



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 01:22 AM EST

PDB ID : 4EIW  
Title : Whole cytosolic region of atp-dependent metalloprotease FtsH (G399L)  
Authors : Suno, R.; Niwa, H.; Tsuchiya, D.; Yoshida, M.; Morikawa, K.  
Deposited on : 2012-04-06  
Resolution : 3.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

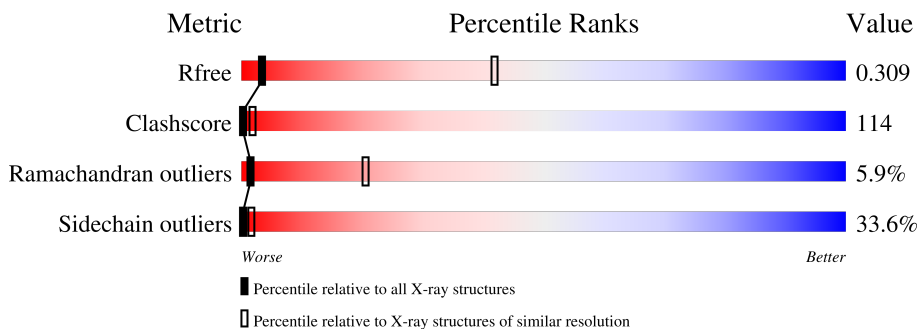
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	508	
1	B	508	
1	C	508	
1	D	508	
1	E	508	
1	F	508	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	B	2001	-	-	X	-
2	ADP	C	1001	-	-	X	-
2	ADP	D	2001	-	-	X	-
2	ADP	E	1001	-	-	X	-
2	ADP	F	2001	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 21429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	458	3578	2245	658	662	13	0	0	0
1	B	446	3511	2206	641	651	13	0	0	0
1	C	458	3578	2245	658	662	13	0	0	0
1	D	446	3511	2206	641	651	13	0	0	0
1	E	458	3578	2245	658	662	13	0	0	0
1	F	446	3511	2206	641	651	13	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	expression tag	UNP Q5SI82
A	118	PRO	-	expression tag	UNP Q5SI82
A	119	LEU	-	expression tag	UNP Q5SI82
A	120	GLY	-	expression tag	UNP Q5SI82
A	121	SER	-	expression tag	UNP Q5SI82
A	122	HIS	-	expression tag	UNP Q5SI82
A	123	MET	-	expression tag	UNP Q5SI82
A	124	GLY	-	expression tag	UNP Q5SI82
A	125	ALA	-	expression tag	UNP Q5SI82
A	399	LEU	GLY	engineered mutation	UNP Q5SI82
B	117	GLY	-	expression tag	UNP Q5SI82
B	118	PRO	-	expression tag	UNP Q5SI82
B	119	LEU	-	expression tag	UNP Q5SI82
B	120	GLY	-	expression tag	UNP Q5SI82
B	121	SER	-	expression tag	UNP Q5SI82
B	122	HIS	-	expression tag	UNP Q5SI82
B	123	MET	-	expression tag	UNP Q5SI82

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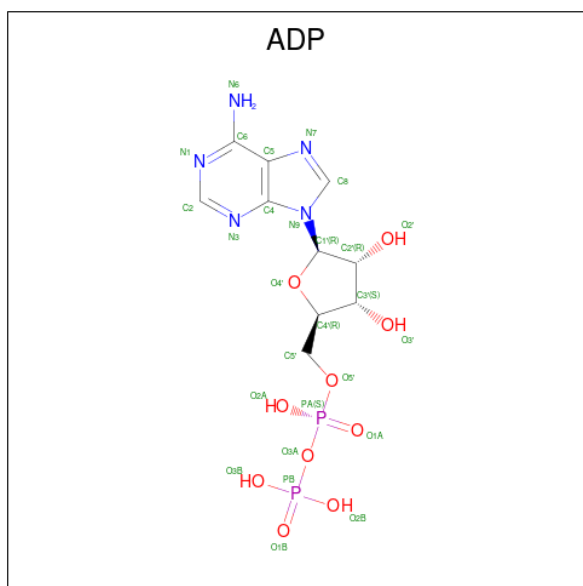
Chain	Residue	Modelled	Actual	Comment	Reference
B	124	GLY	-	expression tag	UNP Q5SI82
B	125	ALA	-	expression tag	UNP Q5SI82
B	399	LEU	GLY	engineered mutation	UNP Q5SI82
C	117	GLY	-	expression tag	UNP Q5SI82
C	118	PRO	-	expression tag	UNP Q5SI82
C	119	LEU	-	expression tag	UNP Q5SI82
C	120	GLY	-	expression tag	UNP Q5SI82
C	121	SER	-	expression tag	UNP Q5SI82
C	122	HIS	-	expression tag	UNP Q5SI82
C	123	MET	-	expression tag	UNP Q5SI82
C	124	GLY	-	expression tag	UNP Q5SI82
C	125	ALA	-	expression tag	UNP Q5SI82
C	399	LEU	GLY	engineered mutation	UNP Q5SI82
D	117	GLY	-	expression tag	UNP Q5SI82
D	118	PRO	-	expression tag	UNP Q5SI82
D	119	LEU	-	expression tag	UNP Q5SI82
D	120	GLY	-	expression tag	UNP Q5SI82
D	121	SER	-	expression tag	UNP Q5SI82
D	122	HIS	-	expression tag	UNP Q5SI82
D	123	MET	-	expression tag	UNP Q5SI82
D	124	GLY	-	expression tag	UNP Q5SI82
D	125	ALA	-	expression tag	UNP Q5SI82
D	399	LEU	GLY	engineered mutation	UNP Q5SI82
E	117	GLY	-	expression tag	UNP Q5SI82
E	118	PRO	-	expression tag	UNP Q5SI82
E	119	LEU	-	expression tag	UNP Q5SI82
E	120	GLY	-	expression tag	UNP Q5SI82
E	121	SER	-	expression tag	UNP Q5SI82
E	122	HIS	-	expression tag	UNP Q5SI82
E	123	MET	-	expression tag	UNP Q5SI82
E	124	GLY	-	expression tag	UNP Q5SI82
E	125	ALA	-	expression tag	UNP Q5SI82
E	399	LEU	GLY	engineered mutation	UNP Q5SI82
F	117	GLY	-	expression tag	UNP Q5SI82
F	118	PRO	-	expression tag	UNP Q5SI82
F	119	LEU	-	expression tag	UNP Q5SI82
F	120	GLY	-	expression tag	UNP Q5SI82
F	121	SER	-	expression tag	UNP Q5SI82
F	122	HIS	-	expression tag	UNP Q5SI82
F	123	MET	-	expression tag	UNP Q5SI82
F	124	GLY	-	expression tag	UNP Q5SI82
F	125	ALA	-	expression tag	UNP Q5SI82

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Chain	Residue	Modelled	Actual	Comment	Reference
F	399	LEU	GLY	engineered mutation	UNP Q5SI82

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).




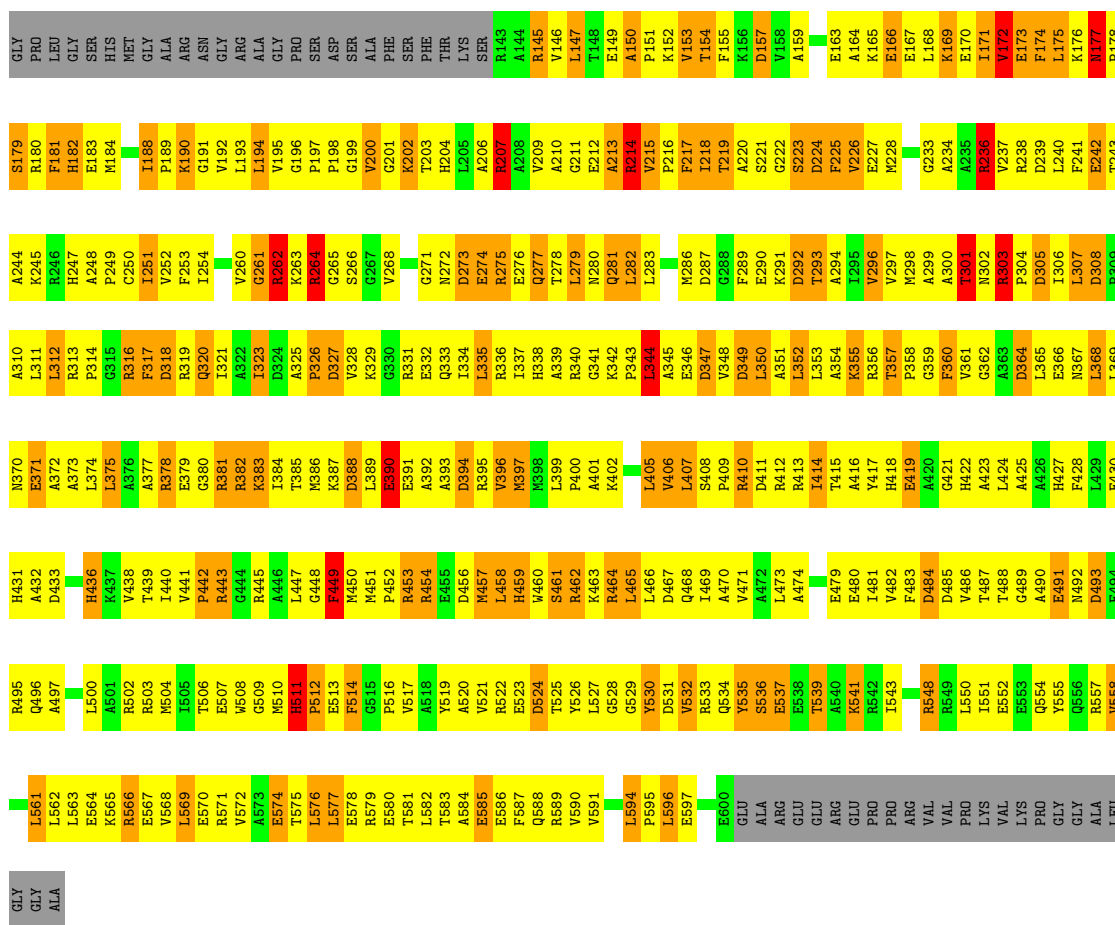
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

### 3 Residue-property plots

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

Chain A: 



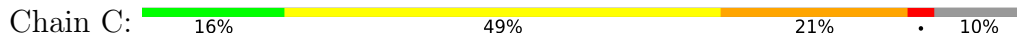
- Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain B: 



V237	V287	T357	H418	E479	K541	GLU
R236	M286	P358	E419	E480	R542	GLU
L240	A299	G359	A300	I481	F543	ARG
F241	A300	F360	G421	V482	D544	GLU
E242	N301	G361	H422	F483	V547	PRO
T243	R303	G362	A423	D484	R548	PRO
A244	F304	D364	L424	D485	R549	ARG
K245	G305	D365	H427	V486	R549	VAL
R246	L306	E366	H427	T487	L550	VAL
H247	L307	E367	L429	T488	F551	PRO
A248	L307	N367	L429	G489	E552	ARG
P249	D308	L368	E430	A490	E553	ASN
C250	F309	L369	H431	E491	O554	GLY
I251	A310	N370	A432	N492	Y555	VAL
V252	L311	E371	D433	D493	Q556	PRO
F253	L312	A372	G434	F494	R557	GLY
I254	R313	A373	G434	F494	F558	GLY
D255	P314	A374	H436	R495	V559	ALA
E256	G315	L374	H436	Q496	K560	LEU
I257	R316	L375	K437	A497	A560	GLY
D258	R317	A376	V438	L500	L561	GLY
A259	D318	R377	T439	L500	L562	ALA
V260	R319	R378	I440	A501	L563	ALA
G261	Q320	E379	V441	R502	E564	SER
R262	G321	G380	P442	M503	K565	THR
K263	A322	R381	R443	M504	R566	LYS
ARG	I323	R382	G444	L505	E567	SER
GLY	D324	K383	R445	T506	V568	R143
SER	E332	L384	A446	E507	L569	A144
GLY	L335	T385	L447	W508	E570	R145
VAL	Q333	A325	G448	G509	E571	V146
VAL	L334	D327	F449	M510	V572	L147
GLY	V328	V328	M450	R511	L576	T148
GLY	K329	L389	M451	P512	L577	E149
GLY	G330	E390	P452	F513	L578	A150
GLY	R331	E391	R453	E514	R579	P151
D273	Q333	A392	R454	V517	E580	K152
E274	L334	A393	D456	A518	T581	V153
R275	L335	D394	M457	Y519	L582	F154
E276	R336	V396	L458	A520	T583	F155
Q277	L337	M397	H459	V521	A584	R156
T278	H338	M398	R460	R522	E585	D157
L279	A339	L399	S461	E523	E586	G222
N280	R340	P400	R462	D524	F587	V158
Q281	G341	A401	K463	T525	Q588	A159
L282	K342	K402	R464	Y526	R589	E163
V284	P343	K403	L465	L527	R589	A164
E285	L344	S404	L466	G528	V591	K165
E286	A345	L405	D467	G529	E592	E166
D287	E346	V406	Q468	Y530	G593	E167
G288	D347	L407	I469	D531	L594	L168
F289	V348	S408	A470	V532	P595	K169
E290	D349	P409	V471	R533	E596	E170
K291	R350	R410	L472	Q534	L597	I171
K291	A351	D411	L473	A598	E597	V172
D292	L352	R412	A474	Y535	A598	E173
T293	L353	R413	G475	E537	P599	E174
A294	A354	L414	R476	E600	L600	L175
I295	K355	A477	A478	ALA	ALA	K176
V296	R356	Y417	ARG	ARG	ARG	N177
						P178

• Molecule 1: ATP-dependent zinc metalloprotease FtsH



GLY	S179	A244	A310	E371	A432	R486	L561
PRO	R180	K245	L311	A372	D433	A497	L562
LEU	F181	R246	L312	A373	H436	L500	L563
GLY	H182	G247	R313	L374	A437	L501	L564
SER	E183	A248	R316	L375	K438	R502	R565
PRO	M184	P249	F317	A376	V439	R503	R566
ARG		C250	D316	A377	L440	M504	R567
VAL	I188	I251	R319	R378	V441	L505	R568
VAL	P189	V252	R319	E379	V442	L506	R569
ALA	K190	F253	Q320	G380	P442	T506	R570
ARG	G191	I254	L321	R381	R443	E507	L571
ASN	V192	K255	A322	R382	G444	E508	L572
GLY	L193	V260	L323	K383	R445	G509	A573
VAL	L194	G261	R324	I384	A446	M510	A574
PRO	V195	R262	A325	T385	L447	H511	L575
GLY	K196	K263	P326	M386	G448	P512	L576
GLY	P197	R264	D327	R387	F449	E513	L577
ALA	G198	R265	V328	K388	M450	F514	L578
ASP	K199	S266	K329	L389	M451	G515	R579
SER	V200	G267	G330	E390	P452	P516	E580
ALA	G201	V288	R331	E391	L453	V517	E581
PHE	K202	G271	E332	A392	R454	A518	L582
SER	T203	G272	Q333	A393	E455	F519	L583
THR	H204	N272	I334	D394	D456	Y520	L584
LYS	L205	D273	L335	R395	M457	V521	E585
SER	A206	E274	R336	V396	L458	R522	E586
R143	R207	R275	L337	M397	H459	E523	F587
A144	A208	E276	H338	N398	W460	D524	Q588
R145	V209	Q277	A339	L399	S461	R525	R589
V146	A210	T278	R340	P400	R462	V526	V590
L147	G211	L279	G341	A401	K463	L527	V591
T148	E212	N280	K342	K402	R464	G528	L594
E149	A213	Q281	P343	L405	L465	G529	L594
A150	R214	L282	L344	L406	L466	Y530	L594
P151	V215	L283	A345	L407	Q468	D531	L596
K152	K152	M286	E346	L408	V469	R533	E597
V153	T154	D287	V348	P409	A470	Q534	
F155	F155	G288	D349	R410	V471	Y535	
R156	A220	F289	L350	D411	A472	S536	
L154	S221	E290	A351	R412	F483	E537	
F155	G222	K291	L352	R413	F483	E538	
A159	S223	D292	L353	R414	A474	E539	
E163	D224	T293	A354	I414	E479	T539	
A164	F225	A294	K355	T415	E480	A540	
K165	V226	I295	R356	A416	E481	K541	
E166	E227	V296	T357	Y417	V482	R542	
E167	M228	V297	P358	H418	F483	I543	
L168	G233	M298	G359	E419	D484	R543	
K169	A234	A299	F360	A420	D485	R544	
E170	R235	A300	V361	H422	V486	L550	
I171	I171	T301	G362	H423	T487	L551	
V172	R236	N302	A363	L424	T488	E552	
E173	V237	R303	D364	A425	G489	E553	
E174	Q534	A426	L365	A426	F489	O554	
L175	E598	P305	E366	H427	E491	Y555	
K176	E241	I306	M367	F428	M482	R556	
P178	F242	L307	L368	L429	D493	R557	
	T243	E242	L369	F494	F494	V558	
			N370	R495	R495		



GLY  
ALA

- Molecule 1: ATP-dependent zinc metalloprotease FtsH

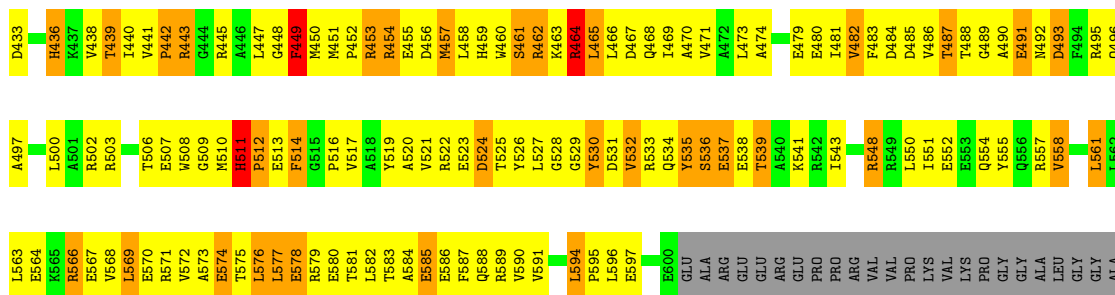
Chain D: 9% 52% 23% 12%

GLY	PRO	LEU	GLY	SER	HIS	MET	GLY	ALA	ALA	GLY	PRO	SER	ASP	ALA	PHE	SER	PHE	THR	LYS	SER	ARG	ALA	VAL	L147	L148	E149	A150	K151	K152	V153	T154	F155	K156	D157	V158	A159	G160	A161	E162	E163	A164	K165	V166	E167	L168	K169	E170	V171	I171	V172	G231	V232	G233	A234	L174	A235	K176																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
M177	P178	S179	R180	F181	H182	E183	M184	G185	A186	R187	I188	K189	G190	V191	L192	L193	L194	L195	V196	G197	P198	P199	G200	K202	T203	H204	G205	A206	R207	A208	V209	G210	E211	A212	A213	R214	V215	P216	F217	T218	T219	N280	S221	G222	D224	F225	V226	E227	M228	F229	V230	G231	V232	G233	A234	L174	A235	K176																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
V237	R238	D239	L240	F241	E242	T243	A244	K245	A186	R246	H247	I188	P249	C250	L251	F253	T254	D255	E256	L257	D258	A259	G261	R262	K263	ARG	GLY	G211	E212	A213	D273	E274	R275	E276	Q277	T278	L279	N280	Q281	L282	L283	V284	E285	K286	D287	G288	F289	G290	K291	D292	T293	A294	L295	V296																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
V297	M298	A299	A300	T301	R302	R303	F304	G305	L306	L307	L308	L309	N370	E371	A310	L311	L312	R313	P314	T254	D255	E256	R316	F317	R318	R319	Q320	I323	D324	P326	K327	V328	K329	G330	R331	E332	Q333	L334	L335	R336	I337	H338	A339	R340	G341	K342	P343	L344	A345	E346	D347	V348	D349	L350	A351	L352	L353	A354	K355	T357																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
P358	G359	F360	V361	G362	A363	D364	L365	E366	N367	L368	L369	N370	E371	A372	A373	L374	L375	A376	A377	R378	E379	G380	R381	Q382	K383	I384	T385	P386	K387	V388	L389	E390	E391	A392	Q393	A394	R395	V396	M397	H398	L399	A400	K402	K403	S404	L405	L406	L407	S408	Q409	R410	D411	R412	L413	I414	T415	K416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000

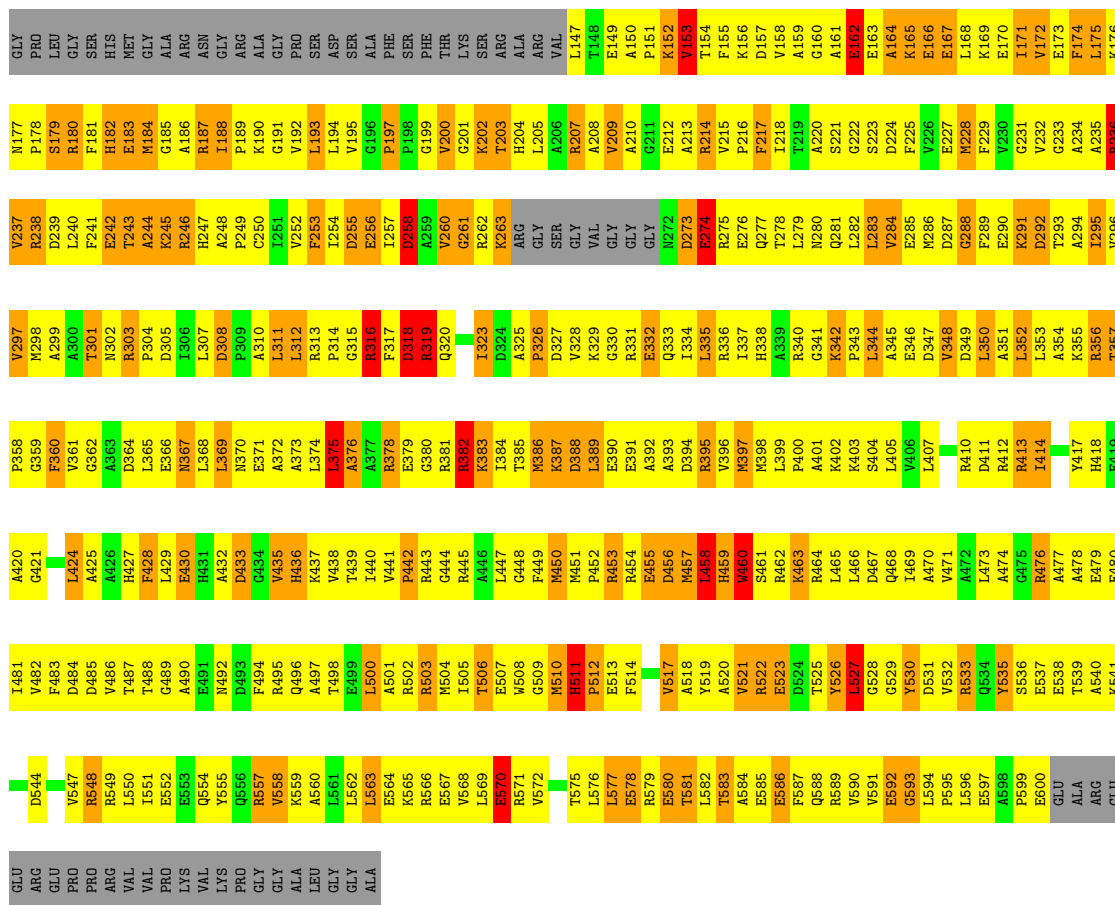
- Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain E: 17% 49% 22% 10%

GLY	PRO	LEU	GLY	SER	HIS	MET	GLY	ALA	ALA	GLY	PRO	SER	ASP	ALA	PHE	SER	PHE	THR	LYS	SER	ARG	ALA	VAL	L147	L148	E149	A150	K151	K152	V153	T154	F155	K156	D157	V158	A159	G160	A161	E162	E163	A164	K165	V166	E167	L168	K169	E170	V171	I171	V172	G231	V232	G233	A234	L174	A235	K176																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
S179	R180	F181	H182	G183	M184	I188	P189	K190	G191	V192	L193	L194	V195	G196	G201	K202	T203	H204	L205	L206	A206	R207	D273	E274	R275	E276	Q277	T278	L279	N280	S221	G222	F225	V226	E227	M228	F229	V230	G231	V232	G233	A234	L235	A236	K237	N302	R303	D304	L305	F306	E307	L308	L309	A310	A311	A312	A313	A314	A315	A316	A317	A318	A319	A320	A321	A322	A323	A324	A325	A326	A327	A328	A329	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A8



• Molecule 1: ATP-dependent zinc metalloprotease FtsH



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.15Å 146.15Å 349.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.53 – 3.90 71.53 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (71.53-3.90) 97.1 (71.53-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.46 (at 3.89Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.299 , 0.312 0.298 , 0.309	Depositor DCC
$R_{free}$ test set	1967 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.1	Xtrriage
Anisotropy	0.272	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 19.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.27$ , $\langle L^2 \rangle = 0.11$	Xtrriage
Estimated twinning fraction	0.237 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	21429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.60	3/3636 (0.1%)	0.95	16/4906 (0.3%)
1	B	0.63	3/3568 (0.1%)	1.01	18/4815 (0.4%)
1	C	0.59	2/3636 (0.1%)	1.03	24/4906 (0.5%)
1	D	0.60	2/3568 (0.1%)	0.98	17/4815 (0.4%)
1	E	0.61	6/3636 (0.2%)	0.96	13/4906 (0.3%)
1	F	0.58	2/3568 (0.1%)	0.96	12/4815 (0.2%)
All	All	0.60	18/21612 (0.1%)	0.98	100/29163 (0.3%)

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	2
1	B	0	5
1	C	0	1
1	D	0	6
1	E	0	1
1	F	0	5
All	All	0	20

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	GLU	CD-OE1	-12.04	1.12	1.25
1	C	214	ARG	CZ-NH2	8.16	1.43	1.33
1	E	214	ARG	CZ-NH2	-8.12	1.22	1.33
1	E	319	ARG	CZ-NH1	-7.39	1.23	1.33
1	D	586	GLU	CD-OE1	-6.72	1.18	1.25
1	A	214	ARG	CZ-NH2	-6.40	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	214	ARG	CZ-NH1	-6.39	1.24	1.33
1	F	586	GLU	CD-OE1	-6.36	1.18	1.25
1	C	214	ARG	CZ-NH1	-6.30	1.24	1.33
1	E	214	ARG	CG-CD	-6.02	1.36	1.51
1	A	301	THR	CB-CG2	-5.76	1.33	1.52
1	B	460	TRP	CD2-CE2	5.54	1.48	1.41
1	A	214	ARG	CD-NE	-5.42	1.37	1.46
1	B	316	ARG	CZ-NH2	-5.36	1.26	1.33
1	E	316	ARG	CZ-NH1	-5.34	1.26	1.33
1	F	460	TRP	CD2-CE2	5.30	1.47	1.41
1	E	214	ARG	CD-NE	-5.23	1.37	1.46
1	D	460	TRP	CD2-CE2	5.20	1.47	1.41

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	319	ARG	NE-CZ-NH2	18.11	129.36	120.30
1	C	207	ARG	NE-CZ-NH1	-15.37	112.61	120.30
1	A	316	ARG	NE-CZ-NH1	-15.14	112.73	120.30
1	B	236	ARG	NE-CZ-NH1	-14.64	112.98	120.30
1	C	207	ARG	NE-CZ-NH2	13.93	127.26	120.30
1	B	236	ARG	NE-CZ-NH2	13.80	127.20	120.30
1	C	316	ARG	NE-CZ-NH2	13.04	126.82	120.30
1	E	316	ARG	NE-CZ-NH1	-11.95	114.33	120.30
1	C	316	ARG	NE-CZ-NH1	-11.85	114.38	120.30
1	A	316	ARG	NE-CZ-NH2	11.58	126.09	120.30
1	C	481	ILE	CG1-CB-CG2	-10.53	88.25	111.40
1	A	214	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	F	316	ARG	NE-CZ-NH1	-9.37	115.62	120.30
1	B	381	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	C	214	ARG	NE-CZ-NH1	-9.09	115.75	120.30
1	F	316	ARG	NE-CZ-NH2	8.93	124.76	120.30
1	E	316	ARG	NE-CZ-NH2	8.61	124.61	120.30
1	B	316	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	D	375	LEU	CA-CB-CG	8.41	134.64	115.30
1	F	236	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	D	289	PHE	CB-CG-CD1	-8.21	115.06	120.80
1	D	236	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	375	LEU	CA-CB-CG	7.99	133.66	115.30
1	D	316	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	C	214	ARG	N-CA-C	7.67	131.72	111.00
1	B	283	LEU	CB-CG-CD1	-7.66	97.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	236	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	207	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	214	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	D	236	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	E	319	ARG	NH1-CZ-NH2	-7.30	111.37	119.40
1	E	335	LEU	CA-CB-CG	7.21	131.88	115.30
1	C	207	ARG	CD-NE-CZ	7.12	133.56	123.60
1	E	207	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	335	LEU	CA-CB-CG	7.09	131.62	115.30
1	C	275	ARG	CB-CA-C	-7.09	96.21	110.40
1	F	375	LEU	CA-CB-CG	7.01	131.43	115.30
1	E	207	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	207	ARG	CG-CD-NE	-6.89	97.33	111.80
1	B	236	ARG	CD-NE-CZ	6.86	133.20	123.60
1	C	335	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	207	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	D	381	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	C	214	ARG	CA-CB-CG	-6.55	98.98	113.40
1	E	214	ARG	N-CA-C	6.44	128.39	111.00
1	B	240	LEU	CA-CB-CG	6.42	130.06	115.30
1	D	289	PHE	N-CA-CB	-6.29	99.28	110.60
1	D	382	ARG	N-CA-CB	-6.22	99.39	110.60
1	C	214	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	D	511	HIS	C-N-CD	6.12	141.25	128.40
1	E	214	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	F	214	ARG	CA-CB-CG	5.99	126.59	113.40
1	B	378	ARG	CG-CD-NE	5.96	124.32	111.80
1	D	285	GLU	CA-CB-CG	5.93	126.44	113.40
1	F	511	HIS	C-N-CD	5.91	140.81	128.40
1	C	496	GLN	CB-CA-C	-5.88	98.64	110.40
1	C	577	LEU	CB-CG-CD1	-5.87	101.02	111.00
1	D	289	PHE	CB-CG-CD2	5.87	124.91	120.80
1	A	177	ASN	CB-CA-C	-5.83	98.74	110.40
1	E	577	LEU	CA-CB-CG	5.82	128.68	115.30
1	C	287	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	344	LEU	CA-CB-CG	5.72	128.45	115.30
1	D	285	GLU	CB-CA-C	-5.71	98.98	110.40
1	A	344	LEU	CA-CB-CG	5.61	128.20	115.30
1	D	382	ARG	CB-CG-CD	-5.58	97.11	111.60
1	D	282	LEU	CA-CB-CG	5.53	128.03	115.30
1	B	369	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	303	ARG	NE-CZ-NH1	5.49	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	458	LEU	N-CA-C	-5.46	96.27	111.00
1	A	301	THR	OG1-CB-CG2	-5.45	97.46	110.00
1	B	511	HIS	C-N-CD	5.42	139.77	128.40
1	E	344	LEU	CA-CB-CG	5.40	127.72	115.30
1	E	464	ARG	CB-CA-C	-5.40	99.61	110.40
1	A	577	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	274	GLU	CB-CG-CD	-5.38	99.68	114.20
1	B	282	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	458	LEU	N-CA-C	-5.36	96.52	111.00
1	C	275	ARG	CA-CB-CG	5.35	125.16	113.40
1	F	282	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	586	GLU	CG-CD-OE2	5.30	128.90	118.30
1	C	378	ARG	CG-CD-NE	5.28	122.89	111.80
1	B	527	LEU	CA-CB-CG	-5.27	103.17	115.30
1	C	378	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	165	LYS	CD-CE-NZ	-5.26	99.61	111.70
1	C	378	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	214	ARG	CG-CD-NE	-5.21	100.87	111.80
1	B	586	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	A	335	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	D	458	LEU	N-CA-C	-5.17	97.04	111.00
1	A	236	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	567	GLU	CA-CB-CG	5.16	124.76	113.40
1	F	318	ASP	N-CA-C	-5.14	97.11	111.00
1	F	369	LEU	CA-CB-CG	5.12	127.08	115.30
1	D	369	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	274	GLU	CB-CA-C	-5.12	100.16	110.40
1	B	318	ASP	N-CA-C	-5.07	97.31	111.00
1	C	236	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	413	ARG	CB-CA-C	-5.06	100.27	110.40
1	A	577	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	E	287	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	ALA	Peptide
1	A	532	VAL	Peptide
1	B	244	ALA	Peptide
1	B	288	GLY	Peptide
1	B	382	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	510	MET	Peptide
1	B	523	GLU	Peptide
1	C	532	VAL	Peptide
1	D	244	ALA	Peptide
1	D	288	GLY	Peptide
1	D	347	ASP	Peptide
1	D	382	ARG	Peptide
1	D	510	MET	Peptide
1	D	523	GLU	Peptide
1	E	532	VAL	Peptide
1	F	244	ALA	Peptide
1	F	288	GLY	Peptide
1	F	382	ARG	Peptide
1	F	510	MET	Peptide
1	F	523	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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	3578	0	3623	862	5
1	B	3511	0	3556	851	3
1	C	3578	0	3623	815	0
1	D	3511	0	3556	851	3
1	E	3578	0	3623	805	3
1	F	3511	0	3556	857	2
2	A	27	0	12	8	0
2	B	27	0	12	9	0
2	C	27	0	12	10	0
2	D	27	0	12	9	0
2	E	27	0	12	11	0
2	F	27	0	12	10	0
All	All	21429	0	21609	4895	8

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 114.

