



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:11 PM BST

PDB ID : 5FJ7
EMDB ID: : EMD-3187
Title : Structure of the P2 polymerase inside in vitro assembled bacteriophage phi6 polymerase complex, with P1 included
Authors : Ilca, S.; Kotecha, A.; Sun, X.; Poranen, M.P.; Stuart, D.I.; Huiskonen, J.T.
Deposited on : 2015-10-06
Resolution : 7.90 Å(reported)
Based on PDB ID : 4K7H,1HHS

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

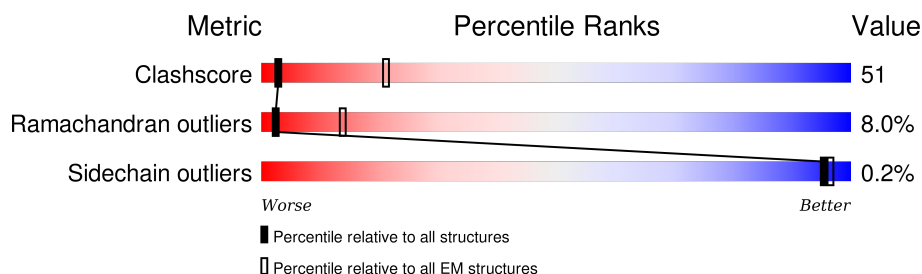
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	761	
1	B	761	
2	C	664	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MAJOR INNER PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		
1	B	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P11126
B	1	GLY	-	EXPRESSION TAG	UNP P11126

- Molecule 2 is a protein called RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	664	Total	C	N	O	S	0	0
			5265	3342	914	977	32		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	456	MET	ILE	CONFLICT	UNP P11124

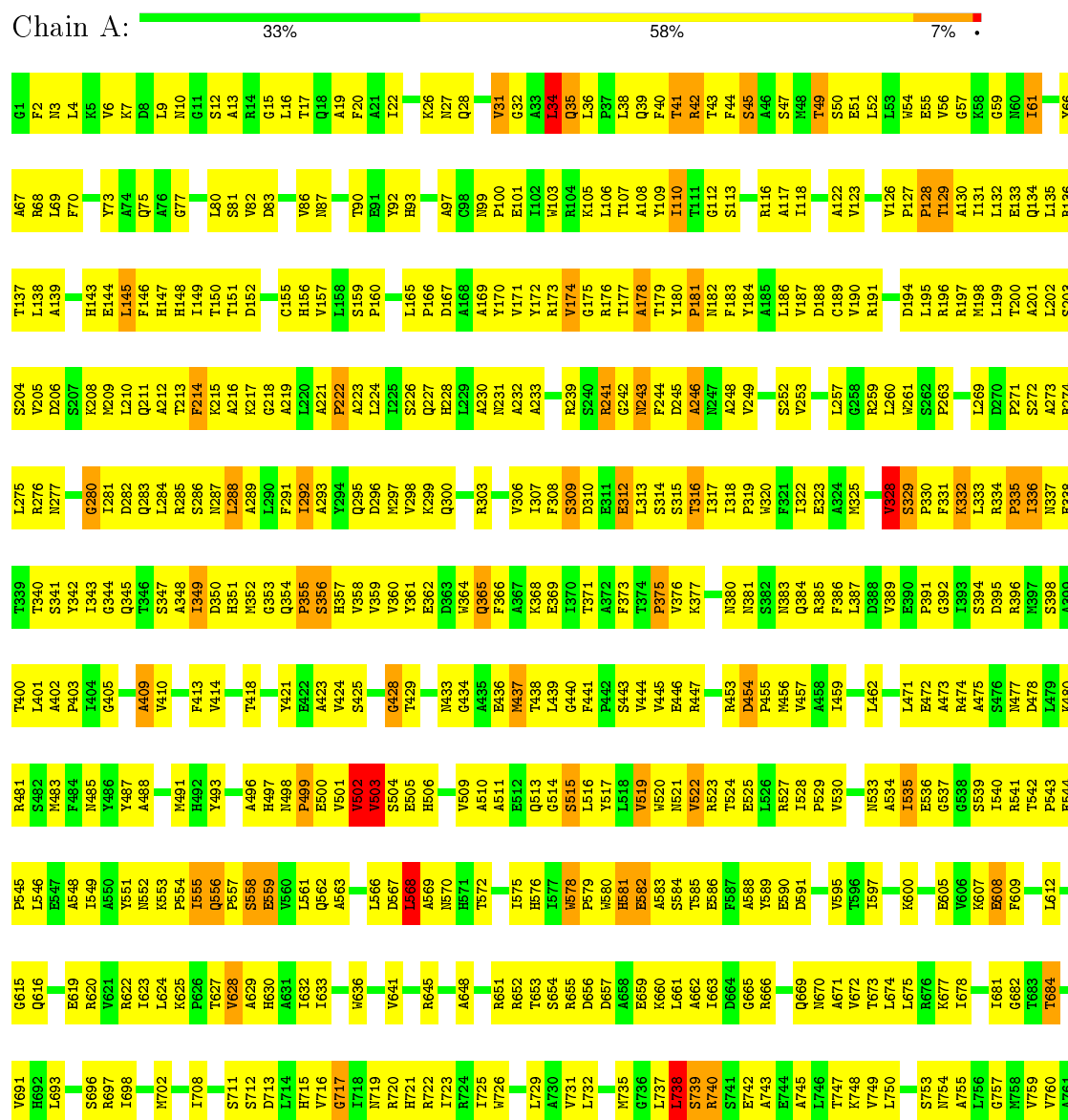
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Mn	0
			1	1	

3 Residue-property plots

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

• Molecule 1: MAJOR INNER PROTEIN P1



• Molecule 1: MAJOR INNER PROTEIN P1



L693	R620	L546	S482	L401	T340	I277	K208	E144	F70	G1
L694	R621	E547	N483	A402	S341	T278	M209	L145	F71	F2
L695	R622	E548	F484	P403	Y342	I279	L210	L146	Y73	N3
L696	R623	I549	N485	I404	I343	G280	Q211	H147	A74	L4
L697	R624	E550	Y486	G405	G344	I281	A212	H148	Q75	V5
L698	K625	Y551	Y487	A409	Q345	D282	T213	I149	A76	V6
L702	R626	N552	A488	A409	T346	Q283	F214	L150	G77	
L703	R627	K553	P554	V410	S347	I284	K215	T151		L9
L708	R628	P554	N491	F413	I349	R285	A216	D152	L80	N10
L711	R629	E555	Y492	V414	D350	I287	Q218	C155	S81	G11
L712	R630	Q556	Y493		R351	L288	A219	H156	V82	S12
L713	R631	P557		T418	H351	I289		D83	D83	A13
L714	R632	S558	A496		K352	A289	L220	V157		R14
L715	R633	E559	H497	Y421	G353	F291	A221	L158	V86	G15
L716	R634	E560	P499	A422	I354	L292	A223	S159		L16
L717	R635	A562	E501	A423	R357	A293	L224	P160	Y92	T17
L718	R636	A563	V501	V424	H357	I294	L225	L165	H93	A19
L719	R637	I566	V502	S425	V358	Q295	S226	P166	A97	F20
L720	R638	D567	V503	G428	V359	D296	Q227	C98	C98	A21
L721	R639	L568	S504	T429	V360	M297	E228	A169	I99	I22
L722	R640	A569	E505		Y361	V298	L229	E168	P100	
L723	R641	N570	H506		E362	K299	A230	V170	E101	K26
L724	R642	E571		N433	L663	Q300	M231	V171	I102	
L725	R643	T572	V509	G434	K364		A232	I172	H103	V31
L726	R644		A510	A435	Q365	R303	A233	H173	R104	G32
L729	R645	I575	A511	E436	F366			V174	K105	A33
L730	R646	H576	E512	M437	A367	V306	F237	G175	L106	L34
L731	R647	I577	Q513	T438	K368	I307	E238	R176	Q35	Q35
L732	R648	M578	Q514	L439	E369	F308	E239	T177	L107	
L733	R649	P579	S515	F440	I370	S309	S240	A178	A108	L36
L734	R650	N580	L516	G441	T371	D310	R241	T179	I110	P37
L735	R651	H581	V517	P442	A372	E311	G242	Y180	T111	Q39
L736	R652	E582	L518	S443	F373	E312	C243	N243	G112	F40
L737	R653	H583	Q519	V444	T374	L313	F244	N382	S113	T41
L738	R654	S584	H520	V445	P375	S314	D245	F133		R42
L739	R655	T585	N521	E446	V376	S315	A246	Y194	R116	T43
L740	R656	E586	V522	R447	K377	T316	N247	A185	A117	F44
L741	R657	F587	R523			I317	A248	L186	I118	S45
L742	R658	A588	T524	R453	N360	T318	V249	V187	A46	A46
L743	R659	Y589	E525	D454	N361	P319		D188	A122	S47
L744	R660	E590	V526	P455	S362	K320	S252	C189	V123	M48
L745	R661	D591	H527	L456	N363	F321	V253	V190	T49	
L746	R662	V595	L528	Q384	Q384	I322	L257	R191	V126	S50
L747	R663	T596	P529	L458	R385	E323	G258	A192	P127	E51
L748	R664	E596	V530	I459	F386	A324	R259	I194	P128	L52
L749	R665	I597		L462	L387	K325	L260	L195	T129	L53
L750	R666		N533		D388		L261	R196	A130	M54
L751	R667	K600	A534	L471	V389	V328	G261	I197	I131	E55
L754	R668	E605	L535	E472	E390	S329	S262	R197	L132	E56
L755	R669	V606	E536	A737	P391	P390	S263	M198	L133	G57
L756	R670	K607	G537	A738	G392	F331		L199	Q134	K58
L757	R671	E608	A538	R474	I393	K332	L269	T200	L135	G59
L758	R672	L609	S539	A475	S394	L333	D270	A201	R136	M60
L759	R673	F609	L540	S476	D395	R334	S271	L202	T137	I61
L760	R674	E610	H541	N477	R396	F335	S272	S203	L138	
L761	R675	L611	T542	D478	M397	L336	A273	S204	S141	Y66
L762	R676	L612	P543	L479	S398	R337	R274	V205	S141	A67
L763	R677		E544	K480	A399	E338	L275	D206	F142	R68
L764	R678		E545	R481	T200	F339	E276	E567	H143	L40

• Molecule 2: RNA-DIRECTED RNA POLYMERASE

Chain C:  23%  74%

P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	P15	P16	P17	P18	P19	P20	P21	P22	P23	P24	P25	P26	P27	P28	P29	P30	P31	P32	P33	P34	P35	P36	P37	P38	P39	P40	P41	P42	P43	P44	P45	P46	P47	P48	P49	P50	P51	P52	P53	P54	P55	P56	P57	P58	P59	P60	P61	P62	P63	P64	P65	P66	P67	P68	P69	P70	P71	P72	P73	P74	P75	P76	P77	P78	P79	P80	P81	P82	P83	P84	P85	P86	P87	P88	P89	P90	P91	P92	P93	P94	P95	P96	P97	P98	P99	1000
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K631	L502	Y439	L379	S318
W632	Y503	W440	G380	L319
E633	D604	Q441	D381	C320
E634	S505	G442	P382	V321
	R506	R443	S383	A322
V637	R507	E444	N384	T323
S638	E508	E445	P385	D324
A639	P509	I446	D386	V325
N640	G510	R447	L387	S326
I641	S511	Q448	E388	D327
H642	A512	I449	V389	H328
E643	I513	S450	G390	D329
V644	F514	K451	L391	T330
L645	V515	S452	S392	F331
M646	G516	D453	S393	W332
H647	N517	D454	G394	P333
G648	I518	A455	Q395	G334
V649	N519	N456	G396	V335
S650	S520	L457	A397	L336
V651	M521	G458	T398	R337
E652	L522	W459	D399	D338
	N523	T460	L400	L339
E655	N524	K461	M401	T340
R656	Q525	G462	G402	C341
F657	P526	R463	T403	D342
L658	S527	A464	L404	E343
R659	P528	L465	M405	L344
S660	E529	Y466	M406	L345
V661			S407	N346
M662	S534	H469	I408	N347
P663	G535	R470	T409	G348
R664	V536	L471	Y410	V349
	R537	F472	L411	A350
	D538		V412	P351
	R539	K476	M413	W352
	S540	E477	Q414	W353
	K541	G478	L415	V354
	R542	K479	D416	T355
	R543	Y480	H417	L356
	R544	N481	T418	P357
	P545	P482	A419	E358
	F546	S483	P420	T359
	P547	P484	H421	S360
	Q548	Y485	L422	L361
	L549	M486	M423	K362
	A550	K487	S424	L363
	W551	T488	R425	P364
	A552	S489	I426	V365
	S553	Y490	K427	Y366
	M554	E491	D428	V367
	K555	H492	M429	G368
	D556	G493	P430	A369
	T557	G494	S431	P370
	Y558	A495	A432	A371
	G559	F496	C433	
	A560	L497	R434	Q374
	C561	G498	F435	G375
	P562	D499	L436	H376
	I563	Y500	D437	T377
	Y564	L501	S438	L378

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.16	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	160000	Depositor
Image detector	GATAN K2 (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.43	0/6040	0.70	7/8206 (0.1%)
1	B	0.43	0/6040	0.70	7/8206 (0.1%)
2	C	1.17	7/5396 (0.1%)	0.66	2/7297 (0.0%)
All	All	0.74	7/17476 (0.0%)	0.69	16/23709 (0.1%)

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	5
1	B	0	5
2	C	0	1
All	All	0	11

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	361	LEU	CG-CD1	52.88	3.47	1.51
2	C	357	PHE	CD1-CE1	26.88	1.93	1.39
2	C	357	PHE	CD2-CE2	26.52	1.92	1.39
2	C	357	PHE	CE2-CZ	25.99	1.86	1.37
2	C	357	PHE	CE1-CZ	25.62	1.86	1.37
2	C	357	PHE	CG-CD2	17.79	1.65	1.38
2	C	357	PHE	CG-CD1	17.00	1.64	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	361	LEU	CB-CG-CD1	11.31	130.23	111.00
1	B	128	PRO	CA-C-N	6.76	132.06	117.20
1	A	128	PRO	CA-C-N	6.75	132.05	117.20
1	A	128	PRO	C-N-CA	6.09	136.93	121.70
1	B	128	PRO	C-N-CA	6.09	136.93	121.70
2	C	361	LEU	CB-CG-CD2	-5.94	100.91	111.00
1	A	568	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	568	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	502	VAL	C-N-CA	5.79	136.19	121.70
1	B	502	VAL	C-N-CA	5.79	136.18	121.70
1	B	128	PRO	N-CA-C	5.33	125.96	112.10
1	A	128	PRO	N-CA-C	5.33	125.94	112.10
1	A	738	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	738	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	128	PRO	CA-C-O	-5.17	107.80	120.20
1	B	128	PRO	CA-C-O	-5.15	107.84	120.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	VAL	Peptide
1	A	34	LEU	Peptide
1	A	35	GLN	Peptide
1	A	365	GLN	Peptide
1	A	437	MET	Peptide
1	B	328	VAL	Peptide
1	B	34	LEU	Peptide
1	B	35	GLN	Peptide
1	B	365	GLN	Peptide
1	B	437	MET	Peptide
2	C	203	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5920	0	5913	504	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5920	0	5907	641	0
2	C	5265	0	5154	718	0
3	C	1	0	0	0	0
All	All	17106	0	16974	1735	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 51.

