL:HG13	1.71	0.72
1:C:120:GLN:HE22	1:C:208:LEU:CB	2.00	0.72
1:C:290:ALA:HB2	1:C:387:LYS:HZ1	1.54	0.72
1:C:428:GLU:HG2	1:C:430:PHE:HE1	1.52	0.72
1:E:348:PHE:CE1	1:E:373:SER:HB2	2.25	0.72
1:C:457:ASN:HD22	1:C:457:ASN:C	1.97	0.72
1:C:538:GLN:HG2	2:D:582:ILE:HD12	1.69	0.72
1:A:274:MET:HG3	1:A:296:ILE:HG12	1.72	0.72
1:A:535:GLU:O	1:A:538:GLN:HB3	1.90	0.72
1:A:544:GLN:HB3	1:C:113:ARG:NH1	2.05	0.72
1:A:357:PHE:HE1	1:A:369:TYR:HD1	1.37	0.71
1:G:181:ASN:O	1:G:407:ARG:NH2	2.22	0.71
1:G:230:VAL:HG23	1:G:512:TRP:HA	1.70	0.71
1:C:272:GLY:HA3	1:C:298:PRO:CD	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ALA:HB3	1:C:270:SER:HB3	1.71	0.71
1:C:398:VAL:HB	1:C:400:ILE:CD1	2.20	0.71
1:A:495:PHE:HB3	1:A:498:ILE:HD11	1.73	0.71
1:C:275:THR:CG2	1:C:478:ARG:NH1	2.53	0.71
1:E:163:ILE:HD12	1:E:163:ILE:N	2.05	0.71
1:C:245:ASP:HB2	1:C:433:LYS:HG2	1.72	0.71
1:C:407:ARG:NH2	1:C:478:ARG:HB2	2.03	0.71
1:G:375:LEU:HB3	1:G:378:SER:HB3	1.71	0.71
1:A:156:ASN:HB3	1:A:206:TYR:O	1.90	0.71
1:C:168:LEU:HG	1:C:173:ARG:HB3	1.72	0.71
1:C:265:ALA:HB2	1:C:404:ALA:N	2.06	0.71
1:G:75:ILE:HG21	1:G:535:GLU:HG2	1.71	0.71
1:A:144:ARG:HD2	1:A:496:TRP:CD1	2.25	0.71
1:C:154:ARG:O	1:C:207:VAL:HG13	1.90	0.71
1:G:49:LEU:HB2	1:G:52:GLU:HG3	1.70	0.71
1:C:275:THR:CG2	1:C:478:ARG:NH2	2.54	0.71
1:C:453:THR:HA	1:C:456:GLU:OE1	1.91	0.71
1:E:250:VAL:HG22	1:E:429:GLN:CG	2.20	0.71
1:G:151:PRO:HB2	1:G:485:GLU:HB3	1.71	0.71
1:A:198:ALA:HA	1:A:388:GLY:O	1.90	0.71
2:B:564:LEU:HD11	2:B:590:VAL:HG22	1.73	0.71
1:C:106:LYS:HE3	1:C:115:SER:OG	1.90	0.71
1:C:229:LYS:H	1:C:485:GLU:CG	2.04	0.71
1:E:444:LYS:O	1:E:444:LYS:HD2	1.91	0.71
1:E:518:ALA:C	1:E:520:SER:H	1.97	0.71
1:A:88:TYR:CE2	1:A:544:GLN:HG3	2.26	0.70
1:A:238:PHE:CG	1:A:432:CYS:HB3	2.26	0.70
2:D:581:VAL:HG12	2:D:585:ILE:CD1	2.21	0.70
1:G:363:THR:HG22	1:G:364:ALA:N	2.04	0.70
1:G:105:SER:OG	1:G:117:ASP:HB2	1.92	0.70
2:H:583:LYS:O	2:H:587:GLN:HG3	1.90	0.70
2:B:563:ALA:O	2:B:567:ILE:HG22	1.91	0.70
1:G:166:GLU:HB3	1:G:201:TRP:CZ2	2.25	0.70
1:A:197:PHE:CZ	1:A:201:TRP:HB3	2.26	0.70
1:C:198:ALA:HB3	1:C:201:TRP:HB2	1.73	0.70
1:C:233:GLY:HA2	1:C:441:VAL:HA	1.74	0.70
1:E:274:MET:HE1	1:E:371:VAL:HG11	1.73	0.70
1:G:75:ILE:CG2	1:G:535:GLU:HG2	2.20	0.70
1:G:543:LEU:O	1:G:546:GLU:HB2	1.91	0.70
1:A:325:ILE:C	1:A:325:ILE:HD12	2.16	0.70
1:E:420:VAL:HG23	1:E:421:THR:H	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:474:ALA:CB	1:E:478:ARG:HD2	2.21	0.70
1:A:207:VAL:HG11	1:A:212:TYR:CD1	2.26	0.70
1:A:363:THR:HB	1:A:366:THR:H	1.57	0.70
1:A:444:LYS:HD3	1:A:450:PHE:HD2	1.56	0.70
1:G:290:ALA:HB2	1:G:387:LYS:HE2	1.72	0.70
1:A:243:LEU:HD12	1:A:243:LEU:C	2.17	0.70
2:D:585:ILE:HD12	2:D:585:ILE:H	1.55	0.70
1:G:84:TRP:O	1:G:85:PHE:C	2.35	0.70
1:G:385:VAL:HG12	1:G:392:SER:HB3	1.74	0.70
1:A:124:VAL:HG11	1:A:206:TYR:HD2	1.57	0.70
1:A:160:LEU:H	1:A:160:LEU:HD12	1.57	0.70
1:C:160:LEU:HD22	1:C:161:ALA:H	1.57	0.70
1:E:187:ARG:NH1	1:E:215:ALA:HA	2.06	0.70
1:E:306:LEU:HA	1:E:333:TRP:HA	1.72	0.70
1:A:424:VAL:O	1:A:427:TYR:HD2	1.75	0.69
1:A:73:GLN:NE2	2:F:578:THR:HG21	2.06	0.69
1:A:419:GLU:HB3	1:A:423:ASN:ND2	2.06	0.69
1:C:371:VAL:CG2	1:C:381:ILE:HB	2.22	0.69
1:E:163:ILE:H	1:E:163:ILE:CD1	2.04	0.69
1:G:143:TRP:CD1	1:G:500:GLN:HA	2.27	0.69
1:E:98:GLY:HA2	1:G:63:MET:HE1	1.75	0.69
1:E:313:THR:HB	1:E:333:TRP:HE1	1.56	0.69
1:A:252:ALA:HB1	1:A:424:VAL:HG11	1.73	0.69
1:C:207:VAL:HG11	1:C:212:TYR:HB2	1.73	0.69
1:C:262:THR:HB	1:E:262:THR:HG21	1.73	0.69
1:G:60:ARG:HG2	1:G:62:THR:O	1.92	0.69
1:G:272:GLY:O	1:G:475:LEU:HD12	1.91	0.69
1:G:198:ALA:HB3	1:G:201:TRP:CB	2.22	0.69
2:B:578:THR:HB	2:B:581:VAL:HG23	1.74	0.69
1:E:168:LEU:HD12	1:E:172:THR:HG22	1.75	0.69
1:E:446:ASN:ND2	1:E:486:ASN:O	2.22	0.69
1:G:263:ILE:HB	1:G:405:VAL:O	1.92	0.69
1:G:360:THR:HB	1:G:368:VAL:HG12	1.74	0.69
1:E:107:VAL:HG23	1:E:230:VAL:HG22	1.73	0.69
1:A:297:THR:HG21	1:A:476:GLY:H	1.56	0.69
1:A:329:VAL:CG1	1:A:330:ASN:N	2.56	0.69
1:C:407:ARG:HD2	1:C:462:GLN:HB2	1.75	0.69
1:G:204:SER:HB3	1:G:206:TYR:OH	1.93	0.69
1:G:290:ALA:O	1:G:326:ASP:HA	1.92	0.69
1:A:148:ILE:HG12	1:A:492:VAL:HG12	1.75	0.69
1:E:225:THR:O	1:E:226:GLN:HB3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:ILE:H	1:G:126:ILE:HD12	1.58	0.69
1:G:228:ARG:HD3	1:G:452:MET:SD	2.33	0.69
1:G:292:ILE:CD1	1:G:325:ILE:HG13	2.22	0.69
1:A:105:SER:HB3	1:A:117:ASP:OD2	1.93	0.69
1:A:186:TRP:CE3	1:A:480:ILE:HG23	2.28	0.69
1:E:130:THR:HG22	1:E:132:SER:N	2.08	0.69
1:E:335:PHE:CE2	1:E:355:THR:HB	2.26	0.69
2:F:606:ALA:O	2:F:610:VAL:HG23	1.93	0.69
1:A:357:PHE:HD1	1:A:371:VAL:HG12	1.58	0.68
1:E:294:TRP:O	1:E:323:VAL:HG23	1.93	0.68
1:C:290:ALA:H	1:C:362:ILE:HD11	1.58	0.68
1:E:44:LEU:HD11	1:E:63:MET:HE3	1.76	0.68
1:A:375:LEU:CB	1:A:378:SER:HB3	2.22	0.68
1:A:416:THR:O	1:A:420:VAL:HG23	1.93	0.68
2:B:564:LEU:O	2:B:567:ILE:HG23	1.94	0.68
1:C:363:THR:HG23	1:C:364:ALA:N	2.09	0.68
1:G:253:HIS:CD2	1:G:549:GLY:HA3	2.28	0.68
1:E:249:TRP:O	1:E:429:GLN:HG2	1.94	0.68
1:A:144:ARG:NH2	1:A:417:THR:OG1	2.26	0.68
1:C:543:LEU:O	1:C:547:LEU:HG	1.94	0.68
2:D:594:GLN:CD	1:E:41:ALA:HB1	2.17	0.68
1:C:297:THR:HG23	1:C:476:GLY:HA2	1.65	0.68
1:E:63:MET:O	1:E:64:ASP:C	2.36	0.68
1:E:199:PRO:HG2	1:E:200:GLY:H	1.59	0.68
1:E:207:VAL:HG21	1:E:212:TYR:CD2	2.28	0.68
1:G:142:LEU:HG	1:G:165:ASN:ND2	2.07	0.68
1:A:297:THR:HG23	1:A:478:ARG:HH21	1.58	0.68
1:C:127:GLU:HA	1:C:503:THR:HG22	1.76	0.68
1:C:148:ILE:HD12	1:C:148:ILE:N	2.09	0.68
2:D:571:LEU:HD12	2:D:585:ILE:HG23	1.75	0.68
1:E:407:ARG:HD2	1:E:460:GLY:HA3	1.76	0.68
1:G:84:TRP:CD1	1:G:230:VAL:HG12	2.29	0.68
1:A:256:VAL:O	1:A:484:PHE:HE2	1.75	0.68
1:C:440:ILE:HG22	1:C:550:VAL:HG12	1.76	0.68
1:G:295:SER:HB3	1:G:322:SER:HA	1.75	0.68
1:A:435:SER:HB2	1:A:552:GLN:HG2	1.76	0.68
1:E:90:ASP:OD2	1:E:93:GLY:HA3	1.94	0.68
1:E:155:LEU:HD12	1:E:156:ASN:H	1.59	0.68
1:A:292:ILE:C	1:A:292:ILE:HD12	2.18	0.67
1:A:353:ASP:OD2	1:A:375:LEU:HB2	1.95	0.67
1:A:371:VAL:O	1:A:381:ILE:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLN:HB3	1:C:113:ARG:HH12	1.59	0.67
1:C:76:ASP:CG	1:C:76:ASP:O	2.37	0.67
1:C:207:VAL:HG12	1:C:208:LEU:N	2.09	0.67
1:C:445:MET:HG2	1:C:445:MET:O	1.92	0.67
1:G:155:LEU:HA	1:G:207:VAL:HG13	1.75	0.67
1:A:136:LEU:HD21	1:A:501:SER:HA	1.76	0.67
1:A:276:VAL:HG22	1:A:294:TRP:CD1	2.30	0.67
1:C:152:ALA:HB3	1:C:155:LEU:HB3	1.76	0.67
1:C:504:ILE:HG22	1:C:506:CYS:SG	2.34	0.67
1:A:277:SER:O	1:A:292:ILE:HB	1.94	0.67
1:A:444:LYS:HD2	1:A:447:ASN:O	1.94	0.67
1:C:206:TYR:N	1:C:206:TYR:CD1	2.59	0.67
1:E:239:ASN:HB3	1:E:503:THR:O	1.93	0.67
1:E:313:THR:HB	1:E:333:TRP:NE1	2.10	0.67
1:A:251:GLY:C	1:A:550:VAL:HG21	2.19	0.67
1:C:446:ASN:O	1:E:111:LEU:HD21	1.94	0.67
1:E:169:THR:HG22	1:E:170:LEU:N	2.10	0.67
1:C:467:GLY:N	1:E:218:GLY:O	2.27	0.67
1:E:241:PRO:O	1:E:243:LEU:N	2.25	0.67
1:C:297:THR:HG21	1:C:476:GLY:CA	2.22	0.67
1:G:198:ALA:HA	1:G:388:GLY:O	1.95	0.67
1:G:243:LEU:C	1:G:245:ASP:H	2.01	0.67
1:G:444:LYS:HG2	1:G:447:ASN:O	1.94	0.67
1:C:151:PRO:O	1:C:485:GLU:HB2	1.95	0.67
1:C:465:TYR:CD1	1:C:466:PRO:HD2	2.29	0.67
1:E:367:VAL:HB	1:E:385:VAL:CG2	2.25	0.67
1:G:408:LEU:HG	1:G:459:GLY:HA3	1.76	0.67
1:A:539:LEU:CD1	1:A:543:LEU:HG	2.25	0.67
1:C:106:LYS:HA	1:C:513:GLU:OE1	1.94	0.67
1:E:168:LEU:HD12	1:E:172:THR:CG2	2.25	0.67
1:A:253:HIS:ND1	1:A:491:ALA:HB2	2.10	0.67
1:C:250:VAL:HB	1:C:429:GLN:HB3	1.75	0.67
1:G:73:GLN:O	1:G:73:GLN:HG2	1.94	0.67
1:A:171:GLU:CD	1:A:171:GLU:N	2.50	0.66
1:C:106:LYS:HG3	1:C:117:ASP:HB3	1.77	0.66
1:C:234:ILE:HB	1:C:508:THR:HG22	1.77	0.66
1:C:292:ILE:HD11	1:C:325:ILE:HD11	1.77	0.66
1:C:319:LYS:HG3	1:C:320:PHE:CD1	2.30	0.66
1:C:341:ILE:HG12	1:C:398:VAL:HG12	1.77	0.66
1:E:444:LYS:HZ2	1:E:444:LYS:HB3	1.60	0.66
1:G:258:PRO:HB2	1:G:408:LEU:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ILE:HG13	1:C:164:ASN:H	1.61	0.66
1:G:89:MET:HE1	1:G:544:GLN:N	2.11	0.66
1:A:230:VAL:HG12	1:A:231:TYR:CD2	2.30	0.66
1:A:480:ILE:H	1:A:480:ILE:CD1	2.05	0.66
1:C:545:MET:HE2	1:C:545:MET:C	2.20	0.66
1:G:369:TYR:CZ	1:G:383:ARG:HB3	2.30	0.66
1:A:448:PRO:HG3	1:C:449:VAL:HG22	1.77	0.66
1:C:176:PHE:CZ	1:C:180:LEU:HD11	2.30	0.66
1:E:308:THR:HB	1:E:332:VAL:HB	1.78	0.66
1:E:474:ALA:HB3	1:E:478:ARG:HD2	1.75	0.66
1:G:332:VAL:HG22	1:G:358:SER:HB2	1.78	0.66
1:G:469:ASP:C	1:G:471:GLU:H	2.03	0.66
1:A:145:VAL:HG12	1:A:498:ILE:HD12	1.78	0.66
1:A:455:GLU:CG	1:E:259:GLN:HB2	2.25	0.66
2:D:567:ILE:HG23	2:D:568:GLY:N	2.09	0.66
1:E:119:GLU:HA	1:E:510:ASP:O	1.94	0.66
1:G:381:ILE:HG23	1:G:383:ARG:HH21	1.61	0.66
1:A:404:ALA:CB	1:E:261:GLU:HB3	2.24	0.66
1:C:137:PRO:O	1:C:501:SER:HB3	1.95	0.66
2:D:578:THR:HB	2:D:581:VAL:HG23	1.78	0.66
1:E:284:GLN:HB3	1:E:289:VAL:HG11	1.77	0.66
2:F:563:ALA:O	2:F:567:ILE:HG22	1.95	0.66
1:G:173:ARG:O	1:G:176:PHE:HB3	1.95	0.66
1:G:304:VAL:HG11	1:G:323:VAL:HG21	1.76	0.66
2:H:564:LEU:HD23	2:H:564:LEU:H	1.59	0.66
1:A:176:PHE:CZ	1:A:180:LEU:HD11	2.29	0.66
1:C:159:ALA:O	1:C:203:TYR:HA	1.96	0.66
1:C:304:VAL:HG22	1:C:335:PHE:HB3	1.78	0.66
1:E:126:ILE:HD13	1:E:506:CYS:SG	2.35	0.66
1:C:248:TRP:HB2	1:C:431:LEU:HD23	1.78	0.66
1:C:475:LEU:HG	1:E:267:GLU:OE2	1.94	0.66
1:G:106:LYS:HA	1:G:513:GLU:OE1	1.95	0.66
1:A:170:LEU:O	1:A:173:ARG:HB3	1.96	0.66
1:A:556:ASN:ND2	1:A:556:ASN:C	2.52	0.66
2:D:564:LEU:CD1	1:E:50:PRO:HG2	2.26	0.66
1:A:87:LYS:HZ2	1:A:95:VAL:HG23	1.60	0.65
1:A:253:HIS:CD2	1:A:549:GLY:HA3	2.31	0.65
1:C:185:ASN:CG	1:C:318:GLY:HA3	2.20	0.65
1:C:357:PHE:CE1	1:C:369:TYR:HB2	2.31	0.65
1:C:421:THR:O	1:G:121:ARG:NH1	2.28	0.65
1:E:228:ARG:HE	1:E:452:MET:HE3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:LEU:HD12	1:E:156:ASN:N	2.11	0.65
1:E:297:THR:N	1:E:478:ARG:HH21	1.94	0.65
1:E:396:VAL:CG1	1:E:397:THR:N	2.58	0.65
1:C:275:THR:HG21	1:C:478:ARG:CZ	2.25	0.65
1:A:255:PRO:HG3	1:C:515:THR:HG21	1.78	0.65
1:C:447:ASN:HB3	1:C:449:VAL:O	1.96	0.65
1:E:173:ARG:HD3	1:E:465:TYR:CD2	2.31	0.65
1:E:256:VAL:HG11	1:E:410:ILE:CG2	2.26	0.65
1:A:244:ILE:HD11	1:A:501:SER:CB	2.27	0.65
1:C:292:ILE:CD1	1:C:325:ILE:HG13	2.27	0.65
1:C:400:ILE:HG22	1:C:401:ASP:N	2.12	0.65
1:C:535:GLU:CD	1:C:535:GLU:H	2.03	0.65
1:A:297:THR:CB	1:A:298:PRO:HD3	2.26	0.65
2:D:569:LEU:O	2:D:569:LEU:HD13	1.96	0.65
1:E:465:TYR:CD1	1:E:466:PRO:HD2	2.32	0.65
1:G:291:ARG:HA	1:G:326:ASP:HA	1.79	0.65
1:G:313:THR:HB	1:G:333:TRP:HE1	1.61	0.65
1:C:79:GLU:HB3	1:C:101:LEU:HD13	1.78	0.65
2:D:560:THR:HG22	2:D:564:LEU:HD21	1.79	0.65
2:D:594:GLN:OE1	1:E:41:ALA:HB1	1.96	0.65
1:E:225:THR:HG23	1:E:517:ASN:HB2	1.77	0.65
1:C:120:GLN:HG2	1:C:210:ASN:OD1	1.97	0.65
1:E:98:GLY:CA	1:G:63:MET:HE1	2.27	0.65
1:E:210:ASN:O	1:E:213:ALA:N	2.30	0.65
1:G:241:PRO:HG2	1:G:244:ILE:HB	1.78	0.65
1:G:297:THR:HB	1:G:298:PRO:HD3	1.77	0.65
1:A:142:LEU:HB3	1:A:498:ILE:O	1.95	0.65
1:C:184:THR:CG2	1:C:295:SER:HB2	2.22	0.65
1:C:238:PHE:CG	1:C:432:CYS:HB3	2.31	0.65
1:C:475:LEU:HD13	1:E:267:GLU:HB2	1.79	0.65
1:E:48:LEU:HD12	1:E:52:GLU:O	1.97	0.65
1:E:297:THR:N	1:E:478:ARG:NH2	2.45	0.65
1:G:174:ASN:HD22	1:G:468:TYR:HD1	1.44	0.65
1:G:291:ARG:HD2	1:G:291:ARG:C	2.22	0.65
1:A:408:LEU:HB2	1:A:461:PHE:HB3	1.78	0.65
1:A:542:ARG:O	1:A:545:MET:HB3	1.96	0.65
1:C:356:SER:OG	1:C:372:SER:HB2	1.97	0.65
1:E:130:THR:HB	1:E:163:ILE:HG12	1.78	0.65
1:G:194:TRP:HA	1:G:194:TRP:CE3	2.32	0.65
1:A:185:ASN:HB2	1:A:188:ASP:OD2	1.97	0.64
1:C:396:VAL:CG1	1:C:397:THR:H	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:PRO:O	1:E:415:LEU:HG	1.97	0.64
2:F:605:LYS:CG	2:F:610:VAL:HG22	2.27	0.64
1:G:474:ALA:HB1	1:G:478:ARG:HD3	1.78	0.64
1:A:114:TYR:O	1:A:115:SER:HB3	1.96	0.64
2:F:597:PRO:O	2:F:599:ILE:N	2.28	0.64
1:G:224:VAL:HG12	1:G:225:THR:N	2.12	0.64
1:G:412:MET:HE2	1:G:463:PHE:CD2	2.32	0.64
1:A:129:PRO:CG	1:A:163:ILE:HG23	2.21	0.64
2:B:570:GLY:O	2:B:574:LYS:HG2	1.98	0.64
1:G:75:ILE:HG21	1:G:535:GLU:CG	2.27	0.64
1:C:259:GLN:HG3	1:E:456:GLU:O	1.97	0.64
1:C:275:THR:CG2	1:C:478:ARG:CZ	2.75	0.64
1:E:241:PRO:C	1:E:243:LEU:H	2.04	0.64
1:E:285:PRO:HG2	1:E:288:THR:HB	1.80	0.64
1:G:286:SER:O	1:G:364:ALA:HA	1.98	0.64
1:G:547:LEU:HD23	1:G:547:LEU:H	1.62	0.64
1:E:183:ILE:O	1:E:479:GLY:N	2.31	0.64
1:E:278:ALA:O	1:E:387:LYS:HA	1.98	0.64
1:E:469:ASP:OD1	1:E:471:GLU:HG2	1.98	0.64
1:A:342:LEU:HB2	1:A:397:THR:HB	1.80	0.64
1:C:246:GLN:OE1	1:C:499:SER:HB2	1.98	0.64
1:C:543:LEU:O	1:C:546:GLU:HB3	1.97	0.64
1:G:403:GLU:O	1:G:405:VAL:HG22	1.98	0.64
1:A:152:ALA:HB3	1:A:155:LEU:HB3	1.78	0.64
1:C:84:TRP:HE1	1:C:230:VAL:CG1	2.10	0.64
1:E:449:VAL:HG12	1:E:450:PHE:H	1.62	0.64
1:G:142:LEU:HA	1:G:500:GLN:N	2.11	0.64
1:G:235:THR:HG23	1:G:507:LYS:HB2	1.80	0.64
1:A:169:THR:HG22	1:A:172:THR:HG23	1.80	0.64
1:A:232:LYS:HB3	1:A:442:HIS:HB2	1.80	0.64
1:A:396:VAL:HG12	1:A:397:THR:N	2.12	0.64
1:A:452:MET:HB2	1:E:446:ASN:O	1.98	0.64
1:C:411:GLU:HG2	1:E:517:ASN:HD22	1.62	0.64
2:D:581:VAL:CG1	2:D:585:ILE:HD11	2.24	0.64
1:E:176:PHE:CE1	1:E:180:LEU:HD11	2.33	0.64
1:E:237:GLU:CG	1:E:507:LYS:HE2	2.24	0.64
1:E:436:GLY:N	1:E:554:ASP:OD2	2.31	0.64
1:A:77:PRO:HA	1:A:533:GLU:OE1	1.97	0.64
1:E:88:TYR:HA	1:E:231:TYR:HB2	1.80	0.64
1:E:144:ARG:HG2	1:E:144:ARG:HH11	1.62	0.64
1:G:435:SER:C	1:G:437:GLY:H	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ILE:HG13	1:E:244:ILE:O	1.98	0.63
1:G:249:TRP:HB3	1:G:495:PHE:CD2	2.33	0.63
1:E:148:ILE:HD12	1:E:148:ILE:N	2.12	0.63
1:E:165:ASN:ND2	1:E:497:GLY:HA2	2.12	0.63
1:E:176:PHE:O	1:E:179:THR:HB	1.97	0.63
1:E:181:ASN:O	1:E:407:ARG:NH2	2.31	0.63
1:G:88:TYR:HA	1:G:231:TYR:CB	2.29	0.63
1:G:129:PRO:HB2	1:G:163:ILE:HD11	1.80	0.63
1:C:443:TYR:HE2	1:E:113:ARG:HD2	1.64	0.63
1:G:145:VAL:HG23	1:G:161:ALA:HB2	1.81	0.63
1:G:224:VAL:HG12	1:G:225:THR:H	1.62	0.63
1:G:542:ARG:HD2	2:H:582:ILE:HG22	1.81	0.63
1:C:287:ASN:O	1:C:362:ILE:HG23	1.99	0.63
1:C:363:THR:HG22	1:C:366:THR:H	1.63	0.63
1:E:87:LYS:O	1:E:91:PRO:HD3	1.98	0.63
1:E:262:THR:HB	1:E:406:ASN:OD1	1.98	0.63
1:A:186:TRP:CZ3	1:A:480:ILE:HG23	2.34	0.63
1:E:274:MET:HG3	1:E:296:ILE:HG12	1.80	0.63
1:G:366:THR:HG22	1:G:386:THR:HG22	1.81	0.63
1:A:412:MET:HE2	1:A:463:PHE:CD2	2.34	0.63
1:C:297:THR:HG22	1:C:298:PRO:CD	2.29	0.63
1:C:363:THR:HG23	1:C:365:ASP:N	2.05	0.63
1:C:400:ILE:HD12	1:C:400:ILE:H	1.62	0.63
1:E:94:ALA:HA	1:E:97:SER:HB3	1.79	0.63
1:E:228:ARG:HD2	1:E:513:GLU:OE1	1.99	0.63
1:G:121:ARG:HH11	1:G:121:ARG:HG3	1.63	0.63
1:G:301:VAL:HA	1:G:321:PHE:HA	1.81	0.63
1:G:485:GLU:C	1:G:487:ASN:H	2.06	0.63
1:A:553:ALA:O	1:A:555:ASP:N	2.32	0.63
1:C:146:SER:HB3	1:C:494:HIS:ND1	2.14	0.63
1:C:290:ALA:HB2	1:C:387:LYS:NZ	2.12	0.63
1:C:475:LEU:HD21	1:E:267:GLU:HB2	1.77	0.63
1:G:181:ASN:C	1:G:407:ARG:HH22	2.06	0.63
1:G:370:SER:HA	1:G:381:ILE:O	1.99	0.63
1:A:182:ASN:HA	1:A:478:ARG:HD2	1.80	0.63
1:A:539:LEU:HD12	1:A:539:LEU:O	1.99	0.63
1:C:105:SER:O	1:C:230:VAL:HG21	1.98	0.63
1:C:114:TYR:HA	1:C:527:HIS:O	1.98	0.63
1:C:407:ARG:HD2	1:C:462:GLN:HB3	1.79	0.63
1:C:446:ASN:OD1	1:C:487:ASN:HA	1.99	0.63
1:G:121:ARG:NH1	1:G:121:ARG:HG3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:PRO:HD2	1:C:490:SER:HB3	1.80	0.63