All (4895) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:ALA:CB	1:E:577:LEU:HD23	1.18	1.63
1:A:416:ALA:HB3	1:A:577:LEU:CD2	1.33	1.58
1:A:416:ALA:CB	1:A:577:LEU:HD23	1.15	1.55
1:F:376:ALA:CA	1:F:381:ARG:HD2	1.31	1.55
1:E:416:ALA:HB3	1:E:577:LEU:CD2	1.35	1.55
1:B:376:ALA:CA	1:B:381:ARG:HD2	1.18	1.54
1:B:376:ALA:HA	1:B:381:ARG:CD	1.38	1.54
1:A:286:MET:HG3	1:A:316:ARG:CD	1.39	1.49
1:B:313:ARG:CD	1:B:314:PRO:HD2	1.42	1.49
1:B:283:LEU:CD1	1:B:316:ARG:NH2	1.77	1.46
1:A:586:GLU:HB2	1:A:589:ARG:NH2	1.18	1.46
1:D:313:ARG:CD	1:D:314:PRO:HD2	1.40	1.46
1:F:311:LEU:HA	1:F:316:ARG:NH1	1.17	1.46
1:A:286:MET:CG	1:A:316:ARG:HD3	1.43	1.45
1:B:283:LEU:CD1	1:B:316:ARG:HH21	1.28	1.45
1:F:313:ARG:CD	1:F:314:PRO:HD2	1.45	1.44
1:E:589:ARG:NH2	1:E:596:LEU:CB	1.82	1.42
1:A:316:ARG:NH1	1:A:317:PHE:CE2	1.90	1.39
1:A:316:ARG:NH1	1:A:317:PHE:CD2	1.91	1.39
1:C:589:ARG:NH2	1:C:596:LEU:CB	1.82	1.39
1:A:286:MET:SD	1:A:316:ARG:HG3	1.65	1.36
1:B:283:LEU:HD11	1:B:316:ARG:NH2	1.06	1.36
1:F:376:ALA:HA	1:F:381:ARG:CD	1.55	1.34
1:A:263:LYS:CE	1:A:276:GLU:OE1	1.77	1.33
1:A:168:LEU:O	1:A:171:ILE:HD13	1.22	1.32
1:A:586:GLU:CB	1:A:589:ARG:HH21	1.43	1.31
1:C:263:LYS:CE	1:C:276:GLU:OE1	1.77	1.31
1:F:311:LEU:CA	1:F:316:ARG:HH12	1.41	1.30
1:E:263:LYS:CE	1:E:276:GLU:OE1	1.80	1.29
1:E:286:MET:HB3	1:E:316:ARG:CG	1.61	1.29
1:A:374:LEU:HD21	1:F:187:ARG:O	1.32	1.28
1:C:303:ARG:HB2	1:C:303:ARG:NH1	1.50	1.26
1:A:311:LEU:HA	1:A:316:ARG:NH2	1.49	1.25
1:C:286:MET:HB3	1:C:316:ARG:CG	1.64	1.25
1:E:303:ARG:HB2	1:E:303:ARG:NH1	1.50	1.25
1:A:303:ARG:HB2	1:A:303:ARG:NH1	1.48	1.25
1:A:416:ALA:CB	1:A:577:LEU:CD2	1.98	1.22
1:A:449:PHE:CZ	1:A:496:GLN:HG2	1.73	1.22
1:D:382:ARG:HH11	1:D:382:ARG:CG	1.50	1.22
1:F:233:GLY:HA2	1:F:236:ARG:NH2	1.54	1.21
1:D:233:GLY:HA2	1:D:236:ARG:NH2	1.53	1.21
1:E:416:ALA:CB	1:E:577:LEU:CD2	2.02	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:ARG:NH2	1:D:388:ASP:OD2	1.72	1.21
1:E:589:ARG:NH2	1:E:596:LEU:HB3	1.40	1.20
1:A:286:MET:CG	1:A:316:ARG:CD	2.05	1.20
1:C:449:PHE:CZ	1:C:496:GLN:HG3	1.75	1.20
1:A:263:LYS:NZ	1:A:276:GLU:OE2	1.75	1.20
1:A:303:ARG:HH11	1:A:303:ARG:CB	1.55	1.20
1:E:449:PHE:CZ	1:E:496:GLN:HG2	1.76	1.20
1:F:283:LEU:HD12	1:F:316:ARG:NH2	1.57	1.20
1:C:286:MET:CG	1:C:316:ARG:HD2	1.70	1.19
1:A:585:GLU:O	1:A:588:GLN:HG2	1.41	1.19
1:C:168:LEU:HB2	1:C:171:ILE:HD11	1.22	1.18
1:C:303:ARG:HH11	1:C:303:ARG:CB	1.57	1.18
1:E:303:ARG:HH11	1:E:303:ARG:CB	1.57	1.18
1:C:263:LYS:NZ	1:C:276:GLU:OE2	1.76	1.18
1:B:395:ARG:HG2	1:B:395:ARG:HH11	1.09	1.17
1:C:413:ARG:HA	1:C:577:LEU:HD22	1.25	1.17
1:C:286:MET:CB	1:C:316:ARG:CD	2.21	1.17
1:C:589:ARG:NH2	1:C:596:LEU:HB3	1.49	1.17
1:A:587:PHE:O	1:A:590:VAL:HG22	1.42	1.16
1:B:318:ASP:O	1:B:319:ARG:HB2	1.46	1.16
1:E:168:LEU:HB2	1:E:171:ILE:HD11	1.18	1.16
1:E:262:ARG:HB3	1:E:275:ARG:HH12	1.10	1.15
1:D:165:LYS:O	1:D:168:LEU:N	1.80	1.15
1:D:311:LEU:O	1:D:316:ARG:HG2	1.44	1.15
1:C:589:ARG:NH2	1:C:596:LEU:HB2	1.45	1.15
1:A:172:VAL:HG23	1:A:213:ALA:HB2	1.29	1.15
1:B:165:LYS:O	1:B:168:LEU:N	1.77	1.14
1:B:233:GLY:HA2	1:B:236:ARG:HH22	1.01	1.14
1:C:428:PHE:CE1	1:C:432:ALA:HA	1.82	1.14
1:F:165:LYS:O	1:F:168:LEU:N	1.79	1.14
1:E:589:ARG:NH2	1:E:596:LEU:HB2	1.53	1.14
1:F:283:LEU:CD1	1:F:316:ARG:HH21	1.60	1.14
1:E:263:LYS:NZ	1:E:276:GLU:OE2	1.79	1.14
1:F:589:ARG:HE	1:F:594:LEU:HD21	1.08	1.14
1:A:524:ASP:HA	1:A:529:GLY:HA2	1.15	1.14
1:C:225:PHE:CZ	1:C:278:THR:HB	1.83	1.14
1:F:283:LEU:CD1	1:F:316:ARG:NH2	2.10	1.14
1:B:589:ARG:HE	1:B:594:LEU:HD21	1.07	1.13
1:E:416:ALA:HB3	1:E:577:LEU:HD21	1.26	1.13
1:A:236:ARG:HG3	1:A:237:VAL:N	1.48	1.13
1:B:165:LYS:HD3	1:B:168:LEU:HD22	1.14	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ALA:CB	1:C:577:LEU:HD23	1.78	1.13
1:C:524:ASP:HA	1:C:529:GLY:HA2	1.14	1.13
1:F:395:ARG:HG2	1:F:395:ARG:HH11	1.08	1.12
1:A:416:ALA:HB3	1:A:577:LEU:HD21	1.21	1.12
1:E:236:ARG:HG3	1:E:237:VAL:N	1.50	1.12
1:E:524:ASP:HA	1:E:529:GLY:HA2	1.13	1.12
1:A:413:ARG:HA	1:A:577:LEU:HD22	1.31	1.12
1:F:165:LYS:HD3	1:F:168:LEU:HD22	1.20	1.12
1:A:170:GLU:O	1:A:174:PHE:HB3	1.49	1.12
1:A:342:LYS:NZ	1:F:184:MET:SD	2.23	1.12
1:B:171:ILE:HD11	1:B:296:VAL:HG11	1.16	1.11
1:C:182:HIS:HB2	1:C:291:LYS:HD2	1.31	1.11
1:C:236:ARG:HG3	1:C:237:VAL:N	1.48	1.11
1:D:165:LYS:HD3	1:D:168:LEU:HD22	1.17	1.11
1:D:412:ARG:HH12	1:D:440:ILE:HG21	1.15	1.11
1:D:291:LYS:HG3	1:D:292:ASP:H	1.13	1.11
1:A:286:MET:HG3	1:A:316:ARG:HD2	1.27	1.11
1:B:413:ARG:HG2	1:B:413:ARG:HH11	1.11	1.11
1:E:170:GLU:O	1:E:174:PHE:HB3	1.50	1.11
1:E:283:LEU:HG	1:E:316:ARG:NH1	1.64	1.11
1:F:286:MET:HE1	1:F:316:ARG:HA	1.11	1.11
1:D:190:LYS:HE3	1:D:289:PHE:CZ	1.85	1.10
1:E:172:VAL:HG23	1:E:213:ALA:HB2	1.24	1.10
1:D:171:ILE:HD11	1:D:296:VAL:HG11	1.15	1.10
1:D:290:GLU:HG2	1:D:293:THR:HG23	1.28	1.10
1:A:416:ALA:HB2	1:A:577:LEU:HD23	1.15	1.10
1:B:286:MET:HE1	1:B:316:ARG:HA	1.17	1.10
1:C:172:VAL:HG23	1:C:213:ALA:HB2	1.28	1.10
1:F:190:LYS:NZ	1:F:289:PHE:HE2	1.49	1.10
1:F:382:ARG:HH11	1:F:382:ARG:HG3	1.11	1.10
1:A:286:MET:SD	1:A:316:ARG:CG	2.39	1.10
1:B:290:GLU:HG2	1:B:293:THR:HG23	1.33	1.10
1:C:264:ARG:HG3	1:C:266:SER:H	1.08	1.10
1:E:182:HIS:HB2	1:E:291:LYS:HD2	1.31	1.10
1:F:356:ARG:HH11	1:F:356:ARG:HG3	1.15	1.10
1:A:262:ARG:HB3	1:A:275:ARG:HH12	1.09	1.10
1:E:147:LEU:HD21	1:E:151:PRO:HB3	1.14	1.10
1:E:264:ARG:HG3	1:E:266:SER:N	1.65	1.10
1:E:428:PHE:CE1	1:E:432:ALA:HA	1.86	1.09
1:F:474:ALA:HA	1:F:558:VAL:HG11	1.34	1.09
1:E:174:PHE:CE1	1:E:188:ILE:HD11	1.86	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LYS:HE2	1:F:205:LEU:HD23	1.24	1.09
1:F:412:ARG:HH12	1:F:440:ILE:HG21	1.16	1.09
1:B:190:LYS:NZ	1:B:289:PHE:HE2	1.49	1.09
1:D:280:ASN:O	1:D:284:VAL:HG12	1.51	1.09
1:A:311:LEU:HD23	1:A:316:ARG:NH2	1.68	1.09
1:A:428:PHE:CE1	1:A:432:ALA:HA	1.86	1.09
1:D:376:ALA:HA	1:D:381:ARG:HG3	1.33	1.09
1:E:145:ARG:NH2	1:E:219:THR:OG1	1.84	1.09
1:F:280:ASN:O	1:F:284:VAL:HG12	1.51	1.09
1:A:286:MET:CB	1:A:316:ARG:HD3	1.81	1.09
1:A:378:ARG:HH22	1:F:170:GLU:HB3	1.06	1.09
1:C:264:ARG:CG	1:C:266:SER:H	1.66	1.09
1:D:589:ARG:HE	1:D:594:LEU:HD21	1.09	1.09
1:E:416:ALA:HB2	1:E:577:LEU:HD23	1.21	1.09
1:F:171:ILE:HD11	1:F:296:VAL:HG11	1.13	1.09
1:A:174:PHE:CE1	1:A:188:ILE:HD11	1.87	1.08
1:A:263:LYS:HE3	1:A:276:GLU:OE1	1.51	1.08
1:D:165:LYS:HE2	1:D:205:LEU:HD23	1.34	1.08
1:C:174:PHE:CE1	1:C:188:ILE:HD11	1.87	1.08
1:C:262:ARG:HB3	1:C:275:ARG:HH12	1.10	1.08
1:D:286:MET:HE1	1:D:316:ARG:HA	1.23	1.08
1:D:413:ARG:HG2	1:D:413:ARG:HH11	1.08	1.08
1:F:318:ASP:O	1:F:319:ARG:HB2	1.50	1.08
1:A:225:PHE:CZ	1:A:278:THR:HB	1.88	1.08
1:E:225:PHE:CZ	1:E:278:THR:HB	1.88	1.08
1:F:283:LEU:HD12	1:F:316:ARG:HH21	0.92	1.08
1:D:276:GLU:HA	1:D:279:LEU:HD13	1.33	1.08
1:E:453:ARG:NH2	1:E:460:TRP:HE1	1.52	1.08
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.10	1.08
1:F:238:ARG:NH1	1:F:239:ASP:N	2.02	1.08
1:F:238:ARG:NH1	1:F:239:ASP:H	1.50	1.08
1:A:182:HIS:HB2	1:A:291:LYS:HD2	1.27	1.07
1:C:170:GLU:O	1:C:174:PHE:HB3	1.50	1.07
1:D:316:ARG:HH11	1:D:316:ARG:HG3	0.99	1.07
1:D:318:ASP:O	1:D:319:ARG:HB2	1.48	1.07
1:E:413:ARG:HA	1:E:577:LEU:HD22	1.32	1.07
1:A:311:LEU:CD2	1:A:316:ARG:NH2	2.17	1.07
1:B:474:ALA:HA	1:B:558:VAL:HG11	1.33	1.07
1:C:453:ARG:NH2	1:C:460:TRP:HE1	1.51	1.07
1:B:276:GLU:HA	1:B:279:LEU:HD13	1.32	1.07
1:B:280:ASN:O	1:B:284:VAL:HG12	1.52	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:HD21	1:C:151:PRO:HB3	1.13	1.07
1:C:264:ARG:HG3	1:C:266:SER:N	1.69	1.07
1:D:190:LYS:HE3	1:D:289:PHE:CE2	1.90	1.07
1:A:342:LYS:HD2	1:A:343:PRO:HD2	1.35	1.06
1:A:453:ARG:NH2	1:A:460:TRP:HE1	1.52	1.06
1:D:459:HIS:ND1	1:D:459:HIS:O	1.88	1.06
1:F:400:PRO:O	1:F:404:SER:N	1.87	1.06
1:A:313:ARG:NH2	1:A:526:TYR:HA	1.70	1.06
1:A:264:ARG:HG3	1:A:266:SER:H	1.12	1.05
1:A:449:PHE:CE2	1:A:496:GLN:HG2	1.90	1.05
1:C:263:LYS:HD2	1:C:276:GLU:CD	1.75	1.05
1:C:449:PHE:CE2	1:C:496:GLN:HG3	1.90	1.05
1:D:313:ARG:CD	1:D:314:PRO:CD	2.34	1.05
1:B:356:ARG:HH11	1:B:356:ARG:HG3	1.16	1.05
1:D:400:PRO:O	1:D:404:SER:N	1.87	1.05
1:B:238:ARG:NH1	1:B:239:ASP:H	1.55	1.05
1:B:412:ARG:NH1	1:B:440:ILE:HG21	1.72	1.05
1:E:313:ARG:NH2	1:E:526:TYR:HA	1.69	1.05
1:D:356:ARG:HG3	1:D:356:ARG:HH11	1.14	1.05
1:D:395:ARG:HG2	1:D:395:ARG:HH11	1.16	1.05
1:D:412:ARG:NH1	1:D:440:ILE:HG21	1.69	1.05
1:E:237:VAL:HG11	1:E:281:GLN:HB3	1.38	1.05
1:E:286:MET:CB	1:E:316:ARG:HG2	1.87	1.05
1:E:342:LYS:HD2	1:E:343:PRO:HD2	1.39	1.05
1:F:412:ARG:NH1	1:F:440:ILE:HG21	1.70	1.05
1:A:262:ARG:HG2	1:A:275:ARG:HH22	1.22	1.04
1:B:376:ALA:C	1:B:381:ARG:HD2	1.76	1.04
1:C:225:PHE:HE1	1:C:233:GLY:CA	1.69	1.04
1:D:474:ALA:HA	1:D:558:VAL:HG11	1.37	1.04
1:E:264:ARG:HG3	1:E:266:SER:H	0.88	1.04
1:F:276:GLU:HA	1:F:279:LEU:HD13	1.35	1.04
1:A:168:LEU:HB2	1:A:171:ILE:HD11	1.38	1.04
1:A:237:VAL:HG11	1:A:281:GLN:HB3	1.35	1.04
1:B:238:ARG:NH1	1:B:239:ASP:N	2.04	1.04
1:C:263:LYS:HE3	1:C:276:GLU:OE1	1.55	1.04
1:C:286:MET:HB2	1:C:316:ARG:HD3	1.39	1.04
1:C:342:LYS:HD2	1:C:343:PRO:HD2	1.37	1.04
1:A:147:LEU:HD21	1:A:151:PRO:CB	1.87	1.04
1:B:400:PRO:O	1:B:404:SER:N	1.89	1.04
1:F:326:PRO:HB3	1:F:360:PHE:O	1.56	1.04
1:A:263:LYS:HD2	1:A:276:GLU:CD	1.77	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ARG:CD	1:B:314:PRO:CD	2.36	1.04
1:C:263:LYS:NZ	1:C:276:GLU:CD	2.10	1.04
1:E:533:ARG:NH2	1:E:534:GLN:O	1.91	1.04
1:F:313:ARG:HD2	1:F:314:PRO:HD2	1.05	1.04
1:A:263:LYS:NZ	1:A:276:GLU:CD	2.11	1.03
1:D:238:ARG:NH1	1:D:239:ASP:N	2.05	1.03
1:A:147:LEU:HD21	1:A:151:PRO:HB3	1.04	1.03
1:A:225:PHE:HE1	1:A:233:GLY:CA	1.71	1.03
1:E:152:LYS:HG3	1:E:153:VAL:HG23	1.39	1.03
1:F:482:VAL:HG13	1:F:483:PHE:HD2	1.24	1.03
1:B:376:ALA:CA	1:B:381:ARG:CD	2.10	1.03
1:B:482:VAL:HG13	1:B:483:PHE:HD2	1.21	1.03
1:E:263:LYS:HD2	1:E:276:GLU:CD	1.79	1.03
1:A:342:LYS:HD3	1:F:184:MET:O	1.58	1.03
1:B:337:ILE:HD12	1:B:340:ARG:HH12	1.19	1.03
1:E:147:LEU:HD21	1:E:151:PRO:CB	1.88	1.03
1:B:237:VAL:O	1:B:240:LEU:HB3	1.57	1.03
1:C:166:GLU:HB2	1:C:169:LYS:HZ2	1.22	1.03
1:D:382:ARG:HH11	1:D:382:ARG:HG3	0.87	1.02
1:A:264:ARG:CG	1:A:266:SER:H	1.71	1.02
1:F:290:GLU:HG2	1:F:293:THR:HG23	1.40	1.02
1:B:412:ARG:HH12	1:B:440:ILE:HG21	1.23	1.02
1:E:225:PHE:HE1	1:E:233:GLY:CA	1.72	1.02
1:E:263:LYS:NZ	1:E:276:GLU:CD	2.12	1.02
1:E:449:PHE:CE2	1:E:496:GLN:HG2	1.93	1.02
1:A:374:LEU:HD11	1:F:187:ARG:H	1.24	1.02
1:C:218:ILE:HD11	1:C:250:CYS:SG	2.00	1.01
1:C:237:VAL:HG11	1:C:281:GLN:HB3	1.37	1.01
1:C:286:MET:HB3	1:C:316:ARG:HG2	1.04	1.01
1:D:326:PRO:HB3	1:D:360:PHE:O	1.58	1.01
1:E:448:GLY:O	1:E:452:PRO:HD2	1.60	1.01
1:C:147:LEU:HD21	1:C:151:PRO:CB	1.88	1.01
1:A:533:ARG:NH2	1:A:534:GLN:O	1.94	1.01
1:B:165:LYS:HE2	1:B:205:LEU:HD23	1.38	1.01
1:B:459:HIS:ND1	1:B:459:HIS:O	1.92	1.01
1:C:152:LYS:HG3	1:C:153:VAL:HG23	1.42	1.01
1:D:348:VAL:CG2	1:D:352:LEU:HD22	1.91	1.01
1:E:263:LYS:HE3	1:E:276:GLU:OE1	1.58	1.01
1:A:218:ILE:HD11	1:A:250:CYS:SG	2.01	1.01
1:D:316:ARG:HH11	1:D:316:ARG:CG	1.71	1.01
1:F:302:ASN:HD21	1:F:443:ARG:HH22	1.05	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:PRO:HB3	1:B:360:PHE:O	1.60	1.01
1:C:589:ARG:NH1	1:C:589:ARG:HB3	1.76	1.01
1:D:453:ARG:CZ	1:D:495:ARG:HH21	1.73	1.01
1:E:286:MET:CB	1:E:316:ARG:CD	2.39	1.01
1:B:311:LEU:HA	1:B:316:ARG:NH1	1.75	1.00
1:C:286:MET:HG3	1:C:316:ARG:CD	1.90	1.00
1:D:313:ARG:HD2	1:D:314:PRO:HD2	1.01	1.00
1:D:348:VAL:HG21	1:D:352:LEU:HD22	1.43	1.00
1:D:382:ARG:HG3	1:D:382:ARG:NH1	1.69	1.00
1:A:152:LYS:HG3	1:A:153:VAL:HG23	1.44	1.00
1:C:416:ALA:HB3	1:C:577:LEU:HD23	1.01	1.00
1:D:238:ARG:NH1	1:D:239:ASP:H	1.56	1.00
1:B:439:THR:HG23	1:B:445:ARG:HH22	1.25	1.00
1:E:286:MET:HG3	1:E:316:ARG:HD2	1.40	1.00
1:E:589:ARG:HH21	1:E:596:LEU:HB3	0.98	1.00
1:C:589:ARG:HH21	1:C:596:LEU:HB3	0.95	1.00
1:B:263:LYS:NZ	1:C:227:GLU:HG3	1.77	1.00
1:A:378:ARG:HH22	1:F:170:GLU:CB	1.75	0.99
1:E:212:GLU:C	1:E:214:ARG:HG3	1.82	0.99
1:B:348:VAL:CG2	1:B:352:LEU:HD22	1.92	0.99
1:D:439:THR:HG23	1:D:445:ARG:HH22	1.23	0.99
1:A:166:GLU:HA	1:A:169:LYS:HG2	1.42	0.99
1:E:173:GLU:HA	1:E:176:LYS:CG	1.92	0.99
1:B:236:ARG:HH12	1:B:278:THR:HG22	1.26	0.99
1:B:262:ARG:HG3	1:B:263:LYS:N	1.77	0.99
1:D:381:ARG:HH22	1:D:388:ASP:CG	1.66	0.99
1:C:263:LYS:CD	1:C:276:GLU:OE1	2.11	0.99
1:F:313:ARG:CD	1:F:314:PRO:CD	2.40	0.99
1:F:190:LYS:NZ	1:F:289:PHE:CE2	2.28	0.99
1:B:313:ARG:HD2	1:B:314:PRO:HD2	1.02	0.98
1:D:313:ARG:CG	1:D:314:PRO:HD2	1.93	0.98
1:F:165:LYS:HE2	1:F:205:LEU:CD2	1.93	0.98
1:A:264:ARG:HG3	1:A:266:SER:N	1.77	0.98
1:C:313:ARG:NH2	1:C:526:TYR:HA	1.77	0.98
1:E:589:ARG:HB3	1:E:589:ARG:NH1	1.78	0.98
1:F:453:ARG:NH1	1:F:495:ARG:HH21	1.59	0.98
1:A:586:GLU:HA	1:A:589:ARG:NE	1.77	0.98
1:F:459:HIS:ND1	1:F:459:HIS:O	1.94	0.98
1:A:311:LEU:CA	1:A:316:ARG:HH22	1.75	0.98
1:A:378:ARG:NH2	1:F:170:GLU:HB3	1.78	0.98
1:D:233:GLY:HA2	1:D:236:ARG:HH22	1.15	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ARG:HG2	1:D:319:ARG:HH11	1.26	0.98
1:E:174:PHE:CZ	1:E:188:ILE:CD1	2.47	0.98
1:D:376:ALA:CA	1:D:381:ARG:HG3	1.92	0.98
1:E:413:ARG:HA	1:E:577:LEU:CD2	1.93	0.98
1:C:190:LYS:HD2	1:C:289:PHE:CE1	1.98	0.98
1:C:286:MET:CG	1:C:316:ARG:CD	2.41	0.98
1:E:262:ARG:HG2	1:E:275:ARG:HH22	1.24	0.98
1:F:262:ARG:HG3	1:F:263:LYS:N	1.78	0.98
1:C:166:GLU:HA	1:C:169:LYS:HG2	1.46	0.98
1:E:218:ILE:HD11	1:E:250:CYS:SG	2.04	0.98
1:A:174:PHE:CZ	1:A:188:ILE:CD1	2.47	0.98
1:A:311:LEU:CA	1:A:316:ARG:NH2	2.26	0.98
1:B:522:ARG:HD2	1:B:530:TYR:HA	1.46	0.98
1:C:286:MET:HG3	1:C:316:ARG:HD2	0.99	0.97
1:D:188:ILE:HG23	1:D:189:PRO:HD2	1.45	0.97
1:D:262:ARG:HG3	1:D:263:LYS:N	1.77	0.97
1:B:348:VAL:HG21	1:B:352:LEU:HD22	1.46	0.97
1:C:416:ALA:HB3	1:C:577:LEU:CD2	1.94	0.97
1:B:313:ARG:CG	1:B:314:PRO:HD2	1.94	0.97
1:C:326:PRO:HB3	1:C:360:PHE:O	1.63	0.97
1:C:145:ARG:NH2	1:C:219:THR:OG1	1.97	0.97
1:A:448:GLY:O	1:A:452:PRO:HD2	1.62	0.97
1:C:262:ARG:HG2	1:C:275:ARG:HH22	1.25	0.97
1:E:524:ASP:HA	1:E:529:GLY:CA	1.94	0.97
1:A:378:ARG:HA	1:F:173:GLU:OE1	1.63	0.97
1:A:571:ARG:HD2	1:A:590:VAL:O	1.64	0.97
1:E:286:MET:HB3	1:E:316:ARG:HG2	0.99	0.97
1:F:171:ILE:CD1	1:F:296:VAL:HG11	1.93	0.97
1:D:337:ILE:HD12	1:D:340:ARG:HH12	1.29	0.97
1:C:448:GLY:O	1:C:452:PRO:HD2	1.64	0.97
1:D:482:VAL:HG13	1:D:483:PHE:HD2	1.25	0.97
1:F:275:ARG:O	1:F:278:THR:OG1	1.82	0.97
1:A:145:ARG:NH2	1:A:219:THR:OG1	1.96	0.97
1:A:316:ARG:NH1	1:A:317:PHE:HD2	1.50	0.97
1:A:286:MET:SD	1:A:316:ARG:CD	2.53	0.96
1:B:187:ARG:O	1:C:374:LEU:HD21	1.63	0.96
1:B:233:GLY:CA	1:B:236:ARG:HH22	1.78	0.96
1:B:453:ARG:CZ	1:B:495:ARG:HH21	1.77	0.96
1:C:215:VAL:HG21	1:C:250:CYS:HA	1.48	0.96
1:E:283:LEU:HG	1:E:316:ARG:HH12	1.29	0.96
1:B:453:ARG:NH1	1:B:495:ARG:HH21	1.62	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASP:HB2	1:B:227:GLU:OE2	1.63	0.96
1:B:171:ILE:CD1	1:B:296:VAL:HG11	1.96	0.96
1:D:171:ILE:CD1	1:D:296:VAL:HG11	1.94	0.96
1:B:188:ILE:HG23	1:B:189:PRO:HD2	1.44	0.96
1:F:291:LYS:HG3	1:F:292:ASP:H	1.31	0.96
1:A:586:GLU:CB	1:A:589:ARG:NH2	2.14	0.96
1:D:184:MET:SD	1:E:342:LYS:NZ	2.39	0.96
1:A:374:LEU:CD2	1:F:187:ARG:O	2.14	0.96
1:B:190:LYS:NZ	1:B:289:PHE:CE2	2.26	0.96
1:C:263:LYS:NZ	1:C:276:GLU:OE1	1.99	0.96
1:D:275:ARG:O	1:D:278:THR:OG1	1.82	0.96
1:D:313:ARG:HD2	1:D:314:PRO:CD	1.93	0.96
1:B:260:VAL:O	1:B:279:LEU:HD11	1.66	0.95
1:F:260:VAL:O	1:F:279:LEU:HD11	1.64	0.95
1:B:165:LYS:HD3	1:B:168:LEU:CD2	1.96	0.95
1:A:227:GLU:HG3	1:F:263:LYS:NZ	1.81	0.95
1:C:174:PHE:CZ	1:C:188:ILE:CD1	2.48	0.95
1:E:215:VAL:HG21	1:E:250:CYS:HA	1.47	0.95
1:E:326:PRO:HB3	1:E:360:PHE:O	1.64	0.95
1:F:337:ILE:HD12	1:F:340:ARG:HH12	1.30	0.95
1:A:166:GLU:HB2	1:A:169:LYS:HZ2	1.31	0.95
1:D:439:THR:HG23	1:D:445:ARG:NH2	1.80	0.95
1:B:578:GLU:HG2	1:B:579:ARG:N	1.81	0.95
1:E:263:LYS:NZ	1:E:276:GLU:OE1	1.99	0.95
1:B:275:ARG:O	1:B:278:THR:OG1	1.83	0.95
1:D:302:ASN:HD21	1:D:443:ARG:HH22	1.06	0.95
1:F:313:ARG:CG	1:F:314:PRO:HD2	1.96	0.95
1:A:263:LYS:CD	1:A:276:GLU:OE1	2.14	0.94
1:A:524:ASP:HA	1:A:529:GLY:CA	1.97	0.94
1:C:520:ALA:HA	1:C:533:ARG:HD3	1.48	0.94
1:D:487:THR:HG22	1:D:488:THR:H	1.30	0.94