All (1735) 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)
2:C:357:PHE:CZ	2:C:357:PHE:CE1	1.86	1.58
2:C:357:PHE:CE2	2:C:357:PHE:CD2	1.92	1.58
2:C:357:PHE:CE2	2:C:357:PHE:CZ	1.86	1.56
2:C:357:PHE:CD1	2:C:357:PHE:CE1	1.93	1.53
1:B:237:PHE:O	2:C:425:ARG:NH2	1.58	1.36
1:B:237:PHE:N	2:C:434:ARG:NH2	1.68	1.35
1:B:313:LEU:N	2:C:466:VAL:HG21	1.45	1.28
1:B:317:ILE:O	2:C:461:LYS:HD2	1.20	1.25
1:B:312:GLU:OE2	2:C:469:HIS:HB2	1.31	1.24
2:C:357:PHE:CD2	2:C:361:LEU:HG	1.75	1.22
1:B:312:GLU:CG	2:C:466:VAL:HG23	1.70	1.21
1:B:312:GLU:CG	2:C:466:VAL:CG2	2.20	1.20
2:C:357:PHE:CG	2:C:361:LEU:HG	1.76	1.20
1:B:237:PHE:N	2:C:434:ARG:HH22	0.93	1.19
1:B:316:THR:HG21	2:C:466:VAL:CA	1.72	1.18
1:B:312:GLU:HG2	2:C:466:VAL:CG2	1.73	1.16
1:B:312:GLU:OE1	2:C:470:ARG:HG3	1.44	1.15
1:B:316:THR:HG23	2:C:469:HIS:CD2	1.82	1.15
1:B:316:THR:O	2:C:465:LEU:HD23	1.48	1.14
1:B:319:PRO:C	2:C:461:LYS:NZ	2.00	1.14
1:B:316:THR:HG21	2:C:466:VAL:N	1.62	1.13
1:B:317:ILE:HD12	2:C:445:GLU:OE2	1.48	1.12
1:B:205:VAL:HG11	2:C:441:GLN:OE1	1.51	1.08
1:B:316:THR:HG23	2:C:469:HIS:NE2	1.68	1.08
1:B:205:VAL:HG13	2:C:441:GLN:CD	1.75	1.06
1:B:313:LEU:N	2:C:466:VAL:CG2	2.18	1.06
1:B:317:ILE:HB	2:C:465:LEU:HB3	1.37	1.04
1:B:317:ILE:HG13	2:C:461:LYS:HA	1.39	1.04
1:B:316:THR:O	2:C:465:LEU:CD2	2.04	1.04
2:C:357:PHE:CE2	2:C:361:LEU:CD1	2.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:H	2:C:466:VAL:CG2	1.71	1.03
1:B:205:VAL:CG1	2:C:441:GLN:CD	2.28	1.02
2:C:357:PHE:CE1	2:C:361:LEU:CD1	2.42	1.01
2:C:357:PHE:CD2	2:C:361:LEU:CD1	2.44	1.01
2:C:357:PHE:CD1	2:C:361:LEU:CD1	2.45	1.00
1:B:205:VAL:HG13	2:C:441:GLN:NE2	1.78	0.99
1:B:205:VAL:CG1	2:C:441:GLN:NE2	2.26	0.99
2:C:357:PHE:CZ	2:C:361:LEU:CD1	2.44	0.99
1:B:317:ILE:O	2:C:461:LYS:CD	2.12	0.96
1:B:317:ILE:CD1	2:C:445:GLU:OE2	2.13	0.96
1:B:237:PHE:H	2:C:434:ARG:NH2	1.45	0.95
1:B:117:ALA:H	1:B:221:ALA:H	1.10	0.95
1:B:237:PHE:C	2:C:425:ARG:NH2	2.12	0.95
1:B:312:GLU:CD	2:C:466:VAL:HG22	1.85	0.95
1:B:312:GLU:CG	2:C:466:VAL:HG22	1.97	0.94
2:C:555:LYS:HD2	2:C:559:GLY:HA3	1.50	0.94
2:C:357:PHE:CG	2:C:361:LEU:CD1	2.50	0.94
1:B:313:LEU:H	2:C:466:VAL:HG21	0.80	0.92
1:B:312:GLU:OE1	2:C:470:ARG:CG	2.18	0.91
2:C:357:PHE:CE2	2:C:361:LEU:CG	2.54	0.91
1:B:312:GLU:OE2	2:C:469:HIS:CB	2.19	0.91
1:B:312:GLU:HG2	2:C:466:VAL:HG23	0.92	0.91
1:B:312:GLU:CB	2:C:466:VAL:CG2	2.49	0.91
1:A:117:ALA:H	1:A:221:ALA:H	1.10	0.90
1:B:321:PHE:CB	2:C:461:LYS:HB3	2.00	0.90
2:C:357:PHE:CD2	2:C:361:LEU:CG	2.55	0.90
1:B:205:VAL:CG1	2:C:441:GLN:OE1	2.19	0.90
2:C:319:LEU:HB3	2:C:459:TRP:HB2	1.53	0.88
2:C:357:PHE:CZ	2:C:361:LEU:CG	2.57	0.88
1:B:316:THR:CG2	2:C:466:VAL:CA	2.54	0.86
2:C:18:PHE:HB3	2:C:24:ALA:HB1	1.57	0.86
2:C:357:PHE:CD1	2:C:361:LEU:CG	2.59	0.86
2:C:357:PHE:CE1	2:C:361:LEU:CG	2.59	0.86
1:B:321:PHE:CD1	2:C:461:LYS:HB3	2.11	0.85
1:B:322:ILE:H	2:C:461:LYS:HZ3	1.23	0.85
1:B:342:TYR:HA	1:B:559:GLU:HG3	1.57	0.85
2:C:60:TYR:O	2:C:64:HIS:ND1	2.08	0.84
1:A:342:TYR:HA	1:A:559:GLU:HG3	1.57	0.84
2:C:332:TRP:HH2	2:C:337:ARG:HB2	1.43	0.84
1:B:108:ALA:HA	1:B:112:GLY:HA3	1.59	0.84
1:B:322:ILE:N	2:C:461:LYS:NZ	2.22	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PHE:H	2:C:434:ARG:HH22	0.85	0.83
1:A:108:ALA:HA	1:A:112:GLY:HA3	1.59	0.83
1:B:316:THR:CG2	2:C:466:VAL:N	2.41	0.83
1:B:316:THR:HG21	2:C:466:VAL:HA	1.60	0.82
1:A:4:LEU:HG	1:A:436:GLU:HB2	1.60	0.82
2:C:554:MET:HG2	2:C:564:TYR:HE1	1.44	0.82
1:B:239:ARG:C	2:C:425:ARG:NH1	2.33	0.82
1:A:527:ARG:HG3	1:A:529:PRO:HD3	1.61	0.82
1:B:527:ARG:HG3	1:B:529:PRO:HD3	1.61	0.82
1:B:4:LEU:HG	1:B:436:GLU:HB2	1.60	0.82
1:A:502:VAL:HA	1:A:503:VAL:HG12	1.62	0.82
1:B:317:ILE:HG13	2:C:461:LYS:CA	2.08	0.82
1:B:316:THR:CG2	2:C:466:VAL:HA	2.09	0.81
1:B:715:HIS:HD2	1:B:716:VAL:HG22	1.43	0.81
1:A:715:HIS:HD2	1:A:716:VAL:HG22	1.44	0.81
2:C:357:PHE:CG	2:C:361:LEU:CG	2.62	0.81
1:B:312:GLU:HB3	2:C:466:VAL:CG2	2.08	0.81
1:B:16:LEU:HA	1:B:487:TYR:HE1	1.46	0.80
1:B:502:VAL:HA	1:B:503:VAL:HG12	1.62	0.80
1:A:582:GLU:O	1:A:625:LYS:NZ	2.15	0.80
1:B:582:GLU:O	1:B:625:LYS:NZ	2.15	0.80
1:A:44:PHE:HA	1:A:333:LEU:HA	1.64	0.80
1:A:173:ARG:HB2	1:A:579:PRO:HG2	1.64	0.80
2:C:206:GLN:HB3	2:C:268:ARG:HB3	1.63	0.80
1:B:651:ARG:HB2	1:B:663:ILE:HD11	1.63	0.80
2:C:357:PHE:CD2	2:C:361:LEU:HD12	2.17	0.79
2:C:83:ASN:HB2	2:C:85:PHE:HD2	1.46	0.79
1:A:651:ARG:HB2	1:A:663:ILE:HD11	1.63	0.79
2:C:627:LYS:O	2:C:631:LYS:N	2.15	0.79
1:B:316:THR:CG2	2:C:465:LEU:HG	2.13	0.79
1:B:436:GLU:OE2	1:B:439:LEU:N	2.12	0.79
1:B:319:PRO:C	2:C:461:LYS:HZ3	1.84	0.79
2:C:146:ARG:NH1	2:C:645:LEU:O	2.16	0.79
1:A:16:LEU:HA	1:A:487:TYR:HE1	1.46	0.79
2:C:357:PHE:CZ	2:C:361:LEU:HD13	2.16	0.78
2:C:226:MET:HB3	2:C:242:LEU:HG	1.64	0.78
1:B:528:ILE:HG12	1:B:536:GLU:HB3	1.65	0.78
2:C:109:ARG:O	2:C:114:LEU:N	2.15	0.78
2:C:466:VAL:HA	2:C:469:HIS:CD2	2.18	0.78
2:C:109:ARG:NH1	2:C:331:PHE:O	2.16	0.78
2:C:115:ALA:N	2:C:484:PRO:O	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ILE:HG12	1:A:536:GLU:HB3	1.65	0.78
1:B:44:PHE:HA	1:B:333:LEU:HA	1.64	0.78
1:A:436:GLU:OE2	1:A:439:LEU:N	2.12	0.78
1:A:197:ARG:HA	1:A:200:THR:HG22	1.66	0.78
2:C:357:PHE:CD1	2:C:361:LEU:HD11	2.17	0.78
1:B:117:ALA:N	1:B:221:ALA:H	1.81	0.78
1:B:316:THR:C	2:C:465:LEU:HD23	2.02	0.77
1:B:317:ILE:HD11	2:C:462:GLY:N	1.99	0.77
1:B:195:LEU:HA	1:B:198:MET:HB3	1.67	0.77
2:C:203:TYR:OH	2:C:269:ARG:NH2	2.17	0.77
1:B:173:ARG:HB2	1:B:579:PRO:HG2	1.64	0.77
1:B:322:ILE:N	2:C:461:LYS:HZ3	1.81	0.77
1:B:321:PHE:HD1	2:C:461:LYS:HB3	1.49	0.77
1:B:320:TRP:N	2:C:461:LYS:NZ	2.32	0.77
1:B:197:ARG:HA	1:B:200:THR:HG22	1.66	0.77
1:B:410:VAL:HA	1:B:413:PHE:HB3	1.67	0.77
2:C:187:ASP:HA	2:C:190:TYR:HB3	1.67	0.77
1:B:189:CYS:HB3	1:B:323:GLU:HG3	1.67	0.77
1:A:588:ALA:HB1	1:A:589:TYR:HB2	1.67	0.76
1:B:321:PHE:HB2	2:C:461:LYS:HB3	1.65	0.76
1:B:316:THR:CG2	2:C:469:HIS:CD2	2.64	0.76
2:C:395:GLN:HE21	2:C:397:ALA:HB3	1.50	0.76
2:C:105:ASN:O	2:C:109:ARG:N	2.19	0.76
1:A:195:LEU:HA	1:A:198:MET:HB3	1.67	0.76
1:B:581:HIS:O	1:B:583:ALA:N	2.17	0.76
1:A:200:THR:HA	1:A:203:SER:HB3	1.67	0.76
2:C:109:ARG:HG2	2:C:114:LEU:HD12	1.68	0.76
1:A:387:LEU:HG	1:A:572:THR:HG21	1.66	0.76
1:B:387:LEU:HG	1:B:572:THR:HG21	1.66	0.76
1:A:410:VAL:HA	1:A:413:PHE:HB3	1.66	0.76
1:A:480:LYS:HA	1:A:483:MET:HG2	1.68	0.76
2:C:446:ILE:HG22	2:C:459:TRP:HE1	1.51	0.76
2:C:55:ASN:HA	2:C:88:ARG:HH12	1.49	0.76
2:C:575:TRP:CG	2:C:583:TYR:HB2	2.20	0.76
1:A:208:LYS:O	1:A:211:GLN:NE2	2.19	0.76
1:A:176:ARG:HH12	1:A:447:ARG:HA	1.49	0.75
1:B:208:LYS:O	1:B:211:GLN:NE2	2.19	0.75
1:B:176:ARG:HH12	1:B:447:ARG:HA	1.49	0.75
2:C:175:GLU:HA	2:C:352:TRP:CD2	2.22	0.75
2:C:395:GLN:HB3	2:C:398:THR:HG23	1.67	0.75
2:C:235:THR:HB	2:C:238:GLU:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LYS:HA	1:B:483:MET:HG2	1.68	0.75
2:C:206:GLN:HE21	2:C:208:THR:H	1.32	0.75
1:B:633:ILE:HD13	1:B:738:LEU:HB3	1.69	0.75
1:A:117:ALA:N	1:A:221:ALA:H	1.81	0.75
1:B:148:HIS:O	1:B:151:THR:OG1	2.04	0.75
1:A:189:CYS:HB3	1:A:323:GLU:HG3	1.67	0.74
1:A:134:GLN:O	1:A:137:THR:OG1	2.06	0.74
1:A:347:SER:HA	1:A:358:VAL:HG13	1.70	0.74
2:C:149:SER:OG	2:C:163:LYS:NZ	2.19	0.74
1:B:588:ALA:HB1	1:B:589:TYR:HB2	1.67	0.74
1:B:317:ILE:HB	2:C:465:LEU:CB	2.17	0.74
1:B:200:THR:HA	1:B:203:SER:HB3	1.67	0.74
2:C:90:MET:N	2:C:265:PHE:O	2.20	0.74
1:A:633:ILE:HD13	1:A:738:LEU:HB3	1.69	0.74
2:C:146:ARG:NH1	2:C:147:LYS:O	2.21	0.74
1:A:581:HIS:O	1:A:583:ALA:N	2.17	0.74
1:B:132:LEU:HD21	1:B:136:ARG:HH21	1.53	0.73
1:B:365:GLN:HA	1:B:562:GLN:HB2	1.70	0.73
1:A:359:VAL:HA	1:A:438:THR:HA	1.71	0.73
1:B:134:GLN:O	1:B:137:THR:OG1	2.05	0.73
1:B:316:THR:HG21	2:C:466:VAL:CB	2.18	0.73
2:C:269:ARG:NH2	2:C:370:PRO:O	2.20	0.73
2:C:88:ARG:NH2	2:C:262:ASP:O	2.21	0.73
1:B:717:GLY:O	1:B:721:HIS:N	2.16	0.73
1:A:365:GLN:HA	1:A:562:GLN:HB2	1.70	0.72
1:A:619:GLU:OE2	1:A:620:ARG:NH1	2.21	0.72
1:B:619:GLU:OE2	1:B:620:ARG:NH1	2.21	0.72
1:A:132:LEU:HD21	1:A:136:ARG:HH21	1.53	0.72
2:C:17:LEU:HD21	2:C:197:GLY:HA3	1.71	0.72
1:A:55:GLU:HG3	1:A:171:VAL:HG22	1.70	0.72
1:A:530:VAL:O	1:A:551:TYR:OH	2.07	0.72
1:B:347:SER:HA	1:B:358:VAL:HG13	1.70	0.72
1:B:359:VAL:HA	1:B:438:THR:HA	1.70	0.72
1:B:533:ASN:HD22	1:B:543:PRO:HD2	1.55	0.72
1:B:272:SER:HB2	1:B:275:LEU:HB3	1.72	0.72
1:B:55:GLU:HG3	1:B:171:VAL:HG22	1.70	0.72
2:C:448:GLN:HA	2:C:457:LEU:HA	1.71	0.72
1:A:148:HIS:O	1:A:151:THR:OG1	2.05	0.72
1:A:334:ARG:HD3	1:A:338:GLU:HB2	1.72	0.71
1:A:272:SER:HB2	1:A:275:LEU:HB3	1.72	0.71
1:A:630:HIS:HB2	1:A:737:LEU:HD22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:MET:N	1:A:353:GLY:HA2	2.05	0.71
1:B:334:ARG:HD3	1:B:338:GLU:HB2	1.72	0.71
2:C:13:LYS:O	2:C:190:TYR:OH	2.08	0.71
2:C:252:LEU:O	2:C:257:GLY:N	2.22	0.71
2:C:250:SER:O	2:C:254:GLU:N	2.23	0.71
1:B:630:HIS:HB2	1:B:737:LEU:HD22	1.72	0.71
2:C:21:ASN:H	2:C:24:ALA:HB3	1.56	0.71
1:A:172:TYR:CD1	1:A:578:TRP:HB2	2.26	0.71
1:B:392:GLY:O	1:B:396:ARG:NH1	2.24	0.71
1:B:172:TYR:CD1	1:B:578:TRP:HB2	2.26	0.71
2:C:106:LEU:HD11	2:C:388:GLU:HG3	1.73	0.71
1:A:242:GLY:O	1:A:244:PHE:N	2.24	0.71
1:B:352:MET:N	1:B:353:GLY:HA2	2.05	0.70
2:C:180:LEU:O	2:C:185:LYS:N	2.23	0.70
1:B:242:GLY:O	1:B:244:PHE:N	2.24	0.70
1:A:392:GLY:O	1:A:396:ARG:NH1	2.24	0.70
1:B:40:PHE:HB2	1:B:288:LEU:HB3	1.73	0.70
2:C:357:PHE:CD1	2:C:361:LEU:HG	2.24	0.70
1:B:316:THR:O	2:C:465:LEU:HD21	1.89	0.70
1:B:530:VAL:O	1:B:551:TYR:OH	2.07	0.70
1:B:655:ARG:N	1:B:656:ASP:HB2	2.07	0.70
2:C:315:LYS:NZ	2:C:511:SER:O	2.24	0.70
2:C:72:TYR:HA	2:C:476:LYS:HD2	1.73	0.70
1:A:655:ARG:N	1:A:656:ASP:HB2	2.07	0.70
1:B:73:TYR:O	1:B:77:GLY:N	2.25	0.70
1:A:73:TYR:O	1:A:77:GLY:N	2.24	0.70
2:C:548:GLY:O	2:C:551:TRP:HB3	1.91	0.70
2:C:503:TYR:HB3	2:C:507:ARG:HA	1.74	0.70
1:A:717:GLY:O	1:A:721:HIS:N	2.16	0.70
1:B:40:PHE:HD2	1:B:289:ALA:HA	1.57	0.70
1:B:317:ILE:CG1	2:C:461:LYS:HA	2.18	0.70
2:C:368:GLY:O	2:C:376:HIS:N	2.24	0.70
2:C:589:ASP:HA	2:C:592:LYS:HD2	1.74	0.70
1:A:533:ASN:HD22	1:A:543:PRO:HD2	1.55	0.70
1:B:316:THR:HG23	2:C:465:LEU:HG	1.73	0.69
1:B:316:THR:HA	2:C:469:HIS:NE2	2.07	0.69
2:C:536:VAL:HG11	2:C:541:LYS:HD2	1.74	0.69
2:C:99:THR:HB	2:C:227:VAL:HB	1.74	0.69
1:B:554:PRO:O	1:B:556:GLN:N	2.22	0.69
1:A:712:SER:O	1:A:715:HIS:ND1	2.22	0.69
1:B:45:SER:OG	1:B:332:LYS:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:180:LEU:HB3	2:C:185:LYS:HB2	1.73	0.69
1:A:453:ARG:NH2	1:A:474:ARG:O	2.26	0.69
1:B:126:VAL:HG13	1:B:166:PRO:HD3	1.75	0.69
1:A:40:PHE:HD2	1:A:289:ALA:HA	1.57	0.69
1:B:321:PHE:HD1	2:C:461:LYS:CB	2.05	0.69
1:A:534:ALA:O	1:A:536:GLU:N	2.26	0.69
1:B:534:ALA:O	1:B:536:GLU:N	2.26	0.69
1:B:312:GLU:CD	2:C:466:VAL:CG2	2.53	0.69
2:C:387:LEU:HB3	2:C:389:VAL:HG13	1.75	0.69
1:B:242:GLY:O	2:C:463:ARG:NH2	2.26	0.69
2:C:454:ASP:OD2	2:C:497:LEU:N	2.24	0.69
1:B:316:THR:CG2	2:C:469:HIS:NE2	2.53	0.69
2:C:466:VAL:HA	2:C:469:HIS:HD2	1.57	0.69
2:C:287:ALA:O	2:C:291:ARG:N	2.23	0.69
1:A:385:ARG:HD2	1:A:580:TRP:HE1	1.57	0.69
1:B:453:ARG:NH2	1:B:474:ARG:O	2.26	0.69
1:A:126:VAL:HG13	1:A:166:PRO:HD3	1.75	0.69
2:C:615:THR:O	2:C:619:LEU:N	2.26	0.69
1:B:312:GLU:OE1	2:C:466:VAL:HG22	1.93	0.69
1:B:51:GLU:HA	1:B:174:VAL:HG21	1.75	0.69
2:C:81:ARG:NH1	2:C:493:GLY:O	2.25	0.69
1:A:296:ASP:O	1:A:300:GLN:N	2.19	0.69
2:C:231:GLU:O	2:C:235:THR:OG1	2.08	0.68
2:C:136:SER:OG	2:C:293:LYS:NZ	2.22	0.68
1:B:385:ARG:HD2	1:B:580:TRP:HE1	1.57	0.68
1:B:317:ILE:CB	2:C:465:LEU:HB3	2.19	0.68
1:A:45:SER:OG	1:A:332:LYS:HB2	1.93	0.68
1:B:97:ALA:HA	1:B:103:TRP:HZ2	1.58	0.68
1:A:112:GLY:HA2	1:A:116:ARG:HD3	1.76	0.68
1:A:40:PHE:HB2	1:A:288:LEU:HB3	1.73	0.68
1:B:321:PHE:CA	2:C:461:LYS:HB3	2.23	0.68
2:C:90:MET:HB3	2:C:93:PHE:HB2	1.74	0.68
1:B:712:SER:O	1:B:715:HIS:ND1	2.22	0.68
2:C:321:VAL:HB	2:C:457:LEU:HB2	1.76	0.68
1:B:31:VAL:HG22	1:B:32:GLY:H	1.58	0.68
1:B:112:GLY:HA2	1:B:116:ARG:HD3	1.76	0.67
2:C:414:GLN:O	2:C:418:THR:OG1	2.07	0.67
1:B:283:GLN:O	1:B:286:SER:OG	2.09	0.67
1:B:240:SER:N	2:C:425:ARG:NH1	2.41	0.67
1:B:238:GLU:HG3	2:C:434:ARG:NH1	2.09	0.67
1:A:97:ALA:HA	1:A:103:TRP:HZ2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:LYS:O	2:C:297:LYS:N	2.22	0.67
1:B:358:VAL:H	1:B:437:MET:HB3	1.60	0.67
1:A:51:GLU:HA	1:A:174:VAL:HG21	1.75	0.67
2:C:70:ASP:O	2:C:492:HIS:NE2	2.28	0.67
2:C:322:ALA:HA	2:C:456:MET:HG2	1.77	0.67
1:A:368:LYS:HG2	1:A:402:ALA:HA	1.77	0.67
1:B:312:GLU:HB3	2:C:466:VAL:HG22	1.74	0.67
1:A:580:TRP:HA	1:A:581:HIS:O	1.95	0.67
2:C:66:PRO:O	2:C:78:ASN:ND2	2.28	0.67
1:A:691:VAL:HG12	1:A:723:ILE:HG12	1.77	0.67
1:B:691:VAL:HG12	1:B:723:ILE:HG12	1.77	0.67
1:B:580:TRP:HA	1:B:581:HIS:O	1.95	0.66
1:B:456:MET:HA	1:B:459:ILE:HD12	1.78	0.66
2:C:627:LYS:HB2	2:C:632:TRP:CZ3	2.29	0.66
1:B:535:ILE:HD12	1:B:541:ARG:H	1.61	0.66
1:B:505:GLU:HG2	1:B:515:SER:H	1.61	0.66
1:A:358:VAL:H	1:A:437:MET:HB3	1.60	0.66
2:C:30:ARG:O	2:C:376:HIS:NE2	2.28	0.66
1:B:521:ASN:O	1:B:539:SER:OG	2.10	0.66
1:B:239:ARG:HD2	2:C:438:SER:OG	1.96	0.66
2:C:248:ASP:OD2	2:C:251:ARG:N	2.27	0.66
1:A:456:MET:HA	1:A:459:ILE:HD12	1.78	0.66
1:B:368:LYS:HG2	1:B:402:ALA:HA	1.76	0.66
1:B:627:THR:O	1:B:629:ALA:N	2.29	0.66
1:A:315:SER:O	1:A:317:ILE:N	2.28	0.66
2:C:634:GLU:O	2:C:642:HIS:NE2	2.29	0.66
1:A:31:VAL:HG22	1:A:32:GLY:H	1.58	0.66
1:B:179:THR:N	1:B:180:TYR:HA	2.11	0.66
1:B:317:ILE:HD12	2:C:460:THR:O	1.96	0.66
2:C:341:CYS:HA	2:C:344:LEU:HD12	1.76	0.66
1:B:315:SER:O	1:B:317:ILE:N	2.28	0.66
1:B:501:VAL:HG23	1:B:502:VAL:HG12	1.78	0.65
2:C:332:TRP:CH2	2:C:337:ARG:HB2	2.29	0.65
2:C:551:TRP:CZ2	2:C:584:ARG:HA	2.31	0.65
1:B:92:TYR:HE2	1:B:150:THR:HG21	1.62	0.65
1:A:627:THR:O	1:A:629:ALA:N	2.29	0.65
2:C:381:ASP:O	2:C:383:SER:N	2.24	0.65
1:B:317:ILE:CD1	2:C:460:THR:O	2.44	0.65
1:A:739:SER:OG	1:A:740:ARG:N	2.28	0.65
1:B:655:ARG:H	1:B:656:ASP:HB2	1.61	0.65
2:C:545:PRO:HG2	2:C:625:PRO:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASP:OD1	1:A:396:ARG:N	2.30	0.65
1:A:535:ILE:HD12	1:A:541:ARG:H	1.60	0.65
1:A:283:GLN:NE2	1:A:286:SER:OG	2.30	0.65
1:B:312:GLU:CB	2:C:466:VAL:HG22	2.22	0.65
2:C:637:VAL:HB	2:C:642:HIS:CD2	2.31	0.65
1:B:739:SER:OG	1:B:740:ARG:N	2.28	0.65
1:B:395:ASP:OD1	1:B:396:ARG:N	2.30	0.65
1:B:283:GLN:NE2	1:B:286:SER:OG	2.30	0.65
2:C:539:ARG:NH1	2:C:542:ARG:HH11	1.95	0.65
1:A:505:GLU:HG2	1:A:515:SER:H	1.61	0.65
2:C:546:PHE:CE2	2:C:598:LEU:HB2	2.31	0.65
2:C:547:PRO:O	2:C:587:ARG:NH2	2.24	0.65
1:A:179:THR:N	1:A:180:TYR:HA	2.11	0.64
1:A:42:ARG:NH2	1:A:283:GLN:HE21	1.95	0.64
1:A:306:VAL:O	1:A:308:PHE:N	2.30	0.64
1:B:57:GLY:H	1:B:170:TYR:HB2	1.62	0.64
1:B:306:VAL:O	1:B:308:PHE:N	2.30	0.64
1:B:715:HIS:CD2	1:B:716:VAL:HG22	2.31	0.64
2:C:536:VAL:O	2:C:542:ARG:NH2	2.30	0.64
1:B:729:LEU:HD21	1:B:743:ALA:HB1	1.79	0.64
1:A:655:ARG:H	1:A:656:ASP:HB2	1.61	0.64
1:A:283:GLN:O	1:A:286:SER:OG	2.09	0.64
2:C:504:ASP:O	2:C:507:ARG:NH1	2.30	0.64
2:C:521:MET:HB2	2:C:558:TYR:HD2	1.63	0.64
1:B:194:ASP:O	1:B:198:MET:N	2.25	0.64
2:C:235:THR:O	2:C:237:GLY:N	2.31	0.64
2:C:94:PRO:HB2	2:C:269:ARG:HD2	1.78	0.64
2:C:534:SER:O	2:C:542:ARG:NH2	2.31	0.64
2:C:277:PHE:O	2:C:280:ASN:N	2.31	0.64
1:A:144:GLU:HG2	1:A:145:LEU:H	1.63	0.64
1:B:358:VAL:N	1:B:437:MET:SD	2.71	0.64
1:A:315:SER:OG	1:A:316:THR:N	2.30	0.64
2:C:587:ARG:NH1	2:C:590:MET:SD	2.71	0.64
2:C:299:ALA:HB1	2:C:303:HIS:HB2	1.80	0.64
2:C:459:TRP:HB3	2:C:465:LEU:HD13	1.79	0.64
1:B:375:PRO:HG3	1:B:622:ARG:HE	1.63	0.64
1:B:520:TRP:H	1:B:542:THR:H	1.46	0.64
1:B:42:ARG:NH2	1:B:283:GLN:HE21	1.96	0.64
1:A:580:TRP:CD2	1:A:581:HIS:HA	2.33	0.63
1:A:554:PRO:O	1:A:556:GLN:N	2.22	0.63
1:A:501:VAL:HG23	1:A:502:VAL:HG12	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:LEU:HD21	1:A:743:ALA:HB1	1.79	0.63
1:B:77:GLY:O	1:B:474:ARG:NH1	2.28	0.63
1:A:520:TRP:H	1:A:542:THR:H	1.46	0.63
1:B:144:GLU:HG2	1:B:145:LEU:H	1.63	0.63
2:C:417:HIS:HB2	2:C:471:LEU:HD22	1.80	0.63
1:A:502:VAL:HA	1:A:503:VAL:CG1	2.28	0.63
1:A:178:ALA:O	1:A:332:LYS:NZ	2.31	0.63
1:B:178:ALA:O	1:B:332:LYS:NZ	2.31	0.63
1:B:45:SER:HB3	1:B:334:ARG:HB2	1.80	0.63
2:C:40:TYR:HB2	2:C:43:LEU:HB3	1.80	0.63
1:A:360:VAL:HG22	1:A:438:THR:HG22	1.80	0.63
2:C:553:SER:O	2:C:557:THR:N	2.32	0.63
1:A:45:SER:HB3	1:A:334:ARG:HB2	1.80	0.63
1:A:194:ASP:O	1:A:198:MET:N	2.25	0.63
1:B:580:TRP:CD2	1:B:581:HIS:HA	2.33	0.63
1:B:666:ARG:HD3	1:B:669:GLN:NE2	2.14	0.63
2:C:91:ASN:HA	2:C:267:GLU:HG3	1.79	0.63
1:A:92:TYR:HE2	1:A:150:THR:HG21	1.62	0.63
1:B:360:VAL:HG22	1:B:438:THR:HG22	1.80	0.63
2:C:86:GLY:O	2:C:89:HIS:NE2	2.31	0.63
2:C:282:PRO:CG	2:C:353:TRP:HE1	2.12	0.63
1:A:607:LYS:O	1:A:609:PHE:N	2.32	0.63
1:B:317:ILE:CG1	2:C:462:GLY:N	2.62	0.63
1:B:190:VAL:HG12	1:B:323:GLU:HB2	1.81	0.63
1:A:375:PRO:HG3	1:A:622:ARG:HE	1.63	0.63
1:A:358:VAL:N	1:A:437:MET:SD	2.71	0.63
2:C:105:ASN:HD21	2:C:331:PHE:HA	1.63	0.63
2:C:369:ALA:HB2	2:C:376:HIS:CE1	2.34	0.63
1:A:190:VAL:HG12	1:A:323:GLU:HB2	1.81	0.63
1:A:597:ILE:HD11	1:A:600:LYS:HE3	1.81	0.63
2:C:449:ILE:HG12	2:C:456:MET:HB2	1.81	0.63
2:C:337:ARG:HD2	2:C:358:GLU:HG3	1.81	0.63
2:C:108:LYS:HE3	2:C:331:PHE:HE1	1.62	0.63
1:B:100:PRO:HA	1:B:103:TRP:HD1	1.63	0.62
1:B:607:LYS:O	1:B:609:PHE:N	2.32	0.62
1:B:10:ASN:HA	1:B:17:THR:HG21	1.81	0.62
1:A:40:PHE:CD2	1:A:289:ALA:HA	2.35	0.62
2:C:616:PRO:HA	2:C:619:LEU:HD12	1.81	0.62
1:A:10:ASN:HA	1:A:17:THR:HG21	1.81	0.62
1:B:296:ASP:O	1:B:300:GLN:N	2.19	0.62
1:A:61:ILE:HD11	1:A:199:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HD11	1:B:199:LEU:HD21	1.80	0.62
1:B:183:PHE:HA	1:B:186:LEU:HD13	1.82	0.62
1:A:183:PHE:HA	1:A:186:LEU:HD13	1.82	0.62
2:C:227:VAL:H	2:C:243:PHE:H	1.48	0.62
1:A:666:ARG:HD3	1:A:669:GLN:NE2	2.14	0.62
2:C:576:TRP:O	2:C:580:GLY:HA2	1.98	0.62
1:B:4:LEU:H	1:B:436:GLU:HB2	1.64	0.62
1:B:498:ASN:HD22	1:B:500:GLU:HG2	1.64	0.62
2:C:333:PRO:HG2	2:C:336:LEU:HB2	1.82	0.62
2:C:369:ALA:HB2	2:C:376:HIS:HE1	1.64	0.62
1:B:317:ILE:HG12	2:C:462:GLY:H	1.65	0.62
2:C:3:ARG:HE	2:C:234:VAL:HG21	1.65	0.62
1:B:296:ASP:HA	1:B:299:LYS:HB3	1.82	0.62
2:C:118:PRO:HA	2:C:127:PHE:HE2	1.64	0.62
1:A:287:ASN:O	1:A:289:ALA:N	2.33	0.62
2:C:115:ALA:HB3	2:C:485:TYR:CE1	2.34	0.62
1:B:173:ARG:HD3	1:B:579:PRO:HG2	1.82	0.62
1:B:205:VAL:CG1	2:C:441:GLN:HE22	2.08	0.62
1:B:287:ASN:O	1:B:289:ALA:N	2.33	0.62
2:C:151:THR:OG1	2:C:157:SER:N	2.32	0.62
1:A:100:PRO:HA	1:A:103:TRP:HD1	1.63	0.62
2:C:38:GLU:HA	2:C:44:LEU:HD23	1.82	0.62
1:A:173:ARG:HD3	1:A:579:PRO:HG2	1.82	0.61
2:C:330:THR:HA	2:C:390:GLY:HA3	1.82	0.61
1:A:116:ARG:HB2	1:A:222:PRO:HA	1.83	0.61
2:C:261:PRO:HB2	2:C:264:PHE:CD2	2.35	0.61
1:B:42:ARG:HH21	1:B:286:SER:HG	1.48	0.61
1:A:498:ASN:HD22	1:A:500:GLU:HG2	1.64	0.61
1:B:666:ARG:HG3	1:B:670:ASN:HD21	1.65	0.61
1:A:349:ILE:HG13	1:A:350:ASP:H	1.66	0.61
1:A:4:LEU:H	1:A:436:GLU:HB2	1.64	0.61
2:C:327:ASP:HB3	2:C:331:PHE:CZ	2.36	0.61
1:B:597:ILE:HD11	1:B:600:LYS:HE3	1.81	0.61
1:A:715:HIS:CD2	1:A:716:VAL:HG22	2.31	0.61
1:A:57:GLY:H	1:A:170:TYR:HB2	1.62	0.61