1:C:177:ILE:CG2	1:C:181:ASN:HD21	2.11	0.63
1:E:129:PRO:HB3	1:E:194:TRP:CD1	2.34	0.63
1:G:123:ILE:HG12	1:G:507:LYS:HA	1.80	0.63
1:G:279:SER:HB3	1:G:291:ARG:HE	1.64	0.63
1:A:169:THR:HG22	1:A:172:THR:CG2	2.29	0.62
1:C:142:LEU:O	1:C:143:TRP:HB3	1.99	0.62
1:C:382:VAL:O	1:C:383:ARG:HD2	1.99	0.62
1:E:230:VAL:HG12	1:E:231:TYR:HD2	1.64	0.62
1:A:455:GLU:O	1:E:259:GLN:HG2	1.99	0.62
1:C:185:ASN:ND2	1:C:318:GLY:HA3	2.14	0.62
1:C:442:HIS:ND1	1:C:489:SER:O	2.32	0.62
1:C:471:GLU:OE1	1:C:471:GLU:HA	1.99	0.62
1:E:93:GLY:O	1:E:97:SER:HB2	1.99	0.62
1:E:160:LEU:HD23	1:E:160:LEU:H	1.64	0.62
1:E:309:GLY:HA3	1:E:331:SER:CA	2.25	0.62
1:G:156:ASN:HB2	1:G:208:LEU:HD23	1.81	0.62
1:C:252:ALA:HB1	1:C:424:VAL:HG11	1.80	0.62
1:C:369:TYR:CE1	1:C:383:ARG:HB2	2.35	0.62
1:G:106:LYS:HB3	1:G:530:ALA:HB2	1.80	0.62
1:A:232:LYS:HE2	1:A:510:ASP:OD2	1.99	0.62
1:A:250:VAL:HG22	1:A:429:GLN:CG	2.29	0.62
1:A:297:THR:HG23	1:A:478:ARG:NE	2.14	0.62
1:C:411:GLU:CG	1:E:517:ASN:HD22	2.12	0.62
1:E:169:THR:H	1:E:172:THR:HB	1.64	0.62
1:E:371:VAL:HB	1:E:381:ILE:HD12	1.80	0.62
2:F:607:ILE:HA	2:F:610:VAL:CG2	2.30	0.62
1:G:443:TYR:CB	1:G:544:GLN:HG2	2.30	0.62
1:C:79:GLU:N	1:C:79:GLU:OE2	2.32	0.62
2:D:592:ALA:O	2:D:593:VAL:HG13	1.99	0.62
1:E:106:LYS:HG3	1:E:117:ASP:OD2	2.00	0.62
1:A:285:PRO:HB2	1:A:288:THR:CB	2.27	0.62
1:C:187:ARG:HD3	1:C:212:TYR:CE1	2.34	0.62
1:C:230:VAL:HG12	1:C:231:TYR:HD2	1.65	0.62
1:C:354:THR:N	1:C:374:SER:HB3	2.13	0.62
1:C:428:GLU:HG2	1:C:430:PHE:CE1	2.34	0.62
1:C:495:PHE:HB3	1:C:498:ILE:CD1	2.30	0.62
1:E:184:THR:HG21	1:E:295:SER:HB2	1.80	0.62
2:H:564:LEU:HD23	2:H:564:LEU:N	2.14	0.62
1:A:228:ARG:HG2	1:A:452:MET:SD	2.39	0.62
1:C:538:GLN:HG3	1:C:542:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:ARG:NH2	1:E:532:GLU:O	2.33	0.62
1:E:224:VAL:HB	1:E:515:THR:O	2.00	0.62
1:A:128:CYS:HA	1:A:143:TRP:CZ3	2.34	0.62
1:E:184:THR:HG21	1:E:295:SER:CB	2.29	0.62
1:G:116:VAL:HG11	1:G:522:VAL:HG11	1.81	0.62
1:A:129:PRO:HG2	1:A:163:ILE:CG2	2.24	0.62
1:A:185:ASN:CG	1:A:318:GLY:HA3	2.25	0.62
1:E:160:LEU:HD23	1:E:160:LEU:N	2.15	0.62
1:E:297:THR:CG2	1:E:298:PRO:CD	2.53	0.62
1:G:127:GLU:O	1:G:194:TRP:NE1	2.32	0.62
1:G:435:SER:O	1:G:437:GLY:N	2.33	0.62
1:A:535:GLU:OE2	2:F:579:PRO:HG2	2.00	0.62
1:G:170:LEU:HD23	1:G:171:GLU:N	2.15	0.62
1:G:342:LEU:CD2	1:G:347:PRO:HA	2.29	0.62
1:A:444:LYS:HB2	1:A:450:PHE:HE2	1.65	0.61
1:C:297:THR:CB	1:C:298:PRO:HD3	2.30	0.61
1:C:425:PRO:CB	1:E:62:THR:HG21	2.28	0.61
1:G:90:ASP:OD2	2:H:561:VAL:HB	2.00	0.61
1:G:127:GLU:HG2	1:G:503:THR:CG2	2.29	0.61
1:G:162:ASN:CG	1:G:166:GLU:HB2	2.25	0.61
1:G:210:ASN:O	1:G:213:ALA:HB3	1.99	0.61
1:G:465:TYR:CD1	1:G:466:PRO:HD2	2.35	0.61
1:A:495:PHE:CB	1:A:498:ILE:HD11	2.30	0.61
1:E:126:ILE:HG12	1:E:147:PHE:HE2	1.64	0.61
1:E:444:LYS:HE3	1:E:450:PHE:HE2	1.65	0.61
1:C:465:TYR:CG	1:C:466:PRO:HD2	2.36	0.61
1:E:295:SER:HA	1:E:322:SER:HA	1.83	0.61
1:E:420:VAL:HG23	1:E:421:THR:N	2.14	0.61
1:E:435:SER:HA	1:E:554:ASP:OD2	1.99	0.61
1:G:299:LEU:HD11	1:G:338:PRO:HG2	1.82	0.61
1:G:396:VAL:HG12	1:G:397:THR:N	2.15	0.61
2:H:569:LEU:O	2:H:572:LEU:HB3	2.00	0.61
1:A:154:ARG:HB3	1:A:211:THR:CG2	2.27	0.61
1:C:128:CYS:SG	1:C:129:PRO:HD2	2.41	0.61
2:F:574:LYS:HG2	2:F:575:SER:H	1.64	0.61
1:G:280:ASN:ND2	1:G:280:ASN:N	2.49	0.61
1:C:97:SER:C	1:C:99:LYS:H	2.07	0.61
1:E:207:VAL:HB	1:E:212:TYR:HB2	1.81	0.61
1:G:116:VAL:O	1:G:513:GLU:HA	1.99	0.61
1:A:281:ALA:O	1:A:282:ILE:C	2.43	0.61
1:C:274:MET:HE2	1:C:394:THR:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD23	1:C:321:PHE:CB	2.30	0.61
1:E:177:ILE:HG22	1:E:181:ASN:HD21	1.65	0.61
1:E:253:HIS:ND1	1:E:491:ALA:HB2	2.16	0.61
1:G:107:VAL:HG11	1:G:450:PHE:CD1	2.36	0.61
1:A:282:ILE:HD13	1:A:282:ILE:H	1.65	0.61
2:B:578:THR:HB	2:B:581:VAL:CG2	2.30	0.61
1:C:421:THR:HG21	1:G:123:ILE:CD1	2.29	0.61
1:E:297:THR:H	1:E:478:ARG:NH2	1.99	0.61
2:F:599:ILE:C	2:F:600:LEU:HG	2.26	0.61
1:C:334:THR:HG22	1:C:356:SER:HA	1.83	0.61
2:D:595:ALA:O	2:D:596:ASN:HB2	2.00	0.61
1:G:411:GLU:HG3	1:G:464:HIS:ND1	2.15	0.61
1:A:162:ASN:ND2	1:A:166:GLU:HB2	2.16	0.61
1:A:276:VAL:HG22	1:A:294:TRP:HB2	1.81	0.61
1:A:535:GLU:CD	2:F:579:PRO:HG2	2.26	0.61
1:A:357:PHE:HE1	1:A:369:TYR:CD1	2.19	0.61
2:B:581:VAL:HG12	2:B:582:ILE:N	2.16	0.61
1:C:273:SER:CB	1:C:475:LEU:HD12	2.18	0.61
1:E:220:ARG:HH12	1:G:218:GLY:HA3	1.65	0.61
1:C:177:ILE:HG22	1:C:181:ASN:ND2	2.16	0.60
1:C:444:LYS:HD2	1:C:447:ASN:O	2.01	0.60
1:E:158:ILE:HG22	1:E:159:ALA:N	2.15	0.60
1:E:299:LEU:HD12	1:E:300:PRO:CD	2.30	0.60
1:E:507:LYS:HE3	1:G:57:SER:HB2	1.82	0.60
1:G:284:GLN:OE1	1:G:289:VAL:HG11	2.00	0.60
1:G:373:SER:C	1:G:375:LEU:H	2.08	0.60
1:C:205:ILE:HD13	1:C:480:ILE:CD1	2.30	0.60
1:E:90:ASP:CB	2:F:561:VAL:HB	2.31	0.60
1:E:178:GLN:HA	1:E:181:ASN:HD22	1.66	0.60
1:G:136:LEU:HD12	1:G:141:LYS:HD3	1.83	0.60
2:H:578:THR:CG2	2:H:581:VAL:H	2.09	0.60
1:A:435:SER:CB	1:A:552:GLN:HG2	2.30	0.60
1:A:180:LEU:HA	1:A:183:ILE:HD11	1.83	0.60
1:A:243:LEU:CD1	1:A:244:ILE:HG23	2.31	0.60
1:A:424:VAL:HG12	1:A:427:TYR:HB3	1.83	0.60
2:D:560:THR:HG22	2:D:564:LEU:CD2	2.31	0.60
1:G:159:ALA:HB2	1:G:206:TYR:HE1	1.66	0.60
1:G:217:ILE:HG23	1:G:319:LYS:NZ	2.15	0.60
1:G:287:ASN:CA	1:G:364:ALA:HB2	2.30	0.60
1:A:329:VAL:HG12	1:A:330:ASN:H	1.66	0.60
1:E:154:ARG:HH11	1:E:154:ARG:HG3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:SER:H	1:C:297:THR:CB	2.14	0.60
1:C:448:PRO:HG3	1:E:449:VAL:CG1	2.31	0.60
1:E:189:LEU:HD12	1:E:205:ILE:HG12	1.82	0.60
1:E:210:ASN:HD22	1:G:524:GLN:HG3	1.64	0.60
1:E:267:GLU:O	1:E:401:ASP:HA	2.02	0.60
1:E:386:THR:O	1:E:389:SER:HB3	2.00	0.60
1:G:290:ALA:CB	1:G:387:LYS:HE2	2.32	0.60
1:A:455:GLU:HG3	1:E:259:GLN:CB	2.32	0.60
1:C:105:SER:HB2	1:C:117:ASP:CB	2.25	0.60
1:C:256:VAL:CG1	1:C:410:ILE:HG23	2.32	0.60
1:C:385:VAL:HG22	1:C:392:SER:OG	2.01	0.60
1:E:210:ASN:HD22	1:G:524:GLN:CD	2.10	0.60
2:F:611:GLY:O	2:F:615:VAL:HG23	2.00	0.60
1:G:277:SER:N	1:G:391:VAL:HG13	2.17	0.60
1:G:288:THR:C	1:G:362:ILE:HD11	2.27	0.60
1:A:180:LEU:HA	1:A:183:ILE:CD1	2.32	0.60
1:C:485:GLU:O	1:C:486:ASN:C	2.44	0.60
1:E:88:TYR:HA	1:E:231:TYR:CB	2.31	0.60
1:E:100:ALA:O	1:E:101:LEU:HB3	2.01	0.60
1:G:194:TRP:CE3	1:G:204:SER:HB2	2.37	0.60
1:G:411:GLU:HG3	1:G:464:HIS:CE1	2.36	0.60
1:E:367:VAL:O	1:E:385:VAL:HG22	2.02	0.60
1:C:177:ILE:O	1:C:180:LEU:N	2.34	0.59
1:C:297:THR:HG22	1:C:298:PRO:N	2.18	0.59
1:E:295:SER:HB3	1:E:322:SER:CB	2.31	0.59
1:E:431:LEU:HD12	1:E:431:LEU:H	1.66	0.59
1:G:121:ARG:HA	1:G:508:THR:O	2.01	0.59
1:G:126:ILE:HG12	1:G:147:PHE:HE1	1.66	0.59
1:G:159:ALA:HB2	1:G:206:TYR:CE1	2.36	0.59
1:G:254:ILE:CG1	1:G:424:VAL:HG21	2.32	0.59
1:C:542:ARG:HD3	2:D:582:ILE:CG2	2.32	0.59
1:E:297:THR:CB	1:E:298:PRO:HD3	2.32	0.59
1:G:485:GLU:HG3	1:G:488:PHE:H	1.67	0.59
1:A:257:LYS:HD3	1:C:456:GLU:HB2	1.83	0.59
1:E:297:THR:HG23	1:E:476:GLY:CA	2.27	0.59
1:G:257:LYS:HE2	1:G:446:ASN:HB3	1.84	0.59
1:G:280:ASN:N	1:G:280:ASN:HD22	1.99	0.59
1:A:128:CYS:HB3	1:A:131:VAL:CG2	2.32	0.59
1:A:306:LEU:CD1	1:A:311:GLY:HA2	2.32	0.59
1:A:366:THR:O	1:A:367:VAL:CG2	2.50	0.59
2:D:561:VAL:HA	2:D:564:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:ASP:HB3	2:F:562:SER:HB3	1.83	0.59
1:E:110:GLY:HA2	1:E:530:ALA:O	2.02	0.59
1:C:205:ILE:HD13	1:C:480:ILE:HD11	1.85	0.59
1:G:342:LEU:HD22	1:G:347:PRO:HA	1.84	0.59
1:A:542:ARG:HE	2:B:583:LYS:HA	1.67	0.59
1:E:229:LYS:HE3	1:E:510:ASP:OD2	2.01	0.59
1:E:297:THR:HG21	1:E:476:GLY:H	1.68	0.59
1:E:552:GLN:C	1:E:554:ASP:H	2.10	0.59
1:G:125:THR:O	1:G:126:ILE:C	2.46	0.59
1:A:315:ASN:HD22	1:A:316:THR:H	1.50	0.59
1:A:445:MET:CE	1:C:113:ARG:HB2	2.32	0.59
1:A:495:PHE:HB3	1:A:498:ILE:CD1	2.32	0.59
1:A:556:ASN:C	1:A:556:ASN:HD22	2.10	0.59
1:E:116:VAL:HG12	1:E:514:GLY:O	2.03	0.59
1:E:153:PHE:HB3	1:E:482:ASP:OD2	2.03	0.59
1:G:82:VAL:O	1:G:83:GLY:C	2.44	0.59
1:G:274:MET:CB	1:G:296:ILE:HG13	2.28	0.59
1:G:329:VAL:HG12	1:G:359:MET:O	2.03	0.59
1:G:538:GLN:HG2	2:H:582:ILE:HG21	1.84	0.59
1:C:89:MET:HE1	1:C:540:ALA:HA	1.85	0.59
1:C:375:LEU:HD12	1:C:376:THR:H	1.66	0.59
1:E:148:ILE:HA	1:E:492:VAL:HG12	1.85	0.59
1:E:190:GLY:C	1:E:192:GLY:H	2.10	0.59
1:E:306:LEU:HD13	1:E:311:GLY:HA2	1.84	0.59
1:G:191:THR:HG21	1:G:193:GLN:OE1	2.03	0.59
1:G:325:ILE:HD12	1:G:333:TRP:CE3	2.37	0.59
1:A:265:ALA:HB2	1:A:404:ALA:N	2.18	0.59
1:A:395:PRO:CB	1:C:267:GLU:HB3	2.32	0.59
1:A:422:THR:O	1:C:523:GLY:HA3	2.03	0.59
1:C:108:PRO:HA	1:C:530:ALA:CB	2.32	0.59
1:C:129:PRO:HA	1:C:194:TRP:CD1	2.38	0.59
1:C:160:LEU:HD22	1:C:161:ALA:N	2.17	0.59
1:C:262:THR:H	1:E:262:THR:HG21	1.68	0.59
1:C:499:SER:O	1:C:500:GLN:C	2.45	0.59
1:E:301:VAL:HA	1:E:321:PHE:HA	1.84	0.59
1:E:313:THR:CB	1:E:325:ILE:HG22	2.33	0.59
1:G:267:GLU:O	1:G:268:ARG:C	2.44	0.59
1:G:360:THR:HG22	1:G:361:THR:OG1	2.02	0.59
1:A:278:ALA:HA	1:A:292:ILE:HG22	1.85	0.58
1:A:408:LEU:H	1:A:461:PHE:HA	1.67	0.58
1:A:451:GLU:HA	1:E:448:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ILE:HD12	1:C:501:SER:OG	2.03	0.58
1:C:545:MET:HE2	1:C:546:GLU:CA	2.32	0.58
1:E:265:ALA:CB	1:E:404:ALA:HB2	2.33	0.58
1:G:313:THR:HB	1:G:325:ILE:HG22	1.85	0.58
1:G:458:PHE:C	1:G:458:PHE:CD1	2.81	0.58
1:G:460:GLY:HA2	1:G:480:ILE:O	2.03	0.58
1:A:297:THR:HG23	1:A:478:ARG:NH2	2.18	0.58
1:C:239:ASN:OD1	1:C:503:THR:OG1	2.21	0.58
1:E:207:VAL:HG11	1:E:212:TYR:CD1	2.38	0.58
1:E:220:ARG:NH1	1:G:215:ALA:CB	2.40	0.58
1:A:424:VAL:O	1:A:427:TYR:CD2	2.57	0.58
1:E:153:PHE:HB2	1:E:227:PHE:CE2	2.38	0.58
1:E:153:PHE:HD2	1:E:154:ARG:NH1	2.00	0.58
2:F:577:ALA:HB1	2:F:582:ILE:HD11	1.85	0.58
1:A:422:THR:O	1:A:422:THR:HG22	2.02	0.58
1:C:84:TRP:HE1	1:C:230:VAL:HG13	1.68	0.58
1:C:87:LYS:C	1:C:89:MET:N	2.55	0.58
1:C:304:VAL:CG1	1:C:305:ALA:H	2.16	0.58
1:E:274:MET:HE3	1:E:296:ILE:HD11	1.84	0.58
2:F:578:THR:HB	2:F:581:VAL:HG23	1.85	0.58
1:G:333:TRP:O	1:G:334:THR:HB	2.04	0.58
1:A:112:LEU:HB3	1:A:114:TYR:O	2.03	0.58
1:A:136:LEU:HD21	1:A:501:SER:CA	2.33	0.58
1:A:226:GLN:NE2	1:A:452:MET:HG2	2.18	0.58
1:A:234:ILE:CG1	1:A:508:THR:HG23	2.19	0.58
1:A:306:LEU:HD13	1:A:311:GLY:HA2	1.86	0.58
1:C:120:GLN:C	1:C:122:PRO:HD3	2.28	0.58
1:C:443:TYR:CE2	1:E:113:ARG:HD2	2.38	0.58
2:F:577:ALA:CB	2:F:582:ILE:HD11	2.34	0.58
1:G:443:TYR:CG	1:G:544:GLN:HG2	2.38	0.58
1:A:106:LYS:HG2	1:A:117:ASP:HB3	1.84	0.58
1:C:542:ARG:HD3	2:D:582:ILE:HG22	1.85	0.58
1:E:168:LEU:CD1	1:E:172:THR:HG22	2.33	0.58
1:E:309:GLY:HA2	1:E:331:SER:HA	1.81	0.58
1:E:342:LEU:O	1:E:343:ALA:HB2	2.02	0.58
1:A:74:SER:O	1:A:75:ILE:HB	2.04	0.58
1:A:144:ARG:HD2	1:A:496:TRP:HD1	1.66	0.58
1:C:275:THR:CG2	1:C:478:ARG:HH12	2.13	0.58
1:E:178:GLN:NE2	1:E:390:GLY:HA2	2.19	0.58
1:G:160:LEU:HD12	1:G:161:ALA:N	2.19	0.58
1:G:162:ASN:OD1	1:G:166:GLU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:475:LEU:O	1:G:476:GLY:O	2.21	0.58
1:C:81:ALA:O	1:C:84:TRP:HB3	2.03	0.58
1:C:246:GLN:HG3	1:G:241:PRO:CB	2.29	0.58
1:E:139:ASP:C	1:E:141:LYS:H	2.08	0.58
1:E:394:THR:O	1:E:395:PRO:C	2.46	0.58
1:A:279:SER:HB3	1:A:388:GLY:HA2	1.85	0.58
1:A:357:PHE:CE1	1:A:369:TYR:HD1	2.19	0.58
1:C:360:THR:HB	1:C:368:VAL:CG1	2.34	0.58
1:E:57:SER:HB3	1:G:237:GLU:OE2	2.04	0.58
1:G:297:THR:HG22	1:G:298:PRO:N	2.17	0.58
1:E:194:TRP:CE3	1:E:194:TRP:HA	2.39	0.58
1:E:228:ARG:HB3	1:E:452:MET:HE3	1.84	0.58
1:E:275:THR:CG2	1:E:478:ARG:HH12	2.17	0.58
1:E:470:PRO:O	1:E:473:ASN:HB2	2.04	0.58
1:C:413:PRO:O	1:C:414:ALA:C	2.47	0.57
1:E:255:PRO:HB3	1:E:445:MET:CG	2.20	0.57
1:E:389:SER:OG	1:E:390:GLY:N	2.36	0.57
1:E:556:ASN:CG	1:E:556:ASN:O	2.46	0.57
1:A:164:ASN:HB2	1:A:166:GLU:HG3	1.85	0.57
1:A:292:ILE:HG13	1:A:325:ILE:HD11	1.85	0.57
1:A:456:GLU:OE1	1:E:257:LYS:HD3	2.04	0.57
1:C:300:PRO:CG	1:C:400:ILE:HG12	2.33	0.57
1:E:304:VAL:HG21	1:E:323:VAL:CG2	2.34	0.57
1:E:313:THR:HA	1:E:325:ILE:HG22	1.86	0.57
2:F:562:SER:O	2:F:566:SER:N	2.31	0.57
1:G:257:LYS:NZ	1:G:257:LYS:HB3	2.18	0.57
1:A:197:PHE:CE2	1:A:201:TRP:HB3	2.39	0.57
1:A:297:THR:HB	1:A:476:GLY:HA3	1.87	0.57
1:C:149:SER:OG	1:C:232:LYS:HE2	2.03	0.57
1:E:238:PHE:CG	1:E:432:CYS:HB3	2.39	0.57
2:H:576:SER:O	2:H:577:ALA:C	2.46	0.57
1:A:539:LEU:HD12	1:A:539:LEU:C	2.29	0.57
1:C:122:PRO:HD2	1:C:508:THR:OG1	2.03	0.57
1:C:363:THR:CG2	1:C:366:THR:N	2.66	0.57
1:E:246:GLN:HE22	1:E:499:SER:HB2	1.70	0.57
1:G:226:GLN:HA	1:G:454:GLY:HA2	1.86	0.57
1:G:261:GLU:O	1:G:406:ASN:HB2	2.05	0.57
1:G:268:ARG:HG2	1:G:268:ARG:HH11	1.69	0.57
1:G:287:ASN:HA	1:G:364:ALA:CB	2.34	0.57
1:A:206:TYR:N	1:A:206:TYR:CD1	2.72	0.57
1:A:350:GLU:C	1:A:352:GLY:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:HB	1:A:366:THR:HG22	1.87	0.57
1:A:545:MET:HE1	1:C:531:GLU:OE2	2.04	0.57
1:C:299:LEU:HD13	1:C:341:ILE:HD11	1.86	0.57
1:E:253:HIS:HD2	1:E:549:GLY:HA3	1.59	0.57
1:G:196:GLN:HB2	1:G:202:TYR:CE2	2.40	0.57
1:G:279:SER:HB3	1:G:291:ARG:NE	2.19	0.57
1:A:262:THR:O	1:A:264:PRO:HD3	2.05	0.57
1:A:346:GLU:OE1	1:A:346:GLU:HA	2.04	0.57
1:E:278:ALA:C	1:E:387:LYS:HA	2.30	0.57
1:E:306:LEU:HD12	1:E:333:TRP:CE2	2.38	0.57
1:E:417:THR:HG22	1:E:418:GLU:OE1	2.05	0.57
1:G:156:ASN:HB3	1:G:206:TYR:O	2.04	0.57
1:G:271:ALA:HA	1:G:397:THR:HA	1.86	0.57
1:G:272:GLY:HA3	1:G:298:PRO:HD3	1.86	0.57
1:G:313:THR:HB	1:G:333:TRP:NE1	2.19	0.57
1:A:217:ILE:HG23	1:E:467:GLY:H	1.68	0.57
1:A:366:THR:HG23	1:A:367:VAL:N	2.19	0.57
1:C:136:LEU:HD12	1:C:137:PRO:O	2.05	0.57
1:C:180:LEU:HA	1:C:183:ILE:CD1	2.35	0.57
1:C:238:PHE:CD2	1:C:432:CYS:HB3	2.39	0.57
1:E:184:THR:HA	1:E:478:ARG:HB2	1.87	0.57
1:E:210:ASN:O	1:E:213:ALA:HB3	2.05	0.57
1:E:238:PHE:CD1	1:E:432:CYS:HB3	2.39	0.57
1:E:538:GLN:HA	1:E:541:ASN:HD22	1.69	0.57
1:G:235:THR:CG2	1:G:507:LYS:HB2	2.35	0.57
1:G:443:TYR:HB3	1:G:544:GLN:HG2	1.86	0.57
1:E:145:VAL:HG23	1:E:161:ALA:HB2	1.86	0.57
1:E:475:LEU:O	1:E:476:GLY:O	2.23	0.57
2:F:575:SER:OG	2:F:581:VAL:HG11	2.04	0.57
1:G:199:PRO:HD3	1:G:388:GLY:CA	2.35	0.57
1:A:306:LEU:HD23	1:A:332:VAL:O	2.05	0.57
1:C:97:SER:C	1:C:99:LYS:N	2.61	0.57
1:C:110:GLY:HA2	1:C:530:ALA:O	2.04	0.57
1:C:435:SER:C	1:C:437:GLY:H	2.11	0.57
2:D:557:PHE:N	2:D:557:PHE:CD2	2.73	0.57
2:F:578:THR:O	2:F:582:ILE:HG12	2.05	0.57
1:G:292:ILE:HD13	1:G:292:ILE:N	2.20	0.57
1:G:296:ILE:HD13	1:G:321:PHE:CD2	2.40	0.57
1:A:299:LEU:HD12	1:A:300:PRO:HD2	1.87	0.57
1:A:531:GLU:CG	2:F:583:LYS:HE3	2.30	0.57
1:E:130:THR:CB	1:E:163:ILE:HG12	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ASN:OD1	1:E:318:GLY:HA3	2.05	0.57
2:F:596:ASN:HB2	2:F:597:PRO:HD2	1.86	0.57
1:G:88:TYR:HA	1:G:231:TYR:HB2	1.87	0.57
1:A:253:HIS:CE1	1:A:442:HIS:HA	2.40	0.56
1:A:553:ALA:C	1:A:555:ASP:H	2.13	0.56
1:C:128:CYS:HA	1:C:143:TRP:CZ3	2.40	0.56
1:C:151:PRO:CD	1:C:490:SER:HB3	2.34	0.56
1:E:253:HIS:NE2	1:E:549:GLY:HA3	2.19	0.56
2:F:607:ILE:HA	2:F:610:VAL:HG23	1.86	0.56
1:G:174:ASN:HD21	1:G:468:TYR:HA	1.66	0.56
1:A:173:ARG:O	1:A:176:PHE:HB3	2.05	0.56
1:A:242:THR:CA	1:A:245:ASP:HB2	2.29	0.56
1:A:412:MET:HG2	1:A:463:PHE:HB3	1.88	0.56
2:B:578:THR:HB	2:B:581:VAL:CB	2.34	0.56
1:C:312:GLY:HA3	1:C:326:ASP:OD1	2.05	0.56