1:A:190:LYS:HD2	1:A:289:PHE:CE1	2.02	0.94
1:B:310:ALA:C	1:B:316:ARG:NH1	2.21	0.94
1:B:313:ARG:HD2	1:B:314:PRO:CD	1.93	0.94
1:E:511:HIS:NE2	1:E:516:PRO:HD3	1.81	0.94
1:F:319:ARG:HG2	1:F:319:ARG:HH11	1.32	0.94
1:A:215:VAL:HG21	1:A:250:CYS:HA	1.49	0.94
1:A:520:ALA:HA	1:A:533:ARG:HD3	1.48	0.94
1:C:275:ARG:HG2	1:C:275:ARG:HH11	1.26	0.94
1:F:311:LEU:CA	1:F:316:ARG:NH1	2.10	0.94
1:F:412:ARG:HH12	1:F:440:ILE:CG2	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:VAL:O	1:D:279:LEU:HD11	1.68	0.94
1:B:203:THR:OG1	2:B:2001:ADP:O2A	1.84	0.94
1:D:190:LYS:NZ	1:D:289:PHE:HE2	1.65	0.94
1:D:453:ARG:NH1	1:D:495:ARG:HH21	1.65	0.94
1:A:413:ARG:HA	1:A:577:LEU:CD2	1.98	0.94
1:A:511:HIS:NE2	1:A:516:PRO:HD3	1.83	0.94
1:A:582:LEU:HD23	1:A:587:PHE:HA	1.49	0.94
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.32	0.94
1:C:533:ARG:NH2	1:C:534:GLN:O	2.01	0.94
1:C:582:LEU:HD23	1:C:587:PHE:HA	1.49	0.94
1:D:263:LYS:NZ	1:E:227:GLU:HG3	1.82	0.94
1:E:166:GLU:HA	1:E:169:LYS:HG2	1.46	0.94
1:E:520:ALA:HA	1:E:533:ARG:HD3	1.50	0.94
1:F:376:ALA:CA	1:F:381:ARG:CD	2.28	0.94
1:F:578:GLU:HG2	1:F:579:ARG:N	1.81	0.94
1:F:188:ILE:HG23	1:F:189:PRO:HD2	1.47	0.94
1:A:586:GLU:HB2	1:A:589:ARG:CZ	1.96	0.94
1:C:524:ASP:HA	1:C:529:GLY:CA	1.97	0.94
1:E:201:GLY:N	2:E:1001:ADP:O1A	2.01	0.94
1:B:579:ARG:O	1:B:579:ARG:HG2	1.65	0.93
1:C:286:MET:CB	1:C:316:ARG:HD3	1.90	0.93
1:D:233:GLY:CA	1:D:236:ARG:HH22	1.80	0.93
1:B:302:ASN:HD21	1:B:443:ARG:HH22	1.06	0.93
1:B:487:THR:HG22	1:B:488:THR:H	1.31	0.93
1:A:173:GLU:HA	1:A:176:LYS:CG	1.98	0.93
1:A:215:VAL:HG23	1:A:216:PRO:HD2	1.48	0.93
1:C:201:GLY:N	2:C:1001:ADP:O1A	1.99	0.93
1:D:190:LYS:CE	1:D:289:PHE:CE2	2.52	0.93
1:D:412:ARG:HH12	1:D:440:ILE:CG2	1.80	0.93
1:B:233:GLY:HA2	1:B:236:ARG:NH2	1.82	0.93
1:D:233:GLY:CA	1:D:236:ARG:NH2	2.32	0.93
1:D:522:ARG:HD2	1:D:530:TYR:HA	1.50	0.93
1:F:376:ALA:CB	1:F:381:ARG:HD2	1.98	0.93
1:F:453:ARG:CZ	1:F:495:ARG:HH21	1.80	0.93
1:A:263:LYS:NZ	1:A:276:GLU:OE1	2.00	0.93
1:B:283:LEU:HD12	1:B:316:ARG:HH21	1.32	0.93
1:C:533:ARG:HD2	1:C:534:GLN:H	1.34	0.93
1:C:215:VAL:HG23	1:C:216:PRO:HD2	1.51	0.93
1:D:385:THR:OG1	1:D:388:ASP:OD1	1.86	0.93
1:A:147:LEU:CD2	1:A:151:PRO:HB3	1.96	0.93
1:B:291:LYS:HG3	1:B:292:ASP:H	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LYS:HG3	1:D:292:ASP:N	1.81	0.93
1:E:236:ARG:HG2	1:E:236:ARG:HH11	1.32	0.93
1:E:589:ARG:HH22	1:E:596:LEU:CB	1.70	0.93
1:B:310:ALA:O	1:B:316:ARG:NH1	2.02	0.93
1:B:352:LEU:HD23	1:B:353:LEU:N	1.82	0.93
1:C:236:ARG:HG2	1:C:236:ARG:HH11	1.32	0.93
1:E:582:LEU:HD23	1:E:587:PHE:HA	1.48	0.93
1:F:237:VAL:O	1:F:240:LEU:HB3	1.69	0.93
1:A:460:TRP:O	1:B:488:THR:HA	1.68	0.92
1:D:165:LYS:HD3	1:D:168:LEU:CD2	1.98	0.92
1:E:263:LYS:CD	1:E:276:GLU:OE1	2.15	0.92
1:E:286:MET:HE1	1:E:297:VAL:HG11	1.50	0.92
1:F:215:VAL:CG2	1:F:216:PRO:HD2	1.99	0.92
1:A:262:ARG:CB	1:A:275:ARG:HH12	1.82	0.92
1:C:586:GLU:HA	1:C:589:ARG:HG3	1.51	0.92
1:F:165:LYS:NZ	1:F:205:LEU:HB3	1.84	0.92
1:B:381:ARG:NH1	1:B:388:ASP:OD2	2.02	0.92
1:D:352:LEU:HD23	1:D:353:LEU:N	1.84	0.92
1:E:166:GLU:HB2	1:E:169:LYS:HZ2	1.31	0.92
1:B:439:THR:HG23	1:B:445:ARG:NH2	1.83	0.92
1:C:173:GLU:HA	1:C:176:LYS:CG	1.98	0.92
1:A:311:LEU:CB	1:A:316:ARG:HH22	1.82	0.92
1:D:190:LYS:NZ	1:D:289:PHE:CE2	2.37	0.92
1:D:190:LYS:CE	1:D:289:PHE:CZ	2.51	0.92
1:F:165:LYS:HD3	1:F:168:LEU:CD2	1.99	0.92
1:F:522:ARG:HD2	1:F:530:TYR:HA	1.49	0.92
1:A:453:ARG:NH1	1:A:460:TRP:CZ2	2.36	0.92
1:D:215:VAL:CG2	1:D:216:PRO:HD2	2.00	0.92
1:D:578:GLU:HG2	1:D:579:ARG:N	1.80	0.92
1:B:153:VAL:HG13	1:B:154:THR:N	1.85	0.92
1:A:316:ARG:NH1	1:A:317:PHE:HE2	1.51	0.91
1:D:454:ARG:NH2	1:D:526:TYR:O	2.02	0.91
1:E:190:LYS:HD2	1:E:289:PHE:CE1	2.05	0.91
1:A:453:ARG:NH1	1:A:460:TRP:HZ2	1.67	0.91
1:A:453:ARG:HH11	1:A:453:ARG:HG3	1.34	0.91
1:B:460:TRP:HE3	1:B:460:TRP:H	1.18	0.91
1:C:286:MET:HE1	1:C:297:VAL:HG11	1.51	0.91
1:F:233:GLY:CA	1:F:236:ARG:HH22	1.81	0.91
1:A:481:ILE:HD12	1:A:563:LEU:HB3	1.51	0.91
1:B:454:ARG:NH2	1:B:526:TYR:O	2.02	0.91
1:C:511:HIS:NE2	1:C:516:PRO:HD3	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:THR:HG23	1:F:445:ARG:HH22	1.34	0.91
1:C:174:PHE:CZ	1:C:188:ILE:HD11	2.06	0.91
1:C:382:ARG:HG3	1:C:383:LYS:N	1.85	0.91
1:D:316:ARG:HG3	1:D:316:ARG:NH1	1.83	0.91
1:F:233:GLY:CA	1:F:236:ARG:NH2	2.32	0.91
1:D:257:ILE:O	1:D:260:VAL:N	2.03	0.91
1:F:313:ARG:HD2	1:F:314:PRO:CD	1.97	0.91
1:C:274:GLU:O	1:C:277:GLN:HB3	1.70	0.91
1:A:174:PHE:CZ	1:A:188:ILE:HD11	2.05	0.91
1:C:313:ARG:NH1	1:C:526:TYR:O	2.04	0.91
1:C:589:ARG:HH22	1:C:596:LEU:CB	1.75	0.91
1:D:346:GLU:HG2	1:D:348:VAL:H	1.36	0.90
1:E:166:GLU:HB2	1:E:169:LYS:NZ	1.86	0.90
1:A:168:LEU:O	1:A:171:ILE:CD1	2.17	0.90
1:B:165:LYS:CD	1:B:168:LEU:HD22	2.01	0.90
1:C:155:PHE:HD2	1:C:212:GLU:OE1	1.54	0.90
1:C:262:ARG:CB	1:C:275:ARG:HH12	1.84	0.90
1:B:283:LEU:HD11	1:B:316:ARG:HH22	1.09	0.90
1:E:274:GLU:O	1:E:277:GLN:HB3	1.70	0.90
1:B:238:ARG:HH12	1:B:239:ASP:HB3	1.35	0.90
1:C:166:GLU:HB2	1:C:169:LYS:NZ	1.85	0.90
1:E:174:PHE:CZ	1:E:188:ILE:HD11	2.05	0.90
1:E:215:VAL:HG23	1:E:216:PRO:HD2	1.51	0.90
1:F:238:ARG:HH12	1:F:239:ASP:HB3	1.36	0.90
1:A:313:ARG:HH22	1:A:526:TYR:C	1.75	0.90
1:B:412:ARG:HH12	1:B:440:ILE:CG2	1.85	0.90
1:E:286:MET:HB2	1:E:316:ARG:HD3	1.54	0.90
1:A:236:ARG:HH11	1:A:236:ARG:HG2	1.33	0.90
1:D:453:ARG:NH1	1:D:495:ARG:NH2	2.20	0.90
1:A:168:LEU:HB2	1:A:171:ILE:CD1	2.01	0.90
1:A:201:GLY:N	2:A:1001:ADP:O1A	2.03	0.90
1:B:376:ALA:CB	1:B:381:ARG:HD2	2.01	0.90
1:B:376:ALA:HA	1:B:381:ARG:NE	1.87	0.89
1:E:262:ARG:CB	1:E:275:ARG:HH12	1.83	0.89
1:F:487:THR:HG22	1:F:488:THR:H	1.36	0.89
1:C:286:MET:CB	1:C:316:ARG:CG	2.47	0.89
1:B:215:VAL:CG2	1:B:216:PRO:HD2	2.01	0.89
1:E:449:PHE:CB	1:E:468:GLN:NE2	2.35	0.89
1:B:395:ARG:HG2	1:B:395:ARG:NH1	1.83	0.89
1:C:292:ASP:HB2	1:D:227:GLU:OE2	1.72	0.89
1:A:236:ARG:CG	1:A:237:VAL:N	2.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:HG2	1:B:413:ARG:NH1	1.78	0.89
1:C:519:TYR:O	1:C:533:ARG:NE	2.05	0.89
1:D:237:VAL:O	1:D:240:LEU:HB3	1.71	0.89
1:D:352:LEU:HD21	1:D:386:MET:HE1	1.55	0.89
1:F:238:ARG:HG2	1:F:281:GLN:NE2	1.88	0.89
1:F:439:THR:HG23	1:F:445:ARG:NH2	1.88	0.89
1:F:454:ARG:NH2	1:F:526:TYR:O	2.05	0.89
1:A:533:ARG:HD2	1:A:534:GLN:H	1.35	0.89
1:B:171:ILE:HD11	1:B:296:VAL:CG1	2.03	0.89
1:D:165:LYS:HE2	1:D:205:LEU:CD2	2.02	0.89
1:D:460:TRP:H	1:D:460:TRP:HE3	1.20	0.89
1:E:588:GLN:O	1:E:591:VAL:HB	1.72	0.89
1:A:412:ARG:NH1	1:A:577:LEU:O	2.05	0.89
1:E:236:ARG:CG	1:E:237:VAL:N	2.36	0.89
1:E:286:MET:CB	1:E:316:ARG:HD3	2.03	0.89
1:A:286:MET:HG3	1:A:316:ARG:HD3	0.99	0.89
1:E:412:ARG:NH1	1:E:577:LEU:O	2.06	0.89
1:F:233:GLY:HA2	1:F:236:ARG:HH22	1.17	0.89
1:C:263:LYS:CD	1:C:276:GLU:CD	2.40	0.89
1:E:533:ARG:HD2	1:E:534:GLN:H	1.36	0.89
1:F:257:ILE:O	1:F:260:VAL:N	2.05	0.89
1:A:456:ASP:OD1	1:A:457:MET:N	2.06	0.88
1:B:238:ARG:HG2	1:B:281:GLN:NE2	1.88	0.88
1:C:155:PHE:CZ	1:C:168:LEU:HD11	2.08	0.88
1:F:171:ILE:HD11	1:F:296:VAL:CG1	2.01	0.88
1:F:190:LYS:HE3	1:F:289:PHE:CE2	2.08	0.88
1:A:311:LEU:HA	1:A:316:ARG:HH21	1.30	0.88
1:A:588:GLN:O	1:A:591:VAL:HB	1.73	0.88
1:C:286:MET:CB	1:C:316:ARG:HG2	1.98	0.88
1:D:327:ASP:OD1	1:D:328:VAL:N	2.06	0.88
1:A:166:GLU:HB2	1:A:169:LYS:NZ	1.89	0.88
1:C:147:LEU:CD2	1:C:151:PRO:HB3	2.02	0.88
1:C:589:ARG:HH21	1:C:596:LEU:CB	1.64	0.88
1:E:313:ARG:HH22	1:E:526:TYR:HA	1.39	0.88
1:C:286:MET:HB3	1:C:316:ARG:CD	1.94	0.88
1:C:313:ARG:HH22	1:C:526:TYR:C	1.77	0.88
1:F:453:ARG:NH1	1:F:495:ARG:NH2	2.20	0.88
1:A:378:ARG:NH2	1:F:170:GLU:CB	2.34	0.88
1:B:356:ARG:HH11	1:B:356:ARG:CG	1.86	0.88
1:D:471:VAL:O	1:D:474:ALA:HB3	1.74	0.88
1:B:184:MET:SD	1:C:342:LYS:NZ	2.46	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LYS:HE2	1:B:578:GLU:O	1.72	0.88
1:C:412:ARG:NH1	1:C:577:LEU:O	2.06	0.88
1:E:176:LYS:HD3	1:E:213:ALA:HA	1.54	0.88
1:E:211:GLY:O	1:E:214:ARG:HD2	1.72	0.88
1:A:326:PRO:HB3	1:A:360:PHE:O	1.73	0.88
1:A:384:ILE:HG23	1:A:388:ASP:HB2	1.56	0.88
1:B:382:ARG:HG3	1:B:382:ARG:NH1	1.74	0.88
1:D:165:LYS:CD	1:D:168:LEU:HD22	2.03	0.88
1:D:168:LEU:O	1:D:171:ILE:HG22	1.73	0.88
1:D:173:GLU:O	1:D:176:LYS:HG2	1.74	0.88
1:A:311:LEU:CD2	1:A:316:ARG:HH22	1.88	0.87
1:A:453:ARG:HH22	1:A:464:ARG:HH12	1.23	0.87
1:B:482:VAL:HG13	1:B:483:PHE:CD2	2.09	0.87
1:F:302:ASN:HD21	1:F:443:ARG:NH2	1.71	0.87
1:C:384:ILE:HG23	1:C:388:ASP:HB2	1.56	0.87
1:E:173:GLU:HA	1:E:176:LYS:HG3	1.52	0.87
1:E:313:ARG:NH1	1:E:526:TYR:O	2.07	0.87
1:B:503:ARG:HH22	1:B:522:ARG:NH2	1.73	0.87
1:E:456:ASP:OD1	1:E:457:MET:N	2.07	0.87
1:A:263:LYS:CD	1:A:276:GLU:CD	2.42	0.87
1:B:173:GLU:O	1:B:176:LYS:HG2	1.74	0.87
1:B:257:ILE:O	1:B:260:VAL:N	2.07	0.87
1:B:453:ARG:NH1	1:B:495:ARG:NH2	2.23	0.87
1:C:430:GLU:O	1:C:431:HIS:HB3	1.75	0.87
1:D:238:ARG:HH12	1:D:239:ASP:HB3	1.36	0.87
1:E:147:LEU:CD2	1:E:151:PRO:HB3	2.02	0.87
1:F:159:ALA:HB3	1:F:334:ILE:HG13	1.57	0.87
1:F:165:LYS:CD	1:F:168:LEU:HD22	2.04	0.87
1:A:449:PHE:CB	1:A:468:GLN:NE2	2.38	0.87
1:E:453:ARG:HH22	1:E:460:TRP:HE1	1.21	0.87
1:F:345:ALA:HB2	1:F:383:LYS:HE3	1.56	0.87
1:F:395:ARG:HG2	1:F:395:ARG:NH1	1.81	0.87
1:E:313:ARG:HH22	1:E:526:TYR:CA	1.87	0.87
1:A:155:PHE:HD2	1:A:212:GLU:OE1	1.58	0.87
1:D:301:THR:HG21	1:D:307:LEU:HD11	1.56	0.87
1:F:460:TRP:HE3	1:F:460:TRP:H	1.19	0.87
1:F:470:ALA:O	1:F:558:VAL:HG21	1.74	0.87
1:C:410:ARG:O	1:C:413:ARG:N	2.07	0.87
1:E:313:ARG:HH22	1:E:526:TYR:C	1.77	0.87
1:D:171:ILE:HD11	1:D:296:VAL:CG1	2.02	0.87
1:D:238:ARG:HG2	1:D:281:GLN:NE2	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:HIS:ND1	1:D:366:GLU:HG3	1.90	0.87
1:F:286:MET:HE1	1:F:316:ARG:CA	2.03	0.87
1:B:175:LEU:HD12	1:B:215:VAL:HG11	1.57	0.86
1:B:291:LYS:HG3	1:B:292:ASP:N	1.89	0.86
1:D:175:LEU:HD12	1:D:215:VAL:HG11	1.57	0.86
1:E:172:VAL:CG2	1:E:213:ALA:HB2	2.05	0.86
1:F:190:LYS:CE	1:F:289:PHE:CE2	2.57	0.86
1:D:153:VAL:HG13	1:D:154:THR:N	1.90	0.86
1:D:253:PHE:HE2	1:D:255:ASP:HB2	1.38	0.86
1:C:176:LYS:HD3	1:C:213:ALA:HA	1.55	0.86
1:B:283:LEU:HD12	1:B:316:ARG:NH2	1.86	0.86
1:B:301:THR:HG21	1:B:307:LEU:HD11	1.57	0.86
1:C:536:SER:OG	1:D:544:ASP:OD2	1.94	0.86
1:D:164:ALA:O	1:D:168:LEU:HD13	1.73	0.86
1:D:370:ASN:OD1	1:D:371:GLU:N	2.08	0.86
1:F:370:ASN:OD1	1:F:371:GLU:N	2.08	0.86
1:A:313:ARG:CZ	1:A:526:TYR:HA	2.05	0.86
1:A:342:LYS:CD	1:A:343:PRO:HD2	2.04	0.86
1:C:308:ASP:OD1	1:C:310:ALA:N	2.09	0.86
1:E:263:LYS:CD	1:E:276:GLU:CD	2.44	0.86
1:F:173:GLU:O	1:F:176:LYS:HG2	1.75	0.86
1:C:467:ASP:OD1	1:C:557:ARG:NH2	2.08	0.86
1:C:588:GLN:O	1:C:591:VAL:HB	1.75	0.86
1:D:345:ALA:HB2	1:D:383:LYS:HE3	1.55	0.86
1:E:428:PHE:CD1	1:E:432:ALA:HA	2.11	0.86
1:E:481:ILE:HD12	1:E:563:LEU:HB3	1.55	0.86
1:A:430:GLU:O	1:A:431:HIS:HB3	1.75	0.86
1:B:346:GLU:HG2	1:B:348:VAL:H	1.41	0.86
1:C:428:PHE:CD1	1:C:432:ALA:HA	2.10	0.86
1:C:456:ASP:OD1	1:C:457:MET:N	2.07	0.86
1:D:174:PHE:HB2	1:D:181:PHE:CE2	2.11	0.86
1:D:356:ARG:HG3	1:D:356:ARG:NH1	1.83	0.86
1:E:155:PHE:CZ	1:E:168:LEU:HD11	2.11	0.86
1:E:264:ARG:CG	1:E:266:SER:H	1.83	0.86
1:F:153:VAL:HG13	1:F:154:THR:N	1.91	0.86
1:F:301:THR:HG21	1:F:307:LEU:HD11	1.56	0.86
1:A:176:LYS:HD3	1:A:213:ALA:HA	1.58	0.85
1:B:164:ALA:O	1:B:168:LEU:HD13	1.76	0.85
1:C:233:GLY:HA2	1:C:236:ARG:NH1	1.91	0.85
1:D:209:VAL:HG13	1:D:210:ALA:H	1.40	0.85
1:D:253:PHE:CE2	1:D:255:ASP:HB2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:GLU:HG2	1:F:348:VAL:H	1.41	0.85
1:F:382:ARG:HG3	1:F:382:ARG:NH1	1.73	0.85
1:A:155:PHE:CZ	1:A:168:LEU:HD11	2.11	0.85
1:A:449:PHE:HB3	1:A:468:GLN:NE2	1.91	0.85
1:D:313:ARG:CG	1:D:314:PRO:CD	2.54	0.85
1:E:155:PHE:HD2	1:E:212:GLU:OE1	1.57	0.85
1:A:174:PHE:CZ	1:A:188:ILE:HD13	2.12	0.85
1:B:382:ARG:HH11	1:B:382:ARG:CG	1.89	0.85
1:F:164:ALA:O	1:F:168:LEU:HD13	1.77	0.85
1:A:509:GLY:O	1:B:476:ARG:NH2	2.09	0.85
1:C:449:PHE:CB	1:C:468:GLN:NE2	2.38	0.85
1:F:238:ARG:HH12	1:F:239:ASP:CB	1.89	0.85
1:C:173:GLU:HA	1:C:176:LYS:HG3	1.59	0.85
1:E:384:ILE:HG23	1:E:388:ASP:HB2	1.58	0.85
1:E:449:PHE:HB3	1:E:468:GLN:NE2	1.91	0.85
1:F:215:VAL:HG22	1:F:216:PRO:HD2	1.57	0.85
1:F:526:TYR:O	1:F:527:LEU:C	2.15	0.85
1:B:327:ASP:OD1	1:B:328:VAL:N	2.08	0.85
1:D:579:ARG:HG2	1:D:579:ARG:O	1.76	0.85
1:A:374:LEU:HD11	1:F:187:ARG:N	1.91	0.85
1:A:453:ARG:HH22	1:A:460:TRP:HE1	1.20	0.85
1:C:202:LYS:HD2	1:C:300:ALA:HB1	1.59	0.85
1:C:453:ARG:HG3	1:C:453:ARG:HH11	1.42	0.85
1:D:159:ALA:HB3	1:D:334:ILE:HG13	1.56	0.85
1:D:311:LEU:O	1:D:316:ARG:CG	2.25	0.85
1:E:173:GLU:HA	1:E:176:LYS:HG2	1.59	0.85
1:F:168:LEU:O	1:F:171:ILE:HG22	1.74	0.85
1:A:316:ARG:HG2	1:A:317:PHE:H	1.41	0.85
1:A:352:LEU:CD1	1:A:356:ARG:HH21	1.90	0.85
1:A:410:ARG:O	1:A:413:ARG:N	2.10	0.85
1:B:168:LEU:O	1:B:171:ILE:HG22	1.76	0.85
1:C:589:ARG:HB3	1:C:589:ARG:CZ	2.07	0.85
1:D:356:ARG:HH11	1:D:356:ARG:CG	1.89	0.85
1:B:238:ARG:HH12	1:B:239:ASP:CB	1.90	0.84
1:E:145:ARG:CZ	1:E:219:THR:OG1	2.25	0.84
1:E:308:ASP:OD1	1:E:310:ALA:N	2.10	0.84
1:E:571:ARG:HD2	1:E:590:VAL:O	1.76	0.84
1:C:473:LEU:HD22	1:C:555:TYR:HB2	1.59	0.84
1:E:342:LYS:CD	1:E:343:PRO:HD2	2.06	0.84
1:E:473:LEU:HD22	1:E:555:TYR:HB2	1.57	0.84
1:F:209:VAL:HG13	1:F:210:ALA:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:ARG:HH11	1:F:382:ARG:CG	1.89	0.84
1:B:190:LYS:CE	1:B:289:PHE:CE2	2.60	0.84
1:B:356:ARG:HG3	1:B:356:ARG:NH1	1.82	0.84
1:C:342:LYS:CD	1:C:343:PRO:HD2	2.06	0.84
1:C:382:ARG:CG	1:C:383:LYS:N	2.41	0.84
1:A:172:VAL:CG2	1:A:213:ALA:HB2	2.07	0.84
1:A:384:ILE:CG2	1:A:388:ASP:HB2	2.08	0.84
1:B:352:LEU:HD21	1:B:386:MET:HE1	1.59	0.84
1:B:460:TRP:HE3	1:B:460:TRP:N	1.74	0.84
1:C:509:GLY:C	1:D:476:ARG:HH22	1.80	0.84
1:D:470:ALA:O	1:D:558:VAL:HG21	1.77	0.84
1:B:345:ALA:HB2	1:B:383:LYS:HE3	1.57	0.84
1:E:163:GLU:N	1:E:163:GLU:OE1	2.11	0.84
1:A:202:LYS:HD2	1:A:300:ALA:HB1	1.59	0.84
1:B:470:ALA:O	1:B:558:VAL:HG21	1.76	0.84
1:C:174:PHE:CZ	1:C:188:ILE:HD13	2.13	0.84
1:D:215:VAL:HG22	1:D:216:PRO:HD2	1.59	0.84
1:D:395:ARG:HG2	1:D:395:ARG:NH1	1.89	0.84
1:E:430:GLU:O	1:E:431:HIS:HB3	1.74	0.84
1:F:253:PHE:CE2	1:F:255:ASP:HB2	2.13	0.84
1:A:163:GLU:OE1	1:A:163:GLU:N	2.11	0.84
1:A:263:LYS:HZ2	1:A:276:GLU:CD	1.79	0.84
1:A:313:ARG:NH1	1:A:526:TYR:O	2.10	0.84
1:C:453:ARG:HH22	1:C:464:ARG:HH12	1.26	0.84
1:A:151:PRO:HD2	1:A:211:GLY:HA2	1.59	0.84
1:F:214:ARG:HH11	1:F:214:ARG:HG3	1.38	0.84
1:A:263:LYS:CE	1:A:276:GLU:CD	2.46	0.84
1:A:428:PHE:CD1	1:A:432:ALA:HA	2.13	0.84
1:F:356:ARG:HH11	1:F:356:ARG:CG	1.88	0.84
1:A:173:GLU:HA	1:A:176:LYS:HG2	1.60	0.84
1:A:308:ASP:OD1	1:A:310:ALA:N	2.11	0.84
1:B:190:LYS:HE3	1:B:289:PHE:CE2	2.12	0.84
1:B:311:LEU:CA	1:B:316:ARG:NH1	2.41	0.84
1:C:236:ARG:CG	1:C:237:VAL:N	2.34	0.84
1:F:355:LYS:HE3	1:F:578:GLU:O	1.76	0.84
1:A:283:LEU:HD11	1:A:311:LEU:HD21	1.59	0.83
1:B:262:ARG:HG3	1:B:263:LYS:H	1.43	0.83
1:B:370:ASN:OD1	1:B:371:GLU:N	2.10	0.83
1:C:453:ARG:HH22	1:C:460:TRP:HE1	1.22	0.83
1:C:571:ARG:HD2	1:C:590:VAL:O	1.78	0.83
1:E:202:LYS:HD2	1:E:300:ALA:HB1	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASN:HD21	1:B:443:ARG:NH2	1.75	0.83
1:D:313:ARG:HG3	1:D:314:PRO:CD	2.07	0.83
1:F:291:LYS:HG3	1:F:292:ASP:N	1.87	0.83
1:A:382:ARG:HG3	1:A:383:LYS:N	1.91	0.83
1:B:159:ALA:HB3	1:B:334:ILE:HG13	1.60	0.83
1:D:589:ARG:NE	1:D:596:LEU:HD11	1.92	0.83
1:A:313:ARG:HH22	1:A:526:TYR:CA	1.90	0.83
1:B:174:PHE:HB2	1:B:181:PHE:CE2	2.13	0.83
1:B:253:PHE:HE2	1:B:255:ASP:HB2	1.42	0.83
1:F:356:ARG:HG3	1:F:356:ARG:NH1	1.83	0.83
1:B:235:ALA:O	1:B:238:ARG:CZ	2.26	0.83
1:E:453:ARG:HH22	1:E:464:ARG:HH12	1.27	0.83
1:F:207:ARG:HB3	1:F:217:PHE:CZ	2.13	0.83
1:A:210:ALA:O	1:A:214:ARG:HA	1.79	0.83
1:A:509:GLY:C	1:B:476:ARG:HH22	1.81	0.83
1:B:165:LYS:HE2	1:B:205:LEU:CD2	2.08	0.83
1:B:257:ILE:H	1:B:257:ILE:HD12	1.43	0.83
1:C:470:ALA:HB1	1:C:558:VAL:HG23	1.59	0.83
1:B:526:TYR:O	1:B:527:LEU:C	2.17	0.83
1:C:384:ILE:CG2	1:C:388:ASP:HB2	2.09	0.83
1:D:302:ASN:HD21	1:D:443:ARG:NH2	1.75	0.83
1:E:470:ALA:HB1	1:E:558:VAL:HG23	1.59	0.83
1:E:589:ARG:HB3	1:E:589:ARG:CZ	2.08	0.83
1:F:175:LEU:HD12	1:F:215:VAL:HG11	1.59	0.83
1:B:207:ARG:HB3	1:B:217:PHE:CZ	2.14	0.83
1:B:313:ARG:CG	1:B:314:PRO:CD	2.57	0.83