1:A:666:ARG:HA	1:A:669:GLN:HE22	1.65	0.61
1:B:205:VAL:HG11	2:C:441:GLN:CD	2.07	0.61
1:B:172:TYR:HD1	1:B:578:TRP:HB2	1.65	0.61
1:B:502:VAL:HA	1:B:503:VAL:CG1	2.28	0.61
1:B:128:PRO:N	1:B:129:THR:HB	2.16	0.61
1:A:666:ARG:HG3	1:A:670:ASN:HD21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:PHE:CG	2:C:461:LYS:HB3	2.36	0.61
1:A:493:TYR:CE2	1:A:549:ILE:HG12	2.36	0.61
1:A:713:ASP:HA	1:A:715:HIS:CE1	2.36	0.61
2:C:38:GLU:HA	2:C:44:LEU:HA	1.82	0.61
1:A:754:ASN:N	1:A:755:ALA:HA	2.16	0.61
1:B:40:PHE:CD2	1:B:289:ALA:HA	2.35	0.61
1:B:173:ARG:HE	1:B:566:LEU:HD21	1.65	0.61
1:A:296:ASP:HA	1:A:299:LYS:HB3	1.82	0.61
1:B:666:ARG:HA	1:B:669:GLN:HE22	1.65	0.61
1:A:77:GLY:O	1:A:474:ARG:NH1	2.28	0.60
1:B:317:ILE:CD1	2:C:462:GLY:N	2.63	0.60
1:B:713:ASP:HA	1:B:715:HIS:CE1	2.36	0.60
2:C:597:GLU:OE2	2:C:601:TYR:OH	2.16	0.60
2:C:40:TYR:HD1	2:C:43:LEU:HD22	1.65	0.60
1:B:181:PRO:HD3	1:B:485:ASN:HD21	1.67	0.60
1:B:319:PRO:CA	2:C:461:LYS:NZ	2.65	0.60
1:B:176:ARG:NH2	1:B:447:ARG:HD2	2.16	0.60
1:A:176:ARG:NH2	1:A:447:ARG:HD2	2.17	0.60
1:A:4:LEU:N	1:A:436:GLU:HB2	2.17	0.60
1:A:173:ARG:HE	1:A:566:LEU:HD21	1.65	0.60
2:C:84:PHE:O	2:C:87:MET:HE3	2.01	0.60
1:B:671:ALA:O	1:B:674:LEU:HG	2.01	0.60
2:C:203:TYR:CE1	2:C:269:ARG:HB3	2.36	0.60
1:B:9:LEU:HA	1:B:12:SER:HB3	1.84	0.60
1:A:9:LEU:HA	1:A:12:SER:HB3	1.84	0.60
1:B:493:TYR:CE2	1:B:549:ILE:HG12	2.36	0.60
1:B:316:THR:HG21	2:C:466:VAL:HB	1.84	0.60
1:B:116:ARG:HB2	1:B:222:PRO:HA	1.83	0.60
1:A:660:LYS:O	1:A:663:ILE:HG13	2.02	0.60
1:B:242:GLY:C	2:C:463:ARG:NH2	2.55	0.60
2:C:307:ARG:NH2	2:C:514:PHE:O	2.35	0.60
2:C:305:THR:H	2:C:309:ASN:HD22	1.50	0.60
2:C:152:CYS:HA	2:C:156:PHE:CD2	2.36	0.60
1:B:237:PHE:CA	2:C:434:ARG:HH22	2.02	0.60
1:A:589:TYR:OH	1:A:740:ARG:NE	2.26	0.60
1:A:505:GLU:HA	1:A:516:LEU:HB3	1.83	0.60
1:B:754:ASN:N	1:B:755:ALA:HA	2.16	0.60
1:B:4:LEU:N	1:B:436:GLU:HB2	2.17	0.60
1:B:739:SER:HG	1:B:742:GLU:CD	2.06	0.60
1:A:135:LEU:HD12	1:A:151:THR:HG22	1.84	0.60
2:C:303:HIS:CG	2:C:309:ASN:HD21	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ILE:N	1:A:559:GLU:OE2	2.34	0.60
2:C:246:SER:O	2:C:251:ARG:NH2	2.35	0.60
1:A:181:PRO:HD3	1:A:485:ASN:HD21	1.67	0.60
2:C:189:ALA:O	2:C:194:GLN:N	2.34	0.59
2:C:279:LEU:HD13	2:C:356:LEU:HB3	1.84	0.59
1:B:135:LEU:HD12	1:B:151:THR:HG22	1.84	0.59
1:B:127:PRO:HG2	1:B:130:ALA:HB2	1.83	0.59
1:A:127:PRO:HG2	1:A:130:ALA:HB2	1.82	0.59
1:B:505:GLU:HA	1:B:516:LEU:HB3	1.83	0.59
1:A:214:PHE:HA	1:A:215:LYS:O	2.02	0.59
2:C:104:SER:HA	2:C:388:GLU:HB2	1.84	0.59
2:C:539:ARG:HG2	2:C:542:ARG:HD2	1.82	0.59
1:A:42:ARG:HH21	1:A:286:SER:HG	1.48	0.59
2:C:25:GLN:O	2:C:28:SER:OG	2.16	0.59
1:B:214:PHE:HA	1:B:215:LYS:O	2.02	0.59
1:A:739:SER:HG	1:A:742:GLU:CD	2.06	0.59
1:A:144:GLU:O	1:A:146:PHE:N	2.36	0.59
2:C:360:SER:HA	2:C:363:LEU:HB2	1.83	0.59
2:C:217:THR:HG23	2:C:219:LYS:HG2	1.85	0.59
2:C:6:ALA:HA	2:C:379:LEU:HD23	1.85	0.59
1:B:349:ILE:HG13	1:B:350:ASP:H	1.65	0.59
1:B:360:VAL:HG13	1:B:438:THR:HG23	1.84	0.59
1:A:715:HIS:CD2	1:A:716:VAL:H	2.21	0.59
1:B:13:ALA:HB1	1:B:16:LEU:HD12	1.83	0.59
1:B:61:ILE:HG13	1:B:66:TYR:HE2	1.68	0.59
1:A:395:ASP:O	1:A:398:SER:OG	2.14	0.59
1:B:505:GLU:OE2	1:B:515:SER:OG	2.15	0.59
1:A:306:VAL:HG12	1:A:309:SER:HA	1.85	0.59
1:A:360:VAL:HG13	1:A:438:THR:HG23	1.84	0.59
1:B:660:LYS:O	1:B:663:ILE:HG13	2.02	0.59
2:C:16:MET:HG3	2:C:191:GLN:HE21	1.65	0.59
1:A:472:GLU:HB3	1:A:475:ALA:HB3	1.83	0.59
1:A:671:ALA:O	1:A:674:LEU:HG	2.01	0.59
1:B:67:ALA:HA	1:B:70:PHE:HD2	1.68	0.59
1:A:61:ILE:HG13	1:A:66:TYR:HE2	1.68	0.59
2:C:73:GLY:HA3	2:C:492:HIS:HA	1.85	0.59
1:B:321:PHE:HA	2:C:461:LYS:HB3	1.85	0.59
1:A:172:TYR:HD1	1:A:578:TRP:HB2	1.65	0.59
2:C:370:PRO:HG2	2:C:374:GLN:HB3	1.85	0.59
2:C:201:VAL:HA	2:C:273:MET:HG2	1.85	0.59
1:B:530:VAL:HG13	1:B:551:TYR:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PRO:N	1:A:129:THR:HB	2.16	0.59
1:B:316:THR:HG22	2:C:465:LEU:HG	1.82	0.59
1:B:347:SER:H	1:B:554:PRO:HB3	1.68	0.59
1:A:210:LEU:HD22	1:A:228:HIS:ND1	2.18	0.59
1:B:210:LEU:HD22	1:B:228:HIS:ND1	2.18	0.59
1:B:144:GLU:O	1:B:146:PHE:N	2.36	0.59
1:B:315:SER:OG	1:B:316:THR:N	2.30	0.58
2:C:199:TYR:HB3	2:C:273:MET:HB3	1.84	0.58
2:C:227:VAL:HG22	2:C:243:PHE:O	2.03	0.58
2:C:152:CYS:O	2:C:156:PHE:N	2.34	0.58
2:C:573:ARG:NH2	2:C:574:CYS:SG	2.76	0.58
2:C:628:LEU:HD11	2:C:634:GLU:HA	1.85	0.58
1:A:97:ALA:HA	1:A:103:TRP:CZ2	2.37	0.58
1:A:678:ILE:HG21	1:A:725:ILE:HG23	1.85	0.58
1:A:47:SER:HB3	1:A:332:LYS:HD3	1.84	0.58
2:C:326:SER:HB2	2:C:487:LYS:HB2	1.85	0.58
2:C:605:MET:HG2	2:C:613:GLU:HG3	1.85	0.58
2:C:597:GLU:HG3	2:C:601:TYR:CE2	2.39	0.58
1:A:13:ALA:HB1	1:A:16:LEU:HD12	1.83	0.58
1:B:47:SER:HB3	1:B:332:LYS:HD3	1.84	0.58
1:B:589:TYR:OH	1:B:740:ARG:NE	2.26	0.58
1:A:702:MET:HG3	1:A:711:SER:HB3	1.86	0.58
1:B:445:VAL:HG13	1:B:455:PRO:HG3	1.85	0.58
1:B:472:GLU:HB3	1:B:475:ALA:HB3	1.83	0.58
2:C:521:MET:HB2	2:C:558:TYR:CD2	2.39	0.58
1:A:180:TYR:CE1	1:A:331:PHE:HA	2.38	0.58
1:B:678:ILE:HG21	1:B:725:ILE:HG23	1.85	0.58
2:C:555:LYS:NZ	2:C:559:GLY:O	2.34	0.58
1:B:715:HIS:CD2	1:B:716:VAL:H	2.21	0.58
1:A:200:THR:O	1:A:204:SER:N	2.37	0.58
1:B:238:GLU:H	2:C:434:ARG:CZ	2.17	0.58
1:B:316:THR:OG1	2:C:466:VAL:HG23	2.04	0.58
2:C:72:TYR:HB2	2:C:74:ARG:HG2	1.86	0.58
1:A:347:SER:H	1:A:554:PRO:HB3	1.68	0.58
1:B:180:TYR:CE1	1:B:331:PHE:HA	2.38	0.58
1:B:200:THR:O	1:B:204:SER:N	2.37	0.58
1:B:732:LEU:HG	1:B:738:LEU:HD11	1.86	0.58
1:A:568:LEU:HD12	1:A:569:ALA:N	2.19	0.58
1:B:568:LEU:HD12	1:B:569:ALA:N	2.19	0.58
2:C:59:ARG:NH2	2:C:262:ASP:OD2	2.36	0.58
1:B:740:ARG:N	1:B:742:GLU:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:VAL:HG13	1:A:551:TYR:CZ	2.38	0.58
1:B:173:ARG:HB2	1:B:579:PRO:CG	2.33	0.58
1:B:97:ALA:HA	1:B:103:TRP:CZ2	2.37	0.57
1:B:306:VAL:HG12	1:B:309:SER:HA	1.85	0.57
1:A:445:VAL:HG13	1:A:455:PRO:HG3	1.85	0.57
1:A:358:VAL:H	1:A:437:MET:CB	2.17	0.57
1:A:284:LEU:HG	1:A:287:ASN:ND2	2.19	0.57
1:A:375:PRO:HB2	1:A:385:ARG:HD3	1.86	0.57
2:C:124:ASN:HA	2:C:127:PHE:CD2	2.39	0.57
2:C:143:LEU:O	2:C:144:LYS:HD3	2.05	0.57
1:B:4:LEU:O	1:B:436:GLU:N	2.37	0.57
2:C:334:GLY:O	2:C:337:ARG:HB3	2.04	0.57
2:C:310:LYS:O	2:C:314:VAL:HG23	2.05	0.57
1:B:433:ASN:HB3	1:B:434:GLY:CA	2.35	0.57
1:A:67:ALA:HA	1:A:70:PHE:HD2	1.68	0.57
2:C:61:LEU:O	2:C:65:PHE:N	2.37	0.57
2:C:151:THR:N	2:C:157:SER:O	2.30	0.57
2:C:105:ASN:HB2	2:C:108:LYS:HB3	1.86	0.57
2:C:657:PHE:O	2:C:660:SER:OG	2.15	0.57
1:A:544:GLU:CD	1:A:546:LEU:H	2.08	0.57
1:A:669:GLN:HA	1:A:672:VAL:HB	1.85	0.57
1:B:702:MET:HG3	1:B:711:SER:HB3	1.86	0.57
1:B:400:THR:HG21	1:B:731:VAL:HG21	1.87	0.57
2:C:176:GLU:O	2:C:180:LEU:HG	2.04	0.57
2:C:575:TRP:HD1	2:C:581:GLU:O	1.87	0.57
2:C:209:ASP:OD1	2:C:210:ALA:N	2.38	0.57
1:A:433:ASN:HB3	1:A:434:GLY:CA	2.34	0.57
1:A:557:PRO:HB2	1:A:559:GLU:HB2	1.87	0.57
1:A:4:LEU:O	1:A:436:GLU:N	2.38	0.57
1:A:732:LEU:HG	1:A:738:LEU:HD11	1.86	0.57
1:A:505:GLU:OE2	1:A:515:SER:OG	2.15	0.57
1:A:400:THR:HG21	1:A:731:VAL:HG21	1.87	0.57
1:B:284:LEU:HG	1:B:287:ASN:ND2	2.19	0.56
2:C:280:ASN:HA	2:C:283:ILE:HD12	1.87	0.56
1:B:375:PRO:HB2	1:B:385:ARG:HD3	1.86	0.56
2:C:299:ALA:O	2:C:301:THR:N	2.38	0.56
2:C:114:LEU:HD22	2:C:485:TYR:C	2.25	0.56
2:C:3:ARG:HG3	2:C:234:VAL:HB	1.85	0.56
1:B:52:LEU:O	1:B:174:VAL:HG13	2.05	0.56
1:B:669:GLN:HA	1:B:672:VAL:HB	1.85	0.56
2:C:477:GLU:HB3	2:C:479:LYS:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:TYR:O	1:B:362:GLU:HG2	2.05	0.56
2:C:621:VAL:HG11	2:C:637:VAL:HG22	1.87	0.56
2:C:180:LEU:HD12	2:C:189:ALA:HB2	1.86	0.56
1:A:591:ASP:OD2	1:A:726:TRP:NE1	2.38	0.56
1:B:337:ASN:ND2	1:B:496:ALA:HB2	2.21	0.56
2:C:518:ILE:HG12	2:C:567:VAL:HG21	1.88	0.56
1:B:358:VAL:H	1:B:437:MET:CB	2.17	0.56
1:B:558:SER:N	1:B:559:GLU:OE1	2.39	0.56
2:C:167:ALA:HB2	2:C:277:PHE:HE2	1.69	0.56
2:C:294:ILE:O	2:C:299:ALA:N	2.26	0.56
2:C:428:ASP:N	2:C:431:SER:OG	2.30	0.56
1:A:661:LEU:O	1:A:665:GLY:N	2.35	0.56
1:A:337:ASN:ND2	1:A:496:ALA:HB2	2.21	0.56
2:C:438:SER:O	2:C:442:GLY:N	2.38	0.56
1:B:312:GLU:CD	2:C:469:HIS:HB2	2.20	0.56
1:B:179:THR:HG21	1:B:488:ALA:HB1	1.87	0.56
1:A:568:LEU:HD12	1:A:569:ALA:H	1.71	0.56
1:A:342:TYR:O	1:A:362:GLU:HG2	2.05	0.56
2:C:481:ASN:ND2	2:C:486:MET:O	2.39	0.56
2:C:32:PHE:CE2	2:C:34:GLU:HB3	2.41	0.56
1:B:473:ALA:O	1:B:477:ASN:ND2	2.39	0.56
1:A:558:SER:N	1:A:559:GLU:OE1	2.39	0.56
2:C:30:ARG:HD2	2:C:33:LYS:HE2	1.88	0.56
1:B:319:PRO:O	2:C:461:LYS:NZ	2.28	0.56
1:A:173:ARG:HB2	1:A:579:PRO:CG	2.33	0.56
1:A:16:LEU:HA	1:A:487:TYR:CE1	2.36	0.56
1:B:274:ARG:HH12	1:B:312:GLU:HG3	1.71	0.56
1:B:349:ILE:HD13	1:B:357:HIS:H	1.71	0.56
1:A:349:ILE:HD13	1:A:357:HIS:H	1.71	0.56
1:B:568:LEU:HD12	1:B:569:ALA:H	1.71	0.56
1:B:544:GLU:CD	1:B:546:LEU:H	2.08	0.56
2:C:69:VAL:HG11	2:C:493:GLY:H	1.70	0.55
1:B:354:GLN:NE2	1:B:525:GLU:OE1	2.38	0.55
1:B:557:PRO:HB2	1:B:559:GLU:HB2	1.87	0.55
2:C:60:TYR:O	2:C:63:ASP:HB3	2.07	0.55
1:A:210:LEU:HG	1:A:213:THR:HA	1.88	0.55
2:C:499:ASP:HB3	2:C:514:PHE:CG	2.41	0.55
2:C:209:ASP:CG	2:C:222:SER:HB2	2.26	0.55
2:C:253:LYS:HB2	2:C:260:VAL:HG23	1.88	0.55
2:C:371:ALA:H	2:C:374:GLN:HB2	1.70	0.55
1:A:740:ARG:N	1:A:742:GLU:OE1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:HH12	1:A:312:GLU:HG3	1.71	0.55
1:B:93:HIS:NE2	1:B:202:LEU:HD13	2.21	0.55
1:B:291:PHE:HZ	1:B:517:TYR:HA	1.71	0.55
1:A:291:PHE:HZ	1:A:517:TYR:HA	1.71	0.55
1:A:196:ARG:HH11	1:A:328:VAL:HG12	1.72	0.55
2:C:199:TYR:HB2	2:C:365:VAL:HG12	1.88	0.55
2:C:168:GLU:O	2:C:172:GLU:HG3	2.06	0.55
2:C:173:LYS:HB2	2:C:193:HIS:CE1	2.41	0.55
1:B:585:THR:N	1:B:586:GLU:HB2	2.22	0.55
2:C:47:ASP:O	2:C:51:LEU:HG	2.05	0.55
2:C:71:GLU:CD	2:C:71:GLU:H	2.07	0.55
1:A:179:THR:HG21	1:A:488:ALA:HB1	1.87	0.55
2:C:214:ASP:HB3	2:C:219:LYS:H	1.72	0.55
1:A:42:ARG:CZ	1:A:283:GLN:HE21	2.20	0.55
1:A:354:GLN:NE2	1:A:525:GLU:OE1	2.38	0.55
1:A:585:THR:N	1:A:586:GLU:HB2	2.22	0.55
2:C:419:ALA:HB1	2:C:422:LEU:HB2	1.89	0.55
1:B:42:ARG:CZ	1:B:283:GLN:HE21	2.20	0.55
1:A:52:LEU:O	1:A:174:VAL:HG13	2.06	0.55
1:B:34:LEU:HG	1:B:35:GLN:HG3	1.89	0.55
1:A:93:HIS:NE2	1:A:202:LEU:HD13	2.21	0.55
1:A:15:GLY:HA2	1:A:20:PHE:CG	2.42	0.55
1:B:22:ILE:HG21	1:B:515:SER:HB2	1.89	0.55
1:A:473:ALA:O	1:A:477:ASN:ND2	2.39	0.55
2:C:205:ALA:HB3	2:C:529:GLU:HG3	1.88	0.55
2:C:395:GLN:HG2	2:C:397:ALA:H	1.72	0.55
2:C:232:TYR:N	2:C:240:GLY:HA3	2.22	0.55
1:B:533:ASN:ND2	1:B:543:PRO:HD2	2.21	0.55
1:B:238:GLU:H	2:C:434:ARG:NH2	2.05	0.54
2:C:197:GLY:H	2:C:363:LEU:HD11	1.71	0.54
1:A:586:GLU:HB3	1:A:623:ILE:HG22	1.89	0.54
1:A:605:GLU:OE1	1:A:605:GLU:N	2.40	0.54
2:C:69:VAL:HG22	2:C:75:VAL:HG22	1.89	0.54
1:B:558:SER:OG	1:B:559:GLU:N	2.40	0.54
1:B:210:LEU:HG	1:B:213:THR:HA	1.88	0.54
1:A:533:ASN:ND2	1:A:543:PRO:HD2	2.21	0.54
1:B:42:ARG:NH2	1:B:283:GLN:O	2.40	0.54
1:B:591:ASP:OD2	1:B:726:TRP:NE1	2.38	0.54
2:C:539:ARG:HE	2:C:545:PRO:HA	1.72	0.54
1:B:196:ARG:HH11	1:B:328:VAL:HG12	1.72	0.54
2:C:397:ALA:HB1	2:C:400:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:HG21	1:A:515:SER:HB2	1.89	0.54
2:C:72:TYR:HD1	2:C:472:PHE:HZ	1.55	0.54
1:B:605:GLU:OE1	1:B:605:GLU:N	2.40	0.54
1:A:45:SER:HB2	1:A:334:ARG:CZ	2.38	0.54
2:C:94:PRO:HG2	2:C:96:ILE:HD11	1.88	0.54
1:A:409:ALA:O	1:A:413:PHE:N	2.38	0.54
1:A:214:PHE:HA	1:A:215:LYS:C	2.28	0.54
1:B:214:PHE:HA	1:B:215:LYS:C	2.28	0.54
2:C:143:LEU:HD12	2:C:285:ALA:HB2	1.89	0.54
2:C:329:ASP:HA	2:C:391:LEU:HD12	1.88	0.54
2:C:357:PHE:CE2	2:C:361:LEU:HG	2.42	0.54
1:B:15:GLY:O	1:B:487:TYR:OH	2.21	0.54
1:B:45:SER:HB2	1:B:334:ARG:CZ	2.38	0.54
2:C:282:PRO:HG3	2:C:353:TRP:HE1	1.72	0.54
1:B:586:GLU:HB3	1:B:623:ILE:HG22	1.89	0.54
1:B:144:GLU:HB2	1:B:147:HIS:HB3	1.90	0.54
1:B:661:LEU:O	1:B:665:GLY:N	2.35	0.54
2:C:85:PHE:O	2:C:211:ILE:HD12	2.08	0.54
2:C:167:ALA:O	2:C:171:LEU:HG	2.08	0.54
2:C:55:ASN:HA	2:C:88:ARG:NH1	2.18	0.54
1:B:446:GLU:HG3	1:B:627:THR:HB	1.90	0.54
1:B:38:LEU:H	1:B:501:VAL:HG21	1.73	0.54
1:A:350:ASP:O	1:A:352:MET:N	2.36	0.54
1:A:558:SER:OG	1:A:559:GLU:N	2.40	0.54
1:A:38:LEU:H	1:A:501:VAL:HG21	1.73	0.54
2:C:502:LEU:HB3	2:C:513:ILE:H	1.73	0.54
1:A:165:LEU:N	1:A:166:PRO:HD2	2.23	0.54
1:A:42:ARG:NH2	1:A:283:GLN:O	2.40	0.54
2:C:38:GLU:HG2	2:C:40:TYR:O	2.08	0.54
2:C:357:PHE:CE2	2:C:361:LEU:CB	2.91	0.54
1:B:317:ILE:HG13	2:C:460:THR:O	2.08	0.54
2:C:528:PRO:HG2	2:C:544:ARG:NH1	2.22	0.54
1:A:366:PHE:HE1	1:A:629:ALA:HB2	1.73	0.54
1:A:34:LEU:HG	1:A:35:GLN:HG3	1.89	0.54
1:A:693:LEU:O	1:A:697:ARG:HG2	2.08	0.54
1:B:343:ILE:N	1:B:559:GLU:OE2	2.34	0.53
1:A:344:GLY:N	1:A:361:TYR:O	2.27	0.53
2:C:190:TYR:O	2:C:194:GLN:HA	2.09	0.53
1:B:641:VAL:O	1:B:645:ARG:HG2	2.08	0.53
2:C:317:TRP:O	2:C:509:PRO:HB2	2.08	0.53
1:A:127:PRO:O	1:A:130:ALA:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:HB2	1:A:147:HIS:HB3	1.90	0.53
1:A:182:ASN:ND2	1:A:184:TYR:HB2	2.23	0.53
2:C:446:ILE:HG22	2:C:459:TRP:NE1	2.20	0.53
2:C:564:TYR:CE1	2:C:568:LEU:HD11	2.44	0.53
1:B:15:GLY:HA2	1:B:20:PHE:CG	2.42	0.53
2:C:481:ASN:ND2	2:C:483:SER:HB3	2.24	0.53
1:B:585:THR:HB	1:B:586:GLU:HA	1.90	0.53
1:A:99:ASN:ND2	1:A:101:GLU:OE2	2.41	0.53
1:B:693:LEU:O	1:B:697:ARG:HG2	2.08	0.53
1:B:316:THR:HG22	2:C:465:LEU:CG	2.37	0.53
2:C:287:ALA:HB1	2:C:400:LEU:HD11	1.91	0.53
1:B:572:THR:HA	1:B:575:ILE:O	2.08	0.53
1:B:272:SER:HB2	1:B:275:LEU:CB	2.38	0.53
2:C:401:MET:O	2:C:404:LEU:HB3	2.09	0.53
1:A:641:VAL:O	1:A:645:ARG:HG2	2.08	0.53
2:C:516:GLY:H	2:C:560:ALA:HB3	1.74	0.53
2:C:268:ARG:HD3	2:C:270:ARG:HE	1.73	0.53
1:B:196:ARG:HD3	1:B:328:VAL:HG12	1.89	0.53
2:C:287:ALA:O	2:C:291:ARG:HG3	2.09	0.53
1:A:446:GLU:HG3	1:A:627:THR:HB	1.90	0.53
2:C:423:ASN:HA	2:C:426:ILE:HD12	1.90	0.53
1:B:527:ARG:HH11	1:B:528:ILE:H	1.56	0.53
1:A:196:ARG:HD3	1:A:328:VAL:HG12	1.89	0.53
1:A:170:TYR:HD1	1:A:576:HIS:CE1	2.27	0.53
2:C:641:ILE:HA	2:C:644:VAL:HB	1.91	0.53
1:B:44:PHE:HE1	1:B:180:TYR:H	1.56	0.53
2:C:141:VAL:HG22	2:C:289:PRO:HG3	1.90	0.53
2:C:179:ASN:OD1	2:C:352:TRP:HB3	2.09	0.53
2:C:616:PRO:O	2:C:620:GLU:HG2	2.08	0.53
1:A:42:ARG:H	1:A:336:ILE:HD13	1.73	0.53
2:C:56:GLU:OE2	2:C:577:ASN:ND2	2.37	0.53
1:B:26:LYS:HE3	1:B:509:VAL:HG22	1.91	0.53
2:C:160:MET:O	2:C:164:ILE:HG12	2.08	0.53
1:B:170:TYR:HD1	1:B:576:HIS:CE1	2.27	0.53
2:C:12:ILE:O	2:C:16:MET:HG2	2.08	0.53
2:C:399:ASP:OD1	2:C:400:LEU:N	2.41	0.53
1:A:143:HIS:CD2	1:A:146:PHE:HE2	2.26	0.53
1:A:159:SER:OG	1:A:160:PRO:HD3	2.09	0.53
1:B:317:ILE:HG12	2:C:462:GLY:N	2.20	0.53
1:B:2:PHE:H	1:B:439:LEU:HD11	1.74	0.53
1:A:572:THR:HA	1:A:575:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLN:HG2	1:B:555:ILE:HG12	1.91	0.53
1:B:99:ASN:ND2	1:B:101:GLU:OE2	2.41	0.53
2:C:650:SER:HB2	2:C:652:GLU:OE1	2.09	0.53
1:B:713:ASP:HA	1:B:715:HIS:ND1	2.24	0.53
1:B:365:GLN:OE1	1:B:563:ALA:HB3	2.09	0.53
1:A:368:LYS:HE2	1:A:402:ALA:HA	1.91	0.53
2:C:306:THR:OG1	2:C:309:ASN:N	2.42	0.53
1:B:182:ASN:ND2	1:B:184:TYR:HB2	2.23	0.53
1:A:157:VAL:O	1:A:160:PRO:HD2	2.09	0.53
1:B:313:LEU:CA	2:C:466:VAL:HG21	2.34	0.53
2:C:508:GLU:HB2	2:C:511:SER:HB3	1.90	0.53
1:A:285:ARG:O	1:A:288:LEU:HD13	2.09	0.53
1:A:713:ASP:HA	1:A:715:HIS:ND1	2.24	0.53
2:C:179:ASN:O	2:C:183:GLN:N	2.37	0.53
1:B:395:ASP:O	1:B:398:SER:OG	2.14	0.53
1:B:42:ARG:H	1:B:336:ILE:HD13	1.73	0.53
1:B:368:LYS:HE2	1:B:402:ALA:HA	1.91	0.53
1:B:366:PHE:HE1	1:B:629:ALA:HB2	1.73	0.53
1:A:26:LYS:HE3	1:A:509:VAL:HG22	1.91	0.53
2:C:273:MET:N	2:C:393:SER:OG	2.35	0.52
1:B:702:MET:HB3	1:B:708:ILE:HA	1.91	0.52
1:B:285:ARG:O	1:B:288:LEU:HD13	2.09	0.52
2:C:504:ASP:CG	2:C:511:SER:HB2	2.29	0.52
1:B:223:ALA:O	1:B:227:GLN:N	2.34	0.52
1:A:527:ARG:HH11	1:A:528:ILE:H	1.56	0.52
1:B:630:HIS:N	1:B:737:LEU:HD13	2.24	0.52
1:B:231:ASN:OD1	1:B:232:ALA:N	2.42	0.52
2:C:74:ARG:HB2	2:C:503:TYR:CD1	2.44	0.52
1:A:287:ASN:C	1:A:289:ALA:H	2.13	0.52
2:C:627:LYS:HB3	2:C:631:LYS:HB3	1.92	0.52
2:C:48:PRO:HA	2:C:51:LEU:HD12	1.91	0.52
2:C:575:TRP:CD2	2:C:583:TYR:HB2	2.44	0.52
1:A:365:GLN:OE1	1:A:563:ALA:HB3	2.09	0.52
1:A:519:VAL:HG22	1:A:542:THR:N	2.25	0.52
1:B:165:LEU:N	1:B:166:PRO:HD2	2.23	0.52
1:A:720:ARG:HD2	1:A:760:VAL:HG21	1.91	0.52
2:C:67:ALA:HA	2:C:80:VAL:HB	1.90	0.52
2:C:142:PRO:HB3	2:C:651:VAL:HB	1.91	0.52
1:B:105:LYS:HE2	1:B:138:LEU:HD11	1.91	0.52
2:C:508:GLU:O	2:C:511:SER:OG	2.18	0.52
2:C:83:ASN:ND2	2:C:211:ILE:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HA	1:B:487:TYR:CE1	2.36	0.52
1:A:44:PHE:HE1	1:A:180:TYR:H	1.56	0.52
2:C:404:LEU:O	2:C:408:ILE:HG12	2.08	0.52
2:C:50:PHE:O	2:C:53:PHE:HB3	2.07	0.52
2:C:357:PHE:CE1	2:C:361:LEU:CD2	2.93	0.52
2:C:206:GLN:HG3	2:C:208:THR:O	2.09	0.52
2:C:180:LEU:HD22	2:C:185:LYS:HD2	1.90	0.52
1:B:580:TRP:CH2	1:B:622:ARG:HD3	2.45	0.52
2:C:592:LYS:O	2:C:596:LEU:HG	2.09	0.52
1:A:580:TRP:CH2	1:A:622:ARG:HD3	2.45	0.52
1:B:720:ARG:HD2	1:B:760:VAL:HG21	1.91	0.52
2:C:132:ARG:NH1	2:C:429:MET:HB3	2.24	0.52
2:C:628:LEU:HA	2:C:632:TRP:HB2	1.92	0.52
2:C:117:GLY:HA2	2:C:335:TRP:CE3	2.44	0.52
1:B:732:LEU:HD21	1:B:738:LEU:HD21	1.92	0.52
1:A:732:LEU:HD21	1:A:738:LEU:HD21	1.91	0.52
1:A:702:MET:HB3	1:A:708:ILE:HA	1.91	0.52
1:A:231:ASN:OD1	1:A:232:ALA:N	2.42	0.52
1:B:239:ARG:NH1	2:C:438:SER:OG	2.43	0.52
1:A:2:PHE:H	1:A:439:LEU:HD11	1.74	0.52
2:C:213:LEU:HD13	2:C:220:PHE:CE1	2.45	0.52
2:C:122:ARG:O	2:C:126:LEU:HG	2.09	0.52
1:B:313:LEU:N	2:C:466:VAL:HG23	2.20	0.52
1:B:472:GLU:HB3	1:B:475:ALA:CB	2.40	0.52
2:C:143:LEU:O	2:C:649:VAL:HB	2.10	0.52
1:A:106:LEU:O	1:A:110:ILE:HG12	2.10	0.52
2:C:438:SER:HA	2:C:441:GLN:HB2	1.90	0.52
1:A:15:GLY:O	1:A:487:TYR:OH	2.21	0.52
1:A:296:ASP:HB2	1:A:300:GLN:HG2	1.92	0.52
2:C:121:GLU:O	2:C:125:LEU:HG	2.10	0.52
1:B:106:LEU:O	1:B:110:ILE:HG12	2.10	0.52
1:B:287:ASN:C	1:B:289:ALA:H	2.13	0.52
1:B:310:ASP:OD2	1:B:313:LEU:N	2.42	0.52
1:B:4:LEU:HG	1:B:436:GLU:CB	2.38	0.52
2:C:180:LEU:O	2:C:184:GLY:N	2.42	0.52
1:A:100:PRO:HA	1:A:103:TRP:CD1	2.45	0.52
1:A:252:SER:HB3	1:A:306:VAL:HG13	1.92	0.52
1:A:17:THR:O	1:A:19:ALA:N	2.38	0.52
1:B:296:ASP:HB2	1:B:300:GLN:HG2	1.92	0.52
2:C:56:GLU:OE2	2:C:573:ARG:NH1	2.43	0.52
2:C:333:PRO:HG2	2:C:336:LEU:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ARG:HB2	1:B:281:ILE:HD11	1.92	0.51
2:C:83:ASN:HB2	2:C:85:PHE:CD2	2.35	0.51
1:B:409:ALA:O	1:B:413:PHE:N	2.38	0.51
2:C:642:HIS:O	2:C:646:MET:N	2.38	0.51
2:C:9:LEU:HD13	2:C:366:TYR:CZ	2.44	0.51
1:A:32:GLY:H	1:A:541:ARG:HH21	1.59	0.51
1:B:143:HIS:CD2	1:B:146:PHE:HE2	2.26	0.51
1:B:159:SER:OG	1:B:160:PRO:HD3	2.09	0.51
2:C:357:PHE:CE1	2:C:361:LEU:HD11	2.43	0.51
1:B:196:ARG:O	1:B:197:ARG:NH1	2.40	0.51
2:C:593:ARG:HA	2:C:596:LEU:HD12	1.93	0.51
1:A:272:SER:HB2	1:A:275:LEU:CB	2.38	0.51
1:A:524:THR:HG21	1:A:540:ILE:HG12	1.92	0.51
2:C:343:GLU:HA	2:C:346:ASN:HB2	1.92	0.51
2:C:588:GLU:O	2:C:592:LYS:HG3	2.10	0.51
1:A:472:GLU:HB3	1:A:475:ALA:CB	2.40	0.51
1:B:310:ASP:OD2	2:C:466:VAL:HG21	2.11	0.51
1:B:39:GLN:HA	1:B:501:VAL:HG11	1.92	0.51
1:A:39:GLN:HA	1:A:501:VAL:HG11	1.92	0.51
1:B:387:LEU:H	1:B:572:THR:HG22	1.76	0.51