1:E:119:GLU:OE2	1:E:509:TYR:HD2	1.87	0.56
1:E:162:ASN:HA	1:E:200:GLY:O	2.04	0.56
2:F:564:LEU:C	2:F:564:LEU:CD2	2.78	0.56
1:G:205:ILE:CD1	1:G:480:ILE:HD11	2.35	0.56
1:A:146:SER:HB2	1:A:160:LEU:HD11	1.86	0.56
1:A:170:LEU:O	1:A:173:ARG:N	2.39	0.56
1:A:177:ILE:O	1:A:181:ASN:ND2	2.39	0.56
1:A:188:ASP:C	1:A:189:LEU:HD12	2.31	0.56
1:A:257:LYS:HD2	1:C:452:MET:O	2.05	0.56
1:A:299:LEU:HD22	1:A:341:ILE:HD11	1.88	0.56
1:C:282:ILE:O	1:C:282:ILE:HG13	2.04	0.56
1:C:342:LEU:CD2	1:C:347:PRO:HA	2.36	0.56
1:C:363:THR:HG21	1:C:366:THR:OG1	2.05	0.56
1:E:121:ARG:HH11	1:E:121:ARG:HG3	1.70	0.56
1:E:538:GLN:HE22	2:F:582:ILE:HG13	1.71	0.56
1:G:179:THR:O	1:G:180:LEU:C	2.48	0.56
1:G:185:ASN:HB3	1:G:318:GLY:HA3	1.86	0.56
1:G:274:MET:HE2	1:G:296:ILE:CD1	2.30	0.56
1:G:276:VAL:HG13	1:G:294:TRP:HB2	1.86	0.56
1:G:299:LEU:HD12	1:G:300:PRO:HD2	1.87	0.56
1:G:301:VAL:HG12	1:G:319:LYS:C	2.30	0.56
1:G:485:GLU:CD	1:G:487:ASN:HB2	2.30	0.56
1:A:235:THR:HG23	1:A:507:LYS:HB3	1.88	0.56
1:A:250:VAL:HG22	1:A:429:GLN:HG3	1.88	0.56
1:C:475:LEU:HD21	1:E:267:GLU:CB	2.35	0.56
1:E:40:GLN:OE1	1:E:70:ILE:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:TYR:N	1:E:206:TYR:CD1	2.73	0.56
1:G:534:ASP:HA	1:G:537:VAL:CB	2.34	0.56
1:A:107:VAL:CG1	1:A:450:PHE:HD1	2.13	0.56
1:A:274:MET:HB3	1:A:394:THR:HB	1.87	0.56
1:C:407:ARG:CD	1:C:462:GLN:HB2	2.36	0.56
1:E:106:LYS:HG3	1:E:117:ASP:CG	2.31	0.56
1:E:107:VAL:HG11	1:E:450:PHE:CD1	2.40	0.56
1:E:163:ILE:HD11	1:E:202:TYR:CD1	2.41	0.56
1:E:163:ILE:HD11	1:E:202:TYR:CE1	2.40	0.56
1:E:253:HIS:CD2	1:E:549:GLY:CA	2.84	0.56
1:A:165:ASN:ND2	1:A:165:ASN:O	2.38	0.56
1:A:539:LEU:HD12	1:A:543:LEU:HG	1.87	0.56
1:C:292:ILE:HD13	1:C:292:ILE:H	1.71	0.56
1:E:302:ALA:HB2	1:E:338:PRO:CG	2.35	0.56
1:G:63:MET:HG3	1:G:64:ASP:N	2.19	0.56
1:G:258:PRO:HB3	1:G:410:ILE:CG1	2.36	0.56
1:A:217:ILE:HG12	1:E:466:PRO:HA	1.88	0.56
1:C:349:ALA:HB2	1:C:373:SER:OG	2.06	0.56
2:D:567:ILE:HG23	2:D:568:GLY:H	1.71	0.56
2:F:617:SER:O	2:F:618:ILE:C	2.49	0.56
1:A:91:PRO:CG	1:A:233:GLY:HA3	2.36	0.56
1:A:380:VAL:CG1	1:A:381:ILE:H	2.15	0.56
1:A:444:LYS:CB	1:A:450:PHE:HE2	2.18	0.56
1:C:273:SER:HA	1:C:396:VAL:HG23	1.88	0.56
1:E:126:ILE:HD12	1:E:126:ILE:N	2.21	0.56
1:E:518:ALA:C	1:E:520:SER:N	2.59	0.56
1:G:131:VAL:O	1:G:132:SER:OG	2.23	0.56
1:G:244:ILE:HG22	1:G:244:ILE:O	2.05	0.56
1:A:126:ILE:O	1:A:126:ILE:HG22	2.06	0.56
1:C:122:PRO:HG3	1:C:209:PRO:HD2	1.87	0.56
1:C:137:PRO:C	1:C:139:ASP:H	2.14	0.56
1:E:555:ASP:O	1:E:556:ASN:C	2.48	0.56
1:G:169:THR:HG22	1:G:172:THR:H	1.71	0.56
1:G:369:TYR:CE1	1:G:383:ARG:HB3	2.41	0.56
1:G:425:PRO:HG2	1:G:426:LYS:H	1.71	0.56
1:A:449:VAL:HG11	1:E:448:PRO:HB2	1.88	0.56
1:C:142:LEU:O	1:C:500:GLN:OE1	2.23	0.56
1:C:250:VAL:O	1:C:250:VAL:HG13	2.04	0.56
1:C:447:ASN:CG	1:E:451:GLU:HG2	2.31	0.56
1:C:453:THR:HG21	1:C:485:GLU:HA	1.88	0.56
1:C:547:LEU:O	1:E:113:ARG:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:ARG:N	1:E:482:ASP:OD1	2.37	0.56
2:F:567:ILE:HD11	2:F:571:LEU:HD21	1.86	0.56
1:A:75:ILE:HD12	2:B:577:ALA:HB2	1.88	0.55
1:A:289:VAL:HG12	1:A:290:ALA:H	1.70	0.55
1:A:342:LEU:O	1:A:396:VAL:HG13	2.06	0.55
1:A:445:MET:HE2	1:C:113:ARG:H	1.71	0.55
1:E:93:GLY:O	1:E:97:SER:N	2.38	0.55
1:E:272:GLY:O	1:E:475:LEU:HD12	2.06	0.55
1:G:122:PRO:HB3	1:G:209:PRO:HG3	1.87	0.55
1:G:207:VAL:HG12	1:G:208:LEU:H	1.70	0.55
1:G:262:THR:O	1:G:264:PRO:HD3	2.06	0.55
1:A:279:SER:HA	1:A:387:LYS:HG2	1.88	0.55
1:E:152:ALA:O	1:E:229:LYS:NZ	2.35	0.55
1:E:295:SER:HB3	1:E:322:SER:HB2	1.89	0.55
1:G:117:ASP:OD2	1:G:117:ASP:N	2.39	0.55
1:G:272:GLY:C	1:G:475:LEU:HD12	2.30	0.55
1:A:465:TYR:CD1	1:A:466:PRO:HD2	2.41	0.55
1:A:537:VAL:HG23	1:A:538:GLN:N	2.20	0.55
1:C:121:ARG:HA	1:C:508:THR:O	2.06	0.55
1:C:440:ILE:HA	1:C:549:GLY:O	2.05	0.55
1:C:495:PHE:HB3	1:C:498:ILE:HD11	1.88	0.55
1:E:220:ARG:CD	1:G:215:ALA:CB	2.77	0.55
1:E:466:PRO:C	1:E:468:TYR:H	2.14	0.55
1:G:142:LEU:N	1:G:142:LEU:HD23	2.21	0.55
1:G:313:THR:CB	1:G:325:ILE:HG22	2.36	0.55
1:A:292:ILE:HG13	1:A:325:ILE:CD1	2.35	0.55
1:A:451:GLU:OE1	1:E:451:GLU:OE1	2.24	0.55
1:C:304:VAL:CG1	1:C:305:ALA:N	2.69	0.55
1:C:329:VAL:HG12	1:C:362:ILE:HB	1.88	0.55
1:E:410:ILE:O	1:E:463:PHE:HA	2.07	0.55
1:G:189:LEU:N	1:G:189:LEU:CD2	2.70	0.55
1:G:203:TYR:CD1	1:G:203:TYR:C	2.83	0.55
1:G:206:TYR:CD1	1:G:206:TYR:N	2.74	0.55
1:G:301:VAL:HG12	1:G:319:LYS:O	2.07	0.55
2:H:578:THR:O	2:H:579:PRO:C	2.50	0.55
1:C:136:LEU:HD11	1:C:138:LEU:HD23	1.87	0.55
1:C:435:SER:HB2	1:C:552:GLN:HG2	1.87	0.55
1:C:475:LEU:CG	1:E:267:GLU:OE2	2.54	0.55
1:C:546:GLU:CG	2:D:590:VAL:HG21	2.37	0.55
1:A:302:ALA:HB3	1:A:321:PHE:CD1	2.41	0.55
1:A:444:LYS:HB2	1:A:450:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLU:C	1:A:487:ASN:H	2.14	0.55
1:C:319:LYS:HG3	1:C:320:PHE:CE1	2.42	0.55
1:E:183:ILE:O	1:E:478:ARG:HB2	2.07	0.55
2:F:572:LEU:HD11	2:F:577:ALA:HB2	1.89	0.55
2:F:578:THR:O	2:F:579:PRO:C	2.44	0.55
2:B:567:ILE:O	2:B:571:LEU:HG	2.07	0.55
1:C:313:THR:CA	1:C:325:ILE:HG22	2.31	0.55
1:E:130:THR:HG22	1:E:132:SER:H	1.72	0.55
1:E:149:SER:HG	1:E:442:HIS:CE1	2.25	0.55
1:G:230:VAL:HG23	1:G:512:TRP:CA	2.37	0.55
1:G:259:GLN:O	1:G:409:SER:HB3	2.07	0.55
2:H:562:SER:HA	2:H:565:ALA:HB3	1.87	0.55
1:C:177:ILE:HG22	1:C:181:ASN:HD21	1.71	0.55
1:E:273:SER:OG	1:E:475:LEU:HG	2.05	0.55
1:G:248:TRP:NE1	1:G:429:GLN:HG2	2.13	0.55
1:A:107:VAL:HG12	1:A:109:ASP:OD1	2.07	0.55
1:A:139:ASP:HB3	1:A:141:LYS:HG3	1.89	0.55
1:A:297:THR:HG21	1:A:476:GLY:N	2.21	0.55
1:E:337:ALA:O	1:E:351:GLU:O	2.25	0.55
1:E:412:MET:HE3	1:E:415:LEU:HD21	1.89	0.55
2:F:601:GLU:CD	2:F:601:GLU:N	2.65	0.55
1:G:185:ASN:CG	1:G:318:GLY:HA3	2.32	0.55
1:E:89:MET:HE1	1:E:540:ALA:HB1	1.89	0.55
1:G:228:ARG:HG3	1:G:228:ARG:O	2.06	0.55
1:A:95:VAL:HG21	1:A:509:TYR:CE2	2.42	0.54
1:A:400:ILE:CG1	1:A:401:ASP:H	2.08	0.54
1:C:86:TYR:OH	2:D:566:SER:HA	2.07	0.54
1:C:145:VAL:HG13	1:C:145:VAL:O	2.06	0.54
1:C:385:VAL:HG22	1:C:392:SER:CB	2.37	0.54
2:D:564:LEU:C	2:D:567:ILE:HG22	2.32	0.54
1:E:190:GLY:C	1:E:192:GLY:N	2.64	0.54
1:E:536:VAL:O	1:E:537:VAL:C	2.49	0.54
1:A:111:LEU:HD22	1:E:448:PRO:HG3	1.89	0.54
1:A:137:PRO:HG2	1:A:137:PRO:O	2.07	0.54
1:A:545:MET:C	1:A:547:LEU:H	2.15	0.54
1:C:207:VAL:CG1	1:C:208:LEU:N	2.69	0.54
1:C:279:SER:HA	1:C:387:LYS:HB2	1.89	0.54
1:G:552:GLN:C	1:G:554:ASP:H	2.14	0.54
1:C:423:ASN:OD1	1:E:520:SER:HB2	2.08	0.54
1:C:443:TYR:HD2	1:E:113:ARG:NH1	2.06	0.54
1:C:522:VAL:C	1:C:524:GLN:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:PHE:HD1	1:E:228:ARG:N	2.06	0.54
1:G:109:ASP:HA	1:G:532:GLU:HA	1.89	0.54
1:G:177:ILE:O	1:G:178:GLN:C	2.50	0.54
1:G:205:ILE:HD13	1:G:480:ILE:CD1	2.38	0.54
1:A:363:THR:HG22	1:A:365:ASP:N	2.13	0.54
1:A:451:GLU:OE1	1:C:451:GLU:OE2	2.26	0.54
1:A:553:ALA:C	1:A:555:ASP:N	2.65	0.54
1:C:191:THR:C	1:C:193:GLN:H	2.14	0.54
1:E:186:TRP:CD1	1:E:481:VAL:HG23	2.42	0.54
1:E:227:PHE:C	1:E:227:PHE:CD1	2.85	0.54
1:A:86:TYR:O	1:A:90:ASP:N	2.27	0.54
1:A:385:VAL:CG2	1:A:392:SER:HB2	2.34	0.54
1:C:131:VAL:CG1	1:C:132:SER:N	2.71	0.54
1:C:250:VAL:HA	1:C:429:GLN:HA	1.89	0.54
1:C:492:VAL:HG11	1:C:494:HIS:NE2	2.21	0.54
1:C:495:PHE:CD2	1:C:498:ILE:HD11	2.42	0.54
1:C:546:GLU:HG3	2:D:590:VAL:HG21	1.89	0.54
2:D:569:LEU:HD13	2:D:569:LEU:C	2.31	0.54
1:E:169:THR:N	1:E:172:THR:HB	2.22	0.54
1:G:86:TYR:HB3	1:G:94:ALA:HB1	1.89	0.54
1:G:88:TYR:HA	1:G:231:TYR:HB3	1.89	0.54
1:G:107:VAL:HG23	1:G:230:VAL:HG13	1.88	0.54
1:G:125:THR:HG23	1:G:505:VAL:HG22	1.89	0.54
2:H:560:THR:O	2:H:563:ALA:HB3	2.07	0.54
1:A:325:ILE:HD12	1:A:325:ILE:O	2.07	0.54
1:A:329:VAL:HG12	1:A:330:ASN:N	2.22	0.54
1:C:97:SER:O	1:C:99:LYS:N	2.41	0.54
1:E:214:MET:HA	1:E:221:THR:HG21	1.88	0.54
1:E:261:GLU:OE1	1:E:409:SER:HB2	2.08	0.54
1:E:443:TYR:O	1:E:445:MET:N	2.41	0.54
2:F:575:SER:OG	2:F:585:ILE:HD11	2.07	0.54
1:G:276:VAL:C	1:G:391:VAL:HG13	2.33	0.54
1:A:293:VAL:HG22	1:A:324:GLU:CB	2.38	0.54
1:C:412:MET:HE2	1:C:415:LEU:HD21	1.88	0.54
1:E:225:THR:CG2	1:E:517:ASN:HB2	2.36	0.54
1:E:297:THR:CA	1:E:478:ARG:HH21	2.21	0.54
1:E:354:THR:N	1:E:374:SER:OG	2.27	0.54
1:G:68:HIS:O	1:G:78:SER:HA	2.08	0.54
1:G:550:VAL:O	1:G:551:TYR:CD2	2.61	0.54
1:A:75:ILE:O	1:A:75:ILE:HG22	2.06	0.54
1:A:363:THR:HB	1:A:366:THR:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:LEU:HD11	1:C:203:TYR:OH	2.08	0.54
1:E:121:ARG:HG3	1:E:121:ARG:NH1	2.23	0.54
1:E:175:THR:O	1:E:178:GLN:HG3	2.08	0.54
1:E:452:MET:CE	1:E:452:MET:HA	2.36	0.54
1:G:74:SER:C	1:G:75:ILE:HG23	2.33	0.54
1:A:157:PHE:CD1	1:A:157:PHE:C	2.86	0.54
1:A:295:SER:HB3	1:A:322:SER:CB	2.38	0.54
1:A:426:LYS:HD2	1:C:113:ARG:O	2.08	0.54
1:C:256:VAL:HG11	1:C:410:ILE:HG23	1.90	0.54
1:E:210:ASN:HD22	1:G:524:GLN:CG	2.20	0.54
1:E:241:PRO:C	1:E:243:LEU:N	2.64	0.54
1:E:295:SER:O	1:E:296:ILE:HG13	2.08	0.54
1:E:518:ALA:O	1:E:520:SER:N	2.41	0.54
1:E:536:VAL:O	1:E:539:LEU:N	2.40	0.54
1:G:296:ILE:H	1:G:321:PHE:HD2	1.54	0.54
1:A:92:ALA:HB3	1:A:556:ASN:HB2	1.89	0.54
1:A:306:LEU:HD11	1:A:310:THR:O	2.09	0.54
1:C:369:TYR:CD1	1:C:369:TYR:C	2.85	0.54
2:D:594:GLN:HA	1:E:42:THR:O	2.08	0.54
1:E:181:ASN:OD1	1:E:463:PHE:N	2.40	0.54
2:F:577:ALA:CA	2:F:582:ILE:HD11	2.38	0.54
1:G:168:LEU:HD22	1:G:173:ARG:CG	2.23	0.54
1:G:238:PHE:CD2	1:G:432:CYS:HB3	2.43	0.54
1:G:444:LYS:CG	1:G:447:ASN:O	2.56	0.54
1:A:169:THR:N	1:A:172:THR:OG1	2.41	0.53
1:A:313:THR:HG1	1:A:333:TRP:HD1	1.50	0.53
1:A:404:ALA:CB	1:E:261:GLU:OE2	2.47	0.53
1:C:145:VAL:HG13	1:C:495:PHE:HB2	1.90	0.53
1:C:336:THR:HG22	1:C:352:GLY:O	2.09	0.53
1:C:553:ALA:C	1:C:555:ASP:H	2.16	0.53
1:E:187:ARG:HG3	1:E:212:TYR:CE1	2.43	0.53
2:F:607:ILE:O	2:F:608:GLY:C	2.50	0.53
1:G:163:ILE:C	1:G:165:ASN:H	2.14	0.53
1:G:272:GLY:HA3	1:G:298:PRO:CD	2.38	0.53
1:G:533:GLU:OE1	1:G:533:GLU:HA	2.07	0.53
1:A:84:TRP:CD1	1:A:230:VAL:HG13	2.43	0.53
1:A:290:ALA:HB2	1:A:387:LYS:HZ3	1.72	0.53
1:A:401:ASP:N	1:A:401:ASP:OD2	2.40	0.53
1:A:403:GLU:HB3	1:A:405:VAL:HG23	1.90	0.53
1:C:128:CYS:HB3	1:C:131:VAL:CG2	2.37	0.53
1:C:295:SER:HB3	1:C:322:SER:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:GLY:HA2	1:G:101:LEU:H	1.73	0.53
1:G:207:VAL:HG12	1:G:208:LEU:N	2.23	0.53
1:A:97:SER:C	1:A:99:LYS:H	2.16	0.53
1:A:178:GLN:HE22	1:A:391:VAL:N	2.06	0.53
1:A:259:GLN:OE1	1:C:456:GLU:O	2.27	0.53
1:A:274:MET:HE1	1:A:381:ILE:HD13	1.89	0.53
1:A:363:THR:CB	1:A:366:THR:HG22	2.38	0.53
1:A:536:VAL:O	1:A:537:VAL:C	2.50	0.53
2:B:572:LEU:C	2:B:572:LEU:HD12	2.33	0.53
1:C:108:PRO:HA	1:C:530:ALA:HB1	1.90	0.53
1:C:128:CYS:HB3	1:C:131:VAL:HG21	1.88	0.53
2:D:580:SER:HB2	1:E:535:GLU:OE1	2.08	0.53
2:D:580:SER:N	1:E:535:GLU:OE1	2.41	0.53
1:E:296:ILE:HD12	1:E:321:PHE:CE2	2.43	0.53
1:E:537:VAL:O	1:E:540:ALA:HB3	2.09	0.53
2:F:605:LYS:HG3	2:F:610:VAL:HG22	1.89	0.53
1:G:109:ASP:O	1:G:111:LEU:N	2.41	0.53
1:G:138:LEU:C	1:G:140:GLY:H	2.17	0.53
1:G:486:ASN:CG	1:G:486:ASN:O	2.50	0.53
1:A:281:ALA:CB	1:A:291:ARG:HB2	2.33	0.53
1:C:144:ARG:CZ	1:C:496:TRP:HZ2	2.22	0.53
1:C:359:MET:HE2	1:C:367:VAL:HG11	1.90	0.53
1:E:69:GLU:CA	1:E:78:SER:HA	2.31	0.53
1:E:116:VAL:HG21	1:E:522:VAL:HG12	1.88	0.53
1:E:348:PHE:CD1	1:E:373:SER:HB2	2.42	0.53
1:E:428:GLU:OE1	1:E:548:THR:HG21	2.08	0.53
1:G:160:LEU:HD11	1:G:201:TRP:CE3	2.43	0.53
1:G:296:ILE:HD13	1:G:321:PHE:CE2	2.43	0.53
1:G:442:HIS:O	1:G:443:TYR:HB3	2.06	0.53
1:G:461:PHE:HE1	1:G:480:ILE:HB	1.73	0.53
2:H:588:GLN:C	2:H:590:VAL:H	2.15	0.53
1:A:371:VAL:N	1:A:381:ILE:HG22	2.17	0.53
1:C:276:VAL:HG11	1:C:369:TYR:CD2	2.44	0.53
1:C:284:GLN:OE1	1:C:289:VAL:HG11	2.09	0.53
1:E:220:ARG:NH1	1:G:221:THR:OG1	2.41	0.53
1:E:256:VAL:CG1	1:E:410:ILE:HG23	2.37	0.53
1:E:370:SER:HA	1:E:381:ILE:O	2.08	0.53
1:E:416:THR:O	1:E:417:THR:C	2.51	0.53
1:E:538:GLN:NE2	2:F:582:ILE:HG13	2.23	0.53
1:G:93:GLY:O	1:G:97:SER:CB	2.56	0.53
1:A:289:VAL:HG13	1:A:327:GLY:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TYR:HE2	1:A:383:ARG:HB3	1.73	0.53
1:C:139:ASP:OD1	1:C:141:LYS:HG3	2.09	0.53
1:C:295:SER:HB3	1:C:322:SER:HB2	1.89	0.53
2:D:563:ALA:C	2:D:565:ALA:H	2.16	0.53
1:E:54:VAL:HG12	1:E:55:ALA:O	2.09	0.53
1:E:304:VAL:HG12	1:E:333:TRP:HB3	1.90	0.53
2:F:593:VAL:HG12	2:F:594:GLN:N	2.23	0.53
2:F:599:ILE:O	2:F:600:LEU:CG	2.47	0.53
1:G:176:PHE:HB2	1:G:197:PHE:CE1	2.44	0.53
1:A:460:GLY:HA2	1:A:481:VAL:HA	1.90	0.53
1:C:215:ALA:CB	1:C:218:GLY:HA2	2.33	0.53
1:C:265:ALA:HB2	1:C:404:ALA:H	1.74	0.53
1:C:292:ILE:HD11	1:C:325:ILE:CD1	2.37	0.53
1:C:297:THR:HG22	1:C:298:PRO:HG3	1.90	0.53
1:E:252:ALA:HB2	1:E:427:TYR:CB	2.38	0.53
1:E:353:ASP:OD1	1:E:375:LEU:HB2	2.09	0.53
1:G:90:ASP:HB3	2:H:562:SER:OG	2.08	0.53
1:G:254:ILE:HD11	1:G:424:VAL:HG21	1.90	0.53
1:A:169:THR:HG22	1:A:172:THR:OG1	2.09	0.53
1:A:249:TRP:CD2	1:A:438:ALA:HB2	2.44	0.53
1:C:195:ALA:HB3	1:C:203:TYR:CE2	2.43	0.53
1:C:363:THR:HG23	1:C:366:THR:H	1.72	0.53
1:E:130:THR:HB	1:E:163:ILE:CG1	2.38	0.53
1:E:348:PHE:CD2	1:E:381:ILE:HD11	2.43	0.53
1:G:81:ALA:O	1:G:84:TRP:HB3	2.09	0.53
1:A:269:PHE:CD1	1:A:399:GLY:HA2	2.44	0.53
1:C:162:ASN:HA	1:C:200:GLY:O	2.09	0.53
1:E:182:ASN:O	1:E:183:ILE:C	2.50	0.53
1:E:194:TRP:HZ3	1:E:204:SER:N	2.06	0.53
1:E:538:GLN:O	1:E:539:LEU:C	2.52	0.53
1:G:262:THR:HA	1:G:406:ASN:HA	1.91	0.53
1:A:120:GLN:HE22	1:A:211:THR:H	1.55	0.53
1:A:297:THR:OG1	1:A:298:PRO:CD	2.56	0.53
1:A:464:HIS:CE1	1:C:455:GLU:OE2	2.62	0.53
1:A:510:ASP:C	1:A:510:ASP:OD1	2.52	0.53
1:C:87:LYS:NZ	1:C:95:VAL:HG23	2.23	0.53
2:D:574:LYS:N	2:D:574:LYS:HD2	2.23	0.53
1:E:256:VAL:HG11	1:E:410:ILE:HG23	1.90	0.53
1:E:534:ASP:O	1:E:535:GLU:C	2.51	0.53
1:G:170:LEU:HA	1:G:173:ARG:HD3	1.91	0.53
1:G:194:TRP:HA	1:G:194:TRP:HE3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:566:SER:O	2:H:567:ILE:C	2.52	0.53
1:A:83:GLY:O	1:A:87:LYS:HG2	2.09	0.52
1:A:267:GLU:OE1	1:A:267:GLU:HA	2.08	0.52
1:A:542:ARG:HH21	2:B:583:LYS:HB2	1.73	0.52
1:C:352:GLY:O	1:C:353:ASP:C	2.52	0.52
1:C:424:VAL:O	1:C:427:TYR:HD2	1.91	0.52
1:C:443:TYR:O	1:C:445:MET:N	2.42	0.52
1:C:461:PHE:HB2	1:C:480:ILE:HB	1.90	0.52
1:G:254:ILE:HG12	1:G:424:VAL:HG21	1.90	0.52
1:A:91:PRO:HG2	1:A:233:GLY:HA3	1.92	0.52
1:A:470:PRO:HA	1:A:473:ASN:OD1	2.09	0.52
1:C:93:GLY:O	1:C:97:SER:N	2.37	0.52
1:C:427:TYR:CD1	1:C:427:TYR:C	2.87	0.52
1:G:142:LEU:HG	1:G:165:ASN:HD21	1.73	0.52
1:G:286:SER:O	1:G:387:LYS:NZ	2.42	0.52
1:A:97:SER:HB3	1:A:99:LYS:HE2	1.91	0.52
1:A:162:ASN:CG	1:A:166:GLU:HB2	2.34	0.52
1:A:543:LEU:O	1:A:544:GLN:C	2.50	0.52
1:C:93:GLY:O	1:C:97:SER:HB3	2.09	0.52
1:E:169:THR:CG2	1:E:170:LEU:N	2.72	0.52
1:E:253:HIS:HA	1:E:491:ALA:CB	2.40	0.52
1:E:350:GLU:O	1:E:351:GLU:C	2.52	0.52
1:G:92:ALA:HB3	1:G:556:ASN:HB2	1.91	0.52
1:G:536:VAL:O	1:G:537:VAL:C	2.52	0.52
1:A:152:ALA:CB	1:A:155:LEU:HB3	2.39	0.52
1:A:282:ILE:O	1:A:283:PHE:HB2	2.09	0.52
1:C:144:ARG:HH12	1:C:168:LEU:HB2	1.74	0.52
1:C:342:LEU:HD22	1:C:347:PRO:HA	1.91	0.52
1:E:40:GLN:O	1:E:41:ALA:HB2	2.09	0.52
1:E:147:PHE:CD2	1:E:159:ALA:HB2	2.44	0.52
1:E:251:GLY:C	1:E:550:VAL:HG21	2.33	0.52
1:E:452:MET:O	1:E:453:THR:C	2.50	0.52
1:G:154:ARG:HA	1:G:211:THR:CG2	2.39	0.52