1:C:332:GLU:OE2	1:C:351:ALA:HA	1.79	0.83
1:C:352:LEU:CD1	1:C:356:ARG:HH21	1.92	0.83
1:C:371:GLU:HG3	1:C:392:ALA:HB1	1.58	0.83
1:D:257:ILE:H	1:D:257:ILE:HD12	1.43	0.83
1:E:215:VAL:CG2	1:E:250:CYS:HA	2.09	0.83
1:F:253:PHE:HE2	1:F:255:ASP:HB2	1.42	0.83
1:A:262:ARG:HB3	1:A:275:ARG:NH1	1.92	0.82
1:B:253:PHE:CE2	1:B:255:ASP:HB2	2.13	0.82
1:D:325:ALA:HB3	1:D:326:PRO:HD3	1.58	0.82
1:D:526:TYR:O	1:D:527:LEU:C	2.16	0.82
1:E:223:SER:O	1:E:225:PHE:N	2.11	0.82
1:F:345:ALA:HB2	1:F:383:LYS:CE	2.08	0.82
1:F:430:GLU:OE1	1:F:430:GLU:HA	1.78	0.82
1:F:482:VAL:HG13	1:F:483:PHE:CD2	2.12	0.82
1:A:342:LYS:CD	1:F:184:MET:O	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ALA:HB1	1:A:577:LEU:HD23	1.56	0.82
1:B:215:VAL:HG22	1:B:216:PRO:HD2	1.61	0.82
1:D:165:LYS:HA	1:D:168:LEU:HD22	1.62	0.82
1:E:233:GLY:HA2	1:E:236:ARG:NH1	1.94	0.82
1:A:233:GLY:O	1:A:236:ARG:HG2	1.79	0.82
1:C:163:GLU:OE1	1:C:163:GLU:N	2.11	0.82
1:C:449:PHE:HB3	1:C:468:GLN:NE2	1.94	0.82
1:D:345:ALA:HB2	1:D:383:LYS:CE	2.08	0.82
1:E:332:GLU:OE2	1:E:351:ALA:HA	1.79	0.82
1:B:345:ALA:HB2	1:B:383:LYS:CE	2.08	0.82
1:E:286:MET:HB3	1:E:316:ARG:CD	2.04	0.82
1:F:174:PHE:HB2	1:F:181:PHE:CE2	2.13	0.82
1:F:214:ARG:HG3	1:F:214:ARG:NH1	1.91	0.82
1:A:449:PHE:CE2	1:A:496:GLN:CG	2.62	0.82
1:D:376:ALA:C	1:D:381:ARG:HG3	1.99	0.82
1:E:197:PRO:HD2	1:E:200:VAL:HG21	1.61	0.82
1:F:257:ILE:H	1:F:257:ILE:HD12	1.44	0.82
1:A:332:GLU:OE2	1:A:351:ALA:HA	1.80	0.82
1:C:263:LYS:HD2	1:C:276:GLU:OE1	1.75	0.82
1:D:529:GLY:O	1:D:530:TYR:HB3	1.78	0.82
1:E:174:PHE:CZ	1:E:188:ILE:HD13	2.12	0.82
1:E:207:ARG:CZ	1:E:207:ARG:HB2	2.10	0.82
1:C:197:PRO:HD2	1:C:200:VAL:HG21	1.59	0.82
1:C:263:LYS:CE	1:C:276:GLU:CD	2.47	0.82
1:D:238:ARG:HH12	1:D:239:ASP:CB	1.92	0.82
1:A:313:ARG:HH22	1:A:526:TYR:HA	1.44	0.82
1:B:529:GLY:O	1:B:530:TYR:HB3	1.79	0.82
1:A:377:ALA:HB1	1:F:181:PHE:CE1	2.15	0.82
1:C:460:TRP:O	1:D:488:THR:HA	1.80	0.82
1:E:223:SER:C	1:E:225:PHE:H	1.81	0.82
1:F:262:ARG:HG3	1:F:263:LYS:H	1.45	0.82
1:F:571:ARG:HD2	1:F:590:VAL:O	1.80	0.82
1:A:470:ALA:HB1	1:A:558:VAL:HG23	1.62	0.82
1:B:343:PRO:HG2	1:B:383:LYS:HA	1.62	0.82
1:C:225:PHE:CE1	1:C:233:GLY:CA	2.60	0.82
1:E:263:LYS:HD2	1:E:276:GLU:OE1	1.78	0.82
1:E:313:ARG:CZ	1:E:526:TYR:HA	2.08	0.81
1:F:327:ASP:OD1	1:F:328:VAL:N	2.12	0.81
1:B:471:VAL:O	1:B:474:ALA:HB3	1.80	0.81
1:F:589:ARG:NE	1:F:596:LEU:HD11	1.95	0.81
1:A:197:PRO:HD2	1:A:200:VAL:HG21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ALA:O	1:A:357:THR:HG23	1.80	0.81
1:A:519:TYR:O	1:A:533:ARG:NE	2.12	0.81
1:B:313:ARG:HG3	1:B:314:PRO:CD	2.10	0.81
1:B:337:ILE:HD12	1:B:340:ARG:NH1	1.96	0.81
1:F:286:MET:CE	1:F:316:ARG:HA	2.04	0.81
1:F:579:ARG:O	1:F:579:ARG:HG2	1.78	0.81
1:A:207:ARG:HB2	1:A:207:ARG:CZ	2.10	0.81
1:A:352:LEU:HD12	1:A:356:ARG:HH21	1.45	0.81
1:B:209:VAL:HG13	1:B:210:ALA:H	1.44	0.81
1:D:378:ARG:C	1:D:380:GLY:H	1.84	0.81
1:D:482:VAL:HG13	1:D:483:PHE:CD2	2.13	0.81
1:E:416:ALA:HB1	1:E:577:LEU:HD23	1.57	0.81
1:F:337:ILE:O	1:F:340:ARG:NH1	2.13	0.81
1:B:523:GLU:HG2	1:B:530:TYR:O	1.81	0.81
1:B:568:VAL:O	1:B:572:VAL:HG23	1.79	0.81
1:C:155:PHE:CD2	1:C:212:GLU:OE1	2.33	0.81
1:C:172:VAL:CG2	1:C:213:ALA:HB2	2.07	0.81
1:C:225:PHE:HE1	1:C:233:GLY:HA2	1.43	0.81
1:B:241:PHE:O	1:B:244:ALA:N	2.13	0.81
1:C:173:GLU:HA	1:C:176:LYS:HG2	1.63	0.81
1:D:243:THR:HA	1:D:246:ARG:HH21	1.45	0.81
1:E:352:LEU:HD21	1:E:386:MET:SD	2.21	0.81
1:E:371:GLU:HG3	1:E:392:ALA:HB1	1.62	0.81
1:F:338:HIS:ND1	1:F:366:GLU:HG3	1.94	0.81
1:F:474:ALA:CA	1:F:558:VAL:HG11	2.11	0.81
1:C:262:ARG:HB3	1:C:275:ARG:NH1	1.93	0.81
1:E:410:ARG:O	1:E:413:ARG:N	2.14	0.81
1:F:155:PHE:CD2	1:F:212:GLU:OE2	2.34	0.81
1:F:238:ARG:HH12	1:F:239:ASP:N	1.78	0.81
1:F:375:LEU:HD11	1:F:388:ASP:HB3	1.61	0.81
1:C:352:LEU:HD12	1:C:356:ARG:HH21	1.46	0.81
1:D:523:GLU:HG2	1:D:530:TYR:O	1.81	0.81
1:E:155:PHE:CD2	1:E:212:GLU:OE1	2.33	0.81
1:F:460:TRP:HE3	1:F:460:TRP:N	1.77	0.81
1:A:178:PRO:HB3	1:A:294:ALA:HB2	1.62	0.80
1:B:430:GLU:HA	1:B:430:GLU:OE1	1.81	0.80
1:C:215:VAL:CG2	1:C:250:CYS:HA	2.10	0.80
1:D:155:PHE:CD2	1:D:212:GLU:OE2	2.34	0.80
1:D:533:ARG:HH11	1:D:533:ARG:HG3	1.45	0.80
1:D:582:LEU:HD21	1:D:590:VAL:HG21	1.62	0.80
1:E:225:PHE:CE1	1:E:233:GLY:CA	2.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:ASP:OD1	1:E:557:ARG:NH2	2.14	0.80
1:F:568:VAL:O	1:F:572:VAL:HG23	1.81	0.80
1:A:173:GLU:HA	1:A:176:LYS:HG3	1.61	0.80
1:B:328:VAL:CG2	1:B:355:LYS:HE3	2.11	0.80
1:B:579:ARG:O	1:B:581:THR:N	2.13	0.80
1:C:223:SER:C	1:C:225:PHE:H	1.84	0.80
1:C:313:ARG:CZ	1:C:526:TYR:HA	2.10	0.80
1:D:331:ARG:NH2	1:D:580:GLU:OE1	2.14	0.80
1:E:236:ARG:HH11	1:E:236:ARG:CG	1.93	0.80
1:F:521:VAL:HG23	1:F:532:VAL:HG13	1.62	0.80
1:D:262:ARG:HG3	1:D:263:LYS:H	1.45	0.80
1:D:355:LYS:HE3	1:D:578:GLU:O	1.81	0.80
1:E:586:GLU:HA	1:E:589:ARG:HG3	1.61	0.80
1:A:168:LEU:C	1:A:171:ILE:HD13	2.02	0.80
1:A:371:GLU:HG3	1:A:392:ALA:HB1	1.62	0.80
1:B:474:ALA:CA	1:B:558:VAL:HG11	2.11	0.80
1:C:533:ARG:HD2	1:C:534:GLN:N	1.96	0.80
1:D:413:ARG:HG2	1:D:413:ARG:NH1	1.77	0.80
1:B:325:ALA:HB3	1:B:326:PRO:HD3	1.62	0.80
1:B:521:VAL:HG23	1:B:532:VAL:HG13	1.62	0.80
1:E:168:LEU:CB	1:E:171:ILE:HD11	2.06	0.80
1:E:225:PHE:HE1	1:E:233:GLY:HA2	1.45	0.80
1:F:471:VAL:O	1:F:474:ALA:HB3	1.80	0.80
1:A:155:PHE:CD2	1:A:212:GLU:OE1	2.34	0.80
1:D:286:MET:CE	1:D:316:ARG:HA	2.09	0.80
1:E:215:VAL:HG11	1:E:250:CYS:HA	1.64	0.80
1:E:352:LEU:CD1	1:E:356:ARG:HH21	1.95	0.80
1:A:225:PHE:HE1	1:A:233:GLY:HA2	1.44	0.80
1:A:233:GLY:HA2	1:A:236:ARG:NH1	1.96	0.80
1:A:339:ALA:HA	1:A:369:LEU:HD21	1.63	0.80
1:D:153:VAL:HG13	1:D:154:THR:H	1.46	0.80
1:E:172:VAL:HG23	1:E:213:ALA:CB	2.08	0.80
1:A:223:SER:C	1:A:225:PHE:H	1.85	0.80
1:F:450:MET:HA	1:F:453:ARG:HD2	1.63	0.80
1:E:210:ALA:HB2	1:E:251:ILE:HD12	1.63	0.79
1:F:468:GLN:O	1:F:471:VAL:HG22	1.82	0.79
1:F:449:PHE:CE2	1:F:453:ARG:NH2	2.50	0.79
1:C:357:THR:HG1	1:C:360:PHE:HD1	1.29	0.79
1:E:382:ARG:HG3	1:E:383:LYS:N	1.98	0.79
1:F:313:ARG:CG	1:F:314:PRO:CD	2.60	0.79
1:D:236:ARG:HG2	1:D:237:VAL:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:VAL:HG21	1:D:352:LEU:CD2	2.12	0.79
1:E:219:THR:HB	1:E:253:PHE:HD2	1.47	0.79
1:E:354:ALA:O	1:E:357:THR:HG23	1.82	0.79
1:E:396:VAL:O	1:E:400:PRO:HD3	1.82	0.79
1:F:582:LEU:HD21	1:F:590:VAL:HG21	1.63	0.79
1:A:225:PHE:CE1	1:A:233:GLY:CA	2.61	0.79
1:C:313:ARG:HH22	1:C:526:TYR:CA	1.96	0.79
1:E:331:ARG:NH1	1:E:354:ALA:O	2.14	0.79
1:F:274:GLU:O	1:F:277:GLN:HG2	1.81	0.79
1:A:223:SER:O	1:A:225:PHE:N	2.15	0.79
1:B:589:ARG:NE	1:B:594:LEU:HD21	1.93	0.79
1:D:235:ALA:O	1:D:238:ARG:HG3	1.83	0.79
1:C:223:SER:O	1:C:225:PHE:N	2.14	0.79
1:C:503:ARG:HG2	1:C:508:TRP:CZ3	2.18	0.79
1:D:241:PHE:O	1:D:244:ALA:N	2.15	0.79
1:D:460:TRP:HE3	1:D:460:TRP:N	1.80	0.79
1:A:274:GLU:O	1:A:277:GLN:HB3	1.81	0.79
1:C:178:PRO:HB3	1:C:294:ALA:HB2	1.65	0.79
1:C:236:ARG:HH11	1:C:236:ARG:CG	1.96	0.79
1:D:286:MET:HE1	1:D:316:ARG:CA	2.08	0.79
1:F:325:ALA:HB3	1:F:326:PRO:HD3	1.65	0.79
1:B:165:LYS:HA	1:B:168:LEU:HD22	1.64	0.79
1:C:168:LEU:CB	1:C:171:ILE:HD11	2.09	0.79
1:E:339:ALA:HA	1:E:369:LEU:HD21	1.63	0.79
1:E:509:GLY:C	1:F:476:ARG:HH22	1.85	0.79
1:A:461:SER:HA	1:B:487:THR:O	1.82	0.79
1:C:354:ALA:O	1:C:357:THR:HG23	1.83	0.79
1:F:376:ALA:C	1:F:381:ARG:HD2	2.03	0.79
1:F:523:GLU:HG2	1:F:530:TYR:O	1.83	0.79
1:A:172:VAL:HG23	1:A:213:ALA:CB	2.11	0.78
1:E:263:LYS:CE	1:E:276:GLU:CD	2.50	0.78
1:F:241:PHE:O	1:F:244:ALA:N	2.16	0.78
1:A:236:ARG:HH11	1:A:236:ARG:CG	1.95	0.78
1:A:449:PHE:CZ	1:A:496:GLN:CG	2.63	0.78
1:B:241:PHE:CE2	1:B:285:GLU:OE2	2.36	0.78
1:B:338:HIS:ND1	1:B:366:GLU:HG3	1.97	0.78
1:D:241:PHE:CE2	1:D:285:GLU:OE2	2.36	0.78
1:E:536:SER:OG	1:F:544:ASP:OD2	2.02	0.78
1:F:378:ARG:C	1:F:380:GLY:H	1.86	0.78
1:B:274:GLU:O	1:B:277:GLN:HG2	1.83	0.78
1:D:376:ALA:O	1:D:381:ARG:CG	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:MET:CB	1:E:316:ARG:CG	2.45	0.78
1:C:396:VAL:O	1:C:400:PRO:HD3	1.83	0.78
1:D:199:GLY:N	2:D:2001:ADP:O2B	2.15	0.78
1:A:215:VAL:CG2	1:A:250:CYS:HA	2.14	0.78
1:A:382:ARG:CG	1:A:383:LYS:N	2.46	0.78
1:D:238:ARG:HH12	1:D:239:ASP:N	1.82	0.78
1:E:262:ARG:HB3	1:E:275:ARG:NH1	1.93	0.78
1:F:313:ARG:HG3	1:F:314:PRO:CD	2.12	0.78
1:A:264:ARG:CD	1:A:266:SER:HB2	2.13	0.78
1:B:235:ALA:O	1:B:238:ARG:HG3	1.84	0.78
1:D:474:ALA:CA	1:D:558:VAL:HG11	2.13	0.78
1:F:238:ARG:HH11	1:F:239:ASP:N	1.77	0.78
1:B:193:LEU:O	1:B:320:GLN:HB2	1.83	0.78
1:D:313:ARG:NE	1:D:314:PRO:HD2	1.97	0.78
1:D:319:ARG:HH11	1:D:319:ARG:CG	1.96	0.78
1:D:382:ARG:CG	1:D:382:ARG:NH1	2.17	0.78
1:F:236:ARG:HG2	1:F:237:VAL:N	1.97	0.78
1:C:346:GLU:N	1:C:346:GLU:OE1	2.17	0.78
1:E:233:GLY:O	1:E:236:ARG:HG2	1.82	0.78
1:E:533:ARG:HD2	1:E:534:GLN:N	1.99	0.78
1:B:313:ARG:NE	1:B:314:PRO:HD2	1.99	0.78
1:C:225:PHE:CE2	1:C:278:THR:HB	2.19	0.78
1:E:465:LEU:HD22	1:E:508:TRP:HZ3	1.50	0.78
1:F:207:ARG:HB3	1:F:217:PHE:CE1	2.19	0.78
1:F:331:ARG:NH2	1:F:580:GLU:OE1	2.15	0.78
1:F:343:PRO:HG2	1:F:383:LYS:HA	1.66	0.78
1:A:263:LYS:HD2	1:A:276:GLU:OE1	1.79	0.77
1:A:396:VAL:O	1:A:400:PRO:HD3	1.84	0.77
1:E:178:PRO:HB3	1:E:294:ALA:HB2	1.66	0.77
1:F:155:PHE:HA	1:F:158:VAL:HG23	1.67	0.77
1:F:235:ALA:O	1:F:238:ARG:HG3	1.84	0.77
1:A:585:GLU:O	1:A:588:GLN:CG	2.27	0.77
1:B:207:ARG:HB3	1:B:217:PHE:CE1	2.20	0.77
1:C:352:LEU:HD21	1:C:386:MET:SD	2.24	0.77
1:C:586:GLU:HA	1:C:589:ARG:CG	2.15	0.77
1:D:283:LEU:HD12	1:D:316:ARG:HH21	1.49	0.77
1:D:337:ILE:O	1:D:340:ARG:NH1	2.18	0.77
1:F:153:VAL:HG13	1:F:154:THR:H	1.48	0.77
1:F:352:LEU:HD11	1:F:386:MET:HE1	1.65	0.77
1:A:346:GLU:OE1	1:A:346:GLU:N	2.17	0.77
1:B:155:PHE:CD2	1:B:212:GLU:OE2	2.36	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:LEU:HD21	1:B:590:VAL:HG21	1.65	0.77
1:E:346:GLU:OE1	1:E:346:GLU:N	2.18	0.77
1:E:357:THR:HG1	1:E:360:PHE:HD1	1.33	0.77
1:F:165:LYS:HA	1:F:168:LEU:HD22	1.66	0.77
1:F:215:VAL:HG21	1:F:249:PRO:O	1.84	0.77
1:A:418:HIS:O	1:A:421:GLY:N	2.18	0.77
1:E:249:PRO:HA	1:E:294:ALA:O	1.85	0.77
1:E:519:TYR:O	1:E:533:ARG:NE	2.17	0.77
1:A:319:ARG:HH21	1:B:402:LYS:NZ	1.82	0.77
1:C:219:THR:HB	1:C:253:PHE:HD2	1.49	0.77
1:C:249:PRO:HA	1:C:294:ALA:O	1.84	0.77
1:D:458:LEU:HD12	1:D:459:HIS:H	1.48	0.77
1:B:414:ILE:HG23	1:B:483:PHE:CE1	2.20	0.77
1:B:450:MET:HA	1:B:453:ARG:HD2	1.65	0.77
1:A:225:PHE:CE2	1:A:278:THR:HB	2.19	0.77
1:B:337:ILE:O	1:B:340:ARG:NH1	2.18	0.77
1:B:413:ARG:HH11	1:B:413:ARG:CG	1.95	0.77
1:E:286:MET:HG3	1:E:316:ARG:CD	2.15	0.77
1:A:352:LEU:HD21	1:A:386:MET:SD	2.25	0.77
1:B:243:THR:HA	1:B:246:ARG:HH21	1.48	0.77
1:E:352:LEU:HD12	1:E:356:ARG:HH21	1.49	0.77
1:F:243:THR:HA	1:F:246:ARG:HH21	1.49	0.77
1:A:533:ARG:HD2	1:A:534:GLN:N	2.00	0.76
1:A:536:SER:OG	1:B:544:ASP:OD2	2.02	0.76
1:B:286:MET:O	1:B:289:PHE:HB2	1.85	0.76
1:D:331:ARG:NH1	1:D:357:THR:O	2.17	0.76
1:E:449:PHE:CE2	1:E:496:GLN:CG	2.67	0.76
1:E:453:ARG:HH11	1:E:453:ARG:HG3	1.50	0.76
1:B:276:GLU:HA	1:B:279:LEU:CD1	2.15	0.76
1:C:313:ARG:HH22	1:C:526:TYR:HA	1.50	0.76
1:C:503:ARG:HD2	1:C:508:TRP:CE2	2.20	0.76
1:D:238:ARG:HH11	1:D:239:ASP:N	1.82	0.76
1:A:174:PHE:CE2	1:A:188:ILE:HD13	2.20	0.76
1:B:331:ARG:NH2	1:B:580:GLU:OE1	2.18	0.76
1:B:348:VAL:HG21	1:B:352:LEU:CD2	2.15	0.76
1:C:461:SER:O	1:C:464:ARG:HB3	1.85	0.76
1:D:274:GLU:O	1:D:277:GLN:HG2	1.85	0.76
1:E:453:ARG:NH1	1:E:460:TRP:HZ2	1.83	0.76
1:A:311:LEU:HD22	1:A:316:ARG:NH2	2.00	0.76
1:B:331:ARG:NH1	1:B:357:THR:O	2.18	0.76
1:B:502:ARG:O	1:B:506:THR:HG23	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ARG:NH2	1:C:526:TYR:O	2.17	0.76
1:E:149:GLU:O	1:E:150:ALA:HB3	1.83	0.76
1:E:225:PHE:CE2	1:E:278:THR:HB	2.20	0.76
1:F:529:GLY:O	1:F:530:TYR:HB3	1.83	0.76
1:B:215:VAL:HG21	1:B:249:PRO:O	1.85	0.76
1:B:238:ARG:HH11	1:B:239:ASP:N	1.82	0.76
1:B:376:ALA:CB	1:B:381:ARG:CD	2.60	0.76
1:C:233:GLY:O	1:C:236:ARG:HG2	1.85	0.76
1:F:588:GLN:O	1:F:591:VAL:HB	1.86	0.76
1:B:328:VAL:HG22	1:B:355:LYS:HE3	1.67	0.76
1:C:210:ALA:HB2	1:C:251:ILE:HD12	1.67	0.76
1:C:453:ARG:NH1	1:C:460:TRP:CZ2	2.54	0.76
1:D:207:ARG:HB2	1:D:217:PHE:CZ	2.20	0.76
1:F:412:ARG:HH22	1:F:440:ILE:HB	1.50	0.76
1:B:238:ARG:HH12	1:B:239:ASP:N	1.82	0.76
1:B:243:THR:HA	1:B:246:ARG:NH2	2.00	0.76
1:E:384:ILE:CG2	1:E:388:ASP:HB2	2.16	0.76
1:F:241:PHE:CE2	1:F:285:GLU:OE2	2.39	0.76
1:A:453:ARG:CZ	1:A:460:TRP:HE1	1.99	0.76
1:A:510:MET:O	1:A:512:PRO:HD2	1.86	0.76
1:B:412:ARG:HH22	1:B:440:ILE:HB	1.51	0.76
1:F:424:LEU:HD11	1:F:569:LEU:HA	1.67	0.76
1:A:211:GLY:HA2	1:A:214:ARG:HE	1.51	0.76
1:A:215:VAL:HG11	1:A:250:CYS:HA	1.67	0.76
1:B:158:VAL:HG22	1:B:204:HIS:CE1	2.21	0.76
1:C:166:GLU:CA	1:C:169:LYS:HG2	2.15	0.76
1:C:453:ARG:NH1	1:C:460:TRP:HZ2	1.82	0.76
1:D:450:MET:HA	1:D:453:ARG:HD2	1.67	0.76
1:F:235:ALA:O	1:F:238:ARG:CZ	2.33	0.76
1:F:238:ARG:HH12	1:F:239:ASP:CA	1.99	0.76
1:F:449:PHE:HE2	1:F:492:ASN:HB3	1.51	0.76
1:A:453:ARG:NH1	1:A:453:ARG:HG3	2.00	0.75
1:B:460:TRP:N	1:B:460:TRP:CE3	2.52	0.75
1:D:588:GLN:O	1:D:591:VAL:HB	1.86	0.75
1:E:339:ALA:CA	1:E:369:LEU:HD21	2.15	0.75
1:F:243:THR:HA	1:F:246:ARG:NH2	2.00	0.75
1:A:342:LYS:HD2	1:A:343:PRO:CD	2.13	0.75
1:B:238:ARG:HH12	1:B:239:ASP:CA	2.00	0.75
1:D:521:VAL:HG23	1:D:532:VAL:HG13	1.67	0.75
1:F:451:MET:HB3	1:F:452:PRO:HD3	1.69	0.75
1:A:219:THR:HB	1:A:253:PHE:HD2	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PRO:HD2	1:B:200:VAL:HG11	1.69	0.75
1:B:247:HIS:HB3	1:B:250:CYS:SG	2.27	0.75
1:C:390:GLU:O	1:C:393:ALA:HB3	1.86	0.75
1:C:584:ALA:O	1:C:587:PHE:HB3	1.85	0.75
1:D:276:GLU:HA	1:D:279:LEU:CD1	2.16	0.75
1:E:174:PHE:CE2	1:E:188:ILE:HD13	2.20	0.75
1:F:233:GLY:O	1:F:278:THR:HG22	1.85	0.75
1:F:474:ALA:HA	1:F:558:VAL:CG1	2.16	0.75
1:A:503:ARG:HG2	1:A:508:TRP:CZ3	2.22	0.75
1:C:339:ALA:CA	1:C:369:LEU:HD21	2.17	0.75
1:C:339:ALA:HA	1:C:369:LEU:HD21	1.66	0.75
1:C:393:ALA:O	1:C:396:VAL:HG12	1.86	0.75
1:B:238:ARG:HB3	1:B:281:GLN:NE2	2.01	0.75
1:F:502:ARG:O	1:F:506:THR:HG23	1.86	0.75
1:A:339:ALA:CA	1:A:369:LEU:HD21	2.15	0.75
1:A:388:ASP:OD1	1:A:388:ASP:N	2.20	0.75
1:C:181:PHE:O	1:C:184:MET:HG2	1.87	0.75
1:C:589:ARG:HH22	1:C:596:LEU:HB2	1.33	0.75
1:E:286:MET:CG	1:E:316:ARG:HD2	2.15	0.75
1:C:449:PHE:CZ	1:C:496:GLN:CG	2.65	0.75
1:D:451:MET:HB3	1:D:452:PRO:HD3	1.69	0.75
1:A:210:ALA:O	1:A:214:ARG:HD3	1.87	0.75
1:C:172:VAL:HG23	1:C:213:ALA:CB	2.12	0.75
1:C:174:PHE:CE2	1:C:188:ILE:HD13	2.22	0.75
1:B:451:MET:HB3	1:B:452:PRO:HD3	1.69	0.74
1:D:412:ARG:HH22	1:D:440:ILE:HB	1.49	0.74
1:E:393:ALA:O	1:E:396:VAL:HG12	1.87	0.74
1:F:319:ARG:HH11	1:F:319:ARG:CG	2.00	0.74
1:F:410:ARG:O	1:F:413:ARG:N	2.20	0.74
1:A:331:ARG:NH1	1:A:354:ALA:O	2.20	0.74
1:C:313:ARG:CZ	1:C:526:TYR:O	2.34	0.74
1:C:381:ARG:HH11	1:C:381:ARG:HG3	1.52	0.74
1:D:233:GLY:O	1:D:278:THR:HG22	1.86	0.74
1:E:286:MET:CG	1:E:316:ARG:CD	2.65	0.74
1:E:335:LEU:CD2	1:E:353:LEU:HD23	2.17	0.74
1:F:337:ILE:HD12	1:F:340:ARG:NH1	2.01	0.74
1:A:166:GLU:CA	1:A:169:LYS:HG2	2.14	0.74
1:A:586:GLU:HA	1:A:589:ARG:HE	1.50	0.74
1:B:233:GLY:O	1:B:278:THR:HG22	1.86	0.74
1:B:310:ALA:C	1:B:316:ARG:HH12	1.86	0.74
1:B:424:LEU:HD11	1:B:569:LEU:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ARG:HH12	1:B:522:ARG:HH21	1.35	0.74
1:E:510:MET:O	1:E:512:PRO:HD2	1.87	0.74
1:E:584:ALA:O	1:E:587:PHE:HB3	1.86	0.74
1:F:503:ARG:HH22	1:F:522:ARG:NH2	1.85	0.74
1:C:196:GLY:N	1:C:202:LYS:NZ	2.35	0.74
1:D:153:VAL:CG1	1:D:154:THR:N	2.51	0.74
1:F:171:ILE:HG13	1:F:296:VAL:HG21	1.69	0.74
1:B:449:PHE:HE2	1:B:492:ASN:HB3	1.52	0.74
1:D:365:LEU:O	1:D:368:LEU:HB3	1.88	0.74
1:E:342:LYS:HD2	1:E:343:PRO:CD	2.16	0.74
1:F:313:ARG:NE	1:F:314:PRO:HD2	2.00	0.74
1:A:236:ARG:O	1:A:237:VAL:C	2.26	0.74
1:A:249:PRO:HA	1:A:294:ALA:O	1.87	0.74
1:A:264:ARG:HG3	1:A:265:GLY:N	2.02	0.74
1:F:331:ARG:NH1	1:F:357:THR:O	2.19	0.74
1:B:378:ARG:C	1:B:380:GLY:H	1.89	0.74
1:C:342:LYS:HD2	1:C:343:PRO:CD	2.16	0.74
1:E:465:LEU:HD22	1:E:508:TRP:CZ3	2.22	0.74
1:A:165:LYS:O	1:A:168:LEU:HG	1.87	0.74
1:C:449:PHE:CE2	1:C:496:GLN:CG	2.68	0.74
1:F:458:LEU:HD12	1:F:459:HIS:H	1.53	0.74
1:A:313:ARG:NH2	1:A:526:TYR:O	2.20	0.74
1:A:390:GLU:O	1:A:393:ALA:HB3	1.88	0.74