1:B:519:VAL:HG22	1:B:542:THR:N	2.25	0.51
1:B:42:ARG:NH2	1:B:286:SER:OG	2.40	0.51
1:A:105:LYS:HE2	1:A:138:LEU:HD11	1.91	0.51
2:C:251:ARG:O	2:C:254:GLU:HB3	2.10	0.51
2:C:395:GLN:HG2	2:C:397:ALA:N	2.25	0.51
1:A:630:HIS:N	1:A:737:LEU:HD13	2.24	0.51
1:B:252:SER:HB3	1:B:306:VAL:HG13	1.93	0.51
2:C:50:PHE:HB2	2:C:579:PHE:CZ	2.45	0.51
2:C:36:ALA:HA	2:C:92:GLY:HA3	1.92	0.51
2:C:552:ALA:HB2	2:C:591:LEU:HD22	1.93	0.51
2:C:539:ARG:HH21	2:C:545:PRO:HA	1.75	0.51
2:C:638:SER:O	2:C:642:HIS:HB2	2.11	0.51
1:A:345:GLN:HG2	1:A:555:ILE:HG12	1.91	0.51
1:B:698:ILE:O	1:B:702:MET:HE2	2.09	0.51
1:B:157:VAL:O	1:B:160:PRO:HD2	2.09	0.51
1:B:350:ASP:O	1:B:352:MET:N	2.36	0.51
2:C:337:ARG:HA	2:C:340:ILE:HD12	1.93	0.51
2:C:96:ILE:HB	2:C:251:ARG:HH12	1.75	0.51
2:C:207:SER:HB3	2:C:528:PRO:O	2.10	0.51
2:C:539:ARG:NH2	2:C:544:ARG:O	2.43	0.51
2:C:366:TYR:OH	2:C:376:HIS:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TRP:CZ3	1:B:174:VAL:HG12	2.46	0.51
2:C:420:PRO:HA	2:C:423:ASN:ND2	2.26	0.51
1:B:312:GLU:HB3	2:C:466:VAL:HG21	1.90	0.51
1:A:352:MET:SD	1:A:355:PRO:HD2	2.51	0.51
2:C:353:TRP:HA	2:C:356:LEU:HD12	1.92	0.51
1:A:585:THR:HB	1:A:586:GLU:HA	1.91	0.51
2:C:662:MET:O	2:C:664:ARG:N	2.44	0.51
1:A:245:ASP:HB2	1:A:248:ALA:HB3	1.93	0.51
1:B:320:TRP:CH2	2:C:460:THR:HB	2.46	0.51
1:B:344:GLY:N	1:B:361:TYR:O	2.27	0.51
1:A:54:TRP:CZ3	1:A:174:VAL:HG12	2.46	0.51
1:A:443:SER:O	1:A:447:ARG:HG2	2.12	0.50
2:C:16:MET:HB2	2:C:190:TYR:CZ	2.45	0.50
2:C:411:LEU:HD21	2:C:435:PHE:CZ	2.46	0.50
1:B:352:MET:SD	1:B:355:PRO:HD2	2.51	0.50
1:B:334:ARG:HD3	1:B:338:GLU:CB	2.41	0.50
2:C:288:GLN:HA	2:C:291:ARG:HD2	1.93	0.50
1:A:387:LEU:H	1:A:572:THR:HG22	1.76	0.50
2:C:298:TYR:HE1	2:C:437:ASP:OD1	1.95	0.50
2:C:333:PRO:O	2:C:336:LEU:HB3	2.11	0.50
1:A:261:TRP:CE2	1:A:288:LEU:HG	2.46	0.50
2:C:99:THR:CB	2:C:227:VAL:HB	2.41	0.50
1:B:524:THR:HG21	1:B:540:ILE:HG12	1.91	0.50
1:A:284:LEU:C	1:A:287:ASN:H	2.14	0.50
1:A:366:PHE:HD2	1:A:405:GLY:HA2	1.77	0.50
1:B:261:TRP:CE2	1:B:288:LEU:HG	2.46	0.50
1:B:502:VAL:HA	1:B:503:VAL:CB	2.42	0.50
1:B:16:LEU:HD11	1:B:462:LEU:HB3	1.94	0.50
2:C:350:ALA:HB1	2:C:352:TRP:CE2	2.46	0.50
2:C:320:CYS:HA	2:C:457:LEU:O	2.12	0.50
1:B:100:PRO:HA	1:B:103:TRP:CD1	2.45	0.50
1:A:698:ILE:O	1:A:702:MET:HE2	2.11	0.50
1:B:81:SER:HB2	1:B:188:ASP:OD2	2.12	0.50
2:C:100:TRP:HB2	2:C:229:ASP:C	2.32	0.50
1:B:321:PHE:HB2	2:C:461:LYS:CB	2.38	0.50
1:B:321:PHE:HA	2:C:461:LYS:CB	2.40	0.50
1:A:276:ARG:HB2	1:A:281:ILE:HD11	1.92	0.50
2:C:273:MET:O	2:C:393:SER:OG	2.29	0.50
2:C:279:LEU:O	2:C:282:PRO:HG2	2.11	0.50
1:A:391:PRO:HA	1:A:394:SER:HB2	1.93	0.50
1:A:103:TRP:O	1:A:226:SER:OG	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ASP:HB2	1:B:248:ALA:HB3	1.92	0.50
1:A:347:SER:O	1:A:358:VAL:HG22	2.11	0.50
2:C:627:LYS:HG2	2:C:630:TYR:CZ	2.47	0.50
2:C:557:THR:OG1	2:C:620:GLU:OE2	2.24	0.50
2:C:15:GLN:HE22	2:C:25:GLN:NE2	2.10	0.50
2:C:554:MET:HG2	2:C:564:TYR:CE1	2.35	0.50
1:B:443:SER:O	1:B:447:ARG:HG2	2.12	0.50
2:C:617:ILE:O	2:C:621:VAL:HG23	2.11	0.50
1:B:391:PRO:HA	1:B:394:SER:HB2	1.93	0.50
2:C:38:GLU:OE2	2:C:42:GLY:N	2.28	0.50
2:C:40:TYR:O	2:C:43:LEU:N	2.45	0.50
2:C:124:ASN:ND2	2:C:128:ARG:HE	2.10	0.50
1:A:196:ARG:O	1:A:197:ARG:NH1	2.40	0.50
1:A:334:ARG:HD3	1:A:338:GLU:CB	2.41	0.50
1:B:61:ILE:HG13	1:B:66:TYR:CE2	2.47	0.50
1:B:42:ARG:H	1:B:336:ILE:CD1	2.25	0.50
2:C:413:MET:HG2	2:C:471:LEU:HD21	1.92	0.50
1:B:284:LEU:C	1:B:287:ASN:H	2.14	0.49
1:A:502:VAL:HA	1:A:503:VAL:CB	2.42	0.49
2:C:250:SER:HA	2:C:253:LYS:HB3	1.94	0.49
2:C:287:ALA:HA	2:C:290:VAL:HB	1.94	0.49
2:C:282:PRO:HB3	2:C:657:PHE:CE2	2.46	0.49
1:B:366:PHE:HD2	1:B:405:GLY:HA2	1.77	0.49
1:A:144:GLU:HG2	1:A:145:LEU:N	2.26	0.49
2:C:295:TYR:O	2:C:299:ALA:HB2	2.12	0.49
1:A:477:ASN:OD1	1:A:478:ASP:N	2.45	0.49
2:C:50:PHE:HB2	2:C:579:PHE:HZ	1.76	0.49
2:C:582:SER:OG	2:C:584:ARG:HB3	2.11	0.49
2:C:58:SER:HA	2:C:84:PHE:HB2	1.94	0.49
2:C:348:GLY:HA3	2:C:663:PRO:HB3	1.92	0.49
2:C:521:MET:O	2:C:525:GLN:HG3	2.12	0.49
1:B:340:THR:O	1:B:343:ILE:HG22	2.12	0.49
1:B:715:HIS:CG	1:B:716:VAL:H	2.29	0.49
2:C:363:LEU:HD12	2:C:364:PRO:HD2	1.94	0.49
1:B:369:GLU:HA	1:B:398:SER:HB2	1.94	0.49
1:B:127:PRO:C	1:B:129:THR:HB	2.33	0.49
2:C:328:HIS:ND1	2:C:453:ASP:HB3	2.27	0.49
1:B:32:GLY:H	1:B:541:ARG:HH21	1.59	0.49
1:A:42:ARG:H	1:A:336:ILE:CD1	2.25	0.49
1:A:155:CYS:O	1:A:159:SER:N	2.45	0.49
2:C:357:PHE:CD1	2:C:361:LEU:HD21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:SER:O	1:B:358:VAL:HG22	2.11	0.49
1:A:16:LEU:HD11	1:A:462:LEU:HB3	1.94	0.49
2:C:117:GLY:O	2:C:485:TYR:OH	2.13	0.49
1:B:567:ASP:O	1:B:569:ALA:N	2.45	0.49
1:A:585:THR:O	1:A:622:ARG:HG2	2.12	0.49
1:A:128:PRO:HG2	1:A:129:THR:OG1	2.12	0.49
1:B:17:THR:O	1:B:19:ALA:N	2.38	0.49
2:C:602:VAL:HG11	2:C:605:MET:HB2	1.95	0.49
1:B:433:ASN:HB3	1:B:434:GLY:C	2.33	0.49
2:C:324:ASP:HB2	2:C:491:GLU:N	2.27	0.49
1:A:81:SER:HB2	1:A:188:ASP:OD2	2.12	0.49
2:C:438:SER:OG	2:C:443:HIS:HB2	2.12	0.49
1:B:317:ILE:HD11	2:C:461:LYS:C	2.32	0.49
1:B:317:ILE:HB	2:C:465:LEU:HD23	1.94	0.49
1:A:196:ARG:HB3	1:A:197:ARG:NH1	2.27	0.49
2:C:352:TRP:O	2:C:356:LEU:HG	2.11	0.49
1:B:585:THR:O	1:B:622:ARG:HG2	2.12	0.49
2:C:551:TRP:CH2	2:C:584:ARG:HA	2.47	0.49
1:B:144:GLU:HG2	1:B:145:LEU:N	2.26	0.49
1:B:477:ASN:OD1	1:B:478:ASP:N	2.45	0.49
1:B:312:GLU:CD	2:C:470:ARG:HG3	2.27	0.49
2:C:336:LEU:O	2:C:340:ILE:HG13	2.12	0.49
1:A:310:ASP:OD2	1:A:313:LEU:N	2.42	0.49
1:B:396:ARG:HE	1:B:612:LEU:HB3	1.77	0.49
1:A:516:LEU:O	1:A:516:LEU:HD12	2.13	0.49
1:A:745:ALA:O	1:A:749:VAL:HG23	2.12	0.49
2:C:316:GLU:HB2	2:C:317:TRP:CD1	2.48	0.49
1:A:340:THR:O	1:A:343:ILE:HG22	2.12	0.49
1:A:61:ILE:HG13	1:A:66:TYR:CE2	2.47	0.49
2:C:27:ALA:HA	2:C:30:ARG:HB2	1.94	0.49
1:B:383:ASN:O	1:B:385:ARG:N	2.38	0.49
1:B:239:ARG:CZ	2:C:438:SER:OG	2.61	0.49
1:B:516:LEU:O	1:B:516:LEU:HD12	2.13	0.49
1:B:257:LEU:HB3	1:B:261:TRP:CZ2	2.48	0.49
2:C:517:ASN:OD1	2:C:519:ASN:N	2.46	0.49
2:C:95:MET:HG2	2:C:268:ARG:HA	1.95	0.49
1:B:196:ARG:HB3	1:B:197:ARG:NH1	2.27	0.49
2:C:395:GLN:HE21	2:C:397:ALA:CB	2.25	0.49
1:B:375:PRO:CG	1:B:622:ARG:HE	2.26	0.49
2:C:310:LYS:HB2	2:C:514:PHE:HE2	1.78	0.49
1:B:103:TRP:O	1:B:226:SER:OG	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:618:ASP:O	2:C:622:LEU:HG	2.12	0.49
1:A:567:ASP:O	1:A:569:ALA:N	2.45	0.49
2:C:199:TYR:CE2	2:C:363:LEU:HB3	2.48	0.49
1:A:410:VAL:CA	1:A:413:PHE:HB3	2.41	0.49
2:C:625:PRO:O	2:C:628:LEU:HB3	2.13	0.48
2:C:288:GLN:HB3	2:C:289:PRO:HD3	1.95	0.48
1:A:375:PRO:CG	1:A:622:ARG:HE	2.26	0.48
1:B:127:PRO:O	1:B:130:ALA:N	2.36	0.48
2:C:416:ASP:HB2	2:C:417:HIS:CD2	2.48	0.48
1:A:418:THR:O	1:A:421:TYR:CD1	2.66	0.48
1:B:556:GLN:OE1	1:B:557:PRO:HD2	2.13	0.48
2:C:249:ALA:HB3	2:C:260:VAL:HG13	1.95	0.48
2:C:350:ALA:O	2:C:354:VAL:HG23	2.13	0.48
2:C:583:TYR:HA	2:C:586:TYR:HB3	1.94	0.48
1:A:369:GLU:HA	1:A:398:SER:HB2	1.93	0.48
1:A:42:ARG:NH2	1:A:286:SER:OG	2.40	0.48
2:C:429:MET:HB2	2:C:430:PRO:HD3	1.95	0.48
2:C:119:VAL:HB	2:C:123:ASP:OD2	2.12	0.48
2:C:123:ASP:HA	2:C:126:LEU:HD12	1.95	0.48
1:A:4:LEU:HG	1:A:436:GLU:CB	2.37	0.48
2:C:39:THR:N	2:C:43:LEU:O	2.46	0.48
2:C:406:MET:HB3	2:C:410:TYR:CZ	2.48	0.48
1:A:715:HIS:CG	1:A:716:VAL:H	2.30	0.48
2:C:277:PHE:CD1	2:C:280:ASN:HB2	2.48	0.48
2:C:547:PRO:HB2	2:C:587:ARG:HH12	1.78	0.48
1:B:128:PRO:HG2	1:B:129:THR:OG1	2.12	0.48
2:C:118:PRO:HA	2:C:127:PHE:CE2	2.46	0.48
1:A:433:ASN:HB3	1:A:434:GLY:C	2.33	0.48
1:A:257:LEU:HB3	1:A:261:TRP:CZ2	2.48	0.48
1:A:127:PRO:C	1:A:129:THR:HB	2.33	0.48
1:A:719:ASN:OD1	1:A:720:ARG:N	2.46	0.48
2:C:339:LEU:O	2:C:342:ASP:HB3	2.14	0.48
1:A:433:ASN:HB3	1:A:434:GLY:HA3	1.95	0.48
1:B:155:CYS:O	1:B:159:SER:N	2.45	0.48
1:A:747:THR:HA	1:A:750:LEU:HG	1.96	0.48
1:B:745:ALA:O	1:B:749:VAL:HG23	2.12	0.48
2:C:555:LYS:HB2	2:C:564:TYR:CZ	2.49	0.48
1:A:556:GLN:OE1	1:A:557:PRO:HD2	2.13	0.48
1:B:335:PRO:HB2	1:B:338:GLU:OE2	2.14	0.48
1:A:729:LEU:O	1:A:732:LEU:HB3	2.14	0.48
2:C:411:LEU:O	2:C:415:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:OG1	1:A:50:SER:N	2.44	0.48
2:C:19:ALA:HB2	2:C:155:TYR:HB3	1.95	0.48
2:C:190:TYR:C	2:C:194:GLN:HA	2.34	0.48
2:C:199:TYR:HE2	2:C:363:LEU:HB3	1.79	0.48
1:A:396:ARG:HE	1:A:612:LEU:HB3	1.77	0.48
2:C:428:ASP:CG	2:C:430:PRO:HD2	2.33	0.48
1:B:418:THR:O	1:B:421:TYR:CD1	2.66	0.48
1:A:83:ASP:OD1	1:A:191:ARG:NE	2.47	0.48
1:A:362:GLU:HB2	1:A:364:TRP:HE1	1.79	0.48
1:A:51:GLU:CA	1:A:174:VAL:HG21	2.44	0.48
2:C:436:LEU:HD21	2:C:440:TRP:CE2	2.48	0.48
1:B:669:GLN:O	1:B:673:THR:N	2.39	0.48
1:A:672:VAL:HA	1:A:675:LEU:HD12	1.96	0.48
1:A:493:TYR:CZ	1:A:549:ILE:HG12	2.49	0.48
1:B:477:ASN:O	1:B:481:ARG:N	2.47	0.48
1:A:253:VAL:HG11	1:A:322:ILE:HD13	1.95	0.48
2:C:476:LYS:HA	2:C:490:TYR:CD1	2.49	0.48
1:A:16:LEU:HD21	1:A:462:LEU:HD13	1.96	0.48
1:B:243:ASN:HD21	2:C:422:LEU:HD22	1.78	0.48
2:C:477:GLU:HB3	2:C:479:LYS:HG3	1.96	0.48
2:C:170:ALA:HB2	2:C:278:ALA:HB1	1.96	0.48
1:B:317:ILE:CG1	2:C:460:THR:O	2.61	0.48
1:B:109:TYR:OH	1:B:130:ALA:HB1	2.14	0.48
1:B:433:ASN:HB3	1:B:434:GLY:HA3	1.95	0.48
1:A:423:ALA:HA	1:A:424:VAL:HA	1.48	0.48
2:C:511:SER:OG	2:C:512:ALA:N	2.46	0.47
1:A:376:VAL:O	1:A:386:PHE:N	2.47	0.47
2:C:250:SER:HA	2:C:260:VAL:HG21	1.96	0.47
1:A:739:SER:OG	1:A:742:GLU:OE1	2.32	0.47
1:B:719:ASN:OD1	1:B:720:ARG:N	2.46	0.47
1:A:441:PHE:HB2	1:A:444:VAL:HG22	1.96	0.47
1:B:747:THR:HA	1:B:750:LEU:HG	1.96	0.47
1:B:253:VAL:HG11	1:B:322:ILE:HD13	1.95	0.47
1:B:349:ILE:HD11	1:B:356:SER:HB2	1.96	0.47
1:B:362:GLU:HB2	1:B:364:TRP:HE1	1.79	0.47
1:B:16:LEU:HD21	1:B:462:LEU:HD13	1.96	0.47
1:A:335:PRO:HB2	1:A:338:GLU:OE2	2.14	0.47
2:C:89:HIS:HE2	2:C:208:THR:HA	1.78	0.47
2:C:641:ILE:O	2:C:645:LEU:N	2.41	0.47
2:C:261:PRO:HB2	2:C:264:PHE:HD2	1.79	0.47
1:B:533:ASN:ND2	1:B:542:THR:OG1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASP:OD1	1:B:191:ARG:NE	2.47	0.47
1:B:757:GLY:HA3	1:B:759:VAL:H	1.79	0.47
1:B:66:TYR:HA	1:B:69:LEU:HD12	1.95	0.47
1:B:729:LEU:O	1:B:732:LEU:HB3	2.14	0.47
2:C:451:LYS:HD3	2:C:497:LEU:HD21	1.96	0.47
1:B:410:VAL:CA	1:B:413:PHE:HB3	2.41	0.47
1:A:349:ILE:HD11	1:A:356:SER:HB2	1.97	0.47
1:A:580:TRP:CE3	1:A:581:HIS:HA	2.49	0.47
1:A:533:ASN:ND2	1:A:542:THR:OG1	2.47	0.47
2:C:499:ASP:HB3	2:C:514:PHE:CD2	2.49	0.47
1:A:535:ILE:HG13	1:A:540:ILE:HG23	1.96	0.47
1:A:146:PHE:HA	1:A:149:ILE:HB	1.97	0.47
1:B:80:LEU:HD21	1:B:477:ASN:HD21	1.79	0.47
1:A:80:LEU:HD21	1:A:477:ASN:HD21	1.79	0.47
1:A:696:SER:OG	1:A:697:ARG:NH1	2.47	0.47
1:A:757:GLY:HA3	1:A:759:VAL:H	1.79	0.47
1:B:189:CYS:O	1:B:193:SER:OG	2.22	0.47
2:C:17:LEU:HB3	2:C:154:PRO:HA	1.96	0.47
1:A:371:THR:HB	1:A:389:VAL:HG23	1.96	0.47
1:B:243:ASN:ND2	2:C:422:LEU:CD2	2.77	0.47
1:A:109:TYR:OH	1:A:130:ALA:HB1	2.14	0.47
1:B:696:SER:OG	1:B:697:ARG:NH1	2.47	0.47
1:A:648:ALA:O	1:A:652:ARG:HG3	2.14	0.47
2:C:503:TYR:HD2	2:C:508:GLU:N	2.13	0.47
2:C:555:LYS:HB2	2:C:564:TYR:OH	2.14	0.47
1:A:282:ASP:N	1:A:282:ASP:OD1	2.48	0.47
1:A:282:ASP:O	1:A:285:ARG:HB3	2.14	0.47
1:B:376:VAL:O	1:B:386:PHE:N	2.47	0.47
2:C:382:PRO:HA	2:C:385:PRO:HG3	1.95	0.47
2:C:1:PRO:HA	2:C:238:GLU:HG3	1.97	0.47
1:B:6:VAL:HG11	1:B:530:VAL:HG23	1.96	0.47
1:B:535:ILE:HG13	1:B:540:ILE:HG23	1.96	0.47
1:B:441:PHE:HB2	1:B:444:VAL:HG22	1.96	0.47
1:B:648:ALA:O	1:B:652:ARG:HG3	2.14	0.47
2:C:564:TYR:O	2:C:568:LEU:HD13	2.15	0.47
2:C:565:SER:O	2:C:568:LEU:HB2	2.15	0.47
1:B:344:GLY:HA2	1:B:557:PRO:HB3	1.96	0.47
1:A:344:GLY:HA2	1:A:557:PRO:HB3	1.96	0.47
2:C:299:ALA:O	2:C:302:PHE:N	2.46	0.47
1:B:146:PHE:HA	1:B:149:ILE:HB	1.97	0.47
1:B:708:ILE:O	1:B:711:SER:OG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:THR:OG1	1:B:50:SER:N	2.44	0.47
2:C:74:ARG:HD2	2:C:507:ARG:HB3	1.96	0.47
2:C:454:ASP:OD2	2:C:497:LEU:HD12	2.15	0.47
1:B:51:GLU:CA	1:B:174:VAL:HG21	2.43	0.47
1:B:493:TYR:CZ	1:B:549:ILE:HG12	2.49	0.47
1:B:745:ALA:O	1:B:748:LYS:HB3	2.15	0.47
1:A:6:VAL:HG11	1:A:530:VAL:HG23	1.96	0.47
2:C:78:ASN:OD1	2:C:79:GLY:N	2.48	0.47
2:C:121:GLU:O	2:C:124:ASN:HB3	2.15	0.47
2:C:28:SER:OG	2:C:29:LYS:HG3	2.15	0.47
1:A:337:ASN:HD21	1:A:496:ALA:HB2	1.80	0.47
1:A:303:ARG:HB2	1:A:513:GLN:OE1	2.15	0.47
1:B:263:PRO:HG3	1:B:504:SER:HA	1.97	0.47
1:B:502:VAL:HG23	1:B:503:VAL:HG12	1.97	0.47
2:C:319:LEU:O	2:C:458:GLY:HA2	2.15	0.47
1:A:117:ALA:H	1:A:221:ALA:N	1.94	0.47
1:A:66:TYR:HA	1:A:69:LEU:HD12	1.95	0.47
1:A:69:LEU:HD22	1:A:172:TYR:HD2	1.80	0.47
2:C:364:PRO:HG2	2:C:382:PRO:HG3	1.97	0.47
1:B:580:TRP:CE3	1:B:581:HIS:HA	2.49	0.47
1:A:308:PHE:HE2	1:A:318:ILE:HG13	1.80	0.47
1:B:316:THR:CA	2:C:469:HIS:NE2	2.78	0.46
1:A:280:GLY:N	1:A:282:ASP:OD1	2.48	0.46
1:A:328:VAL:HG23	1:A:329:SER:HB2	1.97	0.46
1:B:328:VAL:HG23	1:B:329:SER:HB2	1.97	0.46
1:A:149:ILE:HA	1:A:152:ASP:OD2	2.15	0.46
1:B:672:VAL:HA	1:B:675:LEU:HD12	1.96	0.46
2:C:100:TRP:HD1	2:C:229:ASP:HA	1.80	0.46
1:A:502:VAL:HG23	1:A:503:VAL:HG12	1.97	0.46
1:A:503:VAL:HG21	1:A:517:TYR:C	2.36	0.46
2:C:252:LEU:HD22	2:C:256:TYR:CD2	2.50	0.46
1:B:371:THR:HB	1:B:389:VAL:HG23	1.96	0.46
1:A:498:ASN:OD1	1:A:499:PRO:HD2	2.15	0.46
1:A:745:ALA:O	1:A:748:LYS:HB3	2.15	0.46
1:A:418:THR:O	1:A:421:TYR:HD1	1.99	0.46
1:B:320:TRP:HA	1:B:325:MET:HE1	1.97	0.46
1:B:503:VAL:HG21	1:B:517:TYR:C	2.36	0.46
2:C:72:TYR:CD1	2:C:472:PHE:HZ	2.32	0.46
1:A:329:SER:HB3	1:A:331:PHE:HB3	1.98	0.46
2:C:366:TYR:HD1	2:C:378:LEU:HA	1.79	0.46
1:B:385:ARG:HD2	1:B:580:TRP:NE1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:PRO:HB2	1:B:182:ASN:H	1.43	0.46
2:C:129:ALA:O	2:C:133:LEU:HG	2.15	0.46
1:B:282:ASP:O	1:B:285:ARG:HB3	2.14	0.46
1:A:57:GLY:N	1:A:170:TYR:HB2	2.30	0.46
2:C:539:ARG:HH11	2:C:542:ARG:HH11	1.63	0.46
2:C:146:ARG:O	2:C:163:LYS:NZ	2.48	0.46
1:B:308:PHE:HE2	1:B:318:ILE:HG13	1.80	0.46
1:B:280:GLY:N	1:B:282:ASP:OD1	2.48	0.46
1:B:321:PHE:CD1	2:C:461:LYS:C	2.89	0.46
1:B:36:LEU:C	1:B:502:VAL:HG11	2.35	0.46
1:B:69:LEU:HD22	1:B:172:TYR:HD2	1.80	0.46
1:A:212:ALA:HB3	1:A:219:ALA:HB3	1.97	0.46
1:B:149:ILE:HA	1:B:152:ASP:OD2	2.15	0.46
1:B:678:ILE:HA	1:B:681:ILE:HG12	1.97	0.46
2:C:357:PHE:CD1	2:C:361:LEU:CD2	2.99	0.46
1:B:279:ASN:OD1	2:C:506:ARG:HG2	2.16	0.46
2:C:362:LYS:HE3	2:C:388:GLU:OE2	2.16	0.46
1:A:56:VAL:HG13	1:A:66:TYR:CE1	2.50	0.46
2:C:95:MET:HA	2:C:251:ARG:HH22	1.79	0.46
2:C:286:VAL:O	2:C:290:VAL:HG23	2.15	0.46
2:C:306:THR:O	2:C:309:ASN:HB3	2.15	0.46
2:C:15:GLN:HE22	2:C:25:GLN:HE22	1.62	0.46
2:C:525:GLN:HE22	2:C:571:ILE:HD13	1.81	0.46
1:B:176:ARG:C	1:B:447:ARG:HH12	2.19	0.46
1:A:281:ILE:HG22	1:A:319:PRO:HB2	1.98	0.46
1:B:566:LEU:HD12	1:B:568:LEU:HD23	1.98	0.46
1:B:209:MET:O	1:B:210:LEU:HB2	2.16	0.46
1:B:210:LEU:HB3	1:B:212:ALA:O	2.16	0.46
1:B:739:SER:OG	1:B:742:GLU:OE1	2.32	0.46
1:A:580:TRP:HA	1:A:581:HIS:C	2.36	0.46
1:B:498:ASN:OD1	1:B:499:PRO:HD2	2.15	0.46
2:C:73:GLY:CA	2:C:492:HIS:HA	2.45	0.46
1:B:303:ARG:HB2	1:B:513:GLN:OE1	2.15	0.46
1:B:316:THR:CG2	2:C:465:LEU:C	2.84	0.46
1:B:349:ILE:HD12	1:B:349:ILE:HA	1.78	0.46
1:A:559:GLU:OE1	1:A:559:GLU:N	2.49	0.46
1:A:566:LEU:HD12	1:A:568:LEU:HD23	1.98	0.46
2:C:226:MET:HB3	2:C:242:LEU:CG	2.41	0.46
2:C:114:LEU:HD22	2:C:486:MET:N	2.30	0.46
2:C:105:ASN:ND2	2:C:330:THR:O	2.48	0.46
1:B:56:VAL:HG13	1:B:66:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:LEU:HD22	2:C:153:ILE:HG23	1.98	0.46
1:A:365:GLN:CA	1:A:562:GLN:HB2	2.41	0.46
2:C:496:PHE:CE2	2:C:497:LEU:HD13	2.51	0.46
1:B:685:GLY:HA2	1:B:686:ILE:HA	1.53	0.46
2:C:495:ALA:HB2	2:C:500:ILE:HG12	1.98	0.46
1:B:503:VAL:HG22	1:B:504:SER:H	1.81	0.46
1:B:410:VAL:O	1:B:414:VAL:HG23	2.16	0.46
1:B:75:GLN:HE22	1:B:447:ARG:NH2	2.14	0.46
1:A:75:GLN:HE22	1:A:447:ARG:NH2	2.14	0.46
2:C:290:VAL:O	2:C:293:LYS:HB3	2.16	0.46
1:A:678:ILE:HA	1:A:681:ILE:HG12	1.97	0.46
1:B:261:TRP:HE1	1:B:288:LEU:HD11	1.81	0.46
1:A:317:ILE:O	1:A:320:TRP:HB3	2.16	0.46
1:B:712:SER:C	1:B:715:HIS:HD1	2.16	0.46
2:C:326:SER:O	2:C:486:MET:HE1	2.16	0.46
2:C:175:GLU:HG3	2:C:352:TRP:CD1	2.51	0.46
2:C:88:ARG:HG2	2:C:264:PHE:HE1	1.81	0.46
1:B:365:GLN:CA	1:B:562:GLN:HB2	2.41	0.46
2:C:411:LEU:O	2:C:414:GLN:HB2	2.16	0.46
1:B:666:ARG:HA	1:B:669:GLN:NE2	2.31	0.46
1:B:666:ARG:O	1:B:670:ASN:ND2	2.49	0.46
2:C:224:ASP:OD1	2:C:247:LYS:NZ	2.39	0.46
2:C:407:SER:HA	2:C:410:TYR:CD2	2.50	0.46
1:B:281:ILE:HG22	1:B:319:PRO:HB2	1.98	0.45
2:C:315:LYS:HA	2:C:509:PRO:O	2.15	0.45
2:C:518:ILE:O	2:C:522:LEU:HG	2.16	0.45
1:A:36:LEU:C	1:A:502:VAL:HG11	2.36	0.45
2:C:335:TRP:HA	2:C:338:ASP:OD2	2.16	0.45
2:C:481:ASN:HD21	2:C:483:SER:HB3	1.81	0.45
2:C:115:ALA:HB3	2:C:485:TYR:CZ	2.51	0.45
2:C:3:ARG:NH2	2:C:231:GLU:OE2	2.49	0.45
2:C:302:PHE:O	2:C:304:HIS:CD2	2.69	0.45
1:A:454:ASP:HA	1:A:455:PRO:HD2	1.82	0.45
1:A:477:ASN:O	1:A:481:ARG:N	2.47	0.45
2:C:402:GLY:O	2:C:406:MET:HG2	2.16	0.45
1:B:503:VAL:HG11	1:B:517:TYR:O	2.16	0.45
1:B:559:GLU:N	1:B:559:GLU:OE1	2.49	0.45
1:A:350:ASP:N	1:A:350:ASP:OD1	2.49	0.45
1:A:315:SER:O	1:A:319:PRO:HD2	2.16	0.45
1:A:209:MET:O	1:A:210:LEU:HB2	2.16	0.45
1:A:666:ARG:O	1:A:670:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:HIS:O	1:A:159:SER:OG	2.30	0.45
1:B:101:GLU:N	1:B:101:GLU:OE1	2.49	0.45
1:B:317:ILE:O	1:B:320:TRP:HB3	2.16	0.45
1:B:316:THR:HG23	2:C:466:VAL:HA	1.92	0.45
2:C:69:VAL:HA	2:C:75:VAL:HA	1.97	0.45
1:B:117:ALA:H	1:B:221:ALA:N	1.94	0.45
2:C:518:ILE:O	2:C:521:MET:HB3	2.16	0.45
1:A:263:PRO:HG3	1:A:504:SER:HA	1.97	0.45
1:B:45:SER:C	1:B:332:LYS:HD2	2.37	0.45
2:C:199:TYR:HA	2:C:274:GLY:O	2.17	0.45
1:B:371:THR:O	1:B:623:ILE:HD12	2.16	0.45
1:B:201:ALA:HB1	1:B:239:ARG:HD3	1.98	0.45
1:B:282:ASP:OD1	1:B:282:ASP:N	2.48	0.45
2:C:69:VAL:HG22	2:C:75:VAL:HG13	1.98	0.45
1:A:261:TRP:HE1	1:A:288:LEU:HD11	1.81	0.45
2:C:344:LEU:HD13	2:C:354:VAL:HG22	1.98	0.45
1:B:595:VAL:HG12	1:B:597:ILE:HG23	1.99	0.45
2:C:144:LYS:HD2	2:C:648:GLY:HA2	1.99	0.45
1:B:159:SER:HG	1:B:160:PRO:HD3	1.81	0.45
1:A:298:VAL:HG21	1:A:514:GLY:O	2.17	0.45
1:B:315:SER:O	1:B:319:PRO:HD2	2.16	0.45
2:C:521:MET:SD	2:C:554:MET:HG3	2.56	0.45
1:A:176:ARG:C	1:A:447:ARG:HH12	2.19	0.45
1:A:45:SER:C	1:A:332:LYS:HD2	2.37	0.45
1:B:328:VAL:HG23	1:B:329:SER:CB	2.46	0.45
1:A:210:LEU:HB3	1:A:212:ALA:O	2.16	0.45
1:B:156:HIS:O	1:B:159:SER:OG	2.30	0.45
1:A:652:ARG:O	1:A:653:THR:OG1	2.30	0.45
1:A:615:GLY:HA2	1:A:616:GLN:HA	1.64	0.45
1:B:313:LEU:HB3	1:B:314:SER:HB3	1.99	0.45
1:A:313:LEU:HB3	1:A:314:SER:HB3	1.99	0.45
1:A:567:ASP:OD2	1:A:570:ASN:ND2	2.31	0.45
1:A:16:LEU:HD21	1:A:462:LEU:HB3	1.99	0.45
1:B:212:ALA:HB3	1:B:219:ALA:HB3	1.97	0.45
1:A:669:GLN:O	1:A:673:THR:N	2.39	0.45
1:A:101:GLU:N	1:A:101:GLU:OE1	2.49	0.45
2:C:53:PHE:O	2:C:57:LEU:HB2	2.17	0.45
2:C:332:TRP:NE1	2:C:336:LEU:HD23	2.31	0.45
2:C:253:LYS:HD3	2:C:259:ASP:HA	1.97	0.45
1:B:567:ASP:OD2	1:B:570:ASN:ND2	2.31	0.45
2:C:307:ARG:HH22	2:C:513:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:VAL:HG12	1:A:597:ILE:HG23	1.99	0.45
2:C:144:LYS:CD	2:C:648:GLY:HA2	2.47	0.45
1:B:337:ASN:O	1:B:341:SER:N	2.50	0.45