1:G:216:GLU:O	1:G:217:ILE:HG22	2.09	0.52
1:A:153:PHE:CE2	1:A:211:THR:HG23	2.45	0.52
1:A:413:PRO:O	1:A:414:ALA:C	2.52	0.52
1:C:92:ALA:O	1:C:96:GLU:HB2	2.10	0.52
1:C:177:ILE:O	1:C:178:GLN:C	2.51	0.52
1:C:412:MET:CE	1:C:415:LEU:HD21	2.39	0.52
1:C:461:PHE:HB3	1:C:463:PHE:CZ	2.45	0.52
1:E:63:MET:HE1	1:G:101:LEU:CD2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:VAL:HG22	1:E:358:SER:HB2	1.91	0.52
1:G:162:ASN:OD1	1:G:165:ASN:N	2.43	0.52
1:G:334:THR:OG1	1:G:335:PHE:N	2.43	0.52
1:A:144:ARG:N	1:A:165:ASN:HA	2.25	0.52
1:A:433:LYS:HG3	1:A:434:GLU:N	2.25	0.52
1:C:175:THR:O	1:C:178:GLN:HG3	2.08	0.52
1:C:236:PHE:CE1	1:C:493:VAL:HG21	2.44	0.52
1:C:276:VAL:H	1:C:391:VAL:HG13	1.74	0.52
1:C:375:LEU:HB3	1:C:378:SER:CB	2.39	0.52
1:C:522:VAL:O	1:C:524:GLN:N	2.42	0.52
1:G:89:MET:SD	1:G:543:LEU:HD23	2.50	0.52
1:G:287:ASN:HA	1:G:364:ALA:CA	2.39	0.52
1:G:366:THR:HG22	1:G:386:THR:CG2	2.39	0.52
1:G:430:PHE:CE2	1:G:552:GLN:HG2	2.45	0.52
1:G:504:ILE:HG22	1:G:506:CYS:SG	2.49	0.52
2:H:563:ALA:O	2:H:566:SER:HB2	2.10	0.52
1:A:113:ARG:N	1:E:443:TYR:OH	2.42	0.52
1:A:537:VAL:O	1:A:540:ALA:HB3	2.10	0.52
1:C:163:ILE:HG13	1:C:164:ASN:N	2.25	0.52
1:C:292:ILE:HD13	1:C:325:ILE:HG13	1.91	0.52
1:C:538:GLN:HE21	2:D:579:PRO:HB3	1.75	0.52
1:E:194:TRP:CE3	1:E:204:SER:HB2	2.44	0.52
1:E:359:MET:HA	1:E:369:TYR:HA	1.90	0.52
1:G:86:TYR:CD1	1:G:99:LYS:HB3	2.45	0.52
1:G:280:ASN:OD1	1:G:286:SER:HB2	2.09	0.52
1:G:477:LEU:HG	1:G:477:LEU:O	2.09	0.52
1:A:231:TYR:C	1:A:231:TYR:CD1	2.88	0.52
1:A:419:GLU:HB3	1:A:423:ASN:HD22	1.71	0.52
1:E:272:GLY:HA3	1:E:298:PRO:CD	2.39	0.52
1:E:297:THR:HG22	1:E:298:PRO:N	2.15	0.52
1:E:363:THR:HB	1:E:366:THR:H	1.75	0.52
2:F:605:LYS:HG2	2:F:610:VAL:CG2	2.40	0.52
2:F:613:ARG:HD2	3:R:3:U:O2	2.09	0.52
1:A:146:SER:O	1:A:160:LEU:HD12	2.10	0.52
1:A:244:ILE:C	1:A:246:GLN:HG3	2.34	0.52
1:A:340:SER:HA	1:A:349:ALA:O	2.09	0.52
1:A:344:GLU:C	1:A:346:GLU:H	2.16	0.52
1:A:552:GLN:HB2	1:A:555:ASP:OD2	2.10	0.52
1:C:93:GLY:O	1:C:97:SER:CB	2.57	0.52
1:C:544:GLN:C	1:C:546:GLU:N	2.65	0.52
1:E:485:GLU:HG3	1:E:485:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:THR:CB	1:G:298:PRO:HD3	2.40	0.52
1:G:360:THR:HG22	1:G:361:THR:N	2.25	0.52
1:A:297:THR:CB	1:A:298:PRO:CD	2.88	0.52
1:C:144:ARG:NH1	1:C:168:LEU:HB2	2.25	0.52
1:C:222:ASP:CG	1:C:522:VAL:HG23	2.35	0.52
1:C:285:PRO:HB2	1:C:288:THR:HB	1.91	0.52
1:E:100:ALA:C	1:E:101:LEU:HD23	2.35	0.52
1:E:313:THR:HB	1:E:333:TRP:CD1	2.45	0.52
2:F:618:ILE:HG23	2:F:619:LYS:HG3	1.92	0.52
1:G:74:SER:O	1:G:75:ILE:CG2	2.58	0.52
1:G:257:LYS:HB3	1:G:257:LYS:HZ2	1.73	0.52
1:G:278:ALA:CB	1:G:387:LYS:HA	2.35	0.52
1:G:373:SER:HB2	1:G:378:SER:OG	2.10	0.52
1:A:181:ASN:H	1:A:181:ASN:HD22	1.58	0.51
1:A:295:SER:HB3	1:A:322:SER:HB2	1.91	0.51
1:A:365:ASP:O	1:A:387:LYS:HB3	2.10	0.51
1:C:126:ILE:HG22	1:C:126:ILE:O	2.09	0.51
1:C:350:GLU:O	1:C:351:GLU:C	2.53	0.51
1:C:440:ILE:HD12	1:C:491:ALA:HB3	1.92	0.51
1:E:210:ASN:CG	1:G:520:SER:O	2.53	0.51
1:E:444:LYS:HD3	1:E:448:PRO:O	2.10	0.51
2:H:584:GLY:O	2:H:588:GLN:HG3	2.10	0.51
1:A:257:LYS:HG3	1:C:226:GLN:NE2	2.25	0.51
1:A:293:VAL:HG22	1:A:324:GLU:HB2	1.91	0.51
1:C:146:SER:HB3	1:C:494:HIS:CE1	2.44	0.51
1:C:291:ARG:HG2	1:C:291:ARG:HH11	1.75	0.51
1:C:332:VAL:HG22	1:C:358:SER:CB	2.37	0.51
1:C:339:ALA:HB3	1:C:400:ILE:CD1	2.38	0.51
1:G:81:ALA:O	1:G:82:VAL:C	2.51	0.51
1:G:284:GLN:CD	1:G:289:VAL:HG11	2.35	0.51
1:G:453:THR:HG22	1:G:486:ASN:HD22	1.75	0.51
2:H:561:VAL:O	2:H:564:LEU:HG	2.10	0.51
1:A:144:ARG:H	1:A:165:ASN:HA	1.75	0.51
1:A:276:VAL:HG22	1:A:294:TRP:CG	2.44	0.51
1:C:145:VAL:HA	1:C:160:LEU:O	2.10	0.51
1:C:181:ASN:OD1	1:C:463:PHE:O	2.27	0.51
1:C:255:PRO:HB3	1:C:445:MET:SD	2.50	0.51
1:E:544:GLN:OE1	1:E:544:GLN:HA	2.09	0.51
1:G:87:LYS:NZ	1:G:95:VAL:CG1	2.74	0.51
1:G:284:GLN:O	1:G:286:SER:N	2.43	0.51
1:G:412:MET:HB2	1:G:463:PHE:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:NZ	1:A:95:VAL:HG23	2.26	0.51
1:A:461:PHE:CD1	1:A:480:ILE:O	2.64	0.51
1:A:545:MET:HE2	1:A:546:GLU:HB3	1.91	0.51
1:C:285:PRO:C	1:C:287:ASN:H	2.19	0.51
1:C:475:LEU:CG	1:E:267:GLU:HB2	2.37	0.51
1:E:95:VAL:HG13	1:G:63:MET:HB3	1.92	0.51
1:E:150:PHE:O	1:E:152:ALA:N	2.40	0.51
1:E:158:ILE:CG2	1:E:159:ALA:N	2.72	0.51
1:E:396:VAL:HG13	1:E:397:THR:N	2.25	0.51
1:E:554:ASP:HA	1:G:56:PRO:HG3	1.92	0.51
1:G:126:ILE:H	1:G:126:ILE:CD1	2.22	0.51
1:G:542:ARG:NH1	2:H:583:LYS:HB2	2.26	0.51
1:A:289:VAL:HG12	1:A:290:ALA:N	2.26	0.51
1:A:422:THR:HG21	1:C:520:SER:HA	1.93	0.51
1:C:141:LYS:HG2	1:G:136:LEU:HB3	1.93	0.51
1:C:534:ASP:O	1:C:535:GLU:C	2.53	0.51
1:E:173:ARG:O	1:E:177:ILE:HG13	2.10	0.51
1:E:210:ASN:HA	1:E:213:ALA:HB3	1.92	0.51
1:E:435:SER:C	1:E:437:GLY:N	2.59	0.51
2:F:605:LYS:NZ	2:F:610:VAL:HG13	2.26	0.51
1:G:192:GLY:HA2	1:G:205:ILE:O	2.11	0.51
1:G:250:VAL:O	1:G:493:VAL:HA	2.11	0.51
1:A:121:ARG:HA	1:A:508:THR:O	2.11	0.51
1:A:268:ARG:H	1:E:395:PRO:HB3	1.74	0.51
1:A:375:LEU:HB3	1:A:378:SER:CB	2.34	0.51
1:E:107:VAL:CG2	1:E:230:VAL:HG13	2.41	0.51
1:E:154:ARG:H	1:E:482:ASP:CG	2.16	0.51
1:G:447:ASN:CG	1:G:449:VAL:HG12	2.36	0.51
1:A:262:THR:OG1	1:E:262:THR:HG22	2.11	0.51
1:A:263:ILE:HG22	1:A:263:ILE:O	2.11	0.51
1:A:277:SER:HB3	1:A:391:VAL:HG12	1.93	0.51
1:E:90:ASP:O	1:E:91:PRO:C	2.52	0.51
1:E:132:SER:HB2	1:E:141:LYS:NZ	2.25	0.51
1:E:154:ARG:HG3	1:E:154:ARG:NH1	2.26	0.51
1:E:169:THR:H	1:E:172:THR:CB	2.24	0.51
1:E:369:TYR:O	1:E:382:VAL:HA	2.11	0.51
1:G:72:ALA:HB3	1:G:75:ILE:O	2.10	0.51
1:G:330:ASN:OD1	1:G:330:ASN:N	2.43	0.51
1:G:523:GLY:O	1:G:526:ALA:HB3	2.10	0.51
1:A:113:ARG:HG2	1:E:547:LEU:O	2.11	0.51
2:B:578:THR:CB	2:B:581:VAL:HG23	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:THR:CG2	1:G:193:GLN:OE1	2.59	0.51
2:B:578:THR:HB	2:B:581:VAL:HB	1.93	0.51
1:C:176:PHE:O	1:C:179:THR:HB	2.11	0.51
1:C:365:ASP:O	1:C:386:THR:HG23	2.11	0.51
1:C:395:PRO:HB3	1:E:267:GLU:CG	2.40	0.51
1:E:256:VAL:HG11	1:E:410:ILE:HG22	1.92	0.51
1:G:258:PRO:CB	1:G:410:ILE:HG12	2.39	0.51
1:G:281:ALA:CB	1:G:284:GLN:HG3	2.27	0.51
2:B:588:GLN:C	2:B:590:VAL:N	2.68	0.51
1:C:149:SER:HA	1:C:157:PHE:HB3	1.91	0.51
1:C:354:THR:H	1:C:374:SER:CB	2.24	0.51
1:C:537:VAL:O	1:C:538:GLN:C	2.54	0.51
2:D:572:LEU:HA	2:D:575:SER:OG	2.11	0.51
1:E:55:ALA:HB1	1:E:56:PRO:CD	2.35	0.51
1:E:286:SER:HB3	1:E:364:ALA:O	2.11	0.51
1:E:314:ASN:N	1:E:324:GLU:O	2.43	0.51
1:E:380:VAL:HG12	1:E:381:ILE:N	2.26	0.51
1:E:416:THR:O	1:E:418:GLU:N	2.44	0.51
1:E:418:GLU:HA	1:E:421:THR:HG21	1.92	0.51
1:G:417:THR:O	1:G:421:THR:HG23	2.10	0.51
1:A:537:VAL:CG2	1:A:538:GLN:N	2.75	0.50
1:C:191:THR:C	1:C:193:GLN:N	2.69	0.50
1:C:241:PRO:HG2	1:C:244:ILE:HG13	1.93	0.50
1:E:49:LEU:O	1:E:50:PRO:C	2.54	0.50
2:F:567:ILE:CD1	2:F:571:LEU:HD21	2.41	0.50
1:G:117:ASP:O	1:G:118:ALA:HB2	2.10	0.50
1:G:122:PRO:O	1:G:508:THR:HG23	2.10	0.50
1:G:151:PRO:CB	1:G:488:PHE:HB2	2.41	0.50
1:G:226:GLN:O	1:G:227:PHE:HB3	2.10	0.50
1:G:435:SER:C	1:G:437:GLY:N	2.69	0.50
2:H:589:ALA:C	2:H:590:VAL:HG22	2.36	0.50
1:A:177:ILE:O	1:A:178:GLN:C	2.53	0.50
1:A:462:GLN:O	1:A:462:GLN:HG3	2.10	0.50
1:C:251:GLY:C	1:C:550:VAL:HG11	2.36	0.50
1:C:292:ILE:HD11	1:C:325:ILE:CG1	2.40	0.50
1:E:156:ASN:HB3	1:E:206:TYR:O	2.11	0.50
1:E:286:SER:C	1:E:288:THR:H	2.19	0.50
1:E:528:THR:HG22	1:E:529:GLY:O	2.11	0.50
1:E:542:ARG:HD2	2:F:582:ILE:HG22	1.93	0.50
1:G:166:GLU:HB3	1:G:201:TRP:HZ2	1.75	0.50
1:G:232:LYS:O	1:G:442:HIS:HD2	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:ALA:HB2	1:G:338:PRO:HD3	1.94	0.50
1:A:113:ARG:HD3	1:E:547:LEU:O	2.11	0.50
1:A:128:CYS:HB2	1:A:143:TRP:CE2	2.46	0.50
1:A:280:ASN:N	1:A:387:LYS:HD3	2.26	0.50
1:A:325:ILE:C	1:A:325:ILE:CD1	2.84	0.50
1:A:363:THR:C	1:A:365:ASP:N	2.67	0.50
1:C:122:PRO:HG3	1:C:209:PRO:CD	2.41	0.50
1:C:182:ASN:OD1	1:C:474:ALA:N	2.33	0.50
1:C:299:LEU:HD12	1:C:300:PRO:HD2	1.92	0.50
1:C:405:VAL:HG11	1:C:477:LEU:HD22	1.93	0.50
1:E:456:GLU:H	1:E:456:GLU:CD	2.19	0.50
1:G:71:CYS:HA	1:G:76:ASP:HB3	1.93	0.50
1:G:87:LYS:NZ	1:G:95:VAL:HG11	2.26	0.50
1:G:414:ALA:CB	1:G:420:VAL:HG22	2.40	0.50
1:A:268:ARG:HG3	1:A:268:ARG:HH11	1.75	0.50
1:A:439:TYR:HB2	1:A:553:ALA:HA	1.94	0.50
1:C:239:ASN:HB3	1:C:503:THR:O	2.11	0.50
1:C:498:ILE:HD13	1:C:504:ILE:HD11	1.93	0.50
1:E:287:ASN:HB3	1:E:364:ALA:HB2	1.93	0.50
2:F:572:LEU:HD12	2:F:572:LEU:O	2.11	0.50
1:G:82:VAL:O	1:G:85:PHE:HB3	2.11	0.50
1:G:248:TRP:HB2	1:G:431:LEU:CD2	2.41	0.50
1:G:518:ALA:C	1:G:520:SER:H	2.18	0.50
3:R:3:U:C5	3:R:4:U:C5	2.99	0.50
1:A:154:ARG:HG2	1:A:482:ASP:OD1	2.11	0.50
1:A:170:LEU:HG	1:A:174:ASN:OD1	2.11	0.50
1:C:475:LEU:CG	1:E:267:GLU:CD	2.85	0.50
1:E:276:VAL:HG22	1:E:294:TRP:CD1	2.46	0.50
1:E:306:LEU:HD13	1:E:311:GLY:CA	2.41	0.50
1:G:207:VAL:HG21	1:G:212:TYR:CD1	2.47	0.50
1:G:547:LEU:HD23	1:G:547:LEU:N	2.26	0.50
1:A:248:TRP:CZ3	1:A:250:VAL:HG23	2.46	0.50
1:A:319:LYS:HE3	1:A:320:PHE:CE1	2.47	0.50
1:A:449:VAL:CG2	1:C:449:VAL:HG11	2.41	0.50
1:C:400:ILE:HG22	1:C:401:ASP:H	1.77	0.50
2:D:560:THR:C	2:D:564:LEU:HD22	2.37	0.50
2:D:564:LEU:HD13	2:D:564:LEU:N	2.27	0.50
1:E:119:GLU:OE2	1:E:509:TYR:CD2	2.64	0.50
1:G:133:GLU:N	1:G:283:PHE:CZ	2.75	0.50
1:G:135:ASP:CG	1:G:136:LEU:N	2.69	0.50
1:G:232:LYS:HD2	1:G:510:ASP:OD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:N	1:A:189:LEU:CD1	2.72	0.50
1:A:298:PRO:HB2	1:A:398:VAL:HG21	1.94	0.50
1:C:207:VAL:CG1	1:C:212:TYR:HB2	2.39	0.50
2:D:571:LEU:O	2:D:572:LEU:C	2.54	0.50
1:G:109:ASP:O	1:G:110:GLY:C	2.54	0.50
1:G:162:ASN:ND2	1:G:166:GLU:HB2	2.26	0.50
1:G:185:ASN:O	1:G:188:ASP:HB2	2.11	0.50
1:G:189:LEU:C	1:G:191:THR:H	2.20	0.50
1:A:120:GLN:OE1	1:A:208:LEU:HB3	2.12	0.50
1:A:278:ALA:O	1:A:388:GLY:N	2.36	0.50
2:B:579:PRO:HG2	1:C:535:GLU:OE2	2.11	0.50
1:C:297:THR:HG22	1:C:298:PRO:CG	2.41	0.50
1:E:134:SER:HB2	1:E:139:ASP:OD2	2.12	0.50
1:E:226:GLN:NE2	1:E:452:MET:HB3	2.27	0.50
1:E:229:LYS:CB	1:E:485:GLU:HG2	2.35	0.50
1:E:412:MET:HE3	1:E:415:LEU:CD2	2.42	0.50
1:E:504:ILE:HG22	1:E:506:CYS:SG	2.51	0.50
1:G:116:VAL:HG11	1:G:522:VAL:CG1	2.41	0.50
1:G:257:LYS:HE2	1:G:446:ASN:CB	2.41	0.50
1:A:90:ASP:OD1	1:A:93:GLY:N	2.40	0.50
1:A:307:THR:HG23	1:A:308:THR:HG23	1.94	0.50
1:C:77:PRO:HA	1:C:533:GLU:OE2	2.12	0.50
1:C:209:PRO:O	1:C:212:TYR:N	2.45	0.50
1:C:553:ALA:O	1:C:555:ASP:N	2.45	0.50
2:D:567:ILE:CG2	2:D:568:GLY:N	2.75	0.50
2:D:581:VAL:O	2:D:585:ILE:CD1	2.54	0.50
1:E:248:TRP:CA	1:E:431:LEU:HA	2.40	0.50
1:E:275:THR:CG2	1:E:478:ARG:NH1	2.74	0.50
1:G:54:VAL:HG12	1:G:55:ALA:O	2.12	0.50
1:G:84:TRP:CE3	1:G:108:PRO:HD2	2.47	0.50
1:G:248:TRP:CZ2	1:G:429:GLN:HB2	2.47	0.50
1:A:131:VAL:HG21	1:A:500:GLN:HB3	1.94	0.49
1:A:274:MET:HG3	1:A:294:TRP:HE1	1.77	0.49
1:A:447:ASN:HD21	1:A:451:GLU:HB2	1.77	0.49
1:A:498:ILE:HG22	1:A:499:SER:N	2.27	0.49
1:E:436:GLY:H	1:E:554:ASP:CG	2.20	0.49
2:F:609:SER:O	2:F:610:VAL:C	2.55	0.49
1:G:48:LEU:CD2	1:G:54:VAL:HG21	2.42	0.49
1:G:231:TYR:CE2	1:G:511:GLY:HA3	2.47	0.49
1:A:107:VAL:HG12	1:A:109:ASP:CG	2.37	0.49
1:C:299:LEU:HD11	1:C:338:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:571:LEU:N	2:D:571:LEU:HD23	2.27	0.49
1:E:227:PHE:CD1	1:E:228:ARG:N	2.80	0.49
1:E:429:GLN:CD	1:E:429:GLN:C	2.79	0.49
1:E:516:THR:HG21	1:E:523:GLY:HA2	1.94	0.49
1:G:217:ILE:HG23	1:G:319:LYS:HZ1	1.76	0.49
1:G:218:GLY:HA3	1:G:221:THR:OG1	2.11	0.49
1:G:316:THR:HG21	1:G:322:SER:HB3	1.94	0.49
1:G:362:ILE:O	1:G:362:ILE:HG13	2.11	0.49
1:A:146:SER:HB2	1:A:160:LEU:CD1	2.41	0.49
1:A:197:PHE:CD1	1:A:197:PHE:C	2.90	0.49
1:A:248:TRP:HZ3	1:A:250:VAL:CG2	2.25	0.49
1:A:404:ALA:O	1:A:405:VAL:C	2.55	0.49
1:A:406:ASN:OD1	1:A:406:ASN:N	2.45	0.49
1:A:443:TYR:CE2	1:A:445:MET:HE3	2.35	0.49
1:A:464:HIS:C	1:A:464:HIS:CD2	2.90	0.49
1:C:129:PRO:HG2	1:C:163:ILE:HG23	1.94	0.49
1:C:182:ASN:HA	1:C:478:ARG:HD2	1.94	0.49
2:D:582:ILE:HA	2:D:585:ILE:HD13	1.95	0.49
1:E:144:ARG:HG2	1:E:144:ARG:NH1	2.25	0.49
1:E:185:ASN:ND2	1:E:320:PHE:O	2.36	0.49
1:G:39:GLU:O	1:G:71:CYS:N	2.46	0.49
1:G:72:ALA:C	1:G:74:SER:H	2.21	0.49
1:G:133:GLU:O	1:G:134:SER:C	2.56	0.49
1:G:147:PHE:O	1:G:492:VAL:HA	2.12	0.49
1:G:186:TRP:CE3	1:G:480:ILE:HG23	2.47	0.49
1:G:447:ASN:HD21	1:G:449:VAL:CG1	2.19	0.49
1:A:119:GLU:HA	1:A:511:GLY:HA2	1.94	0.49
1:A:136:LEU:HD23	1:A:137:PRO:HD2	1.93	0.49
1:C:428:GLU:HG3	1:E:59:GLY:O	2.12	0.49
1:E:142:LEU:HA	1:E:498:ILE:O	2.13	0.49
1:E:152:ALA:HB3	1:E:155:LEU:HB3	1.94	0.49
1:E:165:ASN:HD21	1:E:497:GLY:HA2	1.74	0.49
1:E:215:ALA:HB3	1:E:221:THR:HB	1.93	0.49
1:E:459:GLY:O	1:E:481:VAL:HA	2.13	0.49
1:E:470:PRO:O	1:E:473:ASN:N	2.38	0.49
1:G:76:ASP:OD1	1:G:76:ASP:N	2.43	0.49
1:G:125:THR:O	1:G:125:THR:HG22	2.13	0.49
1:G:493:VAL:HG12	1:G:495:PHE:CE1	2.47	0.49
1:A:230:VAL:O	1:A:231:TYR:HB3	2.12	0.49
1:A:516:THR:CB	1:E:423:ASN:HB3	2.33	0.49
1:E:78:SER:O	1:E:81:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:GLY:O	1:G:63:MET:HE1	2.11	0.49
1:E:151:PRO:O	1:E:485:GLU:HB3	2.12	0.49
1:E:230:VAL:HG12	1:E:231:TYR:CD2	2.44	0.49
1:G:89:MET:HE1	1:G:544:GLN:H	1.76	0.49
2:H:564:LEU:H	2:H:564:LEU:CD2	2.14	0.49
2:H:564:LEU:O	2:H:565:ALA:C	2.55	0.49
1:A:87:LYS:HB3	1:A:231:TYR:CE2	2.48	0.49
1:A:443:TYR:CE2	1:C:113:ARG:HD3	2.48	0.49
1:C:106:LYS:HE2	1:C:528:THR:O	2.13	0.49
1:C:287:ASN:HA	1:C:363:THR:O	2.12	0.49
1:E:54:VAL:CG1	1:E:55:ALA:N	2.75	0.49
1:G:225:THR:HB	1:G:515:THR:O	2.13	0.49
1:G:281:ALA:O	1:G:284:GLN:HB2	2.13	0.49
1:A:160:LEU:HD12	1:A:160:LEU:N	2.26	0.49
1:A:298:PRO:HB2	1:A:398:VAL:CG2	2.43	0.49
1:C:306:LEU:HD13	1:C:311:GLY:CA	2.39	0.49
1:E:214:MET:HG3	1:G:521:THR:HG22	1.94	0.49
1:E:231:TYR:HA	1:E:488:PHE:CZ	2.48	0.49
1:E:413:PRO:O	1:E:414:ALA:C	2.54	0.49
1:E:485:GLU:HG3	1:E:488:PHE:H	1.78	0.49
1:G:86:TYR:O	1:G:87:LYS:C	2.55	0.49
1:G:153:PHE:O	1:G:208:LEU:HD12	2.13	0.49
1:A:128:CYS:SG	1:A:131:VAL:HG23	2.52	0.49
1:A:164:ASN:C	1:A:166:GLU:H	2.21	0.49
1:A:169:THR:CG2	1:A:172:THR:HG23	2.42	0.49
1:C:75:ILE:HD11	2:D:572:LEU:HG	1.94	0.49
1:C:259:GLN:HB2	1:E:455:GLU:HG2	1.95	0.49
1:C:312:GLY:CA	1:C:326:ASP:OD1	2.61	0.49
2:D:561:VAL:HA	2:D:564:LEU:CD2	2.42	0.49
1:E:248:TRP:HZ3	1:E:250:VAL:CG2	2.25	0.49
1:G:276:VAL:HG22	1:G:294:TRP:HD1	1.78	0.49
1:G:363:THR:CG2	1:G:364:ALA:H	2.21	0.49
1:G:499:SER:O	1:G:500:GLN:C	2.56	0.49
1:A:120:GLN:CD	1:A:208:LEU:HB3	2.38	0.49
1:A:148:ILE:HA	1:A:492:VAL:HG12	1.95	0.49
1:A:170:LEU:O	1:A:171:GLU:C	2.56	0.49
1:C:227:PHE:HA	1:C:514:GLY:HA2	1.95	0.49
1:C:545:MET:HE2	1:C:546:GLU:N	2.26	0.49
1:E:90:ASP:HB2	2:F:561:VAL:CB	2.37	0.49
1:E:107:VAL:HG22	1:E:230:VAL:HG13	1.95	0.49
1:E:175:THR:O	1:E:176:PHE:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:HIS:ND1	1:E:491:ALA:CB	2.76	0.49
1:E:295:SER:C	1:E:296:ILE:HG13	2.37	0.49
1:G:88:TYR:CE1	1:G:544:GLN:NE2	2.80	0.49
1:G:154:ARG:HA	1:G:211:THR:HG22	1.95	0.49
1:G:262:THR:CG2	1:G:263:ILE:N	2.75	0.49
1:A:341:ILE:C	1:A:342:LEU:HD23	2.38	0.49
1:A:370:SER:HB3	1:A:382:VAL:HG13	1.95	0.49
1:A:396:VAL:CG1	1:A:397:THR:N	2.75	0.49
1:A:485:GLU:CG	1:A:488:PHE:H	2.20	0.49
2:B:565:ALA:O	2:B:568:GLY:N	2.46	0.49