1:B:588:GLN:O	1:B:591:VAL:HB	1.88	0.74
1:D:243:THR:HA	1:D:246:ARG:NH2	2.02	0.74
1:D:458:LEU:HD12	1:D:459:HIS:N	2.02	0.74
1:E:418:HIS:O	1:E:421:GLY:N	2.21	0.74
1:F:155:PHE:HD2	1:F:212:GLU:OE2	1.71	0.74
1:A:461:SER:OG	1:B:486:VAL:HG11	1.87	0.74
1:C:236:ARG:HG3	1:C:237:VAL:H	1.52	0.74
1:D:468:GLN:O	1:D:471:VAL:HG22	1.88	0.74
1:F:199:GLY:N	2:F:2001:ADP:O2B	2.17	0.74
1:F:589:ARG:NE	1:F:594:LEU:HD21	1.94	0.74
1:E:236:ARG:HG3	1:E:237:VAL:H	1.52	0.73
1:E:413:ARG:CA	1:E:577:LEU:HD22	2.16	0.73
1:A:181:PHE:O	1:A:184:MET:HG2	1.87	0.73
1:A:381:ARG:HH11	1:A:381:ARG:HG3	1.53	0.73
1:D:235:ALA:O	1:D:238:ARG:CZ	2.36	0.73
1:D:346:GLU:HG3	1:D:386:MET:HG2	1.70	0.73
1:D:571:ARG:HD2	1:D:590:VAL:O	1.88	0.73
1:E:166:GLU:CA	1:E:169:LYS:HG2	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:GLU:O	1:E:393:ALA:HB3	1.87	0.73
1:E:453:ARG:NH1	1:E:460:TRP:CZ2	2.55	0.73
1:A:313:ARG:NH2	1:A:526:TYR:CA	2.46	0.73
1:A:410:ARG:HG3	1:A:411:ASP:N	2.04	0.73
1:B:236:ARG:NH1	1:B:278:THR:HG22	2.00	0.73
1:B:376:ALA:C	1:B:381:ARG:HB2	2.08	0.73
1:B:468:GLN:O	1:B:471:VAL:HG22	1.87	0.73
1:D:155:PHE:HD2	1:D:212:GLU:OE2	1.71	0.73
1:D:589:ARG:NE	1:D:594:LEU:HD21	1.95	0.73
1:E:215:VAL:HG21	1:E:250:CYS:CA	2.17	0.73
1:F:376:ALA:HA	1:F:381:ARG:NE	2.04	0.73
1:F:376:ALA:HA	1:F:381:ARG:HD2	0.74	0.73
1:B:348:VAL:HG22	1:B:352:LEU:HD22	1.70	0.73
1:C:358:PRO:HA	1:C:359:GLY:C	2.08	0.73
1:C:474:ALA:HA	1:C:558:VAL:HG11	1.70	0.73
1:A:441:VAL:O	1:A:441:VAL:HG12	1.88	0.73
1:D:586:GLU:O	1:D:590:VAL:HG23	1.88	0.73
1:F:316:ARG:NH1	1:F:316:ARG:HG2	2.03	0.73
1:F:436:HIS:O	1:F:437:LYS:HG2	1.89	0.73
1:B:589:ARG:HB3	1:B:594:LEU:HD22	1.70	0.73
1:D:158:VAL:HG22	1:D:204:HIS:CE1	2.23	0.73
1:D:191:GLY:HA2	1:D:297:VAL:HG12	1.71	0.73
1:D:430:GLU:OE1	1:D:430:GLU:HA	1.88	0.73
1:D:439:THR:CG2	1:D:445:ARG:HH22	2.00	0.73
1:F:233:GLY:HA2	1:F:236:ARG:HH21	1.52	0.73
1:A:236:ARG:HG3	1:A:237:VAL:H	1.49	0.73
1:A:408:SER:HB2	1:A:409:PRO:HD2	1.71	0.73
1:C:196:GLY:H	1:C:202:LYS:NZ	1.86	0.73
1:F:247:HIS:HB3	1:F:250:CYS:SG	2.28	0.73
1:B:238:ARG:CB	1:B:281:GLN:NE2	2.52	0.73
1:D:238:ARG:HH12	1:D:239:ASP:CA	2.01	0.73
1:D:413:ARG:HH11	1:D:413:ARG:CG	1.96	0.73
1:F:460:TRP:N	1:F:460:TRP:CE3	2.54	0.73
1:A:236:ARG:O	1:A:239:ASP:OD1	2.07	0.73
1:B:501:ALA:HB1	1:B:550:LEU:HD23	1.70	0.73
1:C:215:VAL:HG21	1:C:250:CYS:CA	2.19	0.73
1:D:153:VAL:HB	1:D:207:ARG:HH11	1.54	0.73
1:D:155:PHE:HA	1:D:158:VAL:HG23	1.71	0.73
1:E:382:ARG:HG3	1:E:383:LYS:H	1.51	0.73
1:F:193:LEU:O	1:F:320:GLN:HB2	1.88	0.73
1:A:460:TRP:CD1	1:A:464:ARG:NH1	2.57	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ARG:NH1	1:A:596:LEU:HB3	2.02	0.73
1:F:235:ALA:HA	1:F:238:ARG:CD	2.18	0.73
1:F:316:ARG:HG2	1:F:316:ARG:HH11	1.54	0.73
1:F:503:ARG:HH12	1:F:522:ARG:HH21	1.36	0.73
1:A:393:ALA:O	1:A:396:VAL:HG12	1.88	0.72
1:A:503:ARG:HD2	1:A:508:TRP:CE2	2.23	0.72
1:B:155:PHE:HD2	1:B:212:GLU:OE2	1.72	0.72
1:B:171:ILE:HG13	1:B:296:VAL:HG21	1.71	0.72
1:F:567:GLU:O	1:F:570:GLU:N	2.22	0.72
1:A:587:PHE:O	1:A:590:VAL:CG2	2.32	0.72
1:D:412:ARG:NH2	1:D:440:ILE:HD13	2.03	0.72
1:E:453:ARG:HH21	1:E:464:ARG:NH2	1.86	0.72
1:F:276:GLU:CA	1:F:279:LEU:HD13	2.18	0.72
1:A:586:GLU:CA	1:A:589:ARG:NE	2.52	0.72
1:C:166:GLU:CB	1:C:169:LYS:HZ2	2.02	0.72
1:D:313:ARG:HG3	1:D:314:PRO:N	2.04	0.72
1:D:337:ILE:HD12	1:D:340:ARG:NH1	2.02	0.72
1:D:449:PHE:HE2	1:D:492:ASN:HB3	1.53	0.72
1:E:224:ASP:HA	1:E:227:GLU:OE2	1.88	0.72
1:E:388:ASP:OD1	1:E:388:ASP:N	2.22	0.72
1:E:460:TRP:CD1	1:E:464:ARG:NH1	2.56	0.72
1:B:153:VAL:CG1	1:B:154:THR:N	2.50	0.72
1:B:163:GLU:N	1:B:163:GLU:OE1	2.22	0.72
1:D:378:ARG:O	1:D:380:GLY:N	2.21	0.72
1:E:196:GLY:N	1:E:202:LYS:NZ	2.36	0.72
1:A:196:GLY:N	1:A:202:LYS:NZ	2.38	0.72
1:B:153:VAL:HG13	1:B:154:THR:H	1.54	0.72
1:C:331:ARG:NH1	1:C:354:ALA:O	2.22	0.72
1:D:171:ILE:HG13	1:D:296:VAL:HG21	1.70	0.72
1:D:173:GLU:HA	1:D:176:LYS:HE3	1.71	0.72
1:D:215:VAL:HG21	1:D:249:PRO:O	1.89	0.72
1:D:283:LEU:CD1	1:D:316:ARG:HH21	2.01	0.72
1:D:454:ARG:HH21	1:D:526:TYR:C	1.93	0.72
1:C:165:LYS:O	1:C:168:LEU:HG	1.89	0.72
1:C:215:VAL:HG11	1:C:250:CYS:HA	1.70	0.72
1:C:418:HIS:O	1:C:421:GLY:N	2.22	0.72
1:C:441:VAL:O	1:C:441:VAL:HG12	1.87	0.72
1:E:461:SER:O	1:E:464:ARG:HB2	1.88	0.72
1:F:392:ALA:O	1:F:396:VAL:HG12	1.88	0.72
1:A:149:GLU:O	1:A:150:ALA:HB3	1.90	0.72
1:A:210:ALA:HB2	1:A:251:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:SER:O	1:A:464:ARG:HB3	1.89	0.72
1:C:224:ASP:HA	1:C:227:GLU:OE2	1.89	0.72
1:E:236:ARG:O	1:E:237:VAL:C	2.27	0.72
1:E:441:VAL:O	1:E:441:VAL:HG12	1.89	0.72
1:F:346:GLU:HG3	1:F:386:MET:CG	2.19	0.72
1:F:579:ARG:O	1:F:581:THR:N	2.22	0.72
1:A:439:THR:OG1	1:A:440:ILE:N	2.23	0.72
1:B:474:ALA:HA	1:B:558:VAL:CG1	2.16	0.72
1:A:465:LEU:HD22	1:A:508:TRP:HZ3	1.55	0.72
1:B:392:ALA:O	1:B:396:VAL:HG12	1.89	0.72
1:B:454:ARG:HH21	1:B:526:TYR:C	1.91	0.72
1:C:335:LEU:CD2	1:C:353:LEU:HD23	2.19	0.72
1:C:439:THR:OG1	1:C:440:ILE:N	2.23	0.72
1:D:247:HIS:HB3	1:D:250:CYS:SG	2.29	0.72
1:D:589:ARG:HB3	1:D:594:LEU:HD22	1.71	0.72
1:E:181:PHE:O	1:E:184:MET:HG2	1.90	0.72
1:E:524:ASP:CA	1:E:529:GLY:HA2	2.08	0.72
1:F:466:LEU:HD11	1:F:504:MET:HE1	1.72	0.72
1:A:382:ARG:HG3	1:A:383:LYS:CB	2.20	0.72
1:B:286:MET:HE1	1:B:316:ARG:CA	2.09	0.72
1:B:286:MET:O	1:B:289:PHE:CB	2.37	0.72
1:D:214:ARG:HH11	1:D:214:ARG:HB3	1.54	0.72
1:F:376:ALA:C	1:F:381:ARG:HB2	2.10	0.72
1:A:286:MET:CG	1:A:316:ARG:HD2	1.99	0.71
1:B:170:GLU:HB3	1:C:378:ARG:HH22	1.55	0.71
1:D:414:ILE:HG23	1:D:483:PHE:CE1	2.24	0.71
1:D:567:GLU:O	1:D:570:GLU:N	2.23	0.71
1:D:579:ARG:O	1:D:581:THR:N	2.22	0.71
1:F:153:VAL:CG1	1:F:154:THR:N	2.52	0.71
1:F:190:LYS:CE	1:F:289:PHE:CZ	2.73	0.71
1:F:589:ARG:HB3	1:F:594:LEU:HD22	1.72	0.71
1:B:571:ARG:HD2	1:B:590:VAL:O	1.88	0.71
1:E:263:LYS:HG2	1:E:264:ARG:H	1.56	0.71
1:E:474:ALA:HA	1:E:558:VAL:HG11	1.71	0.71
1:F:346:GLU:HG3	1:F:386:MET:HG2	1.70	0.71
1:F:458:LEU:HD12	1:F:459:HIS:N	2.04	0.71
1:B:184:MET:O	1:C:342:LYS:HD3	1.89	0.71
1:B:238:ARG:HB3	1:B:281:GLN:HE22	1.55	0.71
1:B:284:VAL:O	1:B:288:GLY:N	2.24	0.71
1:C:233:GLY:HA2	1:C:236:ARG:HH12	1.53	0.71
1:C:236:ARG:O	1:C:239:ASP:OD1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ARG:NH2	1:C:460:TRP:NE1	2.33	0.71
1:D:242:GLU:HA	1:D:245:LYS:HB3	1.72	0.71
1:F:286:MET:O	1:F:289:PHE:HB2	1.90	0.71
1:B:376:ALA:HA	1:B:381:ARG:HD2	0.72	0.71
1:E:313:ARG:CZ	1:E:526:TYR:O	2.39	0.71
1:A:239:ASP:OD1	1:A:240:LEU:N	2.22	0.71
1:B:199:GLY:N	2:B:2001:ADP:O2B	2.20	0.71
1:C:149:GLU:O	1:C:150:ALA:HB3	1.88	0.71
1:E:381:ARG:HH11	1:E:381:ARG:HG3	1.53	0.71
1:F:414:ILE:HG23	1:F:483:PHE:CE1	2.26	0.71
1:F:586:GLU:O	1:F:590:VAL:HG23	1.91	0.71
1:A:358:PRO:HA	1:A:359:GLY:C	2.11	0.71
1:B:352:LEU:O	1:B:355:LYS:HB2	1.90	0.71
1:C:586:GLU:O	1:C:589:ARG:HB2	1.90	0.71
1:E:410:ARG:HG3	1:E:411:ASP:N	2.04	0.71
1:F:163:GLU:OE1	1:F:163:GLU:N	2.24	0.71
1:A:467:ASP:OD1	1:A:557:ARG:NH2	2.24	0.71
1:A:474:ALA:HA	1:A:558:VAL:HG11	1.70	0.71
1:A:488:THR:O	1:A:490:ALA:N	2.21	0.71
1:B:233:GLY:O	1:B:236:ARG:NH1	2.23	0.71
1:C:155:PHE:HZ	1:C:168:LEU:HD11	1.55	0.71
1:C:202:LYS:HB2	2:C:1001:ADP:O1B	1.90	0.71
1:C:520:ALA:HA	1:C:533:ARG:CD	2.20	0.71
1:D:163:GLU:OE1	1:D:163:GLU:N	2.23	0.71
1:D:424:LEU:HD11	1:D:569:LEU:HA	1.72	0.71
1:D:465:LEU:O	1:D:469:ILE:HG13	1.89	0.71
1:A:263:LYS:HG2	1:A:264:ARG:H	1.56	0.71
1:A:533:ARG:CD	1:A:534:GLN:H	2.04	0.71
1:D:348:VAL:HG22	1:D:352:LEU:HD22	1.72	0.71
1:F:165:LYS:HZ1	1:F:205:LEU:HB3	1.54	0.71
1:B:155:PHE:HA	1:B:158:VAL:HG23	1.71	0.71
1:B:242:GLU:HA	1:B:245:LYS:HB3	1.72	0.71
1:B:332:GLU:OE1	1:B:351:ALA:HA	1.91	0.71
1:B:533:ARG:HH11	1:B:533:ARG:HG3	1.56	0.71
1:C:521:VAL:HG12	1:D:495:ARG:HD2	1.71	0.71
1:D:502:ARG:O	1:D:506:THR:HG23	1.91	0.71
1:C:453:ARG:HH21	1:C:464:ARG:NH2	1.89	0.71
1:C:493:ASP:O	1:C:496:GLN:HB2	1.91	0.71
1:D:193:LEU:O	1:D:320:GLN:HB2	1.90	0.71
1:B:190:LYS:CE	1:B:289:PHE:CZ	2.74	0.70
1:C:236:ARG:O	1:C:237:VAL:C	2.29	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:PHE:CE1	1:D:432:ALA:HB1	2.26	0.70
1:F:284:VAL:O	1:F:288:GLY:N	2.24	0.70
1:A:178:PRO:HB3	1:A:294:ALA:CB	2.21	0.70
1:A:384:ILE:HG23	1:A:388:ASP:CB	2.21	0.70
1:B:346:GLU:HG3	1:B:386:MET:CG	2.20	0.70
1:D:191:GLY:CA	1:D:297:VAL:HG12	2.21	0.70
1:D:346:GLU:HG3	1:D:386:MET:CG	2.21	0.70
1:E:165:LYS:O	1:E:168:LEU:HG	1.90	0.70
1:E:196:GLY:H	1:E:202:LYS:NZ	1.87	0.70
1:F:153:VAL:HB	1:F:207:ARG:HH11	1.56	0.70
1:F:286:MET:O	1:F:289:PHE:CB	2.39	0.70
1:A:481:ILE:CD1	1:A:563:LEU:HB3	2.21	0.70
1:B:449:PHE:CE2	1:B:453:ARG:NH2	2.59	0.70
1:B:458:LEU:HD12	1:B:459:HIS:H	1.55	0.70
1:D:449:PHE:CE2	1:D:453:ARG:NH2	2.59	0.70
1:E:313:ARG:NH2	1:E:526:TYR:O	2.25	0.70
1:E:419:GLU:OE1	1:E:419:GLU:HA	1.92	0.70
1:A:313:ARG:CZ	1:A:526:TYR:O	2.40	0.70
1:A:340:ARG:C	1:A:342:LYS:H	1.92	0.70
1:B:311:LEU:N	1:B:316:ARG:NH1	2.38	0.70
1:E:503:ARG:HG2	1:E:508:TRP:CZ3	2.27	0.70
1:F:381:ARG:NH1	1:F:388:ASP:OD2	2.25	0.70
1:A:311:LEU:HD22	1:A:316:ARG:CZ	2.22	0.70
1:A:586:GLU:CA	1:A:589:ARG:HE	2.05	0.70
1:E:439:THR:OG1	1:E:440:ILE:N	2.22	0.70
1:A:520:ALA:HA	1:A:533:ARG:CD	2.22	0.70
1:B:365:LEU:O	1:B:368:LEU:HB3	1.92	0.70
1:C:239:ASP:OD1	1:C:240:LEU:N	2.25	0.70
1:C:408:SER:HB2	1:C:409:PRO:HD2	1.73	0.70
1:D:214:ARG:HH11	1:D:214:ARG:CB	2.05	0.70
1:F:238:ARG:HB3	1:F:281:GLN:NE2	2.06	0.70
1:A:335:LEU:CD2	1:A:353:LEU:HD23	2.21	0.70
1:A:465:LEU:HD22	1:A:508:TRP:CZ3	2.26	0.70
1:A:588:GLN:O	1:A:591:VAL:CB	2.39	0.70
1:B:503:ARG:HH22	1:B:522:ARG:CZ	2.05	0.70
1:C:384:ILE:HG23	1:C:388:ASP:CB	2.21	0.70
1:D:284:VAL:O	1:D:288:GLY:N	2.24	0.70
1:D:376:ALA:C	1:D:381:ARG:CG	2.60	0.70
1:D:389:LEU:O	1:D:392:ALA:N	2.25	0.70
1:F:182:HIS:ND1	1:F:182:HIS:N	2.40	0.70
1:F:501:ALA:O	1:F:505:ILE:HD12	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLY:HA2	1:A:443:ARG:HH21	1.55	0.70
1:A:224:ASP:HA	1:A:227:GLU:OE2	1.91	0.70
1:A:227:GLU:HG3	1:F:263:LYS:HZ3	1.57	0.70
1:C:333:GLN:HG3	1:C:336:ARG:NH1	2.06	0.70
1:C:340:ARG:C	1:C:342:LYS:H	1.95	0.70
1:D:165:LYS:O	1:D:168:LEU:HB2	1.91	0.70
1:D:220:ALA:O	1:D:254:ILE:HA	1.91	0.70
1:A:381:ARG:N	1:F:180:ARG:NH2	2.40	0.70
1:A:453:ARG:HH21	1:A:464:ARG:NH2	1.89	0.70
1:B:319:ARG:HH11	1:B:319:ARG:CG	2.02	0.70
1:E:215:VAL:CG1	1:E:250:CYS:HA	2.22	0.70
1:E:286:MET:O	1:E:289:PHE:CZ	2.45	0.70
1:F:376:ALA:HB2	1:F:381:ARG:HH11	1.57	0.70
1:D:215:VAL:HG23	1:D:216:PRO:HD2	1.73	0.70
1:D:428:PHE:CE1	1:D:432:ALA:CB	2.74	0.70
1:D:460:TRP:N	1:D:460:TRP:CE3	2.58	0.70
1:D:568:VAL:O	1:D:572:VAL:HG23	1.92	0.70
1:F:525:THR:HG22	1:F:526:TYR:HD2	1.55	0.70
1:A:196:GLY:H	1:A:202:LYS:NZ	1.89	0.69
1:A:413:ARG:CA	1:A:577:LEU:HD22	2.16	0.69
1:C:275:ARG:HG2	1:C:275:ARG:NH1	2.01	0.69
1:D:262:ARG:CG	1:D:263:LYS:N	2.54	0.69
1:E:236:ARG:NH1	1:E:236:ARG:HB3	2.06	0.69
1:E:340:ARG:C	1:E:342:LYS:H	1.93	0.69
1:E:453:ARG:NH2	1:E:460:TRP:NE1	2.35	0.69
1:F:355:LYS:CE	1:F:578:GLU:O	2.40	0.69
1:F:394:ASP:HA	1:F:397:MET:CE	2.22	0.69
1:F:454:ARG:HH21	1:F:526:TYR:C	1.94	0.69
1:B:215:VAL:HG23	1:B:216:PRO:HD2	1.72	0.69
1:C:460:TRP:CD1	1:C:464:ARG:NH1	2.59	0.69
1:D:201:GLY:O	1:D:205:LEU:HD13	1.92	0.69
1:D:216:PRO:HG3	1:D:247:HIS:ND1	2.07	0.69
1:F:216:PRO:HG3	1:F:247:HIS:ND1	2.06	0.69
1:C:207:ARG:HB2	1:C:207:ARG:CZ	2.21	0.69
1:E:449:PHE:N	1:E:449:PHE:CD2	2.60	0.69
1:E:503:ARG:HD2	1:E:508:TRP:CE2	2.27	0.69
1:A:215:VAL:HG21	1:A:250:CYS:CA	2.21	0.69
1:A:286:MET:HE1	1:A:297:VAL:HG11	1.74	0.69
1:B:187:ARG:H	1:C:374:LEU:HD11	1.58	0.69
1:D:202:LYS:HG2	2:D:2001:ADP:O1A	1.92	0.69
1:D:564:GLU:C	1:D:566:ARG:H	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:VAL:HG22	1:F:204:HIS:CE1	2.26	0.69
1:F:173:GLU:HA	1:F:176:LYS:HE3	1.74	0.69
1:A:283:LEU:HD11	1:A:311:LEU:CD2	2.21	0.69
1:C:303:ARG:HB2	1:C:303:ARG:HH11	0.64	0.69
1:C:533:ARG:CD	1:C:534:GLN:H	2.05	0.69
1:E:358:PRO:HA	1:E:359:GLY:C	2.11	0.69
1:E:382:ARG:HD3	1:E:383:LYS:HB3	1.74	0.69
1:F:253:PHE:HA	1:F:298:MET:HB3	1.74	0.69
1:F:303:ARG:O	1:F:307:LEU:HD13	1.93	0.69
1:A:234:ALA:O	1:A:237:VAL:HG12	1.92	0.69
1:B:238:ARG:CG	1:B:281:GLN:NE2	2.55	0.69
1:B:286:MET:CE	1:B:316:ARG:HA	2.09	0.69
1:B:439:THR:CG2	1:B:445:ARG:HH22	2.01	0.69
1:C:177:ASN:HD22	1:C:180:ARG:HD3	1.58	0.69
1:C:313:ARG:NH2	1:C:526:TYR:CA	2.52	0.69
1:C:453:ARG:HG3	1:C:453:ARG:NH1	2.02	0.69
1:D:225:PHE:CD2	1:D:236:ARG:HD2	2.28	0.69
1:F:424:LEU:O	1:F:427:HIS:N	2.23	0.69
1:A:387:LYS:HA	1:A:390:GLU:HB2	1.73	0.69
1:B:424:LEU:O	1:B:427:HIS:N	2.24	0.69
1:C:234:ALA:HB1	1:C:281:GLN:NE2	2.07	0.69
1:C:469:ILE:HG23	1:C:497:ALA:HB1	1.73	0.69
1:D:155:PHE:O	1:D:158:VAL:N	2.26	0.69
1:D:228:MET:SD	1:D:232:VAL:HG12	2.33	0.69
1:D:233:GLY:HA2	1:D:236:ARG:HH21	1.51	0.69
1:D:337:ILE:HG23	1:D:338:HIS:CD2	2.28	0.69
1:D:355:LYS:CE	1:D:578:GLU:O	2.41	0.69
1:D:424:LEU:O	1:D:427:HIS:N	2.23	0.69
1:E:303:ARG:HB2	1:E:303:ARG:HH11	0.65	0.69
1:E:453:ARG:CZ	1:E:460:TRP:HE1	2.05	0.69
1:E:533:ARG:CZ	1:E:534:GLN:O	2.40	0.69
1:F:238:ARG:CB	1:F:281:GLN:NE2	2.56	0.69
1:F:332:GLU:OE1	1:F:351:ALA:HA	1.91	0.69
1:A:453:ARG:HH22	1:A:464:ARG:NH1	1.90	0.69
1:A:469:ILE:HG23	1:A:497:ALA:HB1	1.75	0.69
1:A:486:VAL:HG21	1:F:463:LYS:HE3	1.73	0.69
1:A:584:ALA:O	1:A:587:PHE:HB3	1.92	0.69
1:B:436:HIS:O	1:B:437:LYS:HG2	1.93	0.69
1:B:567:GLU:O	1:B:570:GLU:N	2.26	0.69
1:C:413:ARG:HA	1:C:577:LEU:CD2	2.15	0.69
1:C:453:ARG:CZ	1:C:460:TRP:HE1	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:PRO:HD2	1:D:200:VAL:HG11	1.75	0.69
1:D:235:ALA:HA	1:D:238:ARG:CD	2.22	0.69
1:E:234:ALA:HB1	1:E:281:GLN:NE2	2.08	0.69
1:E:236:ARG:O	1:E:239:ASP:OD1	2.10	0.69
1:E:239:ASP:OD1	1:E:240:LEU:N	2.26	0.69
1:E:340:ARG:O	1:E:342:LYS:N	2.25	0.69
1:F:242:GLU:HA	1:F:245:LYS:HB3	1.73	0.69
1:F:365:LEU:O	1:F:368:LEU:HB3	1.93	0.69
1:C:357:THR:OG1	1:C:360:PHE:CD1	2.46	0.69
1:D:503:ARG:HH22	1:D:522:ARG:NH2	1.91	0.69
1:F:215:VAL:HG23	1:F:216:PRO:HD2	1.73	0.69
1:A:357:THR:HG1	1:A:360:PHE:HD1	1.37	0.69
1:B:193:LEU:HA	1:B:299:ALA:O	1.92	0.69
1:B:215:VAL:CG2	1:B:249:PRO:O	2.41	0.69
1:C:178:PRO:HB3	1:C:294:ALA:CB	2.23	0.69
1:C:286:MET:O	1:C:289:PHE:CZ	2.46	0.69
1:C:388:ASP:OD1	1:C:388:ASP:N	2.22	0.69
1:D:341:GLY:O	1:D:342:LYS:HB2	1.93	0.69
1:E:196:GLY:O	1:E:302:ASN:HA	1.92	0.69
1:A:197:PRO:HD2	1:A:200:VAL:CG2	2.22	0.68
1:B:313:ARG:HG3	1:B:314:PRO:N	2.08	0.68
1:A:196:GLY:O	1:A:302:ASN:HA	1.94	0.68
1:A:473:LEU:HD22	1:A:555:TYR:HB2	1.76	0.68
1:C:166:GLU:HA	1:C:169:LYS:CG	2.23	0.68
1:C:519:TYR:O	1:C:533:ARG:CD	2.41	0.68
1:E:166:GLU:HA	1:E:169:LYS:CG	2.23	0.68
1:E:453:ARG:HG3	1:E:453:ARG:NH1	2.06	0.68
1:C:481:ILE:HG22	1:C:482:VAL:N	2.07	0.68
1:F:238:ARG:CG	1:F:281:GLN:NE2	2.56	0.68
1:B:220:ALA:O	1:B:254:ILE:HA	1.94	0.68
1:B:235:ALA:HA	1:B:238:ARG:CD	2.23	0.68
1:D:263:LYS:HZ3	1:E:227:GLU:HG3	1.57	0.68
1:E:408:SER:HB2	1:E:409:PRO:HD2	1.76	0.68
1:E:500:LEU:O	1:E:503:ARG:HB3	1.93	0.68
1:F:177:ASN:OD1	1:F:180:ARG:HB2	1.94	0.68
1:F:191:GLY:HA2	1:F:297:VAL:HG12	1.73	0.68
1:F:236:ARG:HH12	1:F:278:THR:HG22	1.57	0.68
1:F:428:PHE:CE1	1:F:432:ALA:CB	2.76	0.68
1:C:234:ALA:O	1:C:237:VAL:HG12	1.94	0.68
1:D:177:ASN:OD1	1:D:180:ARG:HB2	1.92	0.68
1:E:520:ALA:HA	1:E:533:ARG:CD	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:ALA:O	1:F:254:ILE:HA	1.93	0.68
1:F:376:ALA:O	1:F:381:ARG:HG3	1.94	0.68
1:F:412:ARG:NH2	1:F:440:ILE:HD13	2.09	0.68
1:A:166:GLU:HA	1:A:169:LYS:CG	2.21	0.68
1:C:410:ARG:HG3	1:C:411:ASP:N	2.06	0.68
1:D:238:ARG:HB3	1:D:281:GLN:NE2	2.09	0.68
1:D:289:PHE:CD2	1:D:290:GLU:N	2.61	0.68
1:A:319:ARG:HH21	1:B:402:LYS:HZ1	1.39	0.68
1:A:588:GLN:HA	1:A:591:VAL:CG2	2.23	0.68
1:B:216:PRO:HG3	1:B:247:HIS:ND1	2.07	0.68
1:C:357:THR:OG1	1:C:360:PHE:HD1	1.75	0.68
1:D:221:SER:HB2	1:D:256:GLU:OE1	1.93	0.68
1:D:392:ALA:O	1:D:396:VAL:HG12	1.94	0.68
1:E:178:PRO:HB3	1:E:294:ALA:CB	2.23	0.68
1:E:400:PRO:HG2	1:E:405:LEU:HD12	1.76	0.68
1:F:215:VAL:CG2	1:F:249:PRO:O	2.42	0.68
1:F:564:GLU:C	1:F:566:ARG:H	1.95	0.68
1:B:201:GLY:O	1:B:205:LEU:HD13	1.94	0.68
1:B:238:ARG:HG2	1:B:281:GLN:HE22	1.57	0.68
1:B:328:VAL:HG23	1:B:580:GLU:HG3	1.76	0.68
1:B:487:THR:HG22	1:B:488:THR:N	2.06	0.68