2:C:100:TRP:CD1	2:C:229:ASP:HA	2.52	0.45
1:B:510:ALA:HA	1:B:511:ALA:HA	1.72	0.45
2:C:69:VAL:HG11	2:C:493:GLY:N	2.32	0.45
1:A:224:LEU:HA	1:A:227:GLN:HB3	1.99	0.45
1:B:580:TRP:HA	1:B:581:HIS:C	2.36	0.45
1:A:410:VAL:O	1:A:414:VAL:HG23	2.17	0.45
2:C:120:SER:OG	2:C:122:ARG:HB3	2.16	0.45
1:A:428:GLY:HA3	1:A:429:THR:HA	1.59	0.45
1:B:350:ASP:OD1	1:B:350:ASP:N	2.49	0.45
1:A:349:ILE:HA	1:A:349:ILE:HD12	1.79	0.45
1:A:260:LEU:HD11	1:A:285:ARG:HH12	1.82	0.45
1:A:503:VAL:HG22	1:A:504:SER:H	1.81	0.45
1:A:383:ASN:O	1:A:385:ARG:N	2.38	0.45
1:A:371:THR:O	1:A:623:ILE:HD12	2.16	0.45
1:A:666:ARG:HA	1:A:669:GLN:NE2	2.31	0.45
1:B:652:ARG:O	1:B:653:THR:OG1	2.30	0.45
2:C:317:TRP:HH2	2:C:449:ILE:HG23	1.81	0.45
1:B:329:SER:HB3	1:B:331:PHE:HB3	1.98	0.45
2:C:102:LEU:O	2:C:389:VAL:HG12	2.17	0.45
1:A:55:GLU:N	1:A:55:GLU:OE1	2.50	0.45
1:B:366:PHE:O	1:B:368:LYS:HD2	2.17	0.45
1:B:674:LEU:HA	1:B:677:LYS:HG2	1.99	0.45
1:A:337:ASN:O	1:A:341:SER:N	2.50	0.45
1:B:418:THR:O	1:B:421:TYR:HD1	1.99	0.45
1:B:298:VAL:HG21	1:B:514:GLY:O	2.17	0.45
1:B:271:PRO:HA	1:B:276:ARG:HD3	2.00	0.44
2:C:82:THR:HG22	2:C:83:ASN:O	2.17	0.44
1:A:223:ALA:O	1:A:227:GLN:N	2.34	0.44
1:B:116:ARG:HA	1:B:118:ILE:H	1.82	0.44
1:A:328:VAL:HG23	1:A:329:SER:CB	2.46	0.44
1:B:211:GLN:O	1:B:218:GLY:HA3	2.18	0.44
1:B:174:VAL:HB	1:B:175:GLY:H	1.57	0.44
1:A:674:LEU:HA	1:A:677:LYS:NZ	2.32	0.44
1:B:425:SER:OG	1:B:659:GLU:OE2	2.26	0.44
2:C:504:ASP:OD2	2:C:506:ARG:NH2	2.50	0.44
1:A:385:ARG:HD2	1:A:580:TRP:NE1	2.29	0.44
1:B:366:PHE:CD2	1:B:405:GLY:HA2	2.52	0.44
1:A:674:LEU:HA	1:A:677:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ASN:HD21	1:B:496:ALA:HB2	1.80	0.44
1:A:320:TRP:HA	1:A:325:MET:HE1	1.98	0.44
2:C:253:LYS:HB2	2:C:260:VAL:CG2	2.47	0.44
2:C:526:PHE:C	2:C:528:PRO:HD3	2.37	0.44
2:C:146:ARG:HB3	2:C:149:SER:HB3	1.98	0.44
2:C:135:PHE:HB3	2:C:349:TYR:CE1	2.52	0.44
1:A:500:GLU:HB3	1:A:521:ASN:H	1.83	0.44
2:C:554:MET:HB3	2:C:554:MET:HE2	1.83	0.44
2:C:253:LYS:O	2:C:257:GLY:HA2	2.16	0.44
2:C:598:LEU:HA	2:C:601:TYR:CD2	2.53	0.44
2:C:363:LEU:O	2:C:387:LEU:HD12	2.17	0.44
1:B:737:LEU:O	1:B:738:LEU:HG	2.18	0.44
2:C:453:ASP:OD1	2:C:454:ASP:N	2.51	0.44
2:C:222:SER:O	2:C:247:LYS:NZ	2.50	0.44
1:A:216:ALA:HA	1:A:217:LYS:HA	1.72	0.44
1:B:362:GLU:OE1	1:B:443:SER:OG	2.35	0.44
1:B:16:LEU:HD21	1:B:462:LEU:HB3	1.99	0.44
2:C:628:LEU:HD12	2:C:632:TRP:O	2.16	0.44
1:A:201:ALA:HB1	1:A:239:ARG:HD3	1.98	0.44
1:B:260:LEU:HD11	1:B:285:ARG:HH12	1.82	0.44
2:C:637:VAL:HB	2:C:642:HIS:HD2	1.82	0.44
2:C:288:GLN:CA	2:C:291:ARG:HH11	2.30	0.44
1:B:389:VAL:HG13	1:B:391:PRO:HD3	1.99	0.44
2:C:550:ALA:HA	2:C:553:SER:OG	2.17	0.44
1:B:107:THR:OG1	1:B:226:SER:OG	2.18	0.44
2:C:38:GLU:CD	2:C:41:GLU:HA	2.37	0.44
1:B:674:LEU:HA	1:B:677:LYS:NZ	2.32	0.44
1:A:497:HIS:HE2	1:A:548:ALA:C	2.20	0.44
2:C:466:VAL:HG13	2:C:470:ARG:HH12	1.82	0.44
1:B:3:ASN:HA	1:B:436:GLU:HB3	1.98	0.44
1:A:358:VAL:N	1:A:437:MET:HB3	2.31	0.44
1:A:116:ARG:HA	1:A:118:ILE:H	1.82	0.44
1:A:503:VAL:HG11	1:A:517:TYR:O	2.16	0.44
2:C:153:ILE:HG21	2:C:198:ALA:O	2.18	0.44
1:B:55:GLU:N	1:B:55:GLU:OE1	2.51	0.44
2:C:213:LEU:HD11	2:C:218:GLY:HA2	2.00	0.44
1:A:454:ASP:O	1:A:457:VAL:HG12	2.18	0.44
2:C:659:ARG:HA	2:C:664:ARG:O	2.18	0.44
1:A:424:VAL:HG12	1:A:425:SER:O	2.18	0.44
2:C:565:SER:HA	2:C:568:LEU:HD13	1.99	0.44
1:A:362:GLU:OE1	1:A:443:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:HA	1:A:436:GLU:HB3	1.98	0.44
2:C:198:ALA:HA	2:C:364:PRO:O	2.18	0.44
1:A:732:LEU:O	1:A:735:MET:HB3	2.18	0.44
1:A:590:GLU:OE1	1:A:607:LYS:HD3	2.18	0.44
2:C:521:MET:HA	2:C:524:ASN:OD1	2.17	0.44
2:C:555:LYS:HD3	2:C:564:TYR:CE2	2.53	0.44
2:C:337:ARG:CZ	2:C:362:LYS:HD2	2.48	0.44
2:C:528:PRO:HG2	2:C:544:ARG:HH12	1.83	0.44
2:C:584:ARG:O	2:C:588:GLU:HG3	2.18	0.44
1:A:737:LEU:O	1:A:738:LEU:HG	2.18	0.44
1:B:500:GLU:HB3	1:B:521:ASN:H	1.83	0.44
1:B:368:LYS:HE2	1:B:402:ALA:O	2.18	0.44
1:A:59:GLY:HA3	1:A:155:CYS:HB3	2.00	0.44
2:C:75:VAL:O	2:C:503:TYR:N	2.43	0.43
2:C:517:ASN:OD1	2:C:518:ILE:N	2.51	0.43
1:B:177:THR:HA	1:B:447:ARG:HH22	1.83	0.43
2:C:105:ASN:HB2	2:C:108:LYS:HD3	2.00	0.43
1:B:199:LEU:HD23	1:B:203:SER:HB2	1.99	0.43
1:B:66:TYR:HD1	1:B:69:LEU:HD12	1.83	0.43
1:A:211:GLN:O	1:A:218:GLY:HA3	2.18	0.43
1:B:732:LEU:O	1:B:735:MET:HB3	2.18	0.43
1:A:630:HIS:HD2	1:A:633:ILE:HD11	1.83	0.43
1:A:368:LYS:HE2	1:A:402:ALA:O	2.18	0.43
1:B:719:ASN:O	1:B:722:ARG:HB3	2.18	0.43
2:C:152:CYS:N	2:C:156:PHE:HA	2.32	0.43
2:C:300:TYR:CZ	2:C:442:GLY:HA3	2.53	0.43
1:A:271:PRO:HA	1:A:276:ARG:HD3	2.00	0.43
1:B:57:GLY:N	1:B:170:TYR:HB2	2.30	0.43
2:C:411:LEU:HD21	2:C:435:PHE:CE2	2.53	0.43
1:A:366:PHE:CD2	1:A:405:GLY:HA2	2.52	0.43
1:A:521:ASN:O	1:A:539:SER:OG	2.10	0.43
2:C:128:ARG:HA	2:C:339:LEU:HD21	2.00	0.43
1:B:549:ILE:HA	1:B:552:ASN:HB2	2.00	0.43
1:B:754:ASN:HB3	1:B:755:ALA:C	2.39	0.43
1:B:216:ALA:HA	1:B:217:LYS:HA	1.72	0.43
1:A:176:ARG:NH1	1:A:447:ARG:HA	2.26	0.43
1:A:715:HIS:HB2	1:A:716:VAL:HG13	2.01	0.43
2:C:251:ARG:C	2:C:254:GLU:HB3	2.38	0.43
2:C:151:THR:HG23	2:C:157:SER:O	2.19	0.43
2:C:344:LEU:HB3	2:C:349:TYR:HB2	2.00	0.43
2:C:585:ALA:HA	2:C:588:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:328:HIS:CG	2:C:453:ASP:HB3	2.53	0.43
1:B:41:THR:OG1	1:B:42:ARG:N	2.51	0.43
1:A:366:PHE:O	1:A:368:LYS:HD2	2.17	0.43
2:C:40:TYR:CD1	2:C:43:LEU:HD22	2.49	0.43
1:B:590:GLU:OE1	1:B:607:LYS:HD3	2.18	0.43
2:C:652:GLU:O	2:C:655:GLU:HB3	2.18	0.43
1:A:138:LEU:HB3	1:A:139:ALA:H	1.69	0.43
1:B:68:ARG:CZ	1:B:330:PRO:HG3	2.49	0.43
1:B:497:HIS:HE2	1:B:548:ALA:C	2.20	0.43
1:B:221:ALA:HB1	1:B:224:LEU:HB3	1.99	0.43
1:A:199:LEU:HD23	1:A:203:SER:HB2	1.99	0.43
2:C:96:ILE:O	2:C:246:SER:N	2.51	0.43
1:B:204:SER:O	1:B:206:ASP:N	2.52	0.43
2:C:135:PHE:HB3	2:C:349:TYR:CZ	2.52	0.43
1:B:369:GLU:HA	1:B:398:SER:CB	2.49	0.43
1:B:590:GLU:OE2	1:B:607:LYS:HA	2.18	0.43
1:A:345:GLN:HE22	1:A:549:ILE:HG23	1.83	0.43
1:A:754:ASN:H	1:A:755:ALA:HA	1.83	0.43
1:A:682:GLY:O	1:A:684:THR:N	2.51	0.43
2:C:150:SER:HA	2:C:158:ASN:HA	2.00	0.43
1:B:358:VAL:N	1:B:437:MET:HB3	2.31	0.43
1:A:56:VAL:HB	1:A:170:TYR:HB2	2.00	0.43
1:A:66:TYR:HD1	1:A:69:LEU:HD12	1.83	0.43
2:C:154:PRO:HD3	2:C:276:PRO:HA	2.00	0.43
2:C:615:THR:O	2:C:619:LEU:HG	2.18	0.43
1:B:345:GLN:HE22	1:B:549:ILE:HG23	1.83	0.43
2:C:406:MET:HE1	2:C:488:ILE:CD1	2.49	0.43
1:B:441:PHE:HA	1:B:442:PRO:HD2	1.73	0.43
1:A:293:ALA:O	1:A:297:MET:HB2	2.19	0.43
1:A:87:ASN:O	1:A:90:THR:OG1	2.28	0.43
1:B:322:ILE:H	2:C:461:LYS:NZ	1.79	0.43
1:A:359:VAL:HG22	1:A:437:MET:O	2.19	0.43
2:C:279:LEU:HD23	2:C:360:SER:HB3	2.00	0.43
2:C:51:LEU:HB3	2:C:264:PHE:CE2	2.53	0.43
2:C:3:ARG:HH21	2:C:234:VAL:HG21	1.83	0.43
1:B:54:TRP:CH2	1:B:174:VAL:HG12	2.54	0.43
2:C:223:LYS:HD3	2:C:225:ARG:NH1	2.34	0.43
2:C:120:SER:O	2:C:123:ASP:HB2	2.18	0.43
1:B:424:VAL:HG12	1:B:425:SER:O	2.18	0.43
1:A:628:VAL:O	1:A:632:ILE:HD12	2.19	0.43
1:B:38:LEU:HD23	1:B:39:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ALA:O	1:B:349:ILE:HG22	2.18	0.43
1:B:56:VAL:HB	1:B:170:TYR:HB2	2.00	0.43
1:B:566:LEU:CD1	1:B:568:LEU:HB3	2.49	0.43
2:C:171:LEU:HA	2:C:657:PHE:CD1	2.54	0.43
2:C:232:TYR:HB2	2:C:241:SER:N	2.34	0.43
1:A:54:TRP:CH2	1:A:174:VAL:HG12	2.54	0.43
1:A:177:THR:HA	1:A:447:ARG:HH22	1.83	0.43
1:A:291:PHE:O	1:A:292:ILE:HB	2.19	0.43
1:A:566:LEU:CD1	1:A:568:LEU:HB3	2.49	0.43
2:C:146:ARG:HD2	2:C:645:LEU:O	2.19	0.43
1:B:630:HIS:HD2	1:B:633:ILE:HD11	1.83	0.43
1:A:389:VAL:HG13	1:A:391:PRO:HD3	1.99	0.43
1:B:544:GLU:HG2	1:B:545:PRO:HD2	2.01	0.43
2:C:448:GLN:HB3	2:C:457:LEU:HD23	1.99	0.43
1:B:402:ALA:HB3	1:B:403:PRO:HD3	2.01	0.43
1:B:454:ASP:O	1:B:457:VAL:HG12	2.18	0.43
1:A:259:ARG:HG3	1:A:269:LEU:HD13	2.01	0.43
1:B:259:ARG:O	1:B:262:SER:OG	2.23	0.43
1:B:224:LEU:HA	1:B:227:GLN:HB3	1.99	0.43
2:C:596:LEU:O	2:C:599:SER:OG	2.20	0.43
1:A:369:GLU:HA	1:A:398:SER:CB	2.49	0.43
1:B:523:ARG:HA	1:B:539:SER:HB2	2.01	0.43
1:A:41:THR:OG1	1:A:42:ARG:N	2.51	0.43
2:C:413:MET:CE	2:C:482:PRO:HG2	2.49	0.43
2:C:54:LYS:NZ	2:C:91:ASN:HD22	2.17	0.43
1:A:754:ASN:HB3	1:A:755:ALA:C	2.39	0.43
1:B:182:ASN:HD21	1:B:184:TYR:HD2	1.67	0.43
1:A:241:ARG:HG3	1:A:243:ASN:H	1.84	0.43
1:A:204:SER:O	1:A:206:ASP:N	2.52	0.43
2:C:627:LYS:HB2	2:C:632:TRP:HZ3	1.83	0.43
2:C:171:LEU:HD22	2:C:657:PHE:CG	2.54	0.43
2:C:232:TYR:CE2	2:C:237:GLY:HA2	2.54	0.43
2:C:232:TYR:HA	2:C:239:GLN:O	2.18	0.43
1:B:520:TRP:CH2	1:B:545:PRO:HG3	2.54	0.43
1:A:107:THR:OG1	1:A:226:SER:OG	2.18	0.43
2:C:302:PHE:HZ	2:C:440:TRP:CD2	2.36	0.43
1:A:549:ILE:HA	1:A:552:ASN:HB2	2.00	0.43
2:C:210:ALA:HB3	2:C:223:LYS:HB2	2.00	0.43
2:C:520:SER:HA	2:C:523:ASN:ND2	2.34	0.43
1:A:377:LYS:HD2	1:A:380:ASN:HA	2.01	0.43
1:B:82:VAL:O	1:B:86:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:PHE:O	1:B:292:ILE:HB	2.19	0.42
1:A:221:ALA:HB1	1:A:224:LEU:HB3	2.00	0.42
2:C:86:GLY:O	2:C:208:THR:HA	2.18	0.42
2:C:627:LYS:HA	2:C:630:TYR:CE1	2.54	0.42
2:C:124:ASN:HD21	2:C:128:ARG:HE	1.66	0.42
2:C:523:ASN:O	2:C:527:SER:N	2.51	0.42
1:B:377:LYS:HD2	1:B:380:ASN:HA	2.01	0.42
1:B:293:ALA:O	1:B:297:MET:HB2	2.19	0.42
1:A:38:LEU:HD23	1:A:39:GLN:O	2.19	0.42
2:C:181:MET:C	2:C:184:GLY:H	2.23	0.42
1:A:413:PHE:CZ	1:A:636:TRP:HA	2.54	0.42
2:C:235:THR:O	2:C:238:GLU:N	2.36	0.42
1:B:655:ARG:H	1:B:656:ASP:CB	2.30	0.42
1:A:520:TRP:CH2	1:A:545:PRO:HG3	2.54	0.42
2:C:298:TYR:CD2	2:C:440:TRP:HE3	2.38	0.42
1:B:59:GLY:HA3	1:B:155:CYS:HB3	2.00	0.42
1:B:259:ARG:HG3	1:B:269:LEU:HD13	2.01	0.42
1:A:68:ARG:CZ	1:A:330:PRO:HG3	2.49	0.42
2:C:81:ARG:HG3	2:C:82:THR:OG1	2.19	0.42
1:A:331:PHE:O	1:A:332:LYS:HG2	2.19	0.42
2:C:17:LEU:O	2:C:154:PRO:HB2	2.19	0.42
2:C:201:VAL:HG23	2:C:366:TYR:O	2.19	0.42
1:A:373:PHE:CE1	1:A:387:LEU:HD22	2.54	0.42
1:A:182:ASN:HD21	1:A:184:TYR:HD2	1.67	0.42
2:C:566:ASP:HA	2:C:569:GLU:CD	2.39	0.42
1:B:357:HIS:HA	1:B:437:MET:HG2	2.02	0.42
1:A:355:PRO:O	1:A:356:SER:OG	2.28	0.42
1:B:715:HIS:HB2	1:B:716:VAL:HG13	2.01	0.42
2:C:250:SER:HA	2:C:253:LYS:CB	2.50	0.42
1:B:44:PHE:HE1	1:B:180:TYR:N	2.18	0.42
2:C:102:LEU:HD12	2:C:233:ALA:HA	2.00	0.42
1:A:655:ARG:H	1:A:656:ASP:CB	2.30	0.42
1:A:719:ASN:O	1:A:722:ARG:HB3	2.18	0.42
1:B:368:LYS:HA	1:B:401:LEU:HD23	2.01	0.42
1:B:628:VAL:O	1:B:632:ILE:HD12	2.19	0.42
1:A:523:ARG:HA	1:A:539:SER:HB2	2.01	0.42
2:C:413:MET:CG	2:C:417:HIS:HD2	2.33	0.42
1:A:82:VAL:O	1:A:86:VAL:HG23	2.19	0.42
1:B:682:GLY:O	1:B:684:THR:N	2.51	0.42
1:A:510:ALA:HA	1:A:511:ALA:HA	1.72	0.42
1:A:357:HIS:HA	1:A:437:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:151:THR:HG22	2:C:163:LYS:CG	2.49	0.42
1:B:331:PHE:O	1:B:332:LYS:HG2	2.19	0.42
1:B:241:ARG:HG3	1:B:243:ASN:H	1.84	0.42
1:B:80:LEU:HA	1:B:81:SER:HA	1.78	0.42
2:C:5:PRO:HB2	2:C:7:PHE:CE1	2.55	0.42
1:B:359:VAL:HG22	1:B:437:MET:O	2.19	0.42
1:B:413:PHE:CZ	1:B:636:TRP:HA	2.54	0.42
1:A:348:ALA:O	1:A:349:ILE:HG22	2.18	0.42
1:A:289:ALA:C	1:A:291:PHE:H	2.22	0.42
2:C:193:HIS:HB3	2:C:195:MET:HG3	2.00	0.42
2:C:353:TRP:O	2:C:356:LEU:HB2	2.20	0.42
2:C:230:PHE:O	2:C:234:VAL:HG22	2.20	0.42
1:B:133:GLU:O	1:B:137:THR:HG23	2.20	0.42
1:A:590:GLU:OE2	1:A:607:LYS:HA	2.18	0.42
1:B:553:LYS:O	1:B:555:ILE:HG23	2.20	0.42
1:A:43:THR:HA	1:A:289:ALA:CB	2.50	0.42
2:C:26:GLN:O	2:C:30:ARG:N	2.53	0.42
2:C:283:ILE:HG23	2:C:397:ALA:HB2	2.01	0.42
1:A:212:ALA:H	1:A:218:GLY:C	2.23	0.42
1:A:553:LYS:O	1:A:555:ILE:HG23	2.20	0.42
1:A:246:ALA:O	1:A:249:VAL:HG22	2.19	0.42
1:B:289:ALA:C	1:B:291:PHE:H	2.22	0.42
1:A:2:PHE:HE2	1:A:4:LEU:HD23	1.85	0.42
2:C:484:PRO:HG2	2:C:485:TYR:CE2	2.55	0.42
1:B:383:ASN:C	1:B:385:ARG:H	2.22	0.42
1:B:212:ALA:H	1:B:218:GLY:C	2.23	0.42
1:A:608:GLU:HG3	1:A:609:PHE:N	2.35	0.42
2:C:430:PRO:O	2:C:433:CYS:HB2	2.20	0.42
2:C:549:LEU:HA	2:C:591:LEU:HD13	2.01	0.42
1:B:2:PHE:HE2	1:B:4:LEU:HD23	1.85	0.42
1:B:657:ASP:O	1:B:660:LYS:HG2	2.20	0.42
2:C:350:ALA:HA	2:C:351:PRO:HD3	1.71	0.42
1:B:243:ASN:ND2	2:C:422:LEU:HD21	2.35	0.42
2:C:381:ASP:C	2:C:383:SER:H	2.18	0.42
1:A:41:THR:HG23	1:A:286:SER:O	2.20	0.42
1:B:246:ALA:O	1:B:249:VAL:HG22	2.19	0.42
1:A:331:PHE:C	1:A:332:LYS:HG2	2.41	0.42
2:C:96:ILE:H	2:C:251:ARG:HH22	1.68	0.42
2:C:96:ILE:HG12	2:C:269:ARG:NH1	2.35	0.42
2:C:55:ASN:OD1	2:C:59:ARG:NE	2.43	0.42
2:C:414:GLN:NE2	2:C:457:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:HA	1:A:401:LEU:HD23	2.01	0.42
1:B:43:THR:HA	1:B:289:ALA:CB	2.50	0.41
2:C:559:GLY:HA2	2:C:564:TYR:CD1	2.55	0.41
1:B:754:ASN:H	1:B:755:ALA:HA	1.83	0.41
2:C:209:ASP:OD2	2:C:222:SER:HB2	2.20	0.41
1:B:377:LYS:HE3	1:B:377:LYS:HB3	1.86	0.41
1:B:314:SER:HA	1:B:315:SER:C	2.40	0.41
1:B:536:GLU:OE1	1:B:536:GLU:N	2.40	0.41
2:C:551:TRP:HB2	2:C:587:ARG:NH2	2.35	0.41
1:A:133:GLU:O	1:A:137:THR:HG23	2.20	0.41
1:B:498:ASN:C	1:B:500:GLU:H	2.24	0.41
1:A:366:PHE:HA	1:A:366:PHE:HD1	1.75	0.41
2:C:324:ASP:HB3	2:C:489:SER:O	2.20	0.41
2:C:325:VAL:HA	2:C:488:ILE:CD1	2.51	0.41
1:B:659:GLU:O	1:B:662:ALA:HB3	2.20	0.41
1:B:610:GLU:OE1	1:B:610:GLU:N	2.48	0.41
1:B:313:LEU:HA	1:B:314:SER:HA	1.83	0.41
1:B:373:PHE:CE1	1:B:387:LEU:HD22	2.55	0.41
1:B:243:ASN:ND2	2:C:422:LEU:HD22	2.35	0.41
1:A:402:ALA:HB3	1:A:403:PRO:HD3	2.01	0.41
1:B:608:GLU:HG3	1:B:609:PHE:N	2.35	0.41
1:B:3:ASN:HA	1:B:436:GLU:CB	2.50	0.41
2:C:173:LYS:HB3	2:C:176:GLU:HB3	2.02	0.41
2:C:35:GLY:HA2	2:C:93:PHE:HE1	1.85	0.41
1:A:383:ASN:C	1:A:385:ARG:H	2.22	0.41
2:C:414:GLN:O	2:C:419:ALA:N	2.45	0.41
1:A:544:GLU:HG2	1:A:545:PRO:HD2	2.01	0.41
1:B:41:THR:HG23	1:B:286:SER:O	2.20	0.41
1:A:366:PHE:CE1	1:A:629:ALA:HB2	2.54	0.41
1:B:141:SER:HB3	1:B:144:GLU:HA	2.03	0.41
2:C:214:ASP:O	2:C:218:GLY:N	2.43	0.41
1:B:239:ARG:CD	2:C:438:SER:OG	2.67	0.41
1:B:292:ILE:HA	1:B:295:GLN:CG	2.50	0.41
2:C:465:LEU:HG	2:C:469:HIS:NE2	2.35	0.41
1:B:349:ILE:HG21	1:B:354:GLN:O	2.20	0.41
2:C:96:ILE:C	2:C:245:ALA:HB1	2.41	0.41
2:C:536:VAL:HG12	2:C:538:ASP:H	1.85	0.41
2:C:326:SER:OG	2:C:331:PHE:HE2	2.03	0.41
1:B:169:ALA:HB3	1:B:575:ILE:HG13	2.03	0.41
2:C:3:ARG:CZ	2:C:230:PHE:HE2	2.33	0.41
2:C:411:LEU:HD13	2:C:439:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ILE:HD11	1:B:491:MET:HG3	2.02	0.41
1:A:657:ASP:O	1:A:660:LYS:HG2	2.20	0.41
2:C:160:MET:HA	2:C:163:LYS:HE2	2.03	0.41
1:B:183:PHE:O	1:B:187:VAL:HG23	2.21	0.41
2:C:103:ALA:HA	2:C:389:VAL:HG12	2.03	0.41
1:A:186:LEU:O	1:A:190:VAL:HG13	2.21	0.41
1:B:128:PRO:O	1:B:131:ILE:HB	2.21	0.41
2:C:496:PHE:O	2:C:499:ASP:HB2	2.20	0.41
1:B:521:ASN:HA	1:B:540:ILE:O	2.21	0.41
1:A:498:ASN:C	1:A:500:GLU:H	2.24	0.41
2:C:301:THR:HG22	2:C:450:SER:OG	2.21	0.41
1:B:428:GLY:HA3	1:B:429:THR:HA	1.59	0.41
1:A:349:ILE:HG21	1:A:354:GLN:O	2.20	0.41
1:A:436:GLU:CD	1:A:438:THR:H	2.23	0.41
1:A:44:PHE:HE1	1:A:180:TYR:N	2.18	0.41
2:C:539:ARG:HH21	2:C:545:PRO:CA	2.34	0.41
2:C:288:GLN:HA	2:C:291:ARG:HH11	1.85	0.41
1:A:174:VAL:HB	1:A:175:GLY:H	1.57	0.41
1:B:454:ASP:HA	1:B:455:PRO:HD2	1.82	0.41
1:B:381:ASN:OD1	1:B:381:ASN:N	2.54	0.41
2:C:357:PHE:CE2	2:C:361:LEU:HD13	2.47	0.41
2:C:361:LEU:HD23	2:C:361:LEU:N	2.35	0.41
1:B:257:LEU:O	1:B:260:LEU:HB3	2.21	0.41
1:B:284:LEU:HA	1:B:287:ASN:CG	2.41	0.41
1:B:313:LEU:HB2	2:C:466:VAL:HG11	1.96	0.41
1:A:281:ILE:O	1:A:284:LEU:HB2	2.21	0.41
1:A:292:ILE:HA	1:A:295:GLN:CG	2.50	0.41
1:A:292:ILE:HD11	1:A:491:MET:HG3	2.02	0.41
2:C:105:ASN:ND2	2:C:331:PHE:HA	2.34	0.41
2:C:13:LYS:NZ	2:C:187:ASP:OD2	2.46	0.41
1:A:183:PHE:O	1:A:187:VAL:HG23	2.21	0.41
1:A:128:PRO:HD3	1:A:166:PRO:HB2	2.03	0.41
1:A:128:PRO:O	1:A:131:ILE:HB	2.21	0.41
2:C:294:ILE:O	2:C:298:TYR:HB2	2.21	0.41
1:A:7:LYS:N	1:A:433:ASN:OD1	2.25	0.41
1:B:506:HIS:CD2	1:B:517:TYR:CE2	3.09	0.41
1:B:436:GLU:CD	1:B:438:THR:H	2.23	0.41
1:A:349:ILE:CD1	1:A:356:SER:HB2	2.51	0.41
1:A:257:LEU:O	1:A:260:LEU:HB3	2.21	0.41
1:A:284:LEU:HA	1:A:287:ASN:CG	2.41	0.41
2:C:96:ILE:H	2:C:251:ARG:NH2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:335:TRP:O	2:C:338:ASP:HB2	2.20	0.41
1:B:331:PHE:C	1:B:332:LYS:HG2	2.40	0.41
1:B:334:ARG:HG3	1:B:335:PRO:HD2	2.03	0.41
1:B:186:LEU:O	1:B:190:VAL:HG13	2.21	0.41
1:B:629:ALA:HA	1:B:632:ILE:HD13	2.02	0.41
1:B:423:ALA:HA	1:B:424:VAL:HA	1.48	0.41
1:A:230:ALA:HA	1:A:233:ALA:HB3	2.03	0.41
1:B:313:LEU:HD11	2:C:466:VAL:H	1.80	0.41
2:C:565:SER:HA	2:C:568:LEU:HD22	2.03	0.41
1:B:349:ILE:HG13	1:B:353:GLY:O	2.21	0.41
1:B:361:TYR:CG	1:B:414:VAL:HG21	2.56	0.41
1:A:4:LEU:H	1:A:436:GLU:CB	2.34	0.41
1:A:334:ARG:HG3	1:A:335:PRO:HD2	2.03	0.41
2:C:299:ALA:HA	2:C:302:PHE:HB2	2.02	0.41
1:A:753:SER:HA	1:A:754:ASN:HA	1.86	0.41
2:C:561:CYS:HA	2:C:562:PRO:HD3	1.89	0.41
2:C:327:ASP:HB3	2:C:331:PHE:CE2	2.55	0.40
2:C:435:PHE:CE1	2:C:439:TYR:HB2	2.56	0.40
1:B:674:LEU:HA	1:B:677:LYS:HZ2	1.85	0.40
2:C:469:HIS:O	2:C:472:PHE:HB3	2.20	0.40
2:C:74:ARG:HB2	2:C:503:TYR:CE1	2.55	0.40
1:B:349:ILE:CD1	1:B:356:SER:HB2	2.51	0.40
1:A:261:TRP:CZ3	1:A:291:PHE:HD1	2.39	0.40
1:A:313:LEU:HA	1:A:314:SER:HA	1.83	0.40
1:A:506:HIS:CD2	1:A:517:TYR:CE2	3.09	0.40
1:B:657:ASP:HA	1:B:660:LYS:HG2	2.04	0.40
1:B:657:ASP:HA	1:B:660:LYS:HE3	2.03	0.40
1:A:657:ASP:HA	1:A:660:LYS:HE3	2.03	0.40
2:C:546:PHE:HE2	2:C:598:LEU:HD13	1.86	0.40
2:C:575:TRP:CD1	2:C:583:TYR:HB2	2.56	0.40
1:B:720:ARG:HA	1:B:723:ILE:HG22	2.04	0.40
1:B:368:LYS:HG2	1:B:402:ALA:CA	2.49	0.40
2:C:298:TYR:OH	2:C:437:ASP:HA	2.21	0.40
2:C:37:ILE:HG21	2:C:529:GLU:O	2.21	0.40
2:C:663:PRO:O	2:C:664:ARG:HB2	2.22	0.40
1:B:287:ASN:C	1:B:289:ALA:N	2.75	0.40
1:A:436:GLU:O	1:A:438:THR:N	2.54	0.40
1:A:386:PHE:HE1	1:A:576:HIS:H	1.68	0.40
2:C:539:ARG:HG3	2:C:601:TYR:OH	2.21	0.40
1:B:386:PHE:HE1	1:B:576:HIS:H	1.68	0.40
2:C:586:TYR:HD2	2:C:587:ARG:HG2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:O	1:A:147:HIS:N	2.27	0.40
1:B:230:ALA:HA	1:B:233:ALA:HB3	2.03	0.40
1:A:27:ASN:OD1	1:A:28:GLN:N	2.54	0.40
1:A:659:GLU:O	1:A:662:ALA:HB3	2.20	0.40
1:B:281:ILE:O	1:B:284:LEU:HB2	2.21	0.40
1:B:313:LEU:CB	2:C:466:VAL:HG21	2.51	0.40
2:C:472:PHE:CZ	2:C:476:LYS:HD3	2.57	0.40
2:C:332:TRP:HA	2:C:333:PRO:HD2	1.94	0.40
1:A:314:SER:HA	1:A:315:SER:C	2.41	0.40
2:C:175:GLU:HA	2:C:352:TRP:CG	2.55	0.40
1:A:169:ALA:HB3	1:A:575:ILE:HG13	2.03	0.40
1:A:720:ARG:HA	1:A:723:ILE:HG22	2.04	0.40
1:A:521:ASN:HA	1:A:540:ILE:O	2.21	0.40
1:A:500:GLU:HG3	1:A:522:VAL:N	2.36	0.40
1:B:313:LEU:HD21	2:C:466:VAL:HG12	1.49	0.40
1:A:349:ILE:HG13	1:A:353:GLY:O	2.21	0.40
1:A:342:TYR:CD2	1:A:561:LEU:HD22	2.57	0.40
1:B:328:VAL:O	1:B:331:PHE:HD1	2.05	0.40
1:B:173:ARG:HH11	1:B:579:PRO:HG2	1.86	0.40
2:C:364:PRO:HB3	2:C:380:GLY:HA3	2.04	0.40
1:B:389:VAL:HG22	1:B:390:GLU:N	2.37	0.40
1:B:128:PRO:HD3	1:B:166:PRO:HB2	2.03	0.40
2:C:620:GLU:O	2:C:624:ASP:HB3	2.21	0.40
2:C:573:ARG:HG2	2:C:577:ASN:HD21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	759/761 (100%)	594 (78%)	91 (12%)	74 (10%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	759/761 (100%)	594 (78%)	91 (12%)	74 (10%)	1	14
2	C	662/664 (100%)	575 (87%)	61 (9%)	26 (4%)	4	36
All	All	2180/2186 (100%)	1763 (81%)	243 (11%)	174 (8%)	2	19