1:C:443:TYR:CD2	1:E:113:ARG:NH1	2.80	0.49
1:E:164:ASN:C	1:E:166:GLU:H	2.21	0.49
1:E:265:ALA:HB2	1:E:404:ALA:CB	2.37	0.49
1:E:297:THR:HA	1:E:478:ARG:HH21	1.77	0.49
1:E:449:VAL:HG12	1:E:450:PHE:N	2.27	0.49
1:E:520:SER:C	1:E:522:VAL:H	2.20	0.49
2:F:597:PRO:C	2:F:599:ILE:N	2.70	0.49
1:G:273:SER:HB2	1:G:393:ILE:HG22	1.93	0.49
1:G:296:ILE:N	1:G:296:ILE:HD12	2.27	0.49
1:A:106:LYS:HG3	1:A:117:ASP:CG	2.38	0.48
1:A:120:GLN:NE2	1:A:211:THR:H	2.11	0.48
1:C:87:LYS:O	1:C:89:MET:N	2.46	0.48
1:C:146:SER:CB	1:C:494:HIS:ND1	2.76	0.48
1:C:427:TYR:OH	1:G:121:ARG:HD2	2.13	0.48
1:E:194:TRP:HA	1:E:194:TRP:HE3	1.77	0.48
1:E:195:ALA:HB3	1:E:203:TYR:CE2	2.47	0.48
1:E:229:LYS:HB2	1:E:485:GLU:CG	2.38	0.48
1:E:380:VAL:CG1	1:E:381:ILE:N	2.76	0.48
1:G:113:ARG:O	1:G:528:THR:HA	2.12	0.48
1:G:248:TRP:NE1	1:G:429:GLN:CG	2.72	0.48
1:A:148:ILE:HG12	1:A:492:VAL:CG1	2.43	0.48
1:A:363:THR:OG1	1:A:366:THR:HG22	2.13	0.48
1:A:454:GLY:O	1:A:456:GLU:N	2.46	0.48
1:C:193:GLN:O	1:C:204:SER:HB3	2.13	0.48
1:C:241:PRO:O	1:C:244:ILE:N	2.47	0.48
1:C:385:VAL:HG22	1:C:392:SER:HB3	1.95	0.48
2:D:560:THR:O	2:D:564:LEU:HD22	2.13	0.48
1:E:178:GLN:HE22	1:E:391:VAL:H	1.60	0.48
1:E:253:HIS:NE2	1:E:441:VAL:O	2.46	0.48
1:G:189:LEU:C	1:G:191:THR:N	2.70	0.48
1:G:279:SER:OG	1:G:280:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:442:HIS:N	1:G:442:HIS:CD2	2.81	0.48
1:A:257:LYS:O	1:C:455:GLU:HB3	2.12	0.48
1:A:343:ALA:C	1:A:344:GLU:HG2	2.38	0.48
2:B:566:SER:O	2:B:570:GLY:N	2.42	0.48
1:C:84:TRP:O	1:C:85:PHE:C	2.57	0.48
1:C:262:THR:HB	1:E:262:THR:CG2	2.42	0.48
1:E:111:LEU:HD12	1:E:111:LEU:O	2.13	0.48
1:E:214:MET:HG3	1:G:521:THR:CG2	2.43	0.48
1:E:234:ILE:HG12	1:E:508:THR:HB	1.95	0.48
1:E:341:ILE:HA	1:E:397:THR:O	2.13	0.48
1:G:107:VAL:CG2	1:G:230:VAL:HG13	2.44	0.48
1:G:178:GLN:CD	1:G:182:ASN:ND2	2.71	0.48
1:G:343:ALA:HB2	1:G:396:VAL:HG13	1.94	0.48
1:G:407:ARG:HG3	1:G:460:GLY:C	2.38	0.48
1:G:543:LEU:O	1:G:544:GLN:C	2.56	0.48
1:A:297:THR:HB	1:A:298:PRO:HD3	1.94	0.48
1:A:366:THR:C	1:A:367:VAL:HG23	2.39	0.48
1:A:415:LEU:HD12	1:A:415:LEU:N	2.29	0.48
1:A:424:VAL:HG22	1:C:114:TYR:CZ	2.48	0.48
2:B:577:ALA:O	2:B:578:THR:C	2.54	0.48
1:C:90:ASP:C	1:C:92:ALA:H	2.21	0.48
1:C:90:ASP:OD1	1:C:93:GLY:N	2.37	0.48
1:C:245:ASP:O	1:C:246:GLN:C	2.56	0.48
1:C:299:LEU:HD23	1:C:321:PHE:HB3	1.94	0.48
1:C:436:GLY:N	1:C:554:ASP:OD1	2.46	0.48
1:G:143:TRP:CD1	1:G:143:TRP:N	2.79	0.48
2:H:561:VAL:C	2:H:563:ALA:N	2.70	0.48
1:E:329:VAL:HG13	1:E:359:MET:O	2.13	0.48
1:G:193:GLN:HG3	1:G:193:GLN:O	2.13	0.48
1:G:277:SER:CA	1:G:391:VAL:HG13	2.44	0.48
1:A:208:LEU:O	1:A:209:PRO:C	2.56	0.48
1:A:470:PRO:HB2	1:C:403:GLU:CB	2.44	0.48
2:D:561:VAL:CA	2:D:564:LEU:HD22	2.43	0.48
1:E:227:PHE:C	1:E:452:MET:HE2	2.38	0.48
1:E:274:MET:HG3	1:E:296:ILE:CG1	2.43	0.48
1:E:474:ALA:HB1	1:E:478:ARG:HD2	1.94	0.48
2:F:577:ALA:HA	2:F:582:ILE:HD11	1.94	0.48
1:G:78:SER:O	1:G:81:ALA:HB3	2.13	0.48
1:G:178:GLN:HG3	1:G:179:THR:N	2.29	0.48
1:G:230:VAL:O	1:G:231:TYR:HB3	2.13	0.48
1:G:253:HIS:CE1	1:G:442:HIS:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:HB3	1:A:209:PRO:HG3	1.96	0.48
1:A:213:ALA:O	1:A:215:ALA:N	2.47	0.48
2:B:582:ILE:O	2:B:583:LYS:C	2.56	0.48
1:C:170:LEU:O	1:C:171:GLU:C	2.57	0.48
1:C:285:PRO:O	1:C:287:ASN:N	2.43	0.48
1:C:448:PRO:HG3	1:E:449:VAL:HG12	1.94	0.48
1:G:81:ALA:O	1:G:84:TRP:N	2.46	0.48
1:G:316:THR:HG21	1:G:322:SER:CB	2.44	0.48
1:A:180:LEU:O	1:A:479:GLY:HA2	2.13	0.48
1:A:375:LEU:HD12	1:A:376:THR:N	2.29	0.48
1:C:81:ALA:O	1:C:82:VAL:C	2.57	0.48
1:C:136:LEU:HD12	1:C:136:LEU:C	2.39	0.48
1:C:233:GLY:HA2	1:C:440:ILE:O	2.13	0.48
1:C:544:GLN:O	1:C:545:MET:C	2.57	0.48
1:E:87:LYS:HG3	1:E:104:PHE:HB2	1.95	0.48
1:G:108:PRO:HB2	1:G:533:GLU:HB2	1.96	0.48
1:G:146:SER:HB3	1:G:494:HIS:ND1	2.28	0.48
1:G:181:ASN:C	1:G:407:ARG:NH2	2.69	0.48
1:G:181:ASN:N	1:G:181:ASN:OD1	2.47	0.48
1:A:232:LYS:HG3	1:A:510:ASP:HB2	1.96	0.48
1:A:238:PHE:CD1	1:A:432:CYS:HB3	2.47	0.48
1:A:240:ALA:O	1:A:241:PRO:C	2.57	0.48
1:A:267:GLU:HG2	1:E:475:LEU:CG	2.44	0.48
1:E:187:ARG:HG3	1:E:212:TYR:HE1	1.79	0.48
2:F:564:LEU:O	2:F:567:ILE:CG2	2.51	0.48
1:A:533:GLU:HA	1:A:533:GLU:OE2	2.14	0.48
1:C:142:LEU:HD21	1:G:501:SER:O	2.14	0.48
1:C:172:THR:HG21	1:C:201:TRP:CE2	2.49	0.48
1:E:157:PHE:CE2	1:E:206:TYR:CD1	3.02	0.48
1:E:298:PRO:HG2	1:E:398:VAL:CG2	2.44	0.48
1:E:396:VAL:HG13	1:E:397:THR:H	1.79	0.48
1:E:470:PRO:C	1:E:472:ASN:N	2.70	0.48
2:F:561:VAL:O	2:F:564:LEU:HB3	2.12	0.48
1:G:251:GLY:O	1:G:550:VAL:HG21	2.13	0.48
1:G:341:ILE:HG23	1:G:396:VAL:HG11	1.96	0.48
1:G:543:LEU:O	1:G:547:LEU:CD2	2.62	0.48
1:A:113:ARG:CZ	1:E:443:TYR:CD2	2.97	0.47
1:A:126:ILE:HB	1:A:504:ILE:O	2.14	0.47
1:A:128:CYS:O	1:A:130:THR:N	2.47	0.47
1:A:171:GLU:O	1:A:172:THR:C	2.55	0.47
1:A:435:SER:C	1:A:437:GLY:H	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASN:O	1:A:474:ALA:O	2.31	0.47
1:C:74:SER:C	1:C:75:ILE:HG23	2.39	0.47
1:C:87:LYS:HE2	1:C:95:VAL:HG23	1.95	0.47
1:C:131:VAL:HG12	1:C:132:SER:N	2.29	0.47
1:C:238:PHE:HB2	1:C:437:GLY:HA2	1.95	0.47
1:C:545:MET:HE2	1:C:545:MET:O	2.14	0.47
1:E:92:ALA:HB3	1:E:439:TYR:CE1	2.48	0.47
1:E:120:GLN:O	1:E:122:PRO:HD2	2.13	0.47
1:E:157:PHE:N	1:E:157:PHE:CD2	2.82	0.47
1:E:447:ASN:ND2	1:E:449:VAL:H	2.12	0.47
2:F:596:ASN:CB	2:F:597:PRO:CD	2.92	0.47
1:G:142:LEU:HB2	1:G:498:ILE:O	2.14	0.47
1:G:249:TRP:CD2	1:G:438:ALA:HB2	2.49	0.47
1:G:289:VAL:HA	1:G:327:GLY:O	2.14	0.47
1:G:381:ILE:HG23	1:G:383:ARG:NH2	2.27	0.47
2:H:578:THR:CG2	2:H:581:VAL:HG23	2.44	0.47
1:A:251:GLY:O	1:A:550:VAL:HG21	2.13	0.47
1:A:449:VAL:HG23	1:C:449:VAL:HG11	1.96	0.47
1:C:241:PRO:C	1:C:243:LEU:N	2.70	0.47
2:D:579:PRO:HG2	1:E:535:GLU:CD	2.38	0.47
1:E:93:GLY:C	1:E:97:SER:HB2	2.39	0.47
1:E:100:ALA:HB3	1:G:63:MET:HE3	1.96	0.47
1:E:109:ASP:O	1:E:110:GLY:C	2.56	0.47
1:E:313:THR:HB	1:E:325:ILE:HG22	1.96	0.47
1:E:522:VAL:O	1:E:524:GLN:N	2.47	0.47
1:G:290:ALA:HB2	1:G:387:LYS:CE	2.43	0.47
1:G:291:ARG:HD2	1:G:291:ARG:O	2.14	0.47
1:A:97:SER:C	1:A:99:LYS:N	2.73	0.47
1:A:244:ILE:CD1	1:A:501:SER:HB2	2.38	0.47
1:A:363:THR:CB	1:A:366:THR:H	2.26	0.47
1:A:537:VAL:O	1:A:538:GLN:C	2.57	0.47
1:C:187:ARG:C	1:C:189:LEU:N	2.71	0.47
1:C:226:GLN:OE1	1:C:452:MET:HE3	2.14	0.47
1:E:90:ASP:CG	2:F:561:VAL:HB	2.38	0.47
1:E:100:ALA:O	1:G:63:MET:HE3	2.14	0.47
1:E:194:TRP:CZ3	1:E:204:SER:N	2.82	0.47
1:E:266:ALA:CB	1:E:402:THR:HB	2.35	0.47
1:E:270:SER:OG	1:E:402:THR:OG1	2.30	0.47
1:E:297:THR:CG2	1:E:476:GLY:H	2.25	0.47
1:E:302:ALA:HB2	1:E:338:PRO:HG3	1.95	0.47
2:F:613:ARG:O	2:F:616:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:PRO:HG2	1:G:57:SER:N	2.27	0.47
1:G:485:GLU:HG3	1:G:487:ASN:H	1.80	0.47
1:A:230:VAL:HB	1:A:511:GLY:O	2.14	0.47
1:A:235:THR:HG21	1:A:507:LYS:HE2	1.95	0.47
1:A:252:ALA:HB2	1:A:427:TYR:CB	2.39	0.47
1:A:301:VAL:HA	1:A:320:PHE:O	2.15	0.47
1:C:255:PRO:HB2	1:E:226:GLN:OE1	2.14	0.47
1:E:185:ASN:O	1:E:188:ASP:OD1	2.32	0.47
1:E:230:VAL:O	1:E:231:TYR:HB3	2.15	0.47
1:E:343:ALA:O	1:E:344:GLU:C	2.58	0.47
1:G:75:ILE:HG22	1:G:535:GLU:HG2	1.96	0.47
1:G:116:VAL:HG22	1:G:526:ALA:HB2	1.97	0.47
1:G:153:PHE:HB2	1:G:227:PHE:CZ	2.50	0.47
1:G:460:GLY:O	1:G:461:PHE:C	2.57	0.47
1:G:533:GLU:O	1:G:537:VAL:HG23	2.14	0.47
1:A:443:TYR:OH	1:C:112:LEU:HA	2.14	0.47
1:A:482:ASP:CG	1:A:483:THR:H	2.22	0.47
1:A:495:PHE:CE1	1:A:504:ILE:HD13	2.49	0.47
1:C:82:VAL:O	1:C:83:GLY:C	2.56	0.47
1:C:162:ASN:OD1	1:C:166:GLU:O	2.32	0.47
1:C:365:ASP:O	1:C:386:THR:HA	2.15	0.47
1:C:503:THR:C	1:C:504:ILE:HD12	2.40	0.47
1:E:112:LEU:HD21	1:E:452:MET:SD	2.54	0.47
1:E:178:GLN:OE1	1:E:178:GLN:C	2.58	0.47
1:E:228:ARG:HG2	1:E:452:MET:HE1	1.96	0.47
1:E:278:ALA:HA	1:E:292:ILE:CG2	2.40	0.47
1:E:313:THR:CA	1:E:325:ILE:HG22	2.43	0.47
1:G:142:LEU:CD1	1:G:497:GLY:HA2	2.42	0.47
1:G:262:THR:HG22	1:G:263:ILE:N	2.28	0.47
1:A:121:ARG:N	1:A:122:PRO:CD	2.77	0.47
1:A:210:ASN:O	1:A:213:ALA:HB3	2.14	0.47
2:B:564:LEU:O	2:B:567:ILE:CG2	2.61	0.47
1:C:241:PRO:O	1:C:243:LEU:N	2.48	0.47
1:C:357:PHE:HD1	1:C:371:VAL:HG13	1.80	0.47
1:C:535:GLU:CD	1:C:535:GLU:N	2.71	0.47
1:E:105:SER:OG	1:E:117:ASP:OD2	2.28	0.47
1:E:198:ALA:HB1	1:E:199:PRO:CD	2.37	0.47
1:E:239:ASN:HB3	1:E:503:THR:HG23	1.95	0.47
1:E:450:PHE:N	1:E:450:PHE:CD2	2.82	0.47
1:E:453:THR:HG21	1:E:484:PHE:O	2.13	0.47
2:F:614:LEU:HD23	2:F:614:LEU:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:ASP:CA	1:G:532:GLU:HA	2.44	0.47
1:G:440:ILE:HG22	1:G:550:VAL:HG22	1.96	0.47
1:A:87:LYS:NZ	1:A:95:VAL:CG2	2.77	0.47
1:A:235:THR:CG2	1:A:507:LYS:HB3	2.44	0.47
1:A:280:ASN:H	1:A:387:LYS:HD3	1.78	0.47
1:A:424:VAL:CG1	1:A:427:TYR:HB3	2.44	0.47
1:C:108:PRO:HA	1:C:530:ALA:HB3	1.97	0.47
1:C:202:TYR:N	1:C:202:TYR:CD1	2.82	0.47
1:C:227:PHE:HA	1:C:513:GLU:O	2.14	0.47
1:C:232:LYS:HG2	1:C:442:HIS:CE1	2.50	0.47
1:C:292:ILE:HD11	1:C:325:ILE:HG13	1.97	0.47
1:C:303:THR:O	1:C:335:PHE:HB2	2.15	0.47
1:C:346:GLU:OE1	1:C:347:PRO:HD2	2.15	0.47
1:C:359:MET:HA	1:C:368:VAL:O	2.14	0.47
1:C:403:GLU:HG3	1:C:403:GLU:O	2.13	0.47
1:C:418:GLU:HG2	1:C:419:GLU:N	2.30	0.47
1:E:116:VAL:HB	1:E:526:ALA:HB2	1.97	0.47
1:E:134:SER:CB	1:E:139:ASP:HB2	2.44	0.47
1:E:162:ASN:OD1	1:E:166:GLU:HB2	2.15	0.47
1:E:162:ASN:HB2	1:E:201:TRP:CE2	2.50	0.47
1:E:365:ASP:OD1	1:E:365:ASP:N	2.47	0.47
1:E:412:MET:HG2	1:E:463:PHE:HB3	1.97	0.47
1:E:534:ASP:HA	1:E:537:VAL:CG2	2.45	0.47
2:F:598:GLY:O	2:F:599:ILE:HG13	2.14	0.47
1:G:126:ILE:HG12	1:G:147:PHE:CE1	2.49	0.47
1:G:232:LYS:HA	1:G:509:TYR:O	2.15	0.47
1:G:265:ALA:HB2	1:G:404:ALA:N	2.29	0.47
1:G:297:THR:HG21	1:G:476:GLY:N	2.29	0.47
1:G:306:LEU:HD12	1:G:332:VAL:O	2.15	0.47
1:A:307:THR:N	1:A:332:VAL:O	2.40	0.47
1:A:360:THR:HB	1:A:368:VAL:HB	1.95	0.47
1:C:198:ALA:O	1:C:199:PRO:C	2.58	0.47
1:C:287:ASN:HA	1:C:363:THR:C	2.39	0.47
1:G:297:THR:HG22	1:G:298:PRO:CD	2.45	0.47
1:G:350:GLU:HG3	1:G:353:ASP:OD2	2.15	0.47
1:G:539:LEU:O	1:G:543:LEU:HB2	2.14	0.47
1:A:187:ARG:HD3	1:A:212:TYR:CE1	2.50	0.47
1:A:223:SER:O	1:A:516:THR:HG23	2.15	0.47
1:A:243:LEU:HD11	1:A:244:ILE:HG23	1.96	0.47
1:A:461:PHE:CE1	1:A:480:ILE:O	2.68	0.47
1:C:132:SER:C	1:C:134:SER:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:SER:N	1:C:297:THR:HB	2.23	0.47
1:E:95:VAL:O	1:G:47:GLN:HG3	2.15	0.47
1:E:180:LEU:H	1:E:180:LEU:HD12	1.80	0.47
1:E:181:ASN:OD1	1:E:462:GLN:HA	2.14	0.47
1:E:304:VAL:HG21	1:E:323:VAL:HG22	1.97	0.47
1:E:542:ARG:O	1:E:543:LEU:C	2.57	0.47
1:G:95:VAL:HG22	1:G:96:GLU:N	2.30	0.47
1:G:544:GLN:O	1:G:545:MET:C	2.57	0.47
2:H:578:THR:O	2:H:582:ILE:HG13	2.15	0.47
1:A:150:PHE:C	1:A:152:ALA:H	2.22	0.47
1:C:447:ASN:C	1:C:449:VAL:N	2.73	0.47
1:C:475:LEU:HD21	1:E:267:GLU:CA	2.45	0.47
1:C:556:ASN:ND2	1:C:556:ASN:C	2.72	0.47
2:D:564:LEU:HD12	1:E:50:PRO:HG2	1.96	0.47
1:E:95:VAL:HG11	1:G:61:GLY:O	2.15	0.47
1:E:444:LYS:HD3	1:E:447:ASN:O	2.15	0.47
1:G:245:ASP:OD2	1:G:433:LYS:HG2	2.15	0.47
1:G:288:THR:HG22	1:G:288:THR:O	2.15	0.47
1:G:538:GLN:OE1	2:H:579:PRO:HA	2.15	0.47
1:A:329:VAL:HA	1:A:362:ILE:HD11	1.97	0.46
1:C:187:ARG:C	1:C:189:LEU:H	2.22	0.46
1:C:265:ALA:HB2	1:C:404:ALA:HB2	1.97	0.46
2:D:593:VAL:O	1:E:43:ILE:HA	2.15	0.46
1:E:82:VAL:O	1:E:83:GLY:C	2.57	0.46
1:E:154:ARG:NH1	1:E:482:ASP:OD2	2.48	0.46
1:E:445:MET:HE2	1:E:489:SER:CB	2.45	0.46
1:E:548:THR:C	1:E:550:VAL:H	2.21	0.46
1:G:43:ILE:O	1:G:44:LEU:HD23	2.15	0.46
1:G:79:GLU:C	1:G:81:ALA:N	2.73	0.46
1:G:243:LEU:C	1:G:245:ASP:N	2.69	0.46
1:G:424:VAL:O	1:G:427:TYR:HD2	1.97	0.46
2:H:580:SER:O	2:H:581:VAL:C	2.58	0.46
1:A:113:ARG:NH1	1:E:544:GLN:O	2.48	0.46
1:A:181:ASN:OD1	1:A:463:PHE:N	2.49	0.46
1:A:403:GLU:OE1	1:A:405:VAL:HG23	2.15	0.46
1:A:405:VAL:CG1	1:A:477:LEU:HD13	2.45	0.46
1:A:455:GLU:HG3	1:E:259:GLN:CG	2.45	0.46
1:C:178:GLN:CB	1:C:472:ASN:ND2	2.78	0.46
1:C:400:ILE:CG2	1:C:401:ASP:N	2.78	0.46
2:D:565:ALA:C	2:D:567:ILE:N	2.71	0.46
1:E:416:THR:C	1:E:418:GLU:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:569:LEU:C	2:F:569:LEU:HD13	2.40	0.46
1:G:133:GLU:H	1:G:283:PHE:HE2	1.52	0.46
1:G:428:GLU:HB3	1:G:430:PHE:HE1	1.81	0.46
1:G:464:HIS:ND1	1:G:464:HIS:C	2.73	0.46
1:A:85:PHE:CD2	2:B:569:LEU:HD22	2.50	0.46
1:C:127:GLU:HA	1:C:503:THR:CG2	2.45	0.46
1:C:168:LEU:HD13	1:C:201:TRP:CH2	2.49	0.46
1:C:236:PHE:HD2	1:C:506:CYS:HG	1.61	0.46
1:C:278:ALA:O	1:C:387:LYS:HA	2.16	0.46
1:C:418:GLU:HG2	1:C:419:GLU:H	1.79	0.46
1:E:70:ILE:HG22	1:E:71:CYS:N	2.29	0.46
1:E:114:TYR:CD1	1:E:114:TYR:C	2.93	0.46
1:E:261:GLU:OE1	1:E:409:SER:CB	2.63	0.46
1:E:447:ASN:ND2	1:E:449:VAL:O	2.41	0.46
1:G:292:ILE:N	1:G:325:ILE:O	2.39	0.46
1:G:313:THR:HA	1:G:325:ILE:HA	1.97	0.46
1:A:180:LEU:HD23	1:A:183:ILE:HD11	1.97	0.46
1:A:195:ALA:HB3	1:A:203:TYR:CE2	2.50	0.46
1:C:84:TRP:NE1	1:C:230:VAL:CG1	2.77	0.46
1:C:450:PHE:C	1:C:451:GLU:O	2.57	0.46
1:E:99:LYS:O	1:E:101:LEU:CD2	2.63	0.46
1:E:272:GLY:C	1:E:475:LEU:HD12	2.41	0.46
1:E:323:VAL:HG12	1:E:325:ILE:HG23	1.98	0.46
1:E:369:TYR:O	1:E:382:VAL:HG13	2.15	0.46
1:E:391:VAL:HG12	1:E:392:SER:N	2.30	0.46
1:E:539:LEU:O	1:E:540:ALA:C	2.58	0.46
1:G:373:SER:C	1:G:375:LEU:N	2.71	0.46
1:A:249:TRP:CE2	1:A:438:ALA:HB2	2.50	0.46
1:A:369:TYR:H	1:A:369:TYR:HD2	1.63	0.46
1:C:176:PHE:O	1:C:177:ILE:C	2.59	0.46
2:D:576:SER:O	2:D:577:ALA:HB3	2.16	0.46
1:E:99:LYS:O	1:E:101:LEU:HD23	2.15	0.46
1:E:233:GLY:HA2	1:E:440:ILE:O	2.15	0.46
1:E:276:VAL:HG11	1:E:369:TYR:CD2	2.51	0.46
1:E:402:THR:O	1:E:402:THR:HG22	2.13	0.46
1:E:474:ALA:HB1	1:E:478:ARG:NH1	2.31	0.46
2:F:605:LYS:CG	2:F:610:VAL:CG2	2.94	0.46
1:G:84:TRP:O	1:G:87:LYS:N	2.49	0.46
1:G:110:GLY:H	1:G:531:GLU:C	2.24	0.46
1:G:248:TRP:HB2	1:G:431:LEU:HD23	1.97	0.46
1:A:128:CYS:HB3	1:A:131:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LEU:O	1:A:540:ALA:C	2.59	0.46
1:C:539:LEU:O	1:C:540:ALA:C	2.59	0.46
2:D:588:GLN:O	2:D:591:GLY:N	2.49	0.46
1:E:69:GLU:HB2	1:E:76:ASP:O	2.14	0.46
1:E:265:ALA:CA	1:E:404:ALA:HB2	2.46	0.46
1:E:445:MET:HE2	1:E:489:SER:OG	2.16	0.46
1:E:453:THR:HB	1:E:485:GLU:OE1	2.16	0.46
1:G:254:ILE:CD1	1:G:424:VAL:HG21	2.45	0.46
1:G:257:LYS:CE	1:G:446:ASN:HB3	2.46	0.46
1:G:380:VAL:CG1	1:G:381:ILE:N	2.78	0.46
1:A:257:LYS:HG3	1:C:226:GLN:HE21	1.81	0.46
1:A:539:LEU:HA	1:A:542:ARG:HB2	1.97	0.46
1:C:79:GLU:CB	1:C:101:LEU:HD13	2.46	0.46
1:C:275:THR:HB	1:C:391:VAL:CG1	2.35	0.46
1:C:553:ALA:C	1:C:555:ASP:N	2.73	0.46
1:E:43:ILE:HB	1:E:67:VAL:CB	2.41	0.46
1:E:54:VAL:HG12	1:E:55:ALA:N	2.31	0.46
1:E:124:VAL:HG11	1:E:206:TYR:CD2	2.51	0.46
1:E:145:VAL:HA	1:E:161:ALA:HA	1.97	0.46
1:E:393:ILE:HG22	1:E:394:THR:N	2.30	0.46
1:G:89:MET:CE	1:G:543:LEU:HB3	2.45	0.46
1:G:142:LEU:O	1:G:165:ASN:ND2	2.48	0.46
1:G:273:SER:HA	1:G:396:VAL:HG23	1.96	0.46
1:G:461:PHE:CE1	1:G:480:ILE:HB	2.50	0.46
1:G:534:ASP:HA	1:G:537:VAL:CG2	2.46	0.46
2:H:564:LEU:O	2:H:568:GLY:N	2.42	0.46
2:H:582:ILE:O	2:H:583:LYS:C	2.59	0.46
1:A:262:THR:H	1:C:262:THR:HG21	1.81	0.46
2:B:563:ALA:C	2:B:565:ALA:N	2.73	0.46
1:C:87:LYS:HE3	1:C:95:VAL:HG23	1.93	0.46
1:C:195:ALA:O	1:C:202:TYR:HA	2.16	0.46
1:C:205:ILE:CD1	1:C:480:ILE:HD11	2.46	0.46