1:C:195:VAL:HG11	1:C:304:PRO:HD3	1.74	0.68
1:C:581:THR:O	1:C:582:LEU:HD12	1.94	0.68
1:D:165:LYS:NZ	1:D:205:LEU:HB3	2.08	0.68
1:E:197:PRO:HD2	1:E:200:VAL:CG2	2.23	0.68
1:E:283:LEU:CG	1:E:316:ARG:HH12	2.04	0.68
1:B:191:GLY:HA2	1:B:297:VAL:HG12	1.74	0.68
1:B:245:LYS:C	1:B:247:HIS:H	1.97	0.68
1:B:386:MET:O	1:B:389:LEU:HD12	1.93	0.68
1:C:197:PRO:HD2	1:C:200:VAL:CG2	2.23	0.68
1:D:276:GLU:CA	1:D:279:LEU:HD13	2.17	0.68
1:E:449:PHE:CZ	1:E:496:GLN:CG	2.67	0.68
1:E:586:GLU:HA	1:E:589:ARG:CG	2.24	0.68
1:F:193:LEU:HA	1:F:299:ALA:O	1.93	0.68
1:F:283:LEU:HD13	1:F:316:ARG:NH2	2.06	0.68
1:F:386:MET:O	1:F:389:LEU:HD12	1.94	0.68
1:F:389:LEU:O	1:F:392:ALA:N	2.27	0.68
1:A:453:ARG:NH2	1:A:460:TRP:NE1	2.35	0.68
1:B:154:THR:HG23	1:B:156:LYS:HB3	1.76	0.68
1:B:253:PHE:HA	1:B:298:MET:HB3	1.76	0.68
1:B:586:GLU:O	1:B:590:VAL:HG23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ARG:O	1:E:279:LEU:HB2	1.94	0.68
1:E:449:PHE:HB2	1:E:468:GLN:NE2	2.07	0.68
1:F:245:LYS:C	1:F:247:HIS:H	1.97	0.68
1:A:236:ARG:NH1	1:A:236:ARG:HB3	2.09	0.67
1:B:177:ASN:OD1	1:B:180:ARG:HB2	1.94	0.67
1:B:202:LYS:HG2	2:B:2001:ADP:O1A	1.93	0.67
1:B:458:LEU:HD12	1:B:459:HIS:N	2.08	0.67
1:D:174:PHE:CZ	1:D:294:ALA:HB1	2.29	0.67
1:F:191:GLY:CA	1:F:297:VAL:HG12	2.24	0.67
1:B:165:LYS:O	1:B:168:LEU:HB2	1.94	0.67
1:B:466:LEU:HD11	1:B:504:MET:HE1	1.75	0.67
1:C:313:ARG:HH12	1:C:526:TYR:C	1.97	0.67
1:F:225:PHE:HB3	1:F:278:THR:HG21	1.74	0.67
1:A:340:ARG:O	1:A:342:LYS:N	2.26	0.67
1:A:400:PRO:HG2	1:A:405:LEU:HD12	1.76	0.67
1:A:524:ASP:CA	1:A:529:GLY:HA2	2.10	0.67
1:A:585:GLU:OE2	1:A:589:ARG:NE	2.27	0.67
1:B:182:HIS:ND1	1:B:182:HIS:N	2.40	0.67
1:B:276:GLU:CA	1:B:279:LEU:HD13	2.16	0.67
1:B:341:GLY:O	1:B:342:LYS:HB2	1.94	0.67
1:B:395:ARG:HH11	1:B:395:ARG:CG	1.98	0.67
1:C:168:LEU:O	1:C:171:ILE:HD12	1.95	0.67
1:C:263:LYS:HZ1	1:C:276:GLU:CD	1.98	0.67
1:D:188:ILE:HG23	1:D:189:PRO:CD	2.24	0.67
1:D:376:ALA:C	1:D:381:ARG:HB2	2.15	0.67
1:F:174:PHE:CZ	1:F:294:ALA:HB1	2.28	0.67
1:B:564:GLU:C	1:B:566:ARG:H	1.95	0.67
1:C:519:TYR:HA	1:C:533:ARG:NH2	2.09	0.67
1:D:236:ARG:HH12	1:D:278:THR:HG22	1.59	0.67
1:D:253:PHE:HA	1:D:298:MET:HB3	1.76	0.67
1:D:376:ALA:O	1:D:381:ARG:HG3	1.93	0.67
1:E:234:ALA:O	1:E:237:VAL:HG12	1.95	0.67
1:E:449:PHE:CB	1:E:468:GLN:HE22	2.05	0.67
1:B:191:GLY:CA	1:B:297:VAL:HG12	2.24	0.67
1:B:277:GLN:HA	1:B:280:ASN:ND2	2.09	0.67
1:B:362:GLY:HA2	1:B:365:LEU:HD12	1.76	0.67
1:C:264:ARG:HG2	1:C:266:SER:H	1.59	0.67
1:C:447:LEU:HA	1:C:496:GLN:HE21	1.57	0.67
1:C:449:PHE:HB2	1:C:468:GLN:NE2	2.09	0.67
1:E:331:ARG:HD2	1:E:357:THR:HG23	1.77	0.67
1:E:334:ILE:HD13	2:E:1001:ADP:C6	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:GLU:HA	1:F:279:LEU:CD1	2.16	0.67
1:A:586:GLU:CB	1:A:589:ARG:HE	2.07	0.67
1:D:237:VAL:CG2	1:D:281:GLN:HG3	2.24	0.67
1:D:332:GLU:OE1	1:D:351:ALA:HA	1.94	0.67
1:E:263:LYS:HZ2	1:E:276:GLU:CD	1.80	0.67
1:E:387:LYS:HA	1:E:390:GLU:HB2	1.76	0.67
1:F:201:GLY:O	1:F:205:LEU:HD13	1.95	0.67
1:C:168:LEU:O	1:C:171:ILE:CD1	2.43	0.67
1:D:452:PRO:HG3	1:E:402:LYS:HE3	1.77	0.67
1:E:357:THR:OG1	1:E:360:PHE:CD1	2.48	0.67
1:F:190:LYS:HE3	1:F:289:PHE:CZ	2.30	0.67
1:A:378:ARG:HA	1:F:173:GLU:CD	2.14	0.67
1:A:523:GLU:OE1	1:A:523:GLU:N	2.27	0.67
1:C:449:PHE:CB	1:C:468:GLN:HE22	2.08	0.67
1:C:517:VAL:HG23	1:D:498:THR:OG1	1.95	0.67
1:D:154:THR:HG23	1:D:156:LYS:HB3	1.77	0.67
1:F:237:VAL:CG2	1:F:281:GLN:HG3	2.25	0.67
1:F:525:THR:HG22	1:F:526:TYR:CD2	2.29	0.67
1:B:173:GLU:HA	1:B:176:LYS:HE3	1.76	0.67
1:C:196:GLY:O	1:C:302:ASN:HA	1.95	0.67
1:C:273:ASP:OD1	1:C:274:GLU:N	2.28	0.67
1:D:376:ALA:CB	1:D:381:ARG:HH11	2.07	0.67
1:E:335:LEU:HD21	1:E:353:LEU:HD23	1.76	0.67
1:E:491:GLU:O	1:E:493:ASP:N	2.28	0.67
1:A:174:PHE:CE1	1:A:188:ILE:CD1	2.69	0.67
1:A:234:ALA:HB1	1:A:281:GLN:NE2	2.10	0.67
1:B:155:PHE:O	1:B:158:VAL:N	2.27	0.67
1:B:303:ARG:O	1:B:307:LEU:HD13	1.95	0.67
1:B:352:LEU:HD23	1:B:353:LEU:H	1.60	0.67
1:D:238:ARG:CB	1:D:281:GLN:NE2	2.58	0.67
1:D:503:ARG:HH12	1:D:522:ARG:HH21	1.40	0.67
1:E:168:LEU:O	1:E:171:ILE:CD1	2.43	0.67
1:E:333:GLN:HG3	1:E:336:ARG:NH1	2.10	0.67
1:F:503:ARG:HH22	1:F:522:ARG:CZ	2.08	0.67
1:A:333:GLN:HG3	1:A:336:ARG:NH1	2.10	0.66
1:D:153:VAL:HB	1:D:207:ARG:NH1	2.10	0.66
1:D:193:LEU:HA	1:D:299:ALA:O	1.93	0.66
1:D:238:ARG:HG2	1:D:281:GLN:HE22	1.59	0.66
1:E:453:ARG:HH22	1:E:464:ARG:NH1	1.93	0.66
1:F:228:MET:SD	1:F:232:VAL:HG12	2.35	0.66
1:F:311:LEU:C	1:F:311:LEU:HD12	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:LEU:CD1	1:F:365:LEU:HB3	2.24	0.66
1:F:378:ARG:O	1:F:380:GLY:N	2.28	0.66
1:B:200:VAL:HG22	1:B:202:LYS:HD2	1.77	0.66
1:C:264:ARG:CD	1:C:266:SER:HB2	2.25	0.66
1:D:245:LYS:C	1:D:247:HIS:H	1.98	0.66
1:D:436:HIS:O	1:D:437:LYS:HG2	1.94	0.66
1:F:159:ALA:HB3	1:F:334:ILE:CG1	2.24	0.66
1:F:352:LEU:O	1:F:355:LYS:N	2.27	0.66
1:A:215:VAL:HG23	1:A:216:PRO:CD	2.24	0.66
1:A:580:GLU:O	1:A:580:GLU:HG2	1.94	0.66
1:B:228:MET:SD	1:B:232:VAL:HG12	2.35	0.66
1:D:394:ASP:HA	1:D:397:MET:HE3	1.77	0.66
1:E:357:THR:OG1	1:E:360:PHE:HD1	1.77	0.66
1:F:277:GLN:HA	1:F:280:ASN:ND2	2.11	0.66
1:F:333:GLN:O	1:F:336:ARG:HB3	1.96	0.66
1:F:343:PRO:O	1:F:344:LEU:HB3	1.96	0.66
1:F:395:ARG:HH11	1:F:395:ARG:CG	1.96	0.66
1:B:346:GLU:HG3	1:B:386:MET:HG2	1.77	0.66
1:C:387:LYS:HA	1:C:390:GLU:HB2	1.77	0.66
1:E:196:GLY:HA2	1:E:443:ARG:HH21	1.61	0.66
1:E:469:ILE:HG23	1:E:497:ALA:HB1	1.77	0.66
1:F:237:VAL:HG22	1:F:281:GLN:HG3	1.77	0.66
1:F:238:ARG:HG2	1:F:281:GLN:HE22	1.59	0.66
1:F:362:GLY:HA2	1:F:365:LEU:HD12	1.77	0.66
1:A:453:ARG:NH2	1:A:464:ARG:HH22	1.93	0.66
1:C:207:ARG:HH21	1:C:217:PHE:HD2	1.42	0.66
1:C:207:ARG:NH2	1:C:217:PHE:HD2	1.93	0.66
1:D:225:PHE:HB3	1:D:278:THR:HG21	1.77	0.66
1:D:241:PHE:CD2	1:D:285:GLU:HG3	2.31	0.66
1:D:523:GLU:OE2	1:E:264:ARG:NH2	2.29	0.66
1:E:215:VAL:HG11	1:E:250:CYS:CA	2.25	0.66
1:E:585:GLU:O	1:E:588:GLN:HG2	1.94	0.66
1:F:155:PHE:O	1:F:158:VAL:N	2.27	0.66
1:A:225:PHE:CE1	1:A:233:GLY:HA2	2.29	0.66
1:C:340:ARG:O	1:C:342:LYS:N	2.29	0.66
1:C:514:PHE:HB3	1:C:519:TYR:CE1	2.31	0.66
1:C:523:GLU:N	1:C:523:GLU:OE1	2.28	0.66
1:D:237:VAL:HG22	1:D:281:GLN:HG3	1.77	0.66
1:D:428:PHE:CZ	1:D:432:ALA:HB1	2.31	0.66
1:E:533:ARG:CD	1:E:534:GLN:H	2.06	0.66
1:F:209:VAL:HG13	1:F:210:ALA:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:VAL:O	1:C:576:LEU:HB2	1.96	0.66
1:D:277:GLN:HA	1:D:280:ASN:ND2	2.11	0.66
1:D:373:ALA:O	1:D:376:ALA:HB3	1.96	0.66
1:E:460:TRP:O	1:F:488:THR:HA	1.95	0.66
1:A:381:ARG:O	1:F:180:ARG:NH2	2.29	0.66
1:A:449:PHE:CB	1:A:468:GLN:HE22	2.08	0.66
1:A:533:ARG:CZ	1:A:534:GLN:O	2.43	0.66
1:C:290:GLU:OE2	1:D:226:VAL:HG11	1.96	0.66
1:C:382:ARG:HG3	1:C:383:LYS:CB	2.25	0.66
1:C:462:ARG:HB2	1:C:510:MET:SD	2.35	0.66
1:D:241:PHE:CE2	1:D:285:GLU:HG3	2.31	0.66
1:A:155:PHE:HZ	1:A:168:LEU:HD11	1.59	0.66
1:C:585:GLU:O	1:C:588:GLN:HG2	1.94	0.66
1:D:200:VAL:HG22	1:D:202:LYS:HD2	1.78	0.66
1:F:428:PHE:CE1	1:F:432:ALA:HB1	2.30	0.66
1:B:352:LEU:O	1:B:355:LYS:N	2.29	0.66
1:B:378:ARG:O	1:B:380:GLY:N	2.29	0.66
1:B:410:ARG:O	1:B:413:ARG:N	2.29	0.66
1:C:225:PHE:CZ	1:C:278:THR:CB	2.72	0.66
1:C:263:LYS:HG2	1:C:264:ARG:H	1.60	0.66
1:C:467:ASP:O	1:C:470:ALA:HB3	1.96	0.66
1:D:159:ALA:HB3	1:D:334:ILE:CG1	2.25	0.66
1:E:177:ASN:HD22	1:E:180:ARG:HD3	1.61	0.66
1:E:312:LEU:O	1:E:318:ASP:HA	1.95	0.66
1:E:313:ARG:NH2	1:E:526:TYR:CA	2.46	0.66
1:E:586:GLU:O	1:E:589:ARG:HB2	1.96	0.66
1:A:225:PHE:HE1	1:A:233:GLY:C	1.98	0.65
1:B:178:PRO:HG3	1:B:249:PRO:HG3	1.78	0.65
1:B:589:ARG:HB3	1:B:594:LEU:CD2	2.26	0.65
1:C:334:ILE:HD13	2:C:1001:ADP:C6	2.31	0.65
1:C:335:LEU:HD21	1:C:353:LEU:HD23	1.78	0.65
1:D:362:GLY:HA2	1:D:365:LEU:HD12	1.78	0.65
1:E:168:LEU:O	1:E:171:ILE:HD12	1.95	0.65
1:F:225:PHE:CD2	1:F:236:ARG:HD2	2.31	0.65
1:F:283:LEU:HD12	1:F:316:ARG:CZ	2.26	0.65
1:F:313:ARG:HG3	1:F:314:PRO:N	2.11	0.65
1:F:449:PHE:CZ	1:F:453:ARG:CZ	2.79	0.65
1:A:211:GLY:CA	1:A:214:ARG:HE	2.08	0.65
1:B:225:PHE:HB3	1:B:278:THR:HG21	1.78	0.65
1:B:337:ILE:HG23	1:B:338:HIS:CD2	2.31	0.65
1:C:465:LEU:HD22	1:C:508:TRP:HZ3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:LEU:O	1:C:503:ARG:HB3	1.96	0.65
1:D:343:PRO:HG2	1:D:383:LYS:HA	1.79	0.65
1:D:466:LEU:HD11	1:D:504:MET:HE1	1.77	0.65
1:D:508:TRP:HD1	1:E:491:GLU:HG2	1.61	0.65
1:E:155:PHE:HZ	1:E:168:LEU:HD11	1.58	0.65
1:A:169:LYS:O	1:A:172:VAL:HG13	1.96	0.65
1:A:196:GLY:CA	1:A:443:ARG:NH2	2.60	0.65
1:A:202:LYS:HB2	2:A:1001:ADP:O1B	1.96	0.65
1:A:316:ARG:HG2	1:A:317:PHE:N	2.11	0.65
1:A:357:THR:OG1	1:A:360:PHE:CD1	2.49	0.65
1:B:263:LYS:HZ3	1:C:227:GLU:HG3	1.59	0.65
1:C:400:PRO:HG2	1:C:405:LEU:HD12	1.78	0.65
1:C:419:GLU:OE1	1:C:419:GLU:HA	1.95	0.65
1:C:428:PHE:O	1:C:432:ALA:HB2	1.96	0.65
1:D:178:PRO:HG3	1:D:249:PRO:HG3	1.78	0.65
1:D:487:THR:HG22	1:D:488:THR:N	2.07	0.65
1:F:311:LEU:O	1:F:316:ARG:HG2	1.95	0.65
1:A:215:VAL:CG1	1:A:250:CYS:HA	2.27	0.65
1:A:264:ARG:HD2	1:A:266:SER:CB	2.26	0.65
1:C:273:ASP:CG	1:C:274:GLU:N	2.49	0.65
1:C:333:GLN:HA	1:C:336:ARG:CZ	2.26	0.65
1:E:428:PHE:O	1:E:432:ALA:HB2	1.96	0.65
1:F:221:SER:HB2	1:F:256:GLU:OE1	1.97	0.65
1:B:318:ASP:O	1:B:319:ARG:CB	2.32	0.65
1:C:215:VAL:CG1	1:C:250:CYS:HA	2.27	0.65
1:D:238:ARG:CG	1:D:281:GLN:NE2	2.58	0.65
1:E:225:PHE:HE1	1:E:233:GLY:C	2.00	0.65
1:E:313:ARG:HH12	1:E:526:TYR:C	1.99	0.65
1:F:153:VAL:HB	1:F:207:ARG:NH1	2.12	0.65
1:A:512:PRO:HB2	1:A:514:PHE:HD2	1.61	0.65
1:A:519:TYR:O	1:A:533:ARG:CD	2.45	0.65
1:C:533:ARG:CD	1:C:534:GLN:N	2.60	0.65
1:F:160:GLY:H	1:F:333:GLN:NE2	1.95	0.65
1:F:202:LYS:HG2	2:F:2001:ADP:O1A	1.97	0.65
1:A:275:ARG:O	1:A:279:LEU:HB2	1.96	0.65
1:A:419:GLU:OE1	1:A:419:GLU:HA	1.97	0.65
1:B:188:ILE:HG23	1:B:189:PRO:CD	2.24	0.65
1:B:311:LEU:C	1:B:311:LEU:HD12	2.16	0.65
1:C:215:VAL:HG23	1:C:216:PRO:CD	2.27	0.65
1:D:286:MET:CE	1:D:315:GLY:O	2.45	0.65
1:D:352:LEU:O	1:D:355:LYS:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:PHE:HB2	1:F:181:PHE:HE2	1.60	0.65
1:F:348:VAL:HG21	1:F:352:LEU:HD11	1.77	0.65
1:A:305:ASP:OD1	1:A:305:ASP:N	2.27	0.65
1:B:221:SER:HB2	1:B:256:GLU:OE1	1.97	0.65
1:C:312:LEU:O	1:C:318:ASP:HA	1.95	0.65
1:C:414:ILE:HG22	1:C:415:THR:N	2.12	0.65
1:D:463:LYS:O	1:D:466:LEU:N	2.29	0.65
1:F:463:LYS:O	1:F:466:LEU:N	2.30	0.65
1:B:514:PHE:HB3	1:B:519:TYR:HE1	1.62	0.65
1:A:449:PHE:CD2	1:A:449:PHE:N	2.64	0.65
1:D:263:LYS:HZ2	1:E:227:GLU:HG3	1.60	0.65
1:D:394:ASP:HA	1:D:397:MET:CE	2.26	0.65
1:E:195:VAL:HG11	1:E:304:PRO:HD3	1.78	0.65
1:E:233:GLY:HA2	1:E:236:ARG:HH12	1.61	0.65
1:E:510:MET:O	1:E:512:PRO:CD	2.44	0.65
1:A:357:THR:OG1	1:A:360:PHE:HD1	1.77	0.64
1:B:389:LEU:O	1:B:392:ALA:N	2.30	0.64
1:B:412:ARG:NH2	1:B:440:ILE:HD13	2.12	0.64
1:B:463:LYS:O	1:B:466:LEU:N	2.30	0.64
1:C:225:PHE:CE1	1:C:233:GLY:HA2	2.29	0.64
1:C:264:ARG:HG3	1:C:265:GLY:N	2.11	0.64
1:C:488:THR:O	1:C:490:ALA:N	2.28	0.64
1:D:174:PHE:HB2	1:D:181:PHE:HE2	1.58	0.64
1:D:328:VAL:HG23	1:D:580:GLU:HG3	1.79	0.64
1:D:344:LEU:HD22	1:D:346:GLU:OE1	1.97	0.64
1:E:580:GLU:O	1:E:580:GLU:HG2	1.97	0.64
1:B:510:MET:O	1:B:512:PRO:HD2	1.98	0.64
1:D:352:LEU:HD23	1:D:353:LEU:H	1.62	0.64
1:E:179:SER:O	1:E:182:HIS:HD2	1.80	0.64
1:E:263:LYS:HZ1	1:E:276:GLU:CD	1.99	0.64
1:E:283:LEU:CG	1:E:316:ARG:NH1	2.54	0.64
1:F:181:PHE:O	1:F:184:MET:N	2.30	0.64
1:F:188:ILE:HG23	1:F:189:PRO:CD	2.25	0.64
1:A:264:ARG:NE	1:A:266:SER:HB2	2.12	0.64
1:A:335:LEU:HD21	1:A:353:LEU:HD23	1.78	0.64
1:B:154:THR:CG2	1:B:156:LYS:HB3	2.27	0.64
1:B:394:ASP:HA	1:B:397:MET:CE	2.27	0.64
1:C:152:LYS:HG3	1:C:153:VAL:CG2	2.22	0.64
1:C:153:VAL:HA	1:C:157:ASP:OD2	1.98	0.64
1:C:447:LEU:HA	1:C:496:GLN:NE2	2.12	0.64
1:C:580:GLU:O	1:C:580:GLU:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:MET:O	1:D:389:LEU:HD12	1.97	0.64
1:E:567:GLU:HA	1:E:570:GLU:OE1	1.96	0.64
1:B:190:LYS:HE3	1:B:289:PHE:CZ	2.33	0.64
1:B:587:PHE:O	1:B:591:VAL:HG23	1.97	0.64
1:D:273:ASP:OD1	1:D:273:ASP:N	2.29	0.64
1:D:474:ALA:HA	1:D:558:VAL:CG1	2.21	0.64
1:E:470:ALA:O	1:E:558:VAL:HG21	1.98	0.64
1:E:533:ARG:CD	1:E:534:GLN:N	2.60	0.64
1:B:237:VAL:HG22	1:B:281:GLN:HG3	1.79	0.64
1:B:257:ILE:HD12	1:B:257:ILE:N	2.13	0.64
1:C:236:ARG:NH1	1:C:236:ARG:HB3	2.13	0.64
1:C:533:ARG:CZ	1:C:534:GLN:O	2.46	0.64
1:D:154:THR:CG2	1:D:156:LYS:HB3	2.28	0.64
1:D:303:ARG:O	1:D:307:LEU:HD13	1.97	0.64
1:F:341:GLY:O	1:F:342:LYS:HB2	1.98	0.64
1:F:376:ALA:CA	1:F:381:ARG:HH11	2.11	0.64
1:F:439:THR:CG2	1:F:445:ARG:HH22	2.08	0.64
1:F:586:GLU:O	1:F:589:ARG:HB2	1.98	0.64
1:A:453:ARG:NH2	1:A:464:ARG:NH2	2.46	0.64
1:D:207:ARG:HB2	1:D:217:PHE:CE1	2.31	0.64
1:D:209:VAL:HG13	1:D:210:ALA:N	2.10	0.64
1:D:286:MET:O	1:D:289:PHE:CB	2.45	0.64
1:D:414:ILE:O	1:D:417:TYR:N	2.31	0.64
1:E:169:LYS:O	1:E:172:VAL:HG13	1.98	0.64
1:E:520:ALA:CA	1:E:533:ARG:HD3	2.26	0.64
1:A:262:ARG:CG	1:A:275:ARG:HH22	2.07	0.64
1:A:313:ARG:HH12	1:A:526:TYR:C	2.01	0.64
1:B:175:LEU:CD1	1:B:215:VAL:HG11	2.27	0.64
1:C:453:ARG:HH22	1:C:464:ARG:NH1	1.95	0.64
1:D:313:ARG:NE	1:D:314:PRO:CG	2.61	0.64
1:D:369:LEU:O	1:D:372:ALA:N	2.28	0.64
1:F:273:ASP:N	1:F:273:ASP:OD1	2.31	0.64
1:F:465:LEU:O	1:F:469:ILE:HG13	1.98	0.64
1:A:286:MET:O	1:A:289:PHE:CZ	2.50	0.64
1:A:467:ASP:O	1:A:470:ALA:HB3	1.98	0.64
1:B:228:MET:CE	1:B:236:ARG:HD3	2.27	0.64
1:B:237:VAL:CG2	1:B:281:GLN:HG3	2.27	0.64
1:B:379:GLU:OE1	1:B:381:ARG:NE	2.31	0.64
1:B:465:LEU:O	1:B:469:ILE:HG13	1.98	0.64
1:C:190:LYS:HD2	1:C:289:PHE:HE1	1.59	0.64
1:C:449:PHE:CD2	1:C:449:PHE:N	2.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ARG:HH11	1:C:453:ARG:CG	2.10	0.64
1:C:518:ALA:CB	1:D:495:ARG:HA	2.27	0.64
1:D:258:ASP:OD1	1:D:258:ASP:N	2.28	0.64
1:E:481:ILE:CD1	1:E:563:LEU:HB3	2.27	0.64
1:F:385:THR:HB	1:F:388:ASP:OD1	1.98	0.64
1:A:252:VAL:O	1:A:298:MET:N	2.30	0.64
1:B:286:MET:CE	1:B:315:GLY:O	2.46	0.64
1:B:577:LEU:HG	1:B:578:GLU:N	2.13	0.64
1:D:241:PHE:CD1	1:D:242:GLU:N	2.66	0.64
1:F:165:LYS:O	1:F:168:LEU:HB2	1.98	0.64
1:F:175:LEU:CD1	1:F:215:VAL:HG11	2.28	0.64
1:F:253:PHE:HE2	1:F:255:ASP:CB	2.11	0.64
1:A:520:ALA:CA	1:A:533:ARG:HD3	2.27	0.64
1:D:160:GLY:H	1:D:333:GLN:NE2	1.96	0.64
1:D:523:GLU:OE1	1:E:264:ARG:NH2	2.31	0.64
1:A:177:ASN:HD22	1:A:180:ARG:HD3	1.63	0.63
1:B:174:PHE:CZ	1:B:294:ALA:HB1	2.33	0.63
1:B:428:PHE:CE1	1:B:432:ALA:CB	2.81	0.63
1:D:225:PHE:CE2	1:D:236:ARG:HD2	2.32	0.63
1:A:264:ARG:HD2	1:A:266:SER:HB2	1.78	0.63
1:A:567:GLU:HA	1:A:570:GLU:OE1	1.99	0.63
1:B:273:ASP:OD1	1:B:273:ASP:N	2.31	0.63
1:B:400:PRO:HA	1:B:403:LYS:HB2	1.81	0.63
1:C:465:LEU:HD22	1:C:508:TRP:CZ3	2.33	0.63
1:D:420:ALA:O	1:D:424:LEU:HD12	1.99	0.63
1:E:212:GLU:N	1:E:214:ARG:HG3	2.13	0.63
1:E:225:PHE:CE1	1:E:233:GLY:HA2	2.31	0.63
1:E:581:THR:O	1:E:582:LEU:HD12	1.98	0.63
1:F:178:PRO:HG3	1:F:249:PRO:HG3	1.80	0.63
1:F:257:ILE:HD12	1:F:257:ILE:N	2.13	0.63
1:F:376:ALA:CB	1:F:381:ARG:HH11	2.09	0.63
1:B:262:ARG:CG	1:B:263:LYS:N	2.54	0.63
1:C:196:GLY:HA2	1:C:443:ARG:HH21	1.63	0.63
1:E:212:GLU:O	1:E:214:ARG:HG3	1.98	0.63
1:E:292:ASP:C	1:E:292:ASP:OD1	2.36	0.63
1:E:523:GLU:OE1	1:E:523:GLU:N	2.31	0.63
1:F:214:ARG:HH11	1:F:214:ARG:CG	2.11	0.63
1:F:396:VAL:O	1:F:400:PRO:HD2	1.98	0.63
1:A:461:SER:O	1:A:465:LEU:HD12	1.97	0.63
1:A:588:GLN:O	1:A:591:VAL:N	2.31	0.63
1:B:174:PHE:HB2	1:B:181:PHE:HE2	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:ARG:HG2	1:C:508:TRP:CH2	2.33	0.63
1:D:175:LEU:CD1	1:D:215:VAL:HG11	2.28	0.63
1:D:260:VAL:HG23	1:D:279:LEU:HD12	1.81	0.63
1:E:152:LYS:HG3	1:E:153:VAL:CG2	2.20	0.63
1:E:275:ARG:O	1:E:279:LEU:CB	2.47	0.63
1:B:328:VAL:CG2	1:B:355:LYS:CE	2.76	0.63
1:D:526:TYR:HE2	1:E:256:GLU:OE2	1.81	0.63
1:D:577:LEU:HG	1:D:578:GLU:N	2.11	0.63
1:E:252:VAL:O	1:E:298:MET:N	2.30	0.63
1:E:384:ILE:HG23	1:E:388:ASP:CB	2.26	0.63
1:E:467:ASP:O	1:E:470:ALA:HB3	1.98	0.63
1:F:165:LYS:HZ3	1:F:205:LEU:HB3	1.60	0.63
1:F:238:ARG:HB3	1:F:281:GLN:HE22	1.60	0.63
1:A:596:LEU:HG	1:A:597:GLU:N	2.13	0.63
1:C:252:VAL:O	1:C:298:MET:N	2.29	0.63
1:D:215:VAL:CG2	1:D:249:PRO:O	2.45	0.63
1:F:202:LYS:HD3	2:F:2001:ADP:O2B	1.99	0.63
1:F:260:VAL:HG23	1:F:279:LEU:HD12	1.79	0.63
1:F:430:GLU:OE1	1:F:430:GLU:CA	2.46	0.63