All (174) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	41	THR
1	A	129	THR
1	A	145	LEU
1	A	174	VAL
1	A	222	PRO
1	A	243	ASN
1	A	288	LEU
1	A	292	ILE
1	A	307	ILE
1	A	349	ILE
1	A	503	VAL
1	A	535	ILE
1	A	568	LEU
1	A	581	HIS
1	A	582	GLU
1	A	608	GLU
1	A	684	THR
1	A	738	LEU
1	B	31	VAL
1	B	41	THR
1	B	129	THR
1	B	145	LEU
1	B	174	VAL
1	B	222	PRO
1	B	243	ASN
1	B	288	LEU
1	B	292	ILE
1	B	307	ILE
1	B	332	LYS
1	B	349	ILE
1	B	503	VAL
1	B	535	ILE
1	B	568	LEU

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Mol	Chain	Res	Type
1	B	581	HIS
1	B	582	GLU
1	B	608	GLU
1	B	684	THR
1	B	738	LEU
2	C	22	ILE
2	C	154	PRO
2	C	236	GLY
2	C	528	PRO
2	C	564	TYR
1	A	45	SER
1	A	61	ILE
1	A	110	ILE
1	A	122	ALA
1	A	181	PRO
1	A	241	ARG
1	A	277	ASN
1	A	309	SER
1	A	316	THR
1	A	332	LYS
1	A	355	PRO
1	A	356	SER
1	A	381	ASN
1	A	502	VAL
1	A	522	VAL
1	A	537	GLY
1	A	555	ILE
1	A	558	SER
1	A	559	GLU
1	A	717	GLY
1	A	740	ARG
1	B	45	SER
1	B	61	ILE
1	B	110	ILE
1	B	122	ALA
1	B	181	PRO
1	B	241	ARG
1	B	277	ASN
1	B	309	SER
1	B	316	THR
1	B	355	PRO
1	B	356	SER