1:C:257:LYS:HB2	1:E:456:GLU:OE2	2.16	0.46
1:E:70:ILE:O	1:E:76:ASP:HA	2.15	0.46
1:E:266:ALA:HB3	1:E:270:SER:OG	2.16	0.46
2:F:617:SER:O	2:F:619:LYS:N	2.49	0.46
1:G:277:SER:HB3	1:G:391:VAL:HG22	1.97	0.46
1:G:288:THR:O	1:G:289:VAL:HG23	2.15	0.46
1:G:325:ILE:HD12	1:G:333:TRP:CD2	2.51	0.46
1:A:264:PRO:HG2	1:C:264:PRO:CG	2.46	0.46
1:A:275:THR:HG23	1:A:478:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:CG2	1:A:342:LEU:N	2.79	0.46
1:C:75:ILE:HG21	1:C:535:GLU:HG3	1.96	0.46
1:E:274:MET:HB3	1:E:394:THR:HB	1.98	0.46
1:G:142:LEU:HD12	1:G:497:GLY:CA	2.43	0.46
1:G:159:ALA:CB	1:G:206:TYR:HE1	2.28	0.46
1:G:174:ASN:O	1:G:175:THR:C	2.59	0.46
1:G:291:ARG:HA	1:G:326:ASP:CA	2.46	0.46
1:G:360:THR:HB	1:G:368:VAL:CG1	2.45	0.46
1:G:449:VAL:HG13	1:G:450:PHE:N	2.30	0.46
1:G:537:VAL:O	1:G:538:GLN:C	2.59	0.46
2:H:566:SER:O	2:H:570:GLY:N	2.48	0.46
1:A:111:LEU:HD23	1:A:228:ARG:HH12	1.81	0.46
1:A:447:ASN:C	1:A:447:ASN:OD1	2.59	0.46
1:C:127:GLU:HB2	1:C:503:THR:HG21	1.98	0.46
1:C:229:LYS:HB2	1:C:485:GLU:HG3	1.98	0.46
1:C:500:GLN:OE1	1:C:500:GLN:HA	2.15	0.46
2:F:564:LEU:C	2:F:564:LEU:HD23	2.41	0.46
1:G:136:LEU:HD11	1:G:141:LYS:HB2	1.98	0.46
1:G:411:GLU:HG3	1:G:464:HIS:CG	2.51	0.46
1:G:428:GLU:HB2	1:G:550:VAL:HG12	1.97	0.46
1:A:114:TYR:HA	1:A:527:HIS:O	2.16	0.45
1:A:181:ASN:ND2	1:A:181:ASN:H	2.14	0.45
1:A:234:ILE:HG12	1:A:508:THR:CG2	2.22	0.45
1:A:306:LEU:HA	1:A:333:TRP:HA	1.97	0.45
1:A:485:GLU:C	1:A:487:ASN:N	2.74	0.45
1:A:485:GLU:OE1	1:A:487:ASN:HB2	2.16	0.45
1:C:429:GLN:HE22	1:E:58:GLY:C	2.24	0.45
1:E:85:PHE:CE2	2:F:565:ALA:HB1	2.51	0.45
1:E:148:ILE:HG23	1:E:413:PRO:HG3	1.98	0.45
1:E:197:PHE:CE1	1:E:198:ALA:HB2	2.51	0.45
1:G:145:VAL:O	1:G:145:VAL:HG13	2.15	0.45
1:G:173:ARG:NH2	1:G:466:PRO:O	2.49	0.45
1:G:229:LYS:HE3	1:G:510:ASP:OD2	2.16	0.45
1:G:342:LEU:HD23	1:G:347:PRO:HA	1.97	0.45
1:G:428:GLU:HB2	1:G:550:VAL:CG1	2.46	0.45
1:G:429:GLN:C	1:G:430:PHE:CD1	2.94	0.45
2:H:564:LEU:N	2:H:564:LEU:CD2	2.78	0.45
1:A:262:THR:HA	1:A:406:ASN:HB2	1.93	0.45
1:A:282:ILE:HD13	1:A:282:ILE:N	2.29	0.45
1:A:407:ARG:NE	1:A:460:GLY:O	2.49	0.45
2:B:588:GLN:O	2:B:590:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:TYR:O	1:C:88:TYR:CG	2.69	0.45
1:C:155:LEU:HD22	1:C:156:ASN:N	2.31	0.45
1:C:182:ASN:OD1	1:C:474:ALA:CB	2.64	0.45
1:C:363:THR:O	1:C:387:LYS:NZ	2.49	0.45
1:E:157:PHE:N	1:E:157:PHE:HD2	2.13	0.45
1:E:357:PHE:CE1	1:E:369:TYR:HB2	2.51	0.45
1:G:131:VAL:HG23	1:G:163:ILE:CD1	2.47	0.45
1:G:186:TRP:O	1:G:189:LEU:HD23	2.16	0.45
1:G:470:PRO:HA	1:G:473:ASN:OD1	2.15	0.45
2:H:571:LEU:N	2:H:571:LEU:HD23	2.32	0.45
1:A:145:VAL:CG1	1:A:498:ILE:HD12	2.45	0.45
1:A:238:PHE:CD2	1:A:432:CYS:HB3	2.50	0.45
1:A:455:GLU:C	1:E:259:GLN:HG2	2.42	0.45
1:C:228:ARG:O	1:C:228:ARG:HG3	2.17	0.45
1:C:241:PRO:O	1:C:242:THR:C	2.60	0.45
1:C:246:GLN:OE1	1:C:246:GLN:N	2.50	0.45
1:C:405:VAL:HG11	1:C:477:LEU:CD2	2.47	0.45
1:C:407:ARG:NE	1:C:462:GLN:HB2	2.32	0.45
1:C:544:GLN:O	1:C:546:GLU:N	2.50	0.45
1:E:147:PHE:N	1:E:147:PHE:CD1	2.83	0.45
1:E:148:ILE:N	1:E:148:ILE:CD1	2.80	0.45
1:E:543:LEU:O	1:E:547:LEU:N	2.47	0.45
2:F:557:PHE:O	2:F:558:ALA:C	2.57	0.45
1:G:79:GLU:C	1:G:81:ALA:H	2.25	0.45
1:G:185:ASN:CB	1:G:318:GLY:HA3	2.45	0.45
2:H:568:GLY:O	2:H:569:LEU:C	2.58	0.45
1:A:147:PHE:HE1	1:A:495:PHE:CD1	2.35	0.45
1:A:201:TRP:C	1:A:202:TYR:CD1	2.94	0.45
1:A:267:GLU:HB3	1:E:395:PRO:HB3	1.99	0.45
1:A:307:THR:HG22	1:A:308:THR:OG1	2.17	0.45
1:A:350:GLU:O	1:A:352:GLY:N	2.48	0.45
1:A:446:ASN:O	1:C:452:MET:HG3	2.16	0.45
1:C:435:SER:C	1:C:437:GLY:N	2.74	0.45
1:C:461:PHE:HD2	1:C:463:PHE:CZ	2.35	0.45
1:C:544:GLN:O	1:C:547:LEU:N	2.47	0.45
2:D:578:THR:HB	2:D:581:VAL:H	1.80	0.45
1:E:120:GLN:C	1:E:122:PRO:HD2	2.40	0.45
1:E:146:SER:O	1:E:159:ALA:HA	2.17	0.45
1:E:254:ILE:O	1:E:490:SER:HB3	2.16	0.45
1:E:552:GLN:C	1:E:554:ASP:N	2.74	0.45
1:G:110:GLY:H	1:G:532:GLU:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:LEU:C	1:G:165:ASN:ND2	2.75	0.45
1:G:386:THR:O	1:G:387:LYS:C	2.59	0.45
1:A:109:ASP:OD1	1:A:109:ASP:N	2.42	0.45
1:A:356:SER:O	1:A:371:VAL:HA	2.16	0.45
1:E:148:ILE:HG21	1:E:150:PHE:CZ	2.51	0.45
1:G:164:ASN:HD21	1:G:166:GLU:CD	2.25	0.45
1:G:191:THR:HG23	1:G:193:GLN:CG	2.43	0.45
1:A:181:ASN:ND2	1:A:181:ASN:N	2.64	0.45
1:A:255:PRO:HA	1:A:489:SER:HA	1.99	0.45
1:A:307:THR:HG22	1:A:308:THR:N	2.31	0.45
1:A:443:TYR:CE2	1:A:445:MET:HB2	2.52	0.45
1:A:545:MET:HE2	1:A:546:GLU:CA	2.47	0.45
1:A:549:GLY:HA3	1:C:113:ARG:HH21	1.74	0.45
2:B:565:ALA:O	2:B:566:SER:C	2.59	0.45
1:C:197:PHE:CZ	1:C:201:TRP:HB3	2.51	0.45
1:C:225:THR:HB	1:C:515:THR:OG1	2.17	0.45
1:C:259:GLN:HG2	1:E:406:ASN:ND2	2.32	0.45
1:C:484:PHE:O	1:C:486:ASN:N	2.50	0.45
2:D:574:LYS:HD2	2:D:574:LYS:H	1.80	0.45
1:E:173:ARG:HD3	1:E:465:TYR:CE2	2.51	0.45
1:E:275:THR:HG21	1:E:478:ARG:NH1	2.31	0.45
1:E:277:SER:OG	1:E:293:VAL:HB	2.16	0.45
1:E:534:ASP:OD1	1:E:534:ASP:N	2.48	0.45
1:G:176:PHE:CZ	1:G:180:LEU:HD11	2.52	0.45
1:G:297:THR:OG1	1:G:478:ARG:NH1	2.49	0.45
1:G:522:VAL:O	1:G:523:GLY:C	2.58	0.45
2:H:571:LEU:HD23	2:H:571:LEU:H	1.81	0.45
1:A:225:THR:CG2	1:A:517:ASN:HB2	2.29	0.45
1:A:407:ARG:NH2	1:A:462:GLN:HB3	2.31	0.45
1:A:448:PRO:HA	1:C:111:LEU:HD13	1.98	0.45
1:A:456:GLU:HG2	1:A:457:ASN:N	2.32	0.45
1:C:140:GLY:O	1:G:136:LEU:HD23	2.16	0.45
1:C:235:THR:HA	1:C:439:TYR:HA	1.99	0.45
1:E:286:SER:O	1:E:387:LYS:NZ	2.50	0.45
1:E:306:LEU:HD23	1:E:306:LEU:C	2.42	0.45
1:G:90:ASP:HB2	2:H:561:VAL:HB	1.99	0.45
1:G:151:PRO:HB3	1:G:488:PHE:HB2	1.99	0.45
2:H:557:PHE:CD1	2:H:558:ALA:N	2.84	0.45
1:A:143:TRP:NE1	1:A:500:GLN:HA	2.31	0.45
1:A:403:GLU:OE1	1:E:261:GLU:OE2	2.34	0.45
1:C:150:PHE:HE1	1:C:158:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:THR:O	1:C:395:PRO:C	2.57	0.45
1:C:410:ILE:HG22	1:C:411:GLU:O	2.17	0.45
1:C:537:VAL:HG12	1:C:541:ASN:OD1	2.17	0.45
1:E:105:SER:HA	1:E:231:TYR:HE2	1.82	0.45
1:E:445:MET:HE2	1:E:489:SER:HB2	1.98	0.45
1:E:463:PHE:N	1:E:463:PHE:CD1	2.85	0.45
2:H:578:THR:HG23	2:H:580:SER:H	1.82	0.45
1:A:117:ASP:HA	1:A:513:GLU:HA	1.98	0.45
1:A:248:TRP:HB3	1:A:431:LEU:HD22	1.98	0.45
1:A:320:PHE:CE2	1:A:477:LEU:HB3	2.52	0.45
1:A:322:SER:O	1:A:323:VAL:HG23	2.16	0.45
1:A:323:VAL:HG12	1:A:325:ILE:HG23	1.99	0.45
1:C:118:ALA:O	1:C:511:GLY:HA2	2.16	0.45
1:C:122:PRO:CG	1:C:209:PRO:HD2	2.47	0.45
1:C:210:ASN:O	1:C:213:ALA:HB3	2.16	0.45
1:C:285:PRO:CB	1:C:288:THR:HB	2.47	0.45
1:C:334:THR:HG22	1:C:356:SER:CB	2.47	0.45
1:C:400:ILE:N	1:C:400:ILE:CD1	2.75	0.45
1:C:439:TYR:CE1	1:C:441:VAL:HG22	2.52	0.45
2:D:588:GLN:C	2:D:591:GLY:H	2.25	0.45
1:E:77:PRO:HB2	1:E:82:VAL:HG22	1.99	0.45
1:E:272:GLY:HA2	1:E:297:THR:HG21	1.98	0.45
1:E:334:THR:O	1:E:335:PHE:HB3	2.16	0.45
1:E:411:GLU:HB2	1:E:464:HIS:NE2	2.31	0.45
2:F:576:SER:O	2:F:578:THR:N	2.50	0.45
1:G:109:ASP:HA	1:G:532:GLU:HG3	1.97	0.45
1:G:144:ARG:NH1	1:G:201:TRP:HH2	2.15	0.45
1:G:202:TYR:N	1:G:202:TYR:CD1	2.85	0.45
1:G:458:PHE:CD1	1:G:459:GLY:N	2.85	0.45
1:A:164:ASN:C	1:A:166:GLU:N	2.73	0.45
1:A:235:THR:HB	1:A:439:TYR:CD1	2.52	0.45
1:A:268:ARG:HB2	1:E:395:PRO:HB2	1.99	0.45
1:A:531:GLU:OE2	1:A:533:GLU:HG2	2.17	0.45
2:B:578:THR:HB	2:B:581:VAL:H	1.82	0.45
1:C:165:ASN:HB3	1:G:127:GLU:CD	2.42	0.45
1:C:175:THR:O	1:C:176:PHE:C	2.59	0.45
1:C:177:ILE:HG23	1:C:181:ASN:HD21	1.78	0.45
1:C:235:THR:HG21	1:C:556:ASN:CB	2.46	0.45
1:C:316:THR:OG1	1:C:317:SER:N	2.49	0.45
1:C:400:ILE:HG22	1:C:401:ASP:O	2.16	0.45
2:D:572:LEU:CA	2:D:575:SER:OG	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:GLU:HB3	1:E:503:THR:OG1	2.17	0.45
1:E:493:VAL:O	1:E:493:VAL:HG13	2.15	0.45
1:G:88:TYR:OH	1:G:443:TYR:HB2	2.17	0.45
1:G:113:ARG:O	1:G:529:GLY:N	2.49	0.45
1:G:436:GLY:N	1:G:554:ASP:OD2	2.50	0.45
1:A:202:TYR:CD1	1:A:202:TYR:N	2.85	0.44
1:A:235:THR:HA	1:A:439:TYR:HA	1.98	0.44
1:C:250:VAL:CB	1:C:429:GLN:HB3	2.44	0.44
1:E:87:LYS:O	1:E:91:PRO:CD	2.63	0.44
1:E:153:PHE:HB2	1:E:227:PHE:CZ	2.52	0.44
1:E:189:LEU:HB3	1:E:205:ILE:HD11	1.99	0.44
1:G:196:GLN:CG	1:G:197:PHE:N	2.80	0.44
1:G:207:VAL:O	1:G:209:PRO:HD3	2.16	0.44
1:G:274:MET:HA	1:G:295:SER:O	2.17	0.44
2:H:564:LEU:C	2:H:566:SER:N	2.73	0.44
1:A:276:VAL:CG1	1:A:294:TRP:HB2	2.46	0.44
1:A:499:SER:O	1:A:502:ALA:N	2.46	0.44
1:A:538:GLN:HE21	1:A:538:GLN:HA	1.83	0.44
2:B:581:VAL:O	2:B:582:ILE:C	2.60	0.44
1:C:236:PHE:O	1:C:237:GLU:C	2.61	0.44
1:E:186:TRP:O	1:E:187:ARG:C	2.59	0.44
1:E:412:MET:CE	1:E:415:LEU:HD21	2.47	0.44
1:G:443:TYR:O	1:G:444:LYS:C	2.60	0.44
1:A:426:LYS:HE2	1:C:528:THR:OG1	2.16	0.44
1:A:544:GLN:O	1:C:113:ARG:HD2	2.16	0.44
1:A:545:MET:C	1:A:547:LEU:N	2.75	0.44
1:A:550:VAL:O	1:A:551:TYR:CG	2.70	0.44
2:B:575:SER:O	2:B:576:SER:C	2.60	0.44
1:C:243:LEU:HG	1:C:244:ILE:HG23	2.00	0.44
2:D:594:GLN:CD	1:E:41:ALA:CB	2.87	0.44
1:E:106:LYS:NZ	1:E:117:ASP:OD1	2.44	0.44
1:E:210:ASN:OD1	1:G:520:SER:O	2.35	0.44
1:E:450:PHE:N	1:E:450:PHE:HD2	2.14	0.44
1:G:134:SER:O	1:G:135:ASP:O	2.35	0.44
1:G:162:ASN:HB2	1:G:201:TRP:CE3	2.51	0.44
1:G:186:TRP:CD1	1:G:481:VAL:HG23	2.52	0.44
1:G:381:ILE:HD13	1:G:394:THR:HG21	1.98	0.44
1:G:469:ASP:C	1:G:471:GLU:N	2.72	0.44
1:G:527:HIS:O	1:G:528:THR:O	2.35	0.44
1:A:178:GLN:HG3	1:A:472:ASN:HB3	1.99	0.44
1:A:302:ALA:HB3	1:A:321:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:MET:HE3	1:C:528:THR:CG2	2.48	0.44
1:C:88:TYR:HE1	1:C:443:TYR:HA	1.82	0.44
1:C:125:THR:CG2	1:C:505:VAL:HG13	2.48	0.44
1:G:103:GLU:HB3	1:G:117:ASP:OD1	2.18	0.44
1:G:105:SER:O	1:G:117:ASP:CB	2.66	0.44
1:G:203:TYR:CD1	1:G:204:SER:N	2.86	0.44
1:G:363:THR:CG2	1:G:364:ALA:N	2.75	0.44
1:G:481:VAL:O	1:G:482:ASP:CB	2.54	0.44
1:G:498:ILE:O	1:G:498:ILE:HG22	2.17	0.44
2:H:585:ILE:O	2:H:588:GLN:N	2.51	0.44
1:A:334:THR:HG21	1:A:354:THR:HG22	1.99	0.44
1:A:350:GLU:C	1:A:352:GLY:N	2.76	0.44
1:C:313:THR:HG22	1:C:314:ASN:N	2.32	0.44
1:E:109:ASP:O	1:E:111:LEU:N	2.50	0.44
1:E:160:LEU:O	1:E:160:LEU:HG	2.17	0.44
1:E:261:GLU:CD	5:E:557:HOH:O	2.61	0.44
1:G:527:HIS:ND1	1:G:527:HIS:N	2.66	0.44
1:A:198:ALA:HB1	1:A:199:PRO:CD	2.36	0.44
1:C:191:THR:O	1:C:191:THR:HG22	2.17	0.44
1:C:299:LEU:HD12	1:C:300:PRO:CD	2.47	0.44
1:C:300:PRO:HG3	1:C:400:ILE:HG12	1.99	0.44
1:C:369:TYR:C	1:C:369:TYR:HD1	2.26	0.44
1:C:421:THR:CG2	1:G:123:ILE:HD12	2.39	0.44
1:E:230:VAL:N	1:E:511:GLY:O	2.50	0.44
1:E:304:VAL:HG21	1:E:323:VAL:HG21	2.00	0.44
2:F:588:GLN:HG3	2:F:593:VAL:O	2.18	0.44
1:G:119:GLU:HG2	1:G:120:GLN:N	2.33	0.44
1:G:138:LEU:HD22	1:G:244:ILE:CD1	2.47	0.44
1:G:245:ASP:CG	1:G:433:LYS:HG2	2.42	0.44
1:G:265:ALA:HB1	1:G:402:THR:O	2.17	0.44
1:G:291:ARG:C	1:G:291:ARG:CD	2.90	0.44
1:G:420:VAL:O	1:G:421:THR:C	2.60	0.44
1:A:538:GLN:HG2	2:B:582:ILE:CD1	2.30	0.44
1:C:354:THR:N	1:C:374:SER:CB	2.80	0.44
1:C:407:ARG:HH11	1:C:407:ARG:HG3	1.83	0.44
1:E:126:ILE:N	1:E:126:ILE:CD1	2.80	0.44
2:F:613:ARG:NH1	3:R:4:U:C6	2.85	0.44
1:G:236:PHE:HB3	1:G:504:ILE:HG21	2.00	0.44
1:G:248:TRP:HD1	1:G:431:LEU:CD2	2.25	0.44
1:G:276:VAL:H	1:G:391:VAL:HG12	1.81	0.44
1:G:280:ASN:HB3	1:G:286:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:LEU:HD12	1:G:300:PRO:CD	2.48	0.44
1:G:522:VAL:O	1:G:524:GLN:N	2.50	0.44
1:G:547:LEU:N	1:G:547:LEU:CD2	2.81	0.44
2:H:561:VAL:C	2:H:563:ALA:H	2.24	0.44
1:A:110:GLY:HA3	1:A:532:GLU:N	2.33	0.44
1:A:156:ASN:N	1:A:206:TYR:O	2.50	0.44
1:A:419:GLU:O	1:A:423:ASN:N	2.51	0.44
1:C:359:MET:CE	1:C:367:VAL:HG11	2.48	0.44
2:D:563:ALA:C	2:D:565:ALA:N	2.75	0.44
2:D:565:ALA:O	2:D:568:GLY:N	2.51	0.44
1:G:143:TRP:NE1	1:G:498:ILE:HG22	2.32	0.44
1:G:197:PHE:CZ	1:G:201:TRP:HB3	2.53	0.44
1:G:244:ILE:C	1:G:246:GLN:H	2.25	0.44
1:G:341:ILE:HG23	1:G:396:VAL:CG1	2.48	0.44
1:G:407:ARG:CZ	1:G:478:ARG:O	2.66	0.44
1:G:408:LEU:HD21	1:G:458:PHE:O	2.17	0.44
1:G:440:ILE:HA	1:G:549:GLY:O	2.18	0.44
1:G:518:ALA:C	1:G:520:SER:N	2.76	0.44
1:A:297:THR:HG23	1:A:478:ARG:CZ	2.47	0.44
1:A:381:ILE:C	1:A:382:VAL:CG2	2.91	0.44
1:A:534:ASP:O	1:A:537:VAL:HG22	2.18	0.44
1:C:458:PHE:CD2	1:C:458:PHE:C	2.95	0.44
1:C:535:GLU:O	1:C:536:VAL:C	2.60	0.44
2:D:569:LEU:C	2:D:569:LEU:CD1	2.90	0.44
1:E:121:ARG:HA	1:E:508:THR:O	2.17	0.44
1:E:275:THR:HG22	1:E:478:ARG:HH12	1.82	0.44
1:E:407:ARG:NE	1:E:478:ARG:O	2.51	0.44
1:E:447:ASN:HD22	1:E:449:VAL:C	2.24	0.44
1:G:72:ALA:C	1:G:74:SER:N	2.76	0.44
1:G:160:LEU:HA	1:G:203:TYR:HA	2.00	0.44
1:A:225:THR:HB	1:E:255:PRO:O	2.18	0.43
2:B:579:PRO:HA	2:B:582:ILE:HD12	2.00	0.43
1:C:162:ASN:ND2	1:C:164:ASN:O	2.51	0.43
1:C:242:THR:HA	1:C:245:ASP:OD2	2.18	0.43
1:C:257:LYS:CB	1:E:456:GLU:OE2	2.66	0.43
1:C:337:ALA:O	1:C:351:GLU:O	2.35	0.43
1:C:356:SER:HG	1:C:372:SER:HB2	1.80	0.43
2:D:567:ILE:CG2	2:D:568:GLY:H	2.31	0.43
1:E:147:PHE:C	1:E:148:ILE:HD12	2.42	0.43
1:E:173:ARG:HG2	1:E:177:ILE:HD11	2.00	0.43
1:E:250:VAL:HG13	1:E:429:GLN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:LYS:HE3	1:G:117:ASP:CG	2.43	0.43
1:G:139:ASP:OD1	1:G:139:ASP:O	2.35	0.43
1:G:146:SER:OG	1:G:494:HIS:ND1	2.50	0.43
1:G:274:MET:CE	1:G:294:TRP:HE1	2.31	0.43
1:G:537:VAL:HG12	1:G:541:ASN:HD21	1.83	0.43
1:A:128:CYS:HA	1:A:143:TRP:CH2	2.53	0.43
1:A:259:GLN:CB	1:C:455:GLU:HG3	2.43	0.43
1:A:440:ILE:O	1:A:440:ILE:HG13	2.18	0.43
1:A:470:PRO:HB2	1:C:403:GLU:HB3	2.00	0.43
1:C:111:LEU:O	1:C:111:LEU:HG	2.18	0.43
1:C:510:ASP:C	1:C:510:ASP:OD1	2.60	0.43
1:E:77:PRO:HB2	1:E:82:VAL:CG2	2.47	0.43
1:E:184:THR:HG21	1:E:295:SER:OG	2.17	0.43
1:E:300:PRO:O	1:E:338:PRO:HG2	2.18	0.43
1:E:374:SER:O	1:E:375:LEU:C	2.61	0.43
2:F:588:GLN:O	2:F:591:GLY:N	2.51	0.43
1:G:240:ALA:HB1	1:G:241:PRO:HD2	2.00	0.43
1:G:307:THR:OG1	1:G:334:THR:HG22	2.19	0.43
1:G:545:MET:C	1:G:545:MET:SD	3.01	0.43
1:A:276:VAL:HG22	1:A:294:TRP:CB	2.46	0.43
1:A:344:GLU:C	1:A:346:GLU:N	2.76	0.43
1:A:427:TYR:CD1	1:A:427:TYR:C	2.95	0.43
2:B:564:LEU:CD1	2:B:589:ALA:O	2.66	0.43
1:C:126:ILE:N	1:C:126:ILE:CD1	2.81	0.43
1:C:140:GLY:HA3	1:G:138:LEU:CD2	2.47	0.43
1:C:167:ALA:O	1:C:201:TRP:HZ2	2.01	0.43
1:E:120:GLN:NE2	1:E:211:THR:HG23	2.34	0.43
1:E:248:TRP:CB	1:E:431:LEU:HA	2.48	0.43
1:E:364:ALA:O	1:E:387:LYS:HE3	2.18	0.43
2:F:563:ALA:O	2:F:566:SER:HB3	2.18	0.43
2:F:574:LYS:HG2	2:F:575:SER:N	2.33	0.43
1:G:146:SER:CB	1:G:494:HIS:ND1	2.82	0.43
1:G:248:TRP:CH2	1:G:250:VAL:HB	2.54	0.43
1:A:169:THR:HG23	1:A:172:THR:H	1.82	0.43
1:A:178:GLN:NE2	1:A:391:VAL:N	2.67	0.43
1:A:416:THR:C	1:A:418:GLU:N	2.76	0.43
1:A:495:PHE:CG	1:A:498:ILE:HD11	2.54	0.43
1:C:132:SER:C	1:C:134:SER:H	2.25	0.43
1:C:178:GLN:HB3	1:C:472:ASN:ND2	2.33	0.43
1:C:256:VAL:C	1:C:257:LYS:HG2	2.42	0.43
1:C:295:SER:HA	1:C:322:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:VAL:CB	1:C:400:ILE:HD13	2.43	0.43
1:E:253:HIS:HA	1:E:491:ALA:HB2	1.99	0.43
1:E:253:HIS:HB3	1:E:489:SER:OG	2.18	0.43
1:E:371:VAL:HB	1:E:381:ILE:HB	2.00	0.43
1:G:185:ASN:O	1:G:187:ARG:N	2.51	0.43
1:G:295:SER:C	1:G:296:ILE:HD12	2.43	0.43
1:A:97:SER:O	1:A:99:LYS:N	2.51	0.43
1:A:137:PRO:O	1:A:137:PRO:CG	2.65	0.43
1:A:183:ILE:HG22	1:A:186:TRP:HA	2.00	0.43
1:A:224:VAL:HG13	1:A:515:THR:O	2.18	0.43
1:A:227:PHE:CD1	1:A:228:ARG:N	2.86	0.43