1:A:449:PHE:HB2	1:A:468:GLN:NE2	2.12	0.63
1:A:572:VAL:O	1:A:576:LEU:HB2	1.99	0.63
1:B:343:PRO:O	1:B:344:LEU:HB3	1.98	0.63
1:C:292:ASP:C	1:C:292:ASP:OD1	2.37	0.63
1:C:510:MET:O	1:C:512:PRO:HD2	1.98	0.63
1:D:410:ARG:O	1:D:413:ARG:HB2	1.98	0.63
1:E:461:SER:O	1:E:465:LEU:HD12	1.98	0.63
1:E:589:ARG:CZ	1:E:589:ARG:CB	2.77	0.63
1:A:152:LYS:HG3	1:A:153:VAL:CG2	2.25	0.63
1:A:168:LEU:CB	1:A:171:ILE:CD1	2.77	0.63
1:C:169:LYS:O	1:C:172:VAL:HG13	1.99	0.63
1:E:215:VAL:HG23	1:E:216:PRO:CD	2.26	0.63
1:E:273:ASP:CG	1:E:274:GLU:N	2.51	0.63
1:F:376:ALA:CB	1:F:381:ARG:CD	2.70	0.63
1:A:414:ILE:HG22	1:A:415:THR:N	2.13	0.63
1:A:539:THR:O	1:A:543:ILE:HG13	1.99	0.63
1:B:159:ALA:HB3	1:B:334:ILE:CG1	2.29	0.63
1:B:209:VAL:HG13	1:B:210:ALA:N	2.14	0.63
1:D:396:VAL:O	1:D:400:PRO:HD2	1.99	0.63
1:D:597:GLU:O	1:D:599:PRO:HD3	1.98	0.63
1:E:514:PHE:HB3	1:E:519:TYR:CE1	2.34	0.63
1:F:155:PHE:HA	1:F:158:VAL:CG2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:519:TYR:HB3	1:F:535:TYR:HD2	1.64	0.63
1:A:155:PHE:HZ	1:A:209:VAL:HG22	1.64	0.62
1:B:318:ASP:OD1	1:B:318:ASP:N	2.24	0.62
1:D:317:PHE:N	1:D:317:PHE:HD1	1.97	0.62
1:E:447:LEU:HA	1:E:496:GLN:NE2	2.12	0.62
1:E:453:ARG:HH21	1:E:464:ARG:HH22	1.47	0.62
1:F:428:PHE:CZ	1:F:432:ALA:HB1	2.34	0.62
1:B:181:PHE:O	1:B:184:MET:N	2.32	0.62
1:E:149:GLU:O	1:E:150:ALA:CB	2.46	0.62
1:E:212:GLU:CA	1:E:214:ARG:HG3	2.29	0.62
1:E:273:ASP:OD1	1:E:274:GLU:N	2.31	0.62
1:A:586:GLU:CB	1:A:589:ARG:NE	2.63	0.62
1:B:152:LYS:HB2	1:B:207:ARG:NH1	2.14	0.62
1:B:396:VAL:O	1:B:400:PRO:HD2	2.00	0.62
1:B:414:ILE:O	1:B:417:TYR:N	2.32	0.62
1:C:264:ARG:CG	1:C:266:SER:N	2.41	0.62
1:D:318:ASP:O	1:D:319:ARG:CB	2.35	0.62
1:D:400:PRO:HA	1:D:403:LYS:HB2	1.82	0.62
1:F:210:ALA:O	1:F:214:ARG:HA	2.00	0.62
1:F:327:ASP:O	1:F:331:ARG:CZ	2.47	0.62
1:F:420:ALA:O	1:F:424:LEU:HD12	1.99	0.62
1:A:179:SER:O	1:A:182:HIS:HD2	1.82	0.62
1:A:533:ARG:CD	1:A:534:GLN:N	2.61	0.62
1:B:165:LYS:NZ	1:B:205:LEU:HB3	2.15	0.62
1:B:253:PHE:HE2	1:B:255:ASP:CB	2.12	0.62
1:B:313:ARG:NE	1:B:314:PRO:CG	2.63	0.62
1:B:586:GLU:O	1:B:589:ARG:HB2	1.99	0.62
1:C:225:PHE:HZ	1:C:278:THR:HB	1.60	0.62
1:C:414:ILE:CG2	1:C:415:THR:N	2.63	0.62
1:D:510:MET:O	1:D:512:PRO:HD2	1.98	0.62
1:D:589:ARG:HB3	1:D:594:LEU:CD2	2.29	0.62
1:F:258:ASP:OD1	1:F:258:ASP:N	2.31	0.62
1:C:333:GLN:HG3	1:C:336:ARG:HH12	1.63	0.62
1:E:166:GLU:CB	1:E:169:LYS:HZ2	2.09	0.62
1:F:400:PRO:HA	1:F:403:LYS:HB2	1.81	0.62
1:B:165:LYS:O	1:B:168:LEU:CA	2.48	0.62
1:B:328:VAL:HG21	1:B:355:LYS:CE	2.30	0.62
1:C:214:ARG:O	1:C:214:ARG:HG2	1.98	0.62
1:D:586:GLU:O	1:D:589:ARG:HB2	2.00	0.62
1:F:533:ARG:HG3	1:F:533:ARG:HH11	1.65	0.62
1:A:233:GLY:HA2	1:A:236:ARG:HH12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASP:N	1:B:258:ASP:OD1	2.31	0.62
1:C:524:ASP:CA	1:C:529:GLY:HA2	2.09	0.62
1:E:153:VAL:HA	1:E:157:ASP:OD2	1.99	0.62
1:E:191:GLY:HA2	1:E:297:VAL:HG22	1.81	0.62
1:E:286:MET:O	1:E:289:PHE:CE1	2.52	0.62
1:E:453:ARG:NH2	1:E:464:ARG:HH22	1.97	0.62
1:A:195:VAL:HG22	1:A:301:THR:O	1.99	0.62
1:E:397:MET:HG3	1:E:406:VAL:HG13	1.82	0.62
1:E:414:ILE:HG22	1:E:415:THR:N	2.14	0.62
1:A:334:ILE:HD13	2:A:1001:ADP:C6	2.35	0.62
1:B:311:LEU:O	1:B:316:ARG:HD3	1.99	0.62
1:B:373:ALA:O	1:B:376:ALA:HB3	1.99	0.62
1:C:179:SER:O	1:C:182:HIS:HD2	1.82	0.62
1:C:331:ARG:HD2	1:C:357:THR:HG23	1.82	0.62
1:D:181:PHE:O	1:D:184:MET:N	2.33	0.62
1:E:174:PHE:CE1	1:E:188:ILE:CD1	2.69	0.62
1:F:165:LYS:HE2	1:F:205:LEU:CG	2.30	0.62
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.59	0.62
1:A:428:PHE:O	1:A:432:ALA:HB2	2.00	0.62
1:B:225:PHE:HB3	1:B:236:ARG:NH1	2.14	0.62
1:B:355:LYS:NZ	1:B:578:GLU:HG3	2.15	0.62
1:C:191:GLY:HA2	1:C:297:VAL:HG22	1.82	0.62
1:D:165:LYS:O	1:D:168:LEU:CA	2.47	0.62
1:D:255:ASP:O	1:D:256:GLU:HG2	2.00	0.62
1:F:373:ALA:HA	1:F:384:ILE:HD11	1.82	0.62
1:B:382:ARG:HB3	1:B:383:LYS:HB2	1.82	0.61
1:C:177:ASN:ND2	1:C:180:ARG:HD3	2.16	0.61
1:C:276:GLU:OE2	1:C:527:LEU:HD11	2.00	0.61
1:D:238:ARG:HB3	1:D:281:GLN:HE22	1.63	0.61
1:D:517:VAL:HG11	1:D:519:TYR:OH	1.99	0.61
1:E:225:PHE:CZ	1:E:278:THR:CB	2.76	0.61
1:E:519:TYR:O	1:E:533:ARG:CD	2.47	0.61
1:E:572:VAL:O	1:E:576:LEU:HB2	1.99	0.61
1:F:190:LYS:HZ1	1:F:289:PHE:HE2	0.70	0.61
1:F:378:ARG:C	1:F:380:GLY:N	2.52	0.61
1:A:153:VAL:HA	1:A:157:ASP:OD2	2.01	0.61
1:A:193:LEU:HD12	1:A:299:ALA:O	1.99	0.61
1:A:430:GLU:O	1:A:431:HIS:CB	2.48	0.61
1:A:449:PHE:HE2	1:A:496:GLN:NE2	1.97	0.61
1:B:260:VAL:HG23	1:B:279:LEU:HD12	1.82	0.61
1:E:390:GLU:O	1:E:393:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:ASP:O	1:F:256:GLU:HG2	1.99	0.61
1:A:292:ASP:C	1:A:292:ASP:OD1	2.37	0.61
1:A:510:MET:O	1:A:512:PRO:CD	2.47	0.61
1:B:313:ARG:NE	1:B:314:PRO:CD	2.62	0.61
1:C:453:ARG:NH2	1:C:464:ARG:HH22	1.97	0.61
1:D:253:PHE:HE2	1:D:255:ASP:CB	2.11	0.61
1:D:511:HIS:C	1:D:512:PRO:O	2.38	0.61
1:F:215:VAL:HG22	1:F:216:PRO:CD	2.29	0.61
1:F:507:GLU:HG3	1:F:520:ALA:O	2.00	0.61
1:A:166:GLU:CB	1:A:169:LYS:HZ2	2.08	0.61
1:A:440:ILE:HG22	1:A:441:VAL:HG23	1.83	0.61
1:B:241:PHE:CD1	1:B:242:GLU:N	2.68	0.61
1:D:344:LEU:HA	1:D:383:LYS:HG3	1.83	0.61
1:D:382:ARG:NH1	1:D:382:ARG:HG2	2.11	0.61
1:E:338:HIS:CE1	1:E:366:GLU:HG3	2.36	0.61
1:F:159:ALA:HB1	1:F:333:GLN:CG	2.31	0.61
1:F:241:PHE:CD1	1:F:242:GLU:N	2.68	0.61
1:A:333:GLN:HA	1:A:336:ARG:CZ	2.30	0.61
1:A:581:THR:O	1:A:582:LEU:HD12	2.00	0.61
1:B:428:PHE:CE1	1:B:432:ALA:HB1	2.34	0.61
1:D:314:PRO:C	1:D:316:ARG:H	2.02	0.61
1:E:469:ILE:O	1:E:473:LEU:HD12	2.01	0.61
1:F:225:PHE:CE2	1:F:236:ARG:HD2	2.35	0.61
1:F:382:ARG:HB3	1:F:383:LYS:HB2	1.82	0.61
1:F:394:ASP:HA	1:F:397:MET:HE3	1.81	0.61
1:A:215:VAL:HG11	1:A:250:CYS:CA	2.29	0.61
1:A:312:LEU:O	1:A:318:ASP:HA	2.00	0.61
1:F:235:ALA:HA	1:F:238:ARG:CG	2.29	0.61
1:F:376:ALA:HA	1:F:381:ARG:NH1	2.16	0.61
1:A:319:ARG:NH2	1:B:402:LYS:NZ	2.48	0.61
1:A:381:ARG:CG	1:A:382:ARG:H	2.13	0.61
1:B:367:ASN:OD1	1:B:367:ASN:C	2.39	0.61
1:B:391:GLU:O	1:B:395:ARG:HB3	2.01	0.61
1:B:501:ALA:O	1:B:505:ILE:HD12	2.00	0.61
1:C:225:PHE:HE1	1:C:233:GLY:C	2.03	0.61
1:E:150:ALA:HB2	1:E:214:ARG:HH21	1.66	0.61
1:F:317:PHE:N	1:F:317:PHE:HD1	1.99	0.61
1:B:154:THR:HG23	1:B:156:LYS:H	1.66	0.61
1:B:597:GLU:O	1:B:599:PRO:HD3	2.01	0.61
1:C:347:ASP:OD1	1:C:347:ASP:N	2.33	0.61
1:C:428:PHE:HE1	1:C:432:ALA:HA	1.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:587:PHE:O	1:D:591:VAL:HG23	2.00	0.61
1:E:212:GLU:O	1:E:214:ARG:CG	2.49	0.61
1:E:449:PHE:HB2	1:E:468:GLN:HE22	1.66	0.61
1:A:195:VAL:HG11	1:A:304:PRO:HD3	1.81	0.61
1:A:313:ARG:NH2	1:A:526:TYR:C	2.51	0.61
1:A:447:LEU:HA	1:A:496:GLN:NE2	2.15	0.61
1:B:190:LYS:HZ1	1:B:289:PHE:HE2	0.69	0.61
1:B:378:ARG:C	1:B:380:GLY:N	2.54	0.61
1:B:589:ARG:CB	1:B:594:LEU:HD22	2.30	0.61
1:C:520:ALA:CA	1:C:533:ARG:HD3	2.25	0.61
1:D:215:VAL:HG22	1:D:216:PRO:CD	2.31	0.61
1:D:235:ALA:HA	1:D:238:ARG:CG	2.30	0.61
1:D:318:ASP:OD1	1:D:318:ASP:N	2.24	0.61
1:E:223:SER:C	1:E:225:PHE:N	2.48	0.61
1:F:348:VAL:HG21	1:F:352:LEU:CD1	2.31	0.61
1:F:352:LEU:CD1	1:F:353:LEU:N	2.64	0.61
1:A:275:ARG:O	1:A:279:LEU:CB	2.48	0.61
1:A:311:LEU:CD2	1:A:316:ARG:CZ	2.79	0.61
1:B:430:GLU:OE1	1:B:430:GLU:CA	2.48	0.61
1:C:381:ARG:CG	1:C:382:ARG:H	2.14	0.61
1:D:285:GLU:O	1:D:289:PHE:HB2	2.01	0.61
1:A:191:GLY:HA2	1:A:297:VAL:HG22	1.83	0.60
1:A:410:ARG:HG3	1:A:411:ASP:H	1.65	0.60
1:C:337:ILE:HD12	1:C:338:HIS:CD2	2.36	0.60
1:D:171:ILE:CG1	1:D:296:VAL:HG21	2.30	0.60
1:F:328:VAL:HG23	1:F:580:GLU:HG3	1.83	0.60
1:F:369:LEU:O	1:F:372:ALA:N	2.33	0.60
1:F:394:ASP:O	1:F:397:MET:HG2	2.01	0.60
1:A:263:LYS:HZ1	1:A:276:GLU:CD	2.02	0.60
1:A:338:HIS:CE1	1:A:366:GLU:HG3	2.36	0.60
1:B:311:LEU:CA	1:B:316:ARG:HH11	2.11	0.60
1:C:390:GLU:O	1:C:393:ALA:N	2.34	0.60
1:D:327:ASP:O	1:D:331:ARG:CZ	2.49	0.60
1:A:347:ASP:OD1	1:A:347:ASP:N	2.34	0.60
1:B:238:ARG:CG	1:B:281:GLN:HE22	2.13	0.60
1:B:589:ARG:NE	1:B:596:LEU:HD21	2.15	0.60
1:C:166:GLU:O	1:C:169:LYS:CG	2.49	0.60
1:D:367:ASN:C	1:D:367:ASN:OD1	2.40	0.60
1:E:196:GLY:CA	1:E:443:ARG:NH2	2.65	0.60
1:E:371:GLU:OE1	1:E:395:ARG:NH1	2.34	0.60
1:E:488:THR:O	1:E:490:ALA:N	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ASN:C	1:F:367:ASN:OD1	2.39	0.60
1:F:577:LEU:HG	1:F:578:GLU:N	2.15	0.60
1:A:150:ALA:HB2	1:A:214:ARG:NH1	2.17	0.60
1:A:225:PHE:CE1	1:A:233:GLY:C	2.74	0.60
1:B:317:PHE:N	1:B:317:PHE:CD1	2.69	0.60
1:B:317:PHE:N	1:B:317:PHE:HD1	1.99	0.60
1:B:503:ARG:NH2	1:B:522:ARG:CZ	2.64	0.60
1:C:357:THR:N	1:C:358:PRO:HD2	2.16	0.60
1:D:290:GLU:CG	1:D:293:THR:HG23	2.18	0.60
1:B:369:LEU:O	1:B:372:ALA:N	2.33	0.60
1:C:491:GLU:O	1:C:493:ASP:N	2.34	0.60
1:C:567:GLU:HA	1:C:570:GLU:OE1	2.00	0.60
1:C:589:ARG:CZ	1:C:589:ARG:CB	2.78	0.60
1:D:165:LYS:HE2	1:D:205:LEU:CG	2.31	0.60
1:E:166:GLU:O	1:E:169:LYS:HG2	2.01	0.60
1:F:294:ALA:C	1:F:295:ILE:HG12	2.21	0.60
1:A:196:GLY:HA2	1:A:443:ARG:NH2	2.16	0.60
1:B:410:ARG:O	1:B:413:ARG:HB2	2.01	0.60
1:B:467:ASP:O	1:B:470:ALA:HB3	2.01	0.60
1:C:266:SER:C	1:C:268:VAL:H	2.05	0.60
1:C:387:LYS:O	1:C:390:GLU:HB2	2.02	0.60
1:D:257:ILE:HD12	1:D:257:ILE:N	2.13	0.60
1:D:289:PHE:HD2	1:D:290:GLU:N	2.00	0.60
1:D:319:ARG:C	1:D:320:GLN:OE1	2.40	0.60
1:D:343:PRO:O	1:D:344:LEU:HB3	2.00	0.60
1:D:501:ALA:HB1	1:D:550:LEU:HD23	1.83	0.60
1:A:211:GLY:C	1:A:214:ARG:HE	2.05	0.60
1:A:331:ARG:HD2	1:A:357:THR:HG23	1.83	0.60
1:B:159:ALA:HB1	1:B:333:GLN:CG	2.31	0.60
1:B:237:VAL:HG22	1:B:281:GLN:CG	2.31	0.60
1:C:394:ASP:N	1:C:394:ASP:OD1	2.35	0.60
1:E:440:ILE:HG22	1:E:441:VAL:HG23	1.84	0.60
1:E:586:GLU:O	1:E:590:VAL:HG13	2.01	0.60
1:F:171:ILE:CG1	1:F:296:VAL:HG21	2.31	0.60
1:A:275:ARG:NH1	1:A:275:ARG:HG3	2.17	0.60
1:A:514:PHE:HB3	1:A:519:TYR:CE1	2.36	0.60
1:C:430:GLU:O	1:C:431:HIS:CB	2.47	0.60
1:D:239:ASP:HA	1:D:242:GLU:OE1	2.02	0.60
1:E:310:ALA:O	1:E:316:ARG:NH2	2.34	0.60
1:E:333:GLN:HA	1:E:336:ARG:CZ	2.32	0.60
1:E:335:LEU:HD22	1:E:353:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:ARG:NH2	1:E:464:ARG:NH2	2.50	0.60
1:F:276:GLU:HA	1:F:279:LEU:HB2	1.84	0.60
1:A:453:ARG:NH2	1:A:464:ARG:NH1	2.50	0.60
1:B:355:LYS:CE	1:B:578:GLU:O	2.46	0.60
1:B:394:ASP:HA	1:B:397:MET:HE2	1.84	0.60
1:C:519:TYR:HA	1:C:533:ARG:CZ	2.31	0.60
1:D:311:LEU:HD12	1:D:311:LEU:C	2.22	0.60
1:E:166:GLU:O	1:E:169:LYS:CG	2.50	0.60
1:E:346:GLU:CD	1:E:347:ASP:H	2.04	0.60
1:F:337:ILE:HG23	1:F:338:HIS:CD2	2.36	0.60
1:F:461:SER:O	1:F:464:ARG:HB3	2.02	0.60
1:A:303:ARG:HB2	1:A:303:ARG:HH11	0.62	0.60
1:D:410:ARG:O	1:D:413:ARG:N	2.34	0.60
1:E:264:ARG:HE	1:E:266:SER:HB2	1.65	0.60
1:A:191:GLY:HA2	1:A:297:VAL:CG2	2.32	0.59
1:A:286:MET:HB3	1:A:316:ARG:HD3	1.80	0.59
1:C:210:ALA:O	1:C:214:ARG:HG3	2.02	0.59
1:D:394:ASP:O	1:D:397:MET:HG2	2.02	0.59
1:E:318:ASP:OD1	1:E:318:ASP:N	2.34	0.59
1:F:517:VAL:HG11	1:F:519:TYR:OH	2.02	0.59
1:A:337:ILE:HD12	1:A:338:HIS:CD2	2.36	0.59
1:A:346:GLU:CD	1:A:347:ASP:H	2.05	0.59
1:B:165:LYS:HZ2	1:B:168:LEU:HD23	1.67	0.59
1:B:286:MET:HA	1:B:289:PHE:HD1	1.67	0.59
1:B:385:THR:HB	1:B:388:ASP:OD1	2.02	0.59
1:B:390:GLU:O	1:B:393:ALA:HB3	2.02	0.59
1:C:149:GLU:O	1:C:150:ALA:CB	2.50	0.59
1:C:215:VAL:HG11	1:C:250:CYS:CA	2.31	0.59
1:D:294:ALA:C	1:D:295:ILE:HG12	2.23	0.59
1:E:357:THR:N	1:E:358:PRO:HD2	2.17	0.59
1:F:216:PRO:HG2	1:F:250:CYS:HB3	1.83	0.59
1:F:237:VAL:HG22	1:F:281:GLN:CG	2.32	0.59
1:F:583:THR:N	1:F:586:GLU:OE2	2.35	0.59
1:A:274:GLU:HA	1:A:277:GLN:HB3	1.84	0.59
1:B:180:ARG:O	1:B:184:MET:HB3	2.02	0.59
1:B:238:ARG:CB	1:B:281:GLN:HE22	2.13	0.59
1:B:333:GLN:O	1:B:336:ARG:HB3	2.01	0.59
1:C:155:PHE:HZ	1:C:209:VAL:HG22	1.67	0.59
1:C:514:PHE:HB3	1:C:519:TYR:HE1	1.68	0.59
1:D:159:ALA:HB1	1:D:333:GLN:CG	2.32	0.59
1:D:237:VAL:HG22	1:D:281:GLN:CG	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ALA:HB2	1:D:381:ARG:NH1	2.17	0.59
1:D:395:ARG:HH11	1:D:395:ARG:CG	2.02	0.59
1:E:453:ARG:HH11	1:E:453:ARG:CG	2.15	0.59
1:F:239:ASP:HA	1:F:242:GLU:OE1	2.02	0.59
1:A:263:LYS:HG2	1:A:264:ARG:N	2.17	0.59
1:A:264:ARG:HE	1:A:266:SER:HB2	1.66	0.59
1:A:308:ASP:OD1	1:A:308:ASP:C	2.39	0.59
1:A:390:GLU:O	1:A:393:ALA:N	2.35	0.59
1:B:294:ALA:C	1:B:295:ILE:HG12	2.21	0.59
1:B:301:THR:CG2	1:B:303:ARG:H	2.14	0.59
1:B:319:ARG:C	1:B:320:GLN:OE1	2.41	0.59
1:D:390:GLU:O	1:D:393:ALA:HB3	2.01	0.59
1:F:152:LYS:HB2	1:F:207:ARG:NH1	2.18	0.59
1:A:453:ARG:HH11	1:A:453:ARG:CG	2.12	0.59
1:B:428:PHE:CZ	1:B:432:ALA:HB1	2.38	0.59
1:C:313:ARG:NH2	1:C:526:TYR:C	2.52	0.59
1:D:286:MET:HA	1:D:289:PHE:HD1	1.67	0.59
1:F:279:LEU:O	1:F:283:LEU:HB2	2.02	0.59
1:A:511:HIS:HE1	1:B:552:GLU:OE2	1.85	0.59
1:A:589:ARG:HH12	1:A:596:LEU:HB3	1.67	0.59
1:B:157:ASP:HB3	1:B:337:ILE:HG12	1.83	0.59
1:B:160:GLY:H	1:B:333:GLN:NE2	1.99	0.59
1:B:420:ALA:O	1:B:424:LEU:HD12	2.03	0.59
1:C:166:GLU:O	1:C:169:LYS:HG2	2.02	0.59
1:C:318:ASP:OD1	1:C:318:ASP:N	2.33	0.59
1:E:453:ARG:NH2	1:E:464:ARG:HH12	1.99	0.59
1:F:327:ASP:O	1:F:331:ARG:NE	2.35	0.59
1:A:190:LYS:HD2	1:A:289:PHE:HE1	1.66	0.59
1:A:266:SER:C	1:A:268:VAL:H	2.05	0.59
1:D:317:PHE:N	1:D:317:PHE:CD1	2.68	0.59
1:D:331:ARG:O	1:D:335:LEU:HG	2.03	0.59
1:E:264:ARG:CD	1:E:266:SER:HB2	2.32	0.59
1:A:166:GLU:O	1:A:169:LYS:CG	2.51	0.59
1:B:216:PRO:HG2	1:B:250:CYS:HB3	1.84	0.59
1:B:237:VAL:O	1:B:240:LEU:CB	2.44	0.59
1:B:501:ALA:CB	1:B:550:LEU:HD23	2.33	0.59
1:B:507:GLU:HG3	1:B:520:ALA:O	2.02	0.59
1:D:313:ARG:NE	1:D:314:PRO:CD	2.59	0.59
1:F:180:ARG:HH12	1:F:184:MET:HE1	1.68	0.59
1:F:286:MET:CE	1:F:315:GLY:O	2.50	0.59
1:F:418:HIS:NE2	1:F:479:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:597:GLU:O	1:F:599:PRO:HD3	2.03	0.59
1:B:157:ASP:N	1:B:157:ASP:OD1	2.34	0.59
1:B:171:ILE:CG1	1:B:296:VAL:HG21	2.33	0.59
1:C:371:GLU:OE1	1:C:395:ARG:NH1	2.36	0.59
1:D:216:PRO:HG2	1:D:250:CYS:HB3	1.84	0.59
1:D:583:THR:N	1:D:586:GLU:OE2	2.35	0.59
1:E:266:SER:C	1:E:268:VAL:H	2.05	0.59
1:F:257:ILE:H	1:F:257:ILE:CD1	2.14	0.59
1:A:264:ARG:HG2	1:A:266:SER:H	1.65	0.59
1:A:400:PRO:O	1:A:405:LEU:HD11	2.03	0.59
1:A:414:ILE:CG2	1:A:415:THR:N	2.65	0.59
1:B:235:ALA:HA	1:B:238:ARG:CG	2.33	0.59
1:B:449:PHE:CZ	1:B:453:ARG:CZ	2.86	0.59
1:C:440:ILE:HG22	1:C:441:VAL:HG23	1.84	0.59
1:E:191:GLY:HA2	1:E:297:VAL:CG2	2.33	0.59
1:E:479:GLU:OE2	1:E:488:THR:HG23	2.03	0.59
1:F:376:ALA:HA	1:F:381:ARG:CZ	2.32	0.59
1:D:155:PHE:HA	1:D:158:VAL:CG2	2.33	0.58
1:D:438:VAL:HG22	1:D:439:THR:N	2.17	0.58
1:D:449:PHE:CZ	1:D:453:ARG:CZ	2.86	0.58
1:D:517:VAL:CG1	1:D:519:TYR:CZ	2.86	0.58
1:E:465:LEU:CD2	1:E:508:TRP:CZ3	2.86	0.58
1:F:338:HIS:HB3	1:F:369:LEU:CD1	2.33	0.58
1:A:438:VAL:HG23	1:A:439:THR:N	2.18	0.58
1:B:257:ILE:H	1:B:257:ILE:CD1	2.14	0.58
1:C:196:GLY:CA	1:C:443:ARG:NH2	2.66	0.58
1:C:264:ARG:NE	1:C:266:SER:HB2	2.18	0.58
1:C:390:GLU:O	1:C:393:ALA:CB	2.51	0.58
1:C:453:ARG:NH2	1:C:464:ARG:HH12	1.98	0.58
1:D:182:HIS:ND1	1:D:182:HIS:N	2.40	0.58
1:D:301:THR:CG2	1:D:303:ARG:H	2.16	0.58
1:D:589:ARG:CB	1:D:594:LEU:HD22	2.32	0.58
1:E:589:ARG:CZ	1:E:596:LEU:HB2	2.27	0.58
1:F:262:ARG:CG	1:F:263:LYS:N	2.55	0.58
1:A:225:PHE:CZ	1:A:278:THR:CB	2.77	0.58
1:B:153:VAL:HB	1:B:207:ARG:HH11	1.68	0.58
1:B:511:HIS:C	1:B:512:PRO:O	2.41	0.58
1:C:371:GLU:HG3	1:C:392:ALA:CB	2.32	0.58
1:C:449:PHE:HB2	1:C:468:GLN:HE22	1.66	0.58
1:E:145:ARG:NH2	1:E:219:THR:HG1	1.98	0.58
1:F:192:VAL:O	1:F:317:PHE:CE2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:MET:HA	1:F:289:PHE:HD1	1.67	0.58
1:F:317:PHE:N	1:F:317:PHE:CD1	2.70	0.58
1:F:366:GLU:O	1:F:369:LEU:HB2	2.03	0.58
1:F:390:GLU:O	1:F:393:ALA:HB3	2.04	0.58
1:A:286:MET:O	1:A:289:PHE:CE1	2.56	0.58
1:A:513:GLU:O	1:B:548:ARG:NH2	2.37	0.58
1:B:376:ALA:CB	1:B:381:ARG:HD3	2.33	0.58
1:C:397:MET:HG3	1:C:406:VAL:HG13	1.84	0.58
1:C:586:GLU:CA	1:C:589:ARG:HG3	2.30	0.58
1:A:275:ARG:HG3	1:A:275:ARG:HH11	1.69	0.58
1:A:357:THR:N	1:A:358:PRO:HD2	2.17	0.58
1:A:479:GLU:OE2	1:A:488:THR:HG23	2.03	0.58
1:B:153:VAL:HB	1:B:207:ARG:NH1	2.18	0.58
1:B:244:ALA:O	1:B:250:CYS:SG	2.61	0.58
1:B:585:GLU:HA	1:B:588:GLN:OE1	2.04	0.58
1:C:264:ARG:HE	1:C:266:SER:HB2	1.68	0.58
1:C:346:GLU:CD	1:C:347:ASP:H	2.06	0.58
1:D:257:ILE:H	1:D:257:ILE:CD1	2.14	0.58
1:E:337:ILE:HD12	1:E:338:HIS:CD2	2.39	0.58