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Mol	Chain	Res	Type
1	B	381	ASN
1	B	502	VAL
1	B	522	VAL
1	B	537	GLY
1	B	555	ILE
1	B	558	SER
1	B	559	GLU
1	B	717	GLY
1	B	740	ARG
2	C	265	PHE
2	C	300	TYR
2	C	327	ASP
2	C	404	LEU
2	C	511	SER
2	C	545	PRO
1	A	34	LEU
1	A	167	ASP
1	A	205	VAL
1	A	214	PHE
1	A	335	PRO
1	A	351	HIS
1	A	384	GLN
1	A	409	ALA
1	A	584	SER
1	A	654	SER
1	A	739	SER
1	B	34	LEU
1	B	167	ASP
1	B	205	VAL
1	B	214	PHE
1	B	335	PRO
1	B	351	HIS
1	B	384	GLN
1	B	409	ALA
1	B	584	SER
1	B	654	SER
1	B	739	SER
2	C	2	ARG
2	C	382	PRO
2	C	529	GLU
2	C	584	ARG
1	A	113	SER

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Mol	Chain	Res	Type
1	A	178	ALA
1	A	273	ALA
1	A	312	GLU
1	A	375	PRO
1	A	556	GLN
1	B	49	THR
1	B	113	SER
1	B	178	ALA
1	B	273	ALA
1	B	312	GLU
1	B	375	PRO
1	B	556	GLN
2	C	119	VAL
2	C	254	GLU
2	C	464	ALA
1	A	42	ARG
1	A	49	THR
1	A	123	VAL
1	A	328	VAL
1	A	454	ASP
1	A	499	PRO
1	A	515	SER
1	A	624	LEU
1	A	628	VAL
1	B	42	ARG
1	B	123	VAL
1	B	328	VAL
1	B	454	ASP
1	B	499	PRO
1	B	515	SER
1	B	624	LEU
1	B	628	VAL
2	C	217	THR
2	C	484	PRO
2	C	607	ARG
1	A	246	ALA
1	A	329	SER
1	A	471	LEU
1	A	578	TRP
1	B	246	ALA
1	B	329	SER
1	B	471	LEU