2:B:578:THR:HG22	2:B:580:SER:H	1.83	0.43
1:C:153:PHE:CE2	1:C:211:THR:HG23	2.54	0.43
1:C:201:TRP:C	1:C:202:TYR:CD1	2.96	0.43
1:E:408:LEU:HD12	1:E:461:PHE:CE2	2.53	0.43
1:E:458:PHE:CD2	1:E:458:PHE:C	2.97	0.43
2:F:567:ILE:HG13	2:F:568:GLY:N	2.34	0.43
1:G:74:SER:C	1:G:75:ILE:CG2	2.91	0.43
1:G:224:VAL:CG1	1:G:225:THR:N	2.81	0.43
1:G:274:MET:HG3	1:G:274:MET:O	2.17	0.43
1:G:375:LEU:HD23	1:G:376:THR:O	2.19	0.43
1:G:554:ASP:O	1:G:555:ASP:OD2	2.37	0.43
1:A:111:LEU:HD13	1:E:448:PRO:HA	2.01	0.43
1:A:122:PRO:HB3	1:A:209:PRO:CG	2.49	0.43
1:A:156:ASN:OD1	1:A:156:ASN:C	2.60	0.43
1:A:253:HIS:CE1	1:A:491:ALA:HB2	2.54	0.43
1:A:407:ARG:O	1:A:408:LEU:HD23	2.19	0.43
1:A:532:GLU:HG2	1:E:542:ARG:NH2	2.34	0.43
1:A:538:GLN:OE1	1:A:542:ARG:NH1	2.47	0.43
1:C:75:ILE:HD12	1:C:535:GLU:HG3	2.00	0.43
1:C:254:ILE:CG2	1:E:225:THR:HG21	2.48	0.43
1:C:299:LEU:HA	1:C:300:PRO:HD3	1.92	0.43
1:C:431:LEU:HD23	1:C:431:LEU:HA	1.90	0.43
1:C:442:HIS:O	1:C:443:TYR:HB3	2.17	0.43
2:D:578:THR:HB	2:D:581:VAL:CG2	2.47	0.43
1:E:130:THR:OG1	1:E:163:ILE:HG12	2.18	0.43
1:E:396:VAL:HG12	1:E:397:THR:N	2.32	0.43
1:E:537:VAL:HG12	1:E:541:ASN:HD21	1.83	0.43
1:E:555:ASP:O	1:E:556:ASN:O	2.37	0.43
1:G:74:SER:O	1:G:75:ILE:HG23	2.19	0.43
1:G:122:PRO:HB3	1:G:209:PRO:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:GLN:HA	1:G:468:TYR:OH	2.17	0.43
1:E:249:TRP:HB3	1:E:495:PHE:CD2	2.54	0.43
1:E:291:ARG:HG2	1:E:291:ARG:O	2.18	0.43
1:G:142:LEU:HB3	1:G:499:SER:HA	2.01	0.43
1:G:217:ILE:HG23	1:G:319:LYS:HZ2	1.84	0.43
1:A:108:PRO:HG2	1:A:537:VAL:HG12	2.01	0.43
1:A:269:PHE:CE1	1:A:399:GLY:HA2	2.54	0.43
1:A:475:LEU:HD12	1:A:475:LEU:HA	1.76	0.43
1:C:144:ARG:O	1:C:161:ALA:HA	2.19	0.43
1:C:229:LYS:CB	1:C:485:GLU:HG3	2.49	0.43
1:C:234:ILE:HG22	1:C:508:THR:HB	2.00	0.43
1:C:246:GLN:HE22	1:C:499:SER:CB	2.31	0.43
1:C:356:SER:O	1:C:371:VAL:HA	2.19	0.43
1:E:174:ASN:OD1	1:E:468:TYR:HA	2.19	0.43
1:E:245:ASP:OD1	1:E:245:ASP:N	2.52	0.43
1:G:304:VAL:CG1	1:G:323:VAL:HG21	2.46	0.43
1:A:116:VAL:HG22	1:A:526:ALA:HB2	2.01	0.43
1:C:230:VAL:O	1:C:231:TYR:HB3	2.19	0.43
1:C:360:THR:HB	1:C:368:VAL:HG11	1.99	0.43
1:E:87:LYS:NZ	1:E:95:VAL:CG2	2.81	0.43
1:E:117:ASP:O	1:E:118:ALA:HB2	2.19	0.43
1:E:120:GLN:C	1:E:122:PRO:CD	2.91	0.43
1:E:248:TRP:CZ3	1:E:250:VAL:HG23	2.53	0.43
1:E:286:SER:C	1:E:364:ALA:HA	2.44	0.43
1:E:304:VAL:HA	1:E:334:THR:O	2.19	0.43
1:E:521:THR:C	1:G:210:ASN:OD1	2.62	0.43
1:G:48:LEU:HD22	1:G:54:VAL:HG21	2.01	0.43
1:G:130:THR:HG22	1:G:282:ILE:HG21	2.01	0.43
1:G:256:VAL:HG12	1:G:410:ILE:HG23	2.01	0.43
1:G:339:ALA:O	1:G:341:ILE:HG13	2.18	0.43
1:A:85:PHE:CE2	2:B:565:ALA:HB1	2.54	0.43
1:A:198:ALA:HB3	1:A:201:TRP:CB	2.35	0.43
1:A:256:VAL:HG22	1:C:225:THR:CG2	2.49	0.43
1:A:279:SER:OG	1:A:291:ARG:NH2	2.52	0.43
1:A:282:ILE:O	1:A:283:PHE:CB	2.66	0.43
1:A:435:SER:OG	1:A:552:GLN:HG2	2.19	0.43
1:C:148:ILE:N	1:C:148:ILE:CD1	2.79	0.43
1:C:215:ALA:O	1:C:216:GLU:C	2.62	0.43
1:C:291:ARG:NE	1:C:324:GLU:OE1	2.45	0.43
1:C:370:SER:HB2	1:C:381:ILE:O	2.19	0.43
1:E:79:GLU:HB3	1:E:101:LEU:CD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:SER:O	1:E:160:LEU:HD23	2.19	0.43
1:E:174:ASN:O	1:E:175:THR:C	2.59	0.43
1:E:212:TYR:C	1:E:214:MET:H	2.27	0.43
1:E:228:ARG:CB	1:E:452:MET:CE	2.92	0.43
1:G:522:VAL:O	1:G:525:PHE:N	2.48	0.43
1:G:533:GLU:C	1:G:535:GLU:N	2.75	0.43
1:A:152:ALA:HA	1:A:483:THR:O	2.19	0.42
1:A:398:VAL:HG12	1:A:399:GLY:N	2.34	0.42
1:A:456:GLU:HG2	1:A:457:ASN:H	1.83	0.42
2:B:588:GLN:C	2:B:590:VAL:H	2.26	0.42
1:C:82:VAL:HB	1:C:101:LEU:HD11	2.01	0.42
1:C:87:LYS:HE3	1:C:94:ALA:HB3	2.02	0.42
1:C:88:TYR:OH	1:C:443:TYR:HB2	2.19	0.42
1:C:142:LEU:O	1:C:143:TRP:CB	2.67	0.42
1:C:451:GLU:HG2	1:C:452:MET:H	1.83	0.42
2:D:580:SER:O	2:D:583:LYS:HB3	2.18	0.42
1:E:144:ARG:NH1	1:E:201:TRP:HH2	2.17	0.42
1:E:214:MET:HE2	1:G:521:THR:CB	2.42	0.42
1:E:507:LYS:HE3	1:G:57:SER:C	2.44	0.42
2:F:593:VAL:CG1	2:F:594:GLN:N	2.81	0.42
1:G:89:MET:HE2	1:G:543:LEU:HD23	2.01	0.42
1:G:292:ILE:HD13	1:G:325:ILE:O	2.19	0.42
1:G:292:ILE:HG12	1:G:325:ILE:CG1	2.49	0.42
1:G:539:LEU:O	1:G:543:LEU:N	2.52	0.42
2:H:582:ILE:O	2:H:585:ILE:HB	2.19	0.42
1:A:240:ALA:HB2	1:A:502:ALA:HB1	2.00	0.42
1:A:256:VAL:HG22	1:C:225:THR:HG21	2.00	0.42
1:A:359:MET:HE2	1:A:367:VAL:CG1	2.50	0.42
1:A:359:MET:HA	1:A:369:TYR:HA	2.02	0.42
1:A:375:LEU:CG	1:A:378:SER:HB3	2.49	0.42
1:A:485:GLU:HG3	1:A:487:ASN:H	1.83	0.42
1:C:492:VAL:CG1	1:C:494:HIS:NE2	2.81	0.42
1:E:281:ALA:HB1	1:E:284:GLN:CD	2.44	0.42
1:G:56:PRO:O	1:G:57:SER:C	2.62	0.42
1:G:87:LYS:HG3	1:G:104:PHE:CD1	2.53	0.42
2:H:588:GLN:C	2:H:590:VAL:N	2.73	0.42
1:A:121:ARG:HG2	1:A:509:TYR:CE2	2.54	0.42
1:A:143:TRP:HB2	1:A:162:ASN:O	2.19	0.42
1:A:205:ILE:C	1:A:206:TYR:CD1	2.96	0.42
1:A:231:TYR:C	1:A:231:TYR:HD1	2.27	0.42
1:A:405:VAL:HG12	1:A:477:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:PHE:HB2	1:C:197:PHE:CE1	2.53	0.42
1:E:116:VAL:HG22	1:G:525:PHE:HE2	1.85	0.42
1:E:207:VAL:HB	1:E:212:TYR:CB	2.48	0.42
1:E:267:GLU:O	1:E:401:ASP:OD2	2.37	0.42
1:E:471:GLU:HG3	1:E:472:ASN:N	2.34	0.42
1:E:480:ILE:HG22	1:E:481:VAL:N	2.34	0.42
1:G:155:LEU:HD12	1:G:156:ASN:H	1.85	0.42
1:G:274:MET:HA	1:G:296:ILE:HA	2.01	0.42
1:G:276:VAL:HG22	1:G:294:TRP:CD1	2.54	0.42
1:G:299:LEU:HA	1:G:300:PRO:HD3	1.83	0.42
1:G:442:HIS:CD2	1:G:442:HIS:H	2.37	0.42
1:A:435:SER:C	1:A:437:GLY:N	2.75	0.42
1:C:107:VAL:HG23	1:C:230:VAL:HG22	1.99	0.42
1:C:162:ASN:CG	1:C:164:ASN:O	2.63	0.42
1:E:60:ARG:NH2	1:E:64:ASP:OD1	2.52	0.42
1:E:64:ASP:O	1:E:65:PRO:C	2.63	0.42
1:E:177:ILE:C	1:E:179:THR:N	2.78	0.42
1:E:178:GLN:HE22	1:E:391:VAL:HG23	1.84	0.42
1:E:284:GLN:OE1	1:E:284:GLN:N	2.41	0.42
2:F:567:ILE:HD12	2:F:567:ILE:O	2.20	0.42
2:F:578:THR:C	2:F:580:SER:N	2.74	0.42
1:G:154:ARG:O	1:G:208:LEU:HG	2.19	0.42
2:H:569:LEU:O	2:H:570:GLY:C	2.61	0.42
1:A:114:TYR:HA	1:A:528:THR:HA	2.00	0.42
1:A:370:SER:CB	1:A:381:ILE:O	2.61	0.42
1:C:177:ILE:C	1:C:181:ASN:HD22	2.28	0.42
1:C:248:TRP:CE2	1:G:505:VAL:HG11	2.54	0.42
1:C:295:SER:C	1:C:296:ILE:HG13	2.44	0.42
1:C:375:LEU:CB	1:C:378:SER:HB3	2.42	0.42
1:E:160:LEU:N	1:E:160:LEU:CD2	2.82	0.42
1:E:178:GLN:CA	1:E:181:ASN:HD22	2.33	0.42
1:E:270:SER:CB	1:E:402:THR:OG1	2.68	0.42
1:E:400:ILE:O	1:E:400:ILE:HG23	2.19	0.42
1:G:176:PHE:HB2	1:G:197:PHE:HE1	1.83	0.42
1:G:178:GLN:NE2	1:G:182:ASN:ND2	2.67	0.42
1:G:196:GLN:HG2	1:G:197:PHE:N	2.34	0.42
1:G:299:LEU:HD13	1:G:341:ILE:HD11	2.00	0.42
1:A:89:MET:HE2	1:A:543:LEU:CD1	2.50	0.42
1:A:98:GLY:C	1:A:100:ALA:H	2.27	0.42
1:A:349:ALA:HA	1:A:353:ASP:OD2	2.19	0.42
1:A:485:GLU:HG2	1:A:488:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:GLY:O	2:B:560:THR:C	2.63	0.42
1:C:93:GLY:O	1:C:94:ALA:C	2.61	0.42
1:C:140:GLY:HA3	1:G:138:LEU:HD21	2.01	0.42
1:C:211:THR:HA	1:C:214:MET:SD	2.59	0.42
1:C:241:PRO:HG2	1:C:244:ILE:CG1	2.50	0.42
1:C:272:GLY:HA3	1:C:298:PRO:CG	2.49	0.42
1:C:326:ASP:O	1:C:333:TRP:HZ2	2.02	0.42
1:E:95:VAL:HG13	1:G:63:MET:CB	2.50	0.42
1:E:111:LEU:HD12	1:E:111:LEU:C	2.45	0.42
1:E:274:MET:CE	1:E:296:ILE:HD11	2.48	0.42
1:G:177:ILE:CD1	1:G:465:TYR:HB2	2.49	0.42
1:G:194:TRP:HE3	1:G:204:SER:HB2	1.80	0.42
1:G:224:VAL:CG1	1:G:225:THR:H	2.32	0.42
1:G:263:ILE:O	1:G:404:ALA:HA	2.19	0.42
1:G:453:THR:HG23	1:G:487:ASN:ND2	2.35	0.42
1:A:83:GLY:HA3	1:A:104:PHE:HB3	2.00	0.42
1:A:329:VAL:HG13	1:A:330:ASN:N	2.31	0.42
1:A:334:THR:CG2	1:A:354:THR:HG22	2.49	0.42
1:A:454:GLY:O	1:A:455:GLU:C	2.61	0.42
1:C:238:PHE:CD1	1:C:432:CYS:HB3	2.55	0.42
1:C:259:GLN:HG2	1:E:406:ASN:HD21	1.84	0.42
1:C:306:LEU:HD11	1:C:310:THR:O	2.20	0.42
1:C:548:THR:HB	1:C:550:VAL:CG2	2.50	0.42
1:E:106:LYS:HE3	1:E:115:SER:OG	2.20	0.42
1:E:274:MET:HE2	1:E:294:TRP:CE2	2.54	0.42
1:G:238:PHE:CE2	1:G:240:ALA:HB3	2.55	0.42
1:G:526:ALA:C	1:G:527:HIS:ND1	2.78	0.42
2:H:570:GLY:O	2:H:571:LEU:C	2.63	0.42
1:A:395:PRO:CB	1:C:268:ARG:HB2	2.50	0.42
1:A:552:GLN:O	1:A:553:ALA:C	2.62	0.42
1:C:141:LYS:NZ	1:G:133:GLU:O	2.53	0.42
1:C:254:ILE:O	1:C:490:SER:O	2.37	0.42
1:C:334:THR:HG22	1:C:356:SER:CA	2.49	0.42
1:E:180:LEU:HD12	1:E:180:LEU:N	2.35	0.42
1:E:424:VAL:HG12	1:E:427:TYR:HB3	2.01	0.42
1:E:524:GLN:HG3	1:E:525:PHE:CD1	2.54	0.42
2:F:583:LYS:O	2:F:587:GLN:HG3	2.19	0.42
1:G:134:SER:O	1:G:135:ASP:C	2.61	0.42
1:G:208:LEU:HA	1:G:209:PRO:HD2	1.68	0.42
1:G:538:GLN:O	1:G:539:LEU:C	2.62	0.42
2:H:562:SER:HA	2:H:565:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:O	1:A:89:MET:HG2	2.19	0.42
1:E:43:ILE:HG22	1:E:44:LEU:N	2.34	0.42
1:E:65:PRO:HA	1:E:66:PRO:HD2	1.74	0.42
1:E:111:LEU:HD23	1:E:228:ARG:NH2	2.35	0.42
1:E:134:SER:HB3	1:E:139:ASP:HB2	2.02	0.42
1:E:272:GLY:CA	1:E:298:PRO:HD3	2.50	0.42
1:E:274:MET:HE1	1:E:371:VAL:CG1	2.47	0.42
1:E:306:LEU:HD21	1:E:309:GLY:C	2.45	0.42
1:E:369:TYR:CD1	1:E:369:TYR:C	2.97	0.42
1:E:543:LEU:O	1:E:544:GLN:C	2.62	0.42
2:F:570:GLY:O	2:F:573:GLY:N	2.53	0.42
2:F:584:GLY:O	2:F:588:GLN:HB2	2.20	0.42
1:G:196:GLN:HB2	1:G:202:TYR:CD2	2.54	0.42
1:G:275:THR:C	1:G:276:VAL:CG2	2.92	0.42
1:G:307:THR:N	1:G:332:VAL:O	2.53	0.42
1:G:313:THR:HA	1:G:325:ILE:HG22	2.02	0.42
1:A:180:LEU:HA	1:A:183:ILE:HG13	2.01	0.42
1:A:185:ASN:O	1:A:187:ARG:N	2.53	0.42
1:A:239:ASN:OD1	1:A:503:THR:OG1	2.38	0.42
1:A:357:PHE:CE1	1:A:369:TYR:HB2	2.55	0.42
1:C:87:LYS:O	1:C:91:PRO:CD	2.63	0.42
1:C:313:THR:CG2	1:C:314:ASN:N	2.82	0.42
1:E:149:SER:OG	1:E:442:HIS:CE1	2.73	0.42
1:E:197:PHE:HD2	1:E:203:TYR:CD2	2.38	0.42
1:E:231:TYR:CD1	1:E:231:TYR:C	2.97	0.42
1:E:522:VAL:C	1:E:524:GLN:N	2.77	0.42
1:G:138:LEU:HD22	1:G:244:ILE:HD11	2.02	0.42
1:G:236:PHE:O	1:G:237:GLU:C	2.62	0.42
1:G:280:ASN:HD22	1:G:280:ASN:H	1.62	0.42
1:G:282:ILE:O	1:G:283:PHE:HB2	2.19	0.42
1:G:350:GLU:HG3	1:G:375:LEU:HD12	2.01	0.42
2:H:572:LEU:O	2:H:574:LYS:N	2.52	0.42
1:A:74:SER:O	1:A:75:ILE:CB	2.65	0.41
1:A:249:TRP:HB3	1:A:495:PHE:CD2	2.55	0.41
1:A:500:GLN:C	1:A:502:ALA:H	2.28	0.41
1:C:148:ILE:HG12	1:C:412:MET:CE	2.50	0.41
1:C:174:ASN:OD1	1:C:468:TYR:HA	2.19	0.41
1:C:297:THR:CB	1:C:298:PRO:CD	2.98	0.41
1:C:313:THR:OG1	1:C:333:TRP:CD1	2.73	0.41
1:C:499:SER:O	1:C:502:ALA:N	2.47	0.41
2:D:562:SER:O	2:D:565:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:ASN:C	1:E:214:MET:HE3	2.45	0.41
1:E:232:LYS:HG2	1:E:442:HIS:HD2	1.85	0.41
1:E:304:VAL:HG22	1:E:321:PHE:HE1	1.85	0.41
1:E:386:THR:O	1:E:387:LYS:C	2.61	0.41
1:G:92:ALA:C	1:G:95:VAL:HG13	2.43	0.41
1:G:143:TRP:CD1	1:G:498:ILE:HG22	2.54	0.41
1:G:162:ASN:HB2	1:G:201:TRP:CD2	2.55	0.41
1:G:231:TYR:CD1	1:G:231:TYR:C	2.98	0.41
1:G:444:LYS:O	1:G:444:LYS:CD	2.68	0.41
1:A:118:ALA:HB3	1:A:512:TRP:CE2	2.55	0.41
1:A:235:THR:HG23	1:A:507:LYS:CB	2.50	0.41
1:A:542:ARG:NE	2:B:583:LYS:HA	2.32	0.41
1:C:306:LEU:HA	1:C:333:TRP:HA	2.03	0.41
1:C:482:ASP:CG	1:C:483:THR:H	2.28	0.41
1:E:354:THR:H	1:E:374:SER:HG	1.59	0.41
1:E:393:ILE:HG22	1:E:395:PRO:HD3	2.01	0.41
1:G:208:LEU:O	1:G:210:ASN:N	2.52	0.41
1:G:243:LEU:O	1:G:245:ASP:OD1	2.38	0.41
1:G:292:ILE:CG1	1:G:325:ILE:HG13	2.50	0.41
1:G:444:LYS:O	1:G:444:LYS:HD3	2.20	0.41
1:G:552:GLN:C	1:G:554:ASP:N	2.78	0.41
1:A:193:GLN:HG2	1:A:194:TRP:O	2.20	0.41
1:A:230:VAL:O	1:A:231:TYR:CB	2.68	0.41
1:A:543:LEU:O	1:A:547:LEU:HB2	2.21	0.41
1:C:137:PRO:C	1:C:139:ASP:N	2.77	0.41
1:C:232:LYS:O	1:C:233:GLY:O	2.37	0.41
1:C:235:THR:HG22	1:C:439:TYR:CG	2.54	0.41
1:C:245:ASP:O	1:C:247:GLY:N	2.54	0.41
1:C:421:THR:HG21	1:G:123:ILE:CG1	2.49	0.41
1:C:448:PRO:CG	1:E:449:VAL:CG1	2.98	0.41
1:E:47:GLN:N	1:E:47:GLN:CD	2.77	0.41
1:E:90:ASP:HB2	2:F:561:VAL:CG1	2.51	0.41
1:E:217:ILE:HD13	1:E:217:ILE:H	1.85	0.41
1:E:276:VAL:HG11	1:E:369:TYR:CE2	2.55	0.41
1:E:522:VAL:O	1:E:525:PHE:N	2.50	0.41
1:G:47:GLN:CD	1:G:63:MET:HA	2.40	0.41
1:G:281:ALA:HB3	1:G:284:GLN:CG	2.29	0.41
1:A:131:VAL:CG2	1:A:500:GLN:HB3	2.49	0.41
1:A:248:TRP:CZ3	1:A:250:VAL:CG2	3.04	0.41
1:A:293:VAL:HG22	1:A:324:GLU:CG	2.51	0.41
1:A:532:GLU:HB3	1:E:542:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:564:LEU:C	2:B:567:ILE:CG2	2.93	0.41
2:B:583:LYS:HB3	2:B:583:LYS:HE2	1.89	0.41
1:C:107:VAL:O	1:C:530:ALA:HB3	2.21	0.41
1:C:405:VAL:HG13	1:C:406:ASN:N	2.35	0.41
1:C:418:GLU:O	1:C:419:GLU:C	2.62	0.41
1:C:428:GLU:HG3	1:E:59:GLY:C	2.45	0.41
1:C:450:PHE:O	1:C:451:GLU:O	2.39	0.41
1:E:444:LYS:HD3	1:E:448:PRO:C	2.45	0.41
1:G:170:LEU:HD23	1:G:170:LEU:C	2.45	0.41
1:G:533:GLU:C	1:G:537:VAL:HG23	2.44	0.41
1:A:113:ARG:NH2	1:E:443:TYR:HD2	2.17	0.41
1:A:158:ILE:HG22	1:A:159:ALA:N	2.35	0.41
1:A:178:GLN:O	1:A:182:ASN:ND2	2.54	0.41
1:A:289:VAL:HG13	1:A:327:GLY:CA	2.50	0.41
1:A:460:GLY:CA	1:A:481:VAL:HG22	2.50	0.41
1:C:106:LYS:HG3	1:C:117:ASP:CB	2.49	0.41
1:C:447:ASN:C	1:C:449:VAL:H	2.28	0.41
1:E:455:GLU:O	1:E:456:GLU:C	2.63	0.41
1:E:474:ALA:HB1	1:E:478:ARG:HH11	1.86	0.41
2:F:607:ILE:CA	2:F:610:VAL:HG23	2.49	0.41
2:F:614:LEU:HD23	2:F:617:SER:OG	2.21	0.41
1:G:84:TRP:NE1	1:G:230:VAL:HG12	2.35	0.41
1:G:133:GLU:N	1:G:283:PHE:CE2	2.66	0.41
1:G:150:PHE:O	1:G:152:ALA:N	2.48	0.41
1:G:366:THR:C	1:G:367:VAL:HG23	2.45	0.41
1:A:82:VAL:O	1:A:83:GLY:C	2.63	0.41
1:A:156:ASN:ND2	1:A:508:THR:HG21	2.36	0.41
1:A:299:LEU:HD11	1:A:338:PRO:HD2	2.02	0.41
1:A:369:TYR:OH	1:A:392:SER:HB3	2.20	0.41
1:C:250:VAL:CG2	1:C:429:GLN:HB3	2.50	0.41
1:C:286:SER:O	1:C:364:ALA:HA	2.21	0.41
2:D:565:ALA:O	2:D:567:ILE:N	2.54	0.41
1:E:149:SER:OG	1:E:442:HIS:NE2	2.43	0.41
1:E:195:ALA:O	1:E:203:TYR:CD2	2.73	0.41
1:E:534:ASP:HA	1:E:537:VAL:HB	2.02	0.41
1:E:554:ASP:O	2:F:557:PHE:N	2.54	0.41
1:G:201:TRP:C	1:G:202:TYR:CD1	2.98	0.41
1:G:237:GLU:HB2	1:G:507:LYS:HE3	2.01	0.41
1:G:332:VAL:CG2	1:G:358:SER:HB2	2.49	0.41
1:G:412:MET:SD	1:G:413:PRO:CD	3.04	0.41
1:A:182:ASN:OD1	1:A:474:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:HD11	1:E:465:TYR:O	2.21	0.41
1:A:334:THR:HG23	1:A:355:THR:O	2.21	0.41
1:A:348:PHE:CZ	1:A:372:SER:HA	2.55	0.41
1:A:410:ILE:O	1:A:463:PHE:HA	2.20	0.41
1:A:420:VAL:HG21	1:A:494:HIS:CD2	2.56	0.41
1:C:90:ASP:O	1:C:92:ALA:N	2.54	0.41
1:C:155:LEU:HD22	1:C:155:LEU:C	2.44	0.41
1:C:181:ASN:OD1	1:C:463:PHE:N	2.53	0.41
1:C:363:THR:CG2	1:C:365:ASP:H	2.12	0.41
1:C:363:THR:HG21	1:C:365:ASP:OD2	2.20	0.41
1:C:366:THR:HA	1:C:386:THR:HA	2.01	0.41
1:E:44:LEU:HD11	1:E:63:MET:CE	2.47	0.41
1:E:162:ASN:CG	1:E:164:ASN:O	2.64	0.41
1:E:250:VAL:CG1	1:E:427:TYR:CD2	3.03	0.41
1:E:253:HIS:HD2	1:E:549:GLY:CA	2.27	0.41
1:E:304:VAL:CG2	1:E:321:PHE:HE1	2.33	0.41
1:E:306:LEU:HD21	1:E:309:GLY:O	2.20	0.41
2:F:562:SER:O	2:F:566:SER:HB2	2.19	0.41
1:G:137:PRO:HG2	1:G:140:GLY:HA3	2.03	0.41
1:G:170:LEU:O	1:G:171:GLU:C	2.64	0.41
1:G:449:VAL:HG22	1:G:450:PHE:H	1.86	0.41
1:G:541:ASN:C	1:G:543:LEU:N	2.75	0.41
1:A:106:LYS:CG	1:A:117:ASP:HB3	2.50	0.41
1:A:162:ASN:HA	1:A:200:GLY:O	2.19	0.41
1:A:262:THR:HG22	1:A:263:ILE:N	2.36	0.41
1:A:267:GLU:HG2	1:E:475:LEU:HD11	2.03	0.41
1:A:422:THR:O	1:A:422:THR:CG2	2.67	0.41
1:A:522:VAL:O	1:A:523:GLY:C	2.64	0.41
1:C:177:ILE:O	1:C:181:ASN:ND2	2.48	0.41
1:C:194:TRP:CZ3	1:C:204:SER:OG	2.72	0.41
1:C:297:THR:CG2	1:C:298:PRO:HD3	2.50	0.41
1:C:362:ILE:O	1:C:362:ILE:CG2	2.69	0.41