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Mol	Chain	Res	Type
1	B	578	TRP
2	C	640	ASN
1	A	336	ILE
1	A	440	GLY
1	B	336	ILE
1	B	440	GLY
2	C	408	ILE
2	C	420	PRO
1	A	428	GLY
1	B	428	GLY
1	A	280	GLY
1	B	280	GLY
2	C	663	PRO
2	C	97	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/629 (100%)	627 (100%)	2 (0%)	94	96
1	B	629/629 (100%)	627 (100%)	2 (0%)	94	96
2	C	557/557 (100%)	557 (100%)	0	100	100
All	All	1815/1815 (100%)	1811 (100%)	4 (0%)	95	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	VAL
1	A	519	VAL
1	B	503	VAL
1	B	519	VAL

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

Mol	Chain	Res	Type
1	A	156	HIS
1	A	283	GLN
1	A	337	ASN
1	A	345	GLN
1	A	380	ASN
1	A	485	ASN
1	A	492	HIS
1	A	506	HIS
1	A	670	ASN
1	A	695	GLN
1	B	156	HIS
1	B	243	ASN
1	B	283	GLN
1	B	337	ASN
1	B	345	GLN
1	B	485	ASN
1	B	492	HIS
1	B	506	HIS
1	B	670	ASN
1	B	695	GLN
2	C	15	GLN
2	C	91	ASN
2	C	105	ASN
2	C	158	ASN
2	C	191	GLN
2	C	193	HIS
2	C	304	HIS
2	C	309	ASN
2	C	395	GLN
2	C	417	HIS
2	C	448	GLN
2	C	469	HIS
2	C	481	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.