1:C:413:PRO:HB2	1:C:492:VAL:CG2	2.50	0.41
1:C:446:ASN:ND2	1:E:226:GLN:OE1	2.54	0.41
1:C:453:THR:HG22	1:C:485:GLU:OE1	2.20	0.41
1:E:79:GLU:CB	1:E:101:LEU:HD12	2.44	0.41
1:E:84:TRP:O	1:E:85:PHE:C	2.62	0.41
1:E:296:ILE:HB	1:E:321:PHE:HD2	1.86	0.41
2:F:569:LEU:HD13	2:F:569:LEU:O	2.20	0.41
1:G:150:PHE:HB3	1:G:484:PHE:CE1	2.56	0.41
1:G:197:PHE:CG	1:G:198:ALA:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:TRP:CD1	1:G:431:LEU:CD2	2.97	0.41
1:G:249:TRP:NE1	1:G:430:PHE:HB2	2.35	0.41
1:G:400:ILE:HG12	1:G:401:ASP:N	2.35	0.41
1:G:537:VAL:HG12	1:G:541:ASN:ND2	2.36	0.41
1:G:552:GLN:O	1:G:554:ASP:N	2.49	0.41
1:A:151:PRO:HB2	1:A:485:GLU:CB	2.44	0.41
1:A:325:ILE:HB	1:A:333:TRP:CE2	2.56	0.41
1:A:359:MET:CE	1:A:367:VAL:HG11	2.51	0.41
1:A:425:PRO:HG3	1:C:526:ALA:O	2.21	0.41
1:A:436:GLY:N	1:A:554:ASP:OD1	2.54	0.41
1:A:550:VAL:C	1:A:551:TYR:CD1	2.99	0.41
2:B:582:ILE:O	2:B:585:ILE:HB	2.21	0.41
1:C:106:LYS:HA	1:C:513:GLU:CD	2.46	0.41
1:C:117:ASP:OD2	1:C:117:ASP:N	2.53	0.41
1:C:210:ASN:O	1:C:214:MET:HG3	2.20	0.41
1:C:266:ALA:HB3	1:C:270:SER:CB	2.47	0.41
1:C:297:THR:CG2	1:C:298:PRO:CD	2.97	0.41
1:C:342:LEU:HD23	1:C:347:PRO:HA	2.02	0.41
1:C:453:THR:CG2	1:C:485:GLU:OE1	2.68	0.41
1:C:469:ASP:OD2	1:C:471:GLU:CB	2.69	0.41
1:C:481:VAL:O	1:C:481:VAL:HG12	2.19	0.41
1:C:535:GLU:O	1:C:538:GLN:HB3	2.19	0.41
1:E:100:ALA:N	1:G:63:MET:HE3	2.36	0.41
1:E:116:VAL:HG22	1:E:117:ASP:N	2.36	0.41
1:E:182:ASN:O	1:E:478:ARG:HD3	2.21	0.41
1:E:235:THR:O	1:E:506:CYS:HA	2.21	0.41
1:E:460:GLY:HA2	1:E:480:ILE:O	2.20	0.41
1:E:466:PRO:C	1:E:468:TYR:N	2.77	0.41
1:E:528:THR:HG22	1:E:529:GLY:N	2.35	0.41
1:E:535:GLU:OE2	2:F:577:ALA:HB3	2.21	0.41
1:G:160:LEU:HD11	1:G:201:TRP:CZ3	2.56	0.41
1:G:263:ILE:O	1:G:263:ILE:HG22	2.20	0.41
1:A:178:GLN:HE22	1:A:390:GLY:HA2	1.84	0.41
1:A:248:TRP:NE1	1:A:496:TRP:CE3	2.85	0.41
1:A:267:GLU:HG2	1:E:475:LEU:HG	2.03	0.41
1:A:542:ARG:HD2	2:B:582:ILE:HG22	2.02	0.41
1:C:145:VAL:CG1	1:C:495:PHE:HB2	2.50	0.41
1:C:178:GLN:HB3	1:C:472:ASN:HD21	1.85	0.41
1:C:213:ALA:O	1:C:215:ALA:N	2.54	0.41
1:C:253:HIS:CE1	1:C:442:HIS:HA	2.56	0.41
1:C:296:ILE:HD12	1:C:299:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:MET:O	1:C:445:MET:CG	2.67	0.41
1:E:177:ILE:O	1:E:179:THR:N	2.54	0.41
1:E:522:VAL:O	1:E:523:GLY:C	2.62	0.41
1:G:87:LYS:HZ3	1:G:95:VAL:HG11	1.85	0.41
1:G:182:ASN:OD1	1:G:474:ALA:N	2.54	0.41
1:G:265:ALA:HB2	1:G:404:ALA:HB2	2.01	0.41
1:G:269:PHE:CB	1:G:397:THR:HG23	2.51	0.41
1:G:362:ILE:HG22	1:G:367:VAL:CG1	2.41	0.41
1:G:539:LEU:O	1:G:540:ALA:C	2.64	0.41
1:A:181:ASN:O	1:A:478:ARG:HB2	2.21	0.40
1:A:198:ALA:CB	1:A:199:PRO:HD2	2.33	0.40
1:A:473:ASN:C	1:A:474:ALA:O	2.63	0.40
1:A:486:ASN:O	1:A:486:ASN:CG	2.64	0.40
2:B:581:VAL:CG1	2:B:585:ILE:HD11	2.50	0.40
1:C:251:GLY:O	1:C:252:ALA:HB2	2.21	0.40
1:C:439:TYR:CD2	1:C:556:ASN:HA	2.55	0.40
2:F:596:ASN:C	2:F:598:GLY:N	2.79	0.40
1:G:121:ARG:HH11	1:G:121:ARG:CG	2.28	0.40
1:G:172:THR:HG21	1:G:201:TRP:CE2	2.57	0.40
1:G:174:ASN:ND2	1:G:468:TYR:HD1	2.12	0.40
1:G:183:ILE:HG21	1:G:186:TRP:HA	2.03	0.40
1:G:275:THR:HG23	1:G:478:ARG:NH1	2.36	0.40
1:G:453:THR:HG21	1:G:486:ASN:N	2.36	0.40
1:A:82:VAL:O	1:A:85:PHE:HB3	2.21	0.40
1:A:148:ILE:HG23	1:A:492:VAL:HG12	2.02	0.40
1:A:255:PRO:HB3	1:A:445:MET:SD	2.61	0.40
1:A:412:MET:HG2	1:A:463:PHE:CB	2.50	0.40
1:A:412:MET:HA	1:A:413:PRO:HD2	1.81	0.40
1:A:548:THR:C	1:A:550:VAL:H	2.29	0.40
1:C:101:LEU:HD12	1:C:101:LEU:O	2.22	0.40
1:E:40:GLN:N	1:E:71:CYS:HB2	2.36	0.40
1:E:229:LYS:H	1:E:485:GLU:CD	2.29	0.40
1:E:275:THR:HG22	1:E:478:ARG:HH22	1.86	0.40
1:E:278:ALA:HB2	1:E:385:VAL:CG2	2.45	0.40
1:E:342:LEU:O	1:E:343:ALA:CB	2.68	0.40
2:F:605:LYS:HG2	2:F:610:VAL:HG21	2.03	0.40
1:G:380:VAL:HG12	1:G:381:ILE:N	2.36	0.40
1:G:420:VAL:O	1:G:422:THR:N	2.55	0.40
1:A:198:ALA:HB3	1:A:201:TRP:CD1	2.56	0.40
2:B:580:SER:HB2	1:C:75:ILE:HG22	2.03	0.40
1:C:164:ASN:HD21	1:C:200:GLY:HA3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:GLN:C	1:C:178:GLN:CD	2.90	0.40
1:C:209:PRO:HG2	1:C:210:ASN:OD1	2.21	0.40
1:C:277:SER:OG	1:C:293:VAL:HB	2.22	0.40
1:E:191:THR:OG1	1:E:193:GLN:HG2	2.21	0.40
1:E:210:ASN:C	1:E:213:ALA:H	2.28	0.40
1:E:272:GLY:HA2	1:E:297:THR:CG2	2.51	0.40
2:F:613:ARG:C	2:F:615:VAL:N	2.78	0.40
1:G:49:LEU:HB2	1:G:52:GLU:CG	2.45	0.40
1:G:156:ASN:HB2	1:G:208:LEU:CD2	2.49	0.40
1:G:158:ILE:HG22	1:G:159:ALA:O	2.22	0.40
1:G:185:ASN:HD21	1:G:320:PHE:H	1.70	0.40
1:G:185:ASN:HD21	1:G:320:PHE:HB2	1.86	0.40
1:G:282:ILE:HG22	1:G:283:PHE:CD1	2.57	0.40
1:G:299:LEU:HD23	1:G:321:PHE:CB	2.51	0.40
1:G:397:THR:O	1:G:397:THR:HG22	2.21	0.40
1:G:398:VAL:C	1:G:400:ILE:H	2.29	0.40
1:G:526:ALA:O	1:G:527:HIS:HB3	2.21	0.40
1:G:527:HIS:O	1:G:528:THR:C	2.64	0.40
1:G:542:ARG:HD3	2:H:583:LYS:HA	2.02	0.40
1:C:85:PHE:HE2	2:D:565:ALA:HB1	1.86	0.40
1:C:247:GLY:C	1:C:432:CYS:SG	3.03	0.40
1:C:370:SER:CB	1:C:381:ILE:O	2.70	0.40
1:E:169:THR:HB	1:E:172:THR:CB	2.49	0.40
1:E:412:MET:O	1:E:465:TYR:CE1	2.74	0.40
1:E:484:PHE:O	1:E:486:ASN:N	2.55	0.40
2:F:578:THR:O	2:F:580:SER:N	2.55	0.40
2:F:588:GLN:HG3	2:F:594:GLN:HB3	2.03	0.40
1:G:133:GLU:O	1:G:135:ASP:N	2.55	0.40
1:G:183:ILE:CG2	1:G:186:TRP:HA	2.50	0.40
1:G:408:LEU:HD11	1:G:458:PHE:C	2.46	0.40
1:A:261:GLU:CD	1:C:404:ALA:O	2.65	0.40
1:A:262:THR:HG23	1:A:406:ASN:HB3	2.03	0.40
1:A:335:PHE:CD1	1:A:335:PHE:C	2.99	0.40
1:A:445:MET:O	1:C:111:LEU:HD11	2.21	0.40
1:A:451:GLU:HG3	1:E:447:ASN:OD1	2.21	0.40
1:A:482:ASP:CG	1:A:483:THR:N	2.80	0.40
1:A:528:THR:OG1	1:E:426:LYS:NZ	2.54	0.40
1:C:421:THR:HB	1:G:121:ARG:O	2.21	0.40
1:C:510:ASP:OD1	1:C:511:GLY:N	2.55	0.40
2:D:594:GLN:CG	1:E:41:ALA:HB1	2.52	0.40
1:E:250:VAL:HG13	1:E:427:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:ILE:HD12	1:G:82:VAL:HG21	2.03	0.40
1:G:83:GLY:O	1:G:84:TRP:C	2.62	0.40
1:G:163:ILE:C	1:G:165:ASN:N	2.74	0.40
2:H:582:ILE:O	2:H:585:ILE:N	2.53	0.40
2:H:589:ALA:C	2:H:590:VAL:CG2	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/556 (87%)	357 (74%)	80 (17%)	45 (9%)	0	8
1	C	482/556 (87%)	358 (74%)	74 (15%)	50 (10%)	0	6
1	E	515/556 (93%)	379 (74%)	95 (18%)	41 (8%)	1	10
1	G	516/556 (93%)	373 (72%)	87 (17%)	56 (11%)	0	5
2	B	37/75 (49%)	21 (57%)	12 (32%)	4 (11%)	0	5
2	D	38/75 (51%)	30 (79%)	6 (16%)	2 (5%)	1	16
2	F	65/75 (87%)	47 (72%)	12 (18%)	6 (9%)	0	8
2	H	36/75 (48%)	16 (44%)	16 (44%)	4 (11%)	0	5
All	All	2171/2524 (86%)	1581 (73%)	382 (18%)	208 (10%)	0	7

All (208) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	PRO
1	A	297	THR
1	A	318	GLY
1	A	405	VAL
1	A	455	GLU

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Mol	Chain	Res	Type
1	A	474	ALA
1	C	209	PRO
1	C	260	SER
1	C	286	SER
1	C	351	GLU
1	C	486	ASN
1	C	536	VAL
1	E	223	SER
1	E	395	PRO
1	E	475	LEU
1	E	476	GLY
1	E	537	VAL
2	F	577	ALA
2	F	618	ILE
1	G	133	GLU
1	G	135	ASP
1	G	387	LYS
1	G	475	LEU
1	G	476	GLY
1	G	528	THR
1	A	129	PRO
1	A	214	MET
1	A	231	TYR
1	A	282	ILE
1	A	311	GLY
1	A	414	ALA
1	A	418	GLU
1	A	436	GLY
1	A	534	ASP
1	A	538	GLN
1	A	540	ALA
1	A	554	ASP
2	B	576	SER
2	B	582	ILE
1	C	143	TRP
1	C	176	PHE
1	C	177	ILE
1	C	210	ASN
1	C	218	GLY
1	C	225	THR
1	C	233	GLY
1	C	353	ASP

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Mol	Chain	Res	Type
1	C	436	GLY
1	C	444	LYS
1	C	451	GLU
1	C	485	GLU
1	C	523	GLY
1	E	66	PRO
1	E	110	GLY
1	E	132	SER
1	E	140	GLY
1	E	209	PRO
1	E	434	GLU
1	E	436	GLY
1	E	444	LYS
1	E	485	GLU
2	F	602	GLY
1	G	56	PRO
1	G	57	SER
1	G	110	GLY
1	G	126	ILE
1	G	289	VAL
1	G	329	VAL
1	G	420	VAL
1	G	421	THR
1	G	436	GLY
1	G	454	GLY
1	G	456	GLU
1	G	482	ASP
2	H	590	VAL
1	A	186	TRP
1	A	351	GLU
1	A	422	THR
1	A	446	ASN
1	A	456	GLU
1	A	545	MET
1	A	546	GLU
2	B	572	LEU
2	B	589	ALA
1	C	126	ILE
1	C	184	THR
1	C	214	MET
1	C	242	THR
1	C	250	VAL

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Mol	Chain	Res	Type
1	C	285	PRO
1	C	287	ASN
1	C	414	ALA
1	C	450	PHE
1	C	488	PHE
1	C	532	GLU
1	C	554	ASP
2	D	572	LEU
1	E	50	PRO
1	E	91	PRO
1	E	177	ILE
1	E	199	PRO
1	E	231	TYR
1	E	242	THR
1	E	316	THR
1	E	329	VAL
1	E	343	ALA
1	E	375	LEU
1	E	417	THR
1	E	455	GLU
1	E	519	GLY
1	E	523	GLY
1	E	534	ASP
2	F	620	ALA
1	G	85	PHE
1	G	160	LEU
1	G	182	ASN
1	G	186	TRP
1	G	197	PHE
1	G	209	PRO
1	G	231	TYR
1	G	244	ILE
1	G	285	PRO
1	G	286	SER
1	G	486	ASN
1	G	527	HIS
2	H	573	GLY
1	A	85	PHE
1	A	115	SER
1	A	170	LEU
1	A	177	ILE
1	A	178	GLN

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Mol	Chain	Res	Type
1	A	184	THR
1	A	210	ASN
1	A	264	PRO
1	A	486	ASN
1	C	88	TYR
1	C	91	PRO
1	C	231	TYR
1	C	252	ALA
1	C	305	ALA
1	C	425	PRO
1	C	501	SER
2	D	564	LEU
1	E	64	ASP
1	E	94	ALA
1	E	226	GLN
2	F	596	ASN
1	G	91	PRO
1	G	141	LYS
1	G	219	ASP
1	G	245	ASP
1	G	303	THR
1	G	443	TYR
1	G	544	GLN
2	H	577	ALA
1	A	75	ILE
1	A	134	SER
1	A	173	ARG
1	A	285	PRO
1	A	387	LYS
1	C	82	VAL
1	C	139	ASP
1	C	162	ASN
1	C	199	PRO
1	C	318	GLY
1	C	534	ASP
1	E	103	GLU
1	E	118	ALA
1	E	297	THR
1	E	451	GLU
1	E	536	VAL
1	E	553	ALA
1	G	73	GLN

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Mol	Chain	Res	Type
1	G	82	VAL
1	G	84	TRP
1	G	118	ALA
1	G	134	SER
1	G	164	ASN
1	G	165	ASN
1	G	217	ILE
1	G	297	THR
1	G	318	GLY
1	G	388	GLY
1	G	523	GLY
1	G	553	ALA
1	A	77	PRO
1	A	280	ASN
1	A	524	GLN
1	C	297	THR
2	F	558	ALA
1	G	334	THR
1	G	537	VAL
1	A	217	ILE
1	A	345	GLY
1	E	467	GLY
1	G	163	ILE
1	G	208	LEU
1	E	298	PRO
1	G	466	PRO
1	A	98	GLY
1	C	311	GLY
1	C	312	GLY
1	C	347	PRO
1	E	121	ARG
1	C	98	GLY
1	C	129	PRO
1	G	276	VAL
2	H	581	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/466 (86%)	331 (82%)	72 (18%)	2	12
1	C	403/466 (86%)	347 (86%)	56 (14%)	3	18
1	E	429/466 (92%)	379 (88%)	50 (12%)	5	22
1	G	430/466 (92%)	372 (86%)	58 (14%)	4	19
2	B	25/49 (51%)	20 (80%)	5 (20%)	1	8
2	D	26/49 (53%)	19 (73%)	7 (27%)	0	3
2	F	43/49 (88%)	31 (72%)	12 (28%)	0	2
2	H	25/49 (51%)	21 (84%)	4 (16%)	2	14
All	All	1784/2060 (87%)	1520 (85%)	264 (15%)	3	16

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	79	GLU
1	A	96	GLU
1	A	121	ARG
1	A	124	VAL
1	A	127	GLU
1	A	136	LEU
1	A	142	LEU
1	A	160	LEU
1	A	163	ILE
1	A	165	ASN
1	A	171	GLU
1	A	178	GLN
1	A	181	ASN
1	A	184	THR
1	A	191	THR
1	A	193	GLN
1	A	204	SER
1	A	207	VAL
1	A	210	ASN
1	A	216	GLU
1	A	221	THR
1	A	225	THR
1	A	228	ARG
1	A	230	VAL

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Mol	Chain	Res	Type
1	A	235	THR
1	A	243	LEU
1	A	244	ILE
1	A	246	GLN
1	A	258	PRO
1	A	261	GLU
1	A	264	PRO
1	A	282	ILE
1	A	284	GLN
1	A	289	VAL
1	A	292	ILE
1	A	294	TRP
1	A	295	SER
1	A	307	THR
1	A	310	THR
1	A	315	ASN
1	A	329	VAL
1	A	356	SER
1	A	366	THR
1	A	369	TYR
1	A	371	VAL
1	A	382	VAL
1	A	383	ARG
1	A	386	THR
1	A	401	ASP
1	A	402	THR
1	A	403	GLU
1	A	406	ASN
1	A	412	MET
1	A	417	THR
1	A	433	LYS
1	A	443	TYR
1	A	447	ASN
1	A	449	VAL
1	A	456	GLU
1	A	461	PHE
1	A	480	ILE
1	A	486	ASN
1	A	490	SER
1	A	508	THR
1	A	510	ASP
1	A	532	GLU

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Mol	Chain	Res	Type
1	A	534	ASP
1	A	539	LEU
1	A	548	THR
1	A	554	ASP
1	A	556	ASN
2	B	567	ILE
2	B	572	LEU
2	B	580	SER
2	B	581	VAL
2	B	590	VAL
1	C	75	ILE
1	C	76	ASP
1	C	79	GLU
1	C	96	GLU
1	C	101	LEU
1	C	113	ARG
1	C	121	ARG
1	C	124	VAL
1	C	127	GLU
1	C	136	LEU
1	C	155	LEU
1	C	156	ASN
1	C	160	LEU
1	C	165	ASN
1	C	171	GLU
1	C	178	GLN
1	C	189	LEU
1	C	204	SER
1	C	234	ILE
1	C	244	ILE
1	C	245	ASP
1	C	246	GLN
1	C	262	THR
1	C	263	ILE
1	C	267	GLU
1	C	288	THR
1	C	291	ARG
1	C	292	ILE
1	C	295	SER
1	C	315	ASN
1	C	316	THR
1	C	328	ASN

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Mol	Chain	Res	Type
1	C	336	THR
1	C	359	MET
1	C	361	THR
1	C	371	VAL
1	C	400	ILE
1	C	403	GLU
1	C	405	VAL
1	C	407	ARG
1	C	416	THR
1	C	453	THR
1	C	455	GLU
1	C	457	ASN
1	C	480	ILE
1	C	483	THR
1	C	485	GLU
1	C	501	SER
1	C	516	THR
1	C	525	PHE
1	C	532	GLU
1	C	535	GLU
1	C	545	MET
1	C	548	THR
1	C	550	VAL
1	C	556	ASN
2	D	557	PHE
2	D	564	LEU
2	D	571	LEU
2	D	574	LYS
2	D	582	ILE
2	D	593	VAL
2	D	594	GLN
1	E	48	LEU
1	E	76	ASP
1	E	121	ARG
1	E	124	VAL
1	E	131	VAL
1	E	136	LEU
1	E	157	PHE
1	E	163	ILE
1	E	175	THR
1	E	178	GLN
1	E	189	LEU

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Mol	Chain	Res	Type
1	E	194	TRP
1	E	209	PRO
1	E	217	ILE
1	E	223	SER
1	E	237	GLU
1	E	243	LEU
1	E	245	ASP
1	E	246	GLN
1	E	255	PRO
1	E	259	GLN
1	E	275	THR
1	E	283	PHE
1	E	292	ILE
1	E	297	THR
1	E	313	THR
1	E	323	VAL
1	E	360	THR
1	E	361	THR
1	E	366	THR
1	E	374	SER
1	E	382	VAL
1	E	386	THR
1	E	394	THR
1	E	396	VAL
1	E	397	THR
1	E	412	MET
1	E	440	ILE
1	E	444	LYS
1	E	449	VAL
1	E	452	MET
1	E	462	GLN
1	E	494	HIS
1	E	508	THR
1	E	515	THR
1	E	533	GLU
1	E	547	LEU
1	E	548	THR
1	E	551	TYR
1	E	556	ASN
2	F	560	THR
2	F	564	LEU
2	F	567	ILE

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Mol	Chain	Res	Type
2	F	574	LYS
2	F	590	VAL
2	F	594	GLN
2	F	601	GLU
2	F	604	VAL
2	F	605	LYS
2	F	610	VAL
2	F	618	ILE
2	F	622	ARG
1	G	57	SER
1	G	63	MET
1	G	79	GLU
1	G	95	VAL
1	G	99	LYS
1	G	121	ARG
1	G	142	LEU
1	G	168	LEU
1	G	169	THR
1	G	177	ILE
1	G	178	GLN
1	G	188	ASP
1	G	189	LEU
1	G	191	THR
1	G	194	TRP
1	G	210	ASN
1	G	217	ILE
1	G	220	ARG
1	G	229	LYS
1	G	257	LYS
1	G	274	MET
1	G	280	ASN
1	G	292	ILE
1	G	301	VAL
1	G	308	THR
1	G	313	THR
1	G	315	ASN
1	G	329	VAL
1	G	355	THR
1	G	356	SER
1	G	360	THR
1	G	371	VAL
1	G	376	THR

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Mol	Chain	Res	Type
1	G	385	VAL
1	G	386	THR
1	G	396	VAL
1	G	397	THR
1	G	405	VAL
1	G	417	THR
1	G	419	GLU
1	G	444	LYS
1	G	446	ASN
1	G	456	GLU
1	G	458	PHE
1	G	464	HIS
1	G	486	ASN
1	G	498	ILE
1	G	500	GLN
1	G	508	THR
1	G	524	GLN
1	G	527	HIS
1	G	528	THR
1	G	533	GLU
1	G	536	VAL
1	G	544	GLN
1	G	545	MET
1	G	546	GLU
1	G	547	LEU
2	H	564	LEU
2	H	571	LEU
2	H	578	THR
2	H	590	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	193	GLN
1	A	314	ASN
1	A	429	GLN
1	A	472	ASN
1	C	181	ASN
1	C	447	ASN
1	C	462	GLN
1	C	464	HIS

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Mol	Chain	Res	Type
1	C	524	GLN
1	C	556	ASN
1	E	423	ASN
1	E	524	GLN
1	E	556	ASN
1	G	40	GLN
1	G	47	GLN
1	G	253	HIS
1	G	552	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	3/4 (75%)	3 (100%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	2	U
3	R	3	U
3	R	4	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/556 (87%)	-0.86	0 100 100	7, 20, 30, 48	0
1	C	484/556 (87%)	-0.88	0 100 100	8, 19, 30, 43	0
1	E	517/556 (92%)	-0.88	1 (0%) 91 81	7, 21, 33, 52	0
1	G	518/556 (93%)	-0.86	0 100 100	7, 20, 31, 53	0
2	B	39/75 (52%)	-0.53	0 100 100	10, 20, 36, 40	0
2	D	40/75 (53%)	-0.84	0 100 100	10, 21, 35, 40	0
2	F	67/75 (89%)	-0.81	0 100 100	13, 20, 35, 39	0
2	H	38/75 (50%)	-0.69	0 100 100	11, 18, 29, 38	0
3	R	4/4 (100%)	-0.43	0 100 100	54, 56, 57, 61	0
All	All	2191/2528 (86%)	-0.86	1 (0%) 100 100	7, 20, 32, 61	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	377	GLY	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	G	557	1/1	0.93	0.29	73,73,73,73	0
4	CA	A	557	1/1	0.99	0.05	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.