1:E:507:GLU:CD	1:E:522:ARG:HE	2.07	0.58
1:F:301:THR:CG2	1:F:303:ARG:H	2.15	0.58
1:F:517:VAL:HG13	1:F:519:TYR:CZ	2.39	0.58
1:A:336:ARG:O	1:A:339:ALA:N	2.37	0.58
1:A:509:GLY:C	1:B:476:ARG:NH2	2.56	0.58
1:B:239:ASP:HA	1:B:242:GLU:OE1	2.03	0.58
1:C:438:VAL:HG23	1:C:439:THR:N	2.19	0.58
1:D:463:LYS:O	1:D:464:ARG:C	2.41	0.58
1:E:264:ARG:NE	1:E:266:SER:HB2	2.19	0.58
1:E:336:ARG:O	1:E:339:ALA:N	2.36	0.58
1:F:201:GLY:N	2:F:2001:ADP:O1A	2.33	0.58
1:A:276:GLU:OE2	1:A:527:LEU:HD11	2.03	0.58
1:E:155:PHE:HZ	1:E:209:VAL:HG22	1.69	0.58
1:E:238:ARG:HB2	1:E:238:ARG:CZ	2.34	0.58
1:E:400:PRO:O	1:E:405:LEU:HD11	2.03	0.58
1:E:503:ARG:HG2	1:E:508:TRP:CH2	2.38	0.58
1:F:438:VAL:HG22	1:F:439:THR:N	2.19	0.58
1:A:264:ARG:CG	1:A:266:SER:N	2.47	0.58
1:A:340:ARG:C	1:A:342:LYS:N	2.57	0.58
1:A:548:ARG:NH2	1:A:552:GLU:OE1	2.35	0.58
1:C:319:ARG:O	1:C:320:GLN:NE2	2.37	0.58
1:C:338:HIS:CE1	1:C:366:GLU:HG3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:GLN:O	1:D:336:ARG:HB3	2.04	0.58
1:F:245:LYS:CG	1:F:246:ARG:N	2.66	0.58
1:A:503:ARG:HG2	1:A:508:TRP:CH2	2.39	0.58
1:B:237:VAL:HA	1:B:240:LEU:HD12	1.86	0.58
1:C:349:ASP:OD1	1:C:349:ASP:O	2.22	0.58
1:C:400:PRO:O	1:C:405:LEU:HD11	2.03	0.58
1:D:233:GLY:C	1:D:236:ARG:HH22	2.07	0.58
1:D:526:TYR:O	1:D:528:GLY:N	2.37	0.58
1:E:236:ARG:NH1	1:E:236:ARG:CB	2.67	0.58
1:F:463:LYS:O	1:F:464:ARG:C	2.41	0.58
1:B:236:ARG:HG2	1:B:237:VAL:N	2.17	0.58
1:D:418:HIS:NE2	1:D:479:GLU:OE1	2.37	0.58
1:D:526:TYR:CE2	1:E:256:GLU:OE2	2.57	0.58
1:E:189:PRO:O	1:E:190:LYS:HG2	2.04	0.58
1:E:225:PHE:CE1	1:E:233:GLY:C	2.76	0.58
1:E:381:ARG:CG	1:E:382:ARG:H	2.16	0.58
1:F:159:ALA:CB	1:F:334:ILE:HG13	2.32	0.58
1:F:480:GLU:OE1	1:F:555:TYR:OH	2.21	0.58
1:B:331:ARG:O	1:B:335:LEU:HG	2.04	0.57
1:B:373:ALA:HA	1:B:384:ILE:HD11	1.86	0.57
1:B:512:PRO:HB2	1:B:514:PHE:HD2	1.69	0.57
1:C:514:PHE:CD2	1:C:514:PHE:N	2.72	0.57
1:E:212:GLU:O	1:E:214:ARG:CD	2.52	0.57
1:E:453:ARG:NH2	1:E:464:ARG:NH1	2.51	0.57
1:F:589:ARG:HB3	1:F:594:LEU:CD2	2.33	0.57
1:A:168:LEU:CA	1:A:171:ILE:CD1	2.82	0.57
1:A:286:MET:SD	1:A:316:ARG:HD2	2.36	0.57
1:B:215:VAL:HG22	1:B:216:PRO:CD	2.33	0.57
1:B:245:LYS:CG	1:B:246:ARG:N	2.65	0.57
1:C:585:GLU:OE1	1:C:586:GLU:N	2.37	0.57
1:D:276:GLU:HA	1:D:279:LEU:HB2	1.86	0.57
1:E:210:ALA:O	1:E:214:ARG:HA	2.04	0.57
1:F:373:ALA:O	1:F:376:ALA:HB3	2.05	0.57
1:A:318:ASP:N	1:A:318:ASP:OD1	2.38	0.57
1:A:394:ASP:OD1	1:A:394:ASP:N	2.36	0.57
1:B:337:ILE:CD1	1:B:340:ARG:HH12	2.07	0.57
1:C:335:LEU:HD22	1:C:353:LEU:HD23	1.85	0.57
1:C:453:ARG:NH2	1:C:464:ARG:NH1	2.52	0.57
1:C:479:GLU:OE2	1:C:488:THR:HG23	2.03	0.57
1:D:159:ALA:CB	1:D:334:ILE:HG13	2.32	0.57
1:D:348:VAL:HG13	1:D:350:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:ALA:O	1:D:505:ILE:HD12	2.05	0.57
1:E:347:ASP:N	1:E:347:ASP:OD1	2.37	0.57
1:E:430:GLU:O	1:E:431:HIS:CB	2.48	0.57
1:F:286:MET:HA	1:F:289:PHE:CD1	2.40	0.57
1:F:414:ILE:O	1:F:417:TYR:N	2.38	0.57
1:F:503:ARG:HH12	1:F:522:ARG:NH2	2.00	0.57
1:A:169:LYS:HA	1:A:172:VAL:CG1	2.35	0.57
1:A:188:ILE:O	1:A:190:LYS:NZ	2.35	0.57
1:A:491:GLU:HG2	1:F:508:TRP:HD1	1.68	0.57
1:B:285:GLU:O	1:B:288:GLY:N	2.37	0.57
1:B:290:GLU:CG	1:B:293:THR:HG23	2.23	0.57
1:B:549:ARG:O	1:B:550:LEU:C	2.42	0.57
1:C:191:GLY:HA2	1:C:297:VAL:CG2	2.35	0.57
1:D:549:ARG:O	1:D:550:LEU:C	2.42	0.57
1:E:247:HIS:O	1:E:250:CYS:HB2	2.04	0.57
1:F:165:LYS:O	1:F:168:LEU:CA	2.51	0.57
1:F:233:GLY:C	1:F:236:ARG:HH22	2.07	0.57
1:F:238:ARG:CG	1:F:281:GLN:HE22	2.15	0.57
1:F:244:ALA:O	1:F:250:CYS:SG	2.62	0.57
1:F:413:ARG:HG3	1:F:413:ARG:NH1	2.17	0.57
1:F:517:VAL:CG1	1:F:519:TYR:CZ	2.87	0.57
1:A:200:VAL:CG1	1:A:323:ILE:HG13	2.35	0.57
1:A:378:ARG:CA	1:F:173:GLU:OE1	2.45	0.57
1:A:397:MET:HG3	1:A:406:VAL:HG13	1.86	0.57
1:A:460:TRP:HB3	1:A:465:LEU:HD11	1.85	0.57
1:B:308:ASP:C	1:B:308:ASP:OD1	2.42	0.57
1:B:463:LYS:O	1:B:464:ARG:C	2.41	0.57
1:C:225:PHE:CE1	1:C:233:GLY:C	2.78	0.57
1:D:523:GLU:CD	1:E:264:ARG:NH2	2.58	0.57
1:E:211:GLY:C	1:E:214:ARG:CG	2.72	0.57
1:E:313:ARG:NH2	1:E:526:TYR:C	2.52	0.57
1:E:334:ILE:CD1	2:E:1001:ADP:C6	2.86	0.57
1:E:394:ASP:O	1:E:397:MET:N	2.37	0.57
1:F:512:PRO:HB2	1:F:514:PHE:HD2	1.69	0.57
1:F:526:TYR:O	1:F:528:GLY:N	2.38	0.57
1:F:589:ARG:CB	1:F:594:LEU:HD22	2.34	0.57
1:A:237:VAL:HG11	1:A:281:GLN:CB	2.24	0.57
1:A:371:GLU:HG3	1:A:392:ALA:CB	2.34	0.57
1:A:371:GLU:OE1	1:A:395:ARG:NH1	2.38	0.57
1:B:394:ASP:O	1:B:397:MET:HG2	2.05	0.57
1:C:275:ARG:O	1:C:279:LEU:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ALA:HB3	1:C:385:THR:HA	1.87	0.57
1:D:154:THR:HG23	1:D:156:LYS:H	1.70	0.57
1:D:163:GLU:O	1:D:167:GLU:HB3	2.04	0.57
1:E:371:GLU:HG3	1:E:392:ALA:CB	2.34	0.57
1:E:519:TYR:HA	1:E:533:ARG:CZ	2.35	0.57
1:A:212:GLU:O	1:A:214:ARG:HB2	2.04	0.57
1:B:238:ARG:NH1	1:B:239:ASP:HB3	2.14	0.57
1:B:519:TYR:HB3	1:B:535:TYR:HD2	1.69	0.57
1:C:223:SER:C	1:C:225:PHE:N	2.51	0.57
1:E:275:ARG:NH1	1:E:275:ARG:HG3	2.19	0.57
1:E:382:ARG:HD3	1:E:383:LYS:CB	2.34	0.57
1:E:519:TYR:HA	1:E:533:ARG:NH2	2.20	0.57
1:A:177:ASN:ND2	1:A:180:ARG:HD3	2.19	0.57
1:A:196:GLY:C	1:A:443:ARG:NH2	2.58	0.57
1:A:333:GLN:HG3	1:A:336:ARG:HH12	1.70	0.57
1:B:289:PHE:CD2	1:B:290:GLU:N	2.73	0.57
1:B:335:LEU:CD2	1:B:365:LEU:HB3	2.35	0.57
1:B:512:PRO:HB2	1:B:514:PHE:CD2	2.39	0.57
1:D:235:ALA:C	1:D:238:ARG:HG3	2.25	0.57
1:D:381:ARG:CZ	1:D:388:ASP:OD2	2.48	0.57
1:D:595:PRO:O	1:D:596:LEU:HD12	2.05	0.57
1:E:414:ILE:CG2	1:E:415:THR:N	2.67	0.57
1:F:180:ARG:O	1:F:184:MET:HB3	2.05	0.57
1:A:585:GLU:OE2	1:A:589:ARG:HD3	2.04	0.57
1:C:519:TYR:O	1:C:533:ARG:CG	2.53	0.57
1:D:433:ASP:N	1:D:433:ASP:OD1	2.38	0.57
1:D:519:TYR:HB3	1:D:535:TYR:HD2	1.69	0.57
1:F:391:GLU:O	1:F:394:ASP:OD1	2.22	0.57
1:A:394:ASP:O	1:A:397:MET:N	2.38	0.57
1:B:255:ASP:O	1:B:256:GLU:HG2	2.03	0.57
1:C:470:ALA:O	1:C:558:VAL:HG21	2.05	0.57
1:D:177:ASN:O	1:D:180:ARG:HB3	2.05	0.57
1:D:244:ALA:O	1:D:250:CYS:SG	2.63	0.57
1:D:286:MET:O	1:D:289:PHE:HB3	2.04	0.57
1:E:202:LYS:HB2	2:E:1001:ADP:O1B	2.04	0.57
1:E:236:ARG:CG	1:E:236:ARG:NH1	2.58	0.57
1:E:236:ARG:O	1:E:238:ARG:N	2.37	0.57
1:F:421:GLY:HA2	1:F:562:LEU:HD11	1.86	0.57
1:A:507:GLU:CD	1:A:522:ARG:HE	2.09	0.56
1:A:583:THR:HG22	1:A:586:GLU:CD	2.26	0.56
1:C:263:LYS:HD2	1:C:276:GLU:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ALA:O	1:C:316:ARG:NH2	2.38	0.56
1:C:461:SER:O	1:C:465:LEU:HD12	2.04	0.56
1:C:586:GLU:O	1:C:590:VAL:HG13	2.05	0.56
1:D:308:ASP:C	1:D:308:ASP:OD1	2.42	0.56
1:E:410:ARG:HG3	1:E:411:ASP:H	1.68	0.56
1:F:512:PRO:HB2	1:F:514:PHE:CD2	2.40	0.56
1:F:587:PHE:O	1:F:591:VAL:HG23	2.06	0.56
1:A:469:ILE:O	1:A:473:LEU:HD12	2.05	0.56
1:B:187:ARG:O	1:C:374:LEU:CD2	2.48	0.56
1:B:421:GLY:HA2	1:B:562:LEU:HD11	1.87	0.56
1:C:283:LEU:O	1:C:286:MET:HB2	2.05	0.56
1:D:238:ARG:CG	1:D:281:GLN:HE22	2.17	0.56
1:D:313:ARG:HG3	1:D:314:PRO:CG	2.36	0.56
1:E:150:ALA:HB2	1:E:214:ARG:NH2	2.19	0.56
1:E:331:ARG:HD2	1:E:357:THR:CG2	2.35	0.56
1:E:390:GLU:O	1:E:393:ALA:CB	2.52	0.56
1:F:245:LYS:C	1:F:247:HIS:N	2.58	0.56
1:F:467:ASP:O	1:F:470:ALA:HB3	2.06	0.56
1:A:247:HIS:O	1:A:250:CYS:HB2	2.05	0.56
1:A:305:ASP:O	1:A:307:LEU:N	2.39	0.56
1:A:407:LEU:HD12	1:A:407:LEU:O	2.05	0.56
1:A:453:ARG:NH1	1:A:460:TRP:CE2	2.74	0.56
1:B:170:GLU:HB3	1:C:378:ARG:NH2	2.20	0.56
1:B:245:LYS:C	1:B:247:HIS:N	2.58	0.56
1:B:245:LYS:HG3	1:B:246:ARG:N	2.20	0.56
1:B:279:LEU:O	1:B:283:LEU:HB2	2.05	0.56
1:B:503:ARG:NH2	1:B:522:ARG:NH2	2.49	0.56
1:C:219:THR:HA	1:C:253:PHE:O	2.06	0.56
1:C:334:ILE:CD1	2:C:1001:ADP:C6	2.88	0.56
1:C:394:ASP:O	1:C:397:MET:N	2.37	0.56
1:C:516:PRO:HB2	1:D:494:PHE:CD1	2.40	0.56
1:D:245:LYS:CG	1:D:246:ARG:N	2.68	0.56
1:D:261:GLY:O	1:D:308:ASP:N	2.34	0.56
1:D:286:MET:HA	1:D:289:PHE:CD1	2.40	0.56
1:D:286:MET:HE2	1:D:315:GLY:O	2.05	0.56
1:D:589:ARG:CZ	1:D:596:LEU:HD11	2.35	0.56
1:E:196:GLY:O	1:E:202:LYS:NZ	2.30	0.56
1:E:368:LEU:HD13	1:E:393:ALA:HA	1.88	0.56
1:E:460:TRP:HB3	1:E:465:LEU:HD11	1.86	0.56
1:E:585:GLU:OE1	1:E:586:GLU:N	2.37	0.56
1:F:210:ALA:O	1:F:214:ARG:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:THR:HG22	1:F:526:TYR:H	1.71	0.56
1:B:165:LYS:HE2	1:B:205:LEU:CG	2.36	0.56
1:B:391:GLU:O	1:B:394:ASP:OD1	2.23	0.56
1:B:449:PHE:CE2	1:B:492:ASN:HB3	2.37	0.56
1:B:477:ALA:O	1:B:481:ILE:HG13	2.06	0.56
1:C:263:LYS:HZ2	1:C:276:GLU:CD	1.80	0.56
1:F:447:LEU:O	1:F:450:MET:HG3	2.06	0.56
1:A:238:ARG:CZ	1:A:238:ARG:HB2	2.35	0.56
1:C:407:LEU:O	1:C:407:LEU:HD12	2.05	0.56
1:D:245:LYS:C	1:D:247:HIS:N	2.59	0.56
1:F:180:ARG:NH1	1:F:184:MET:HE1	2.20	0.56
1:F:235:ALA:C	1:F:238:ARG:HG3	2.26	0.56
1:F:503:ARG:NH2	1:F:522:ARG:CZ	2.68	0.56
1:F:592:GLU:O	1:F:594:LEU:N	2.39	0.56
1:A:459:HIS:HB2	1:B:488:THR:HB	1.87	0.56
1:A:500:LEU:O	1:A:504:MET:HG2	2.05	0.56
1:A:525:THR:O	1:A:528:GLY:N	2.39	0.56
1:A:588:GLN:HG3	1:A:589:ARG:N	2.21	0.56
1:B:236:ARG:HH12	1:B:278:THR:CG2	2.11	0.56
1:B:338:HIS:HB3	1:B:369:LEU:CD1	2.35	0.56
1:C:166:GLU:C	1:C:169:LYS:HG2	2.26	0.56
1:C:196:GLY:O	1:C:202:LYS:NZ	2.31	0.56
1:C:275:ARG:O	1:C:279:LEU:CB	2.53	0.56
1:D:327:ASP:O	1:D:331:ARG:NE	2.38	0.56
1:E:345:ALA:HB3	1:E:385:THR:HA	1.88	0.56
1:E:449:PHE:HE2	1:E:496:GLN:NE2	2.03	0.56
1:F:192:VAL:C	1:F:317:PHE:CE2	2.79	0.56
1:A:449:PHE:HB3	1:A:468:GLN:HE22	1.68	0.56
1:B:331:ARG:HD2	1:B:354:ALA:O	2.05	0.56
1:C:199:GLY:O	1:C:361:VAL:HG22	2.06	0.56
1:D:376:ALA:CB	1:D:381:ARG:NH1	2.69	0.56
1:E:147:LEU:HD23	1:E:217:PHE:HB3	1.88	0.56
1:E:263:LYS:HG2	1:E:264:ARG:N	2.20	0.56
1:E:308:ASP:OD1	1:E:308:ASP:C	2.43	0.56
1:E:407:LEU:HD12	1:E:407:LEU:O	2.06	0.56
1:F:397:MET:O	1:F:400:PRO:HG2	2.06	0.56
1:F:487:THR:HG22	1:F:488:THR:N	2.14	0.56
1:A:316:ARG:HH11	1:A:317:PHE:HE2	1.22	0.56
1:A:390:GLU:O	1:A:393:ALA:CB	2.53	0.56
1:A:449:PHE:HB2	1:A:468:GLN:HE22	1.71	0.56
1:B:276:GLU:HA	1:B:279:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ARG:CZ	1:C:219:THR:OG1	2.53	0.56
1:C:305:ASP:OD1	1:C:305:ASP:N	2.28	0.56
1:C:512:PRO:HB2	1:C:514:PHE:HD2	1.71	0.56
1:C:519:TYR:C	1:C:533:ARG:NE	2.59	0.56
1:C:585:GLU:CD	1:C:586:GLU:N	2.59	0.56
1:C:589:ARG:CZ	1:C:596:LEU:HB2	2.28	0.56
1:E:262:ARG:CG	1:E:275:ARG:HH22	2.08	0.56
1:E:514:PHE:HB3	1:E:519:TYR:HE1	1.71	0.56
1:A:438:VAL:HG11	1:A:587:PHE:CD1	2.41	0.56
1:A:536:SER:O	1:A:537:GLU:C	2.44	0.56
1:C:177:ASN:HD22	1:C:180:ARG:CD	2.17	0.56
1:C:234:ALA:HB1	1:C:281:GLN:CD	2.26	0.56
1:C:238:ARG:HB2	1:C:238:ARG:CZ	2.35	0.56
1:C:247:HIS:O	1:C:250:CYS:HB2	2.05	0.56
1:D:335:LEU:CD2	1:D:365:LEU:HB3	2.36	0.56
1:E:196:GLY:HA2	1:E:443:ARG:NH2	2.21	0.56
1:E:554:GLN:O	1:E:557:ARG:HB3	2.06	0.56
1:A:283:LEU:O	1:A:286:MET:HB2	2.05	0.56
1:B:311:LEU:HA	1:B:316:ARG:HH11	1.61	0.56
1:B:438:VAL:HG22	1:B:439:THR:N	2.20	0.56
1:B:537:GLU:O	1:B:540:ALA:HB3	2.05	0.56
1:C:401:ALA:HB3	1:C:405:LEU:HD21	1.88	0.56
1:E:166:GLU:C	1:E:169:LYS:HG2	2.26	0.56
1:F:344:LEU:HA	1:F:383:LYS:HG3	1.88	0.56
1:B:210:ALA:O	1:B:214:ARG:HA	2.07	0.55
1:C:174:PHE:CZ	1:C:294:ALA:HB1	2.41	0.55
1:C:308:ASP:OD1	1:C:308:ASP:C	2.43	0.55
1:C:438:VAL:HG11	1:C:587:PHE:CD1	2.41	0.55
1:E:387:LYS:O	1:E:390:GLU:HB2	2.06	0.55
1:F:216:PRO:HG2	1:F:250:CYS:CB	2.37	0.55
1:F:308:ASP:C	1:F:308:ASP:OD1	2.45	0.55
1:F:521:VAL:HG23	1:F:532:VAL:CG1	2.34	0.55
1:A:196:GLY:O	1:A:202:LYS:NZ	2.31	0.55
1:A:368:LEU:HG	1:A:369:LEU:N	2.20	0.55
1:A:370:ASN:OD1	1:A:374:LEU:HD13	2.06	0.55
1:A:568:VAL:O	1:A:572:VAL:HG23	2.06	0.55
1:B:344:LEU:HA	1:B:383:LYS:HG3	1.88	0.55
1:E:275:ARG:HG3	1:E:275:ARG:HH11	1.70	0.55
1:E:394:ASP:N	1:E:394:ASP:OD1	2.38	0.55
1:B:286:MET:O	1:B:289:PHE:CD1	2.59	0.55
1:B:286:MET:HA	1:B:289:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ALA:HB1	1:B:381:ARG:CD	2.36	0.55
1:D:316:ARG:CG	1:D:316:ARG:NH1	2.42	0.55
1:D:461:SER:O	1:D:464:ARG:HB3	2.06	0.55
1:F:319:ARG:C	1:F:320:GLN:OE1	2.44	0.55
1:A:194:LEU:HA	1:A:321:ILE:O	2.06	0.55
1:A:223:SER:C	1:A:225:PHE:N	2.51	0.55
1:A:514:PHE:CD2	1:A:514:PHE:N	2.75	0.55
1:B:263:LYS:HZ2	1:C:227:GLU:HG3	1.69	0.55
1:C:453:ARG:NH2	1:C:464:ARG:NH2	2.52	0.55
1:D:165:LYS:O	1:D:168:LEU:CB	2.54	0.55
1:E:451:MET:HB2	1:E:452:PRO:HD3	1.88	0.55
1:F:585:GLU:HA	1:F:588:GLN:OE1	2.06	0.55
1:F:589:ARG:HE	1:F:594:LEU:CD2	2.00	0.55
1:A:168:LEU:O	1:A:169:LYS:C	2.45	0.55
1:A:262:ARG:HG2	1:A:275:ARG:NH2	2.06	0.55
1:A:345:ALA:HB3	1:A:385:THR:HA	1.88	0.55
1:B:165:LYS:NZ	1:B:168:LEU:CD2	2.70	0.55
1:B:327:ASP:O	1:B:331:ARG:NE	2.39	0.55
1:B:503:ARG:HH12	1:B:522:ARG:NH2	2.03	0.55
1:C:196:GLY:H	1:C:202:LYS:HZ1	1.55	0.55
1:E:438:VAL:HG11	1:E:587:PHE:CD1	2.41	0.55
1:F:352:LEU:HD13	1:F:353:LEU:N	2.21	0.55
1:A:145:ARG:CZ	1:A:219:THR:OG1	2.54	0.55
1:A:319:ARG:NH2	1:B:402:LYS:HZ3	2.04	0.55
1:A:495:ARG:HD2	1:F:521:VAL:HG12	1.88	0.55
1:A:531:ASP:C	1:A:531:ASP:OD1	2.45	0.55
1:B:194:LEU:HD23	1:B:323:ILE:HD11	1.89	0.55
1:B:239:ASP:O	1:B:242:GLU:OE2	2.24	0.55
1:C:174:PHE:CD2	1:C:175:LEU:N	2.74	0.55
1:D:237:VAL:C	1:D:240:LEU:HB3	2.27	0.55
1:D:449:PHE:CE2	1:D:492:ASN:HB3	2.40	0.55
1:D:511:HIS:O	1:D:512:PRO:O	2.24	0.55
1:D:524:ASP:H	1:E:306:ILE:HD11	1.70	0.55
1:E:340:ARG:C	1:E:342:LYS:N	2.58	0.55
1:F:233:GLY:C	1:F:236:ARG:NH2	2.60	0.55
1:A:166:GLU:O	1:A:169:LYS:HG2	2.07	0.55
1:A:174:PHE:CD2	1:A:175:LEU:N	2.75	0.55
1:B:494:PHE:O	1:B:495:ARG:C	2.45	0.55
1:C:382:ARG:CG	1:C:383:LYS:H	2.19	0.55
1:C:436:HIS:HB3	1:C:584:ALA:HB1	1.88	0.55
1:C:552:GLU:O	1:C:555:TYR:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:ALA:O	1:D:481:ILE:HG13	2.07	0.55
1:D:557:ARG:O	1:D:560:ALA:HB3	2.05	0.55
1:F:245:LYS:HG3	1:F:246:ARG:N	2.21	0.55
1:F:449:PHE:CE2	1:F:492:ASN:HB3	2.37	0.55
1:A:236:ARG:O	1:A:238:ARG:N	2.39	0.55
1:A:589:ARG:NH1	1:A:596:LEU:CB	2.69	0.55
1:C:339:ALA:N	1:C:369:LEU:HD21	2.22	0.55
1:D:467:ASP:OD1	1:D:557:ARG:NH2	2.40	0.55
1:E:197:PRO:C	1:E:302:ASN:OD1	2.45	0.55
1:E:276:GLU:OE2	1:E:527:LEU:HD11	2.06	0.55
1:F:181:PHE:HA	1:F:184:MET:HG2	1.88	0.55
1:F:355:LYS:NZ	1:F:578:GLU:HG3	2.22	0.55
1:A:338:HIS:ND1	1:A:366:GLU:HG3	2.22	0.55
1:A:491:GLU:O	1:A:493:ASP:N	2.40	0.55
1:B:155:PHE:HA	1:B:158:VAL:CG2	2.37	0.55
1:B:257:ILE:O	1:B:260:VAL:HG13	2.07	0.55
1:C:414:ILE:HG22	1:C:415:THR:H	1.71	0.55
1:D:216:PRO:HB2	1:D:218:ILE:HD11	1.88	0.55
1:D:233:GLY:C	1:D:236:ARG:NH2	2.60	0.55
1:D:234:ALA:O	1:D:237:VAL:HG13	2.07	0.55
1:D:236:ARG:O	1:D:239:ASP:OD1	2.25	0.55
1:E:219:THR:HA	1:E:253:PHE:O	2.07	0.55
1:F:241:PHE:CE2	1:F:285:GLU:CG	2.90	0.55
1:F:344:LEU:HG	1:F:346:GLU:OE1	2.06	0.55
1:F:348:VAL:HG21	1:F:386:MET:HE2	1.89	0.55
1:F:459:HIS:O	1:F:459:HIS:CG	2.60	0.55
1:A:500:LEU:O	1:A:503:ARG:HB3	2.06	0.55
1:B:327:ASP:O	1:B:331:ARG:CZ	2.54	0.55
1:C:286:MET:O	1:C:289:PHE:CE1	2.59	0.55
1:C:453:ARG:HH21	1:C:464:ARG:HH22	1.49	0.55
1:C:481:ILE:HD11	1:C:563:LEU:HB3	1.89	0.55
1:D:155:PHE:CE2	1:D:212:GLU:OE2	2.59	0.55
1:D:373:ALA:HA	1:D:384:ILE:HD11	1.88	0.55
1:E:174:PHE:CD2	1:E:175:LEU:N	2.74	0.55
1:E:334:ILE:HD13	2:E:1001:ADP:N1	2.22	0.55
1:F:154:THR:HG23	1:F:156:LYS:H	1.71	0.55
1:A:154:THR:OG1	1:A:155:PHE:N	2.38	0.54
1:A:335:LEU:HD22	1:A:353:LEU:HD23	1.88	0.54
1:A:387:LYS:O	1:A:390:GLU:HB2	2.06	0.54
1:A:462:ARG:HB2	1:A:510:MET:SD	2.47	0.54
1:A:585:GLU:OE1	1:A:586:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:O	1:B:237:VAL:HG13	2.07	0.54
1:B:235:ALA:C	1:B:238:ARG:HG3	2.28	0.54
1:B:525:THR:HG22	1:B:526:TYR:H	1.73	0.54
1:C:179:SER:HA	1:C:182:HIS:NE2	2.23	0.54
1:C:263:LYS:HG2	1:C:264:ARG:N	2.21	0.54
1:C:367:ASN:O	1:C:371:GLU:HB3	2.07	0.54
1:C:463:LYS:HD2	1:D:486:VAL:CG2	2.37	0.54
1:D:253:PHE:C	1:D:253:PHE:CD2	2.80	0.54
1:E:199:GLY:O	1:E:361:VAL:HG22	2.06	0.54
1:F:236:ARG:O	1:F:239:ASP:OD1	2.25	0.54
1:F:501:ALA:HB1	1:F:550:LEU:HD23	1.89	0.54
1:A:234:ALA:HB1	1:A:281:GLN:CD	2.27	0.54
1:C:197:PRO:C	1:C:302:ASN:OD1	2.46	0.54
1:C:336:ARG:CG	1:C:337:ILE:N	2.69	0.54
1:C:336:ARG:O	1:C:339:ALA:N	2.38	0.54
1:D:430:GLU:OE1	1:D:430:GLU:CA	2.54	0.54
1:F:313:ARG:NE	1:F:314:PRO:CD	2.66	0.54
1:F:313:ARG:NE	1:F:314:PRO:CG	2.70	0.54
1:F:394:ASP:HA	1:F:397:MET:HE2	1.88	0.54
1:F:433:ASP:OD1	1:F:433:ASP:N	2.39	0.54
1:A:197:PRO:C	1:A:302:ASN:OD1	2.45	0.54
1:A:199:GLY:O	1:A:361:VAL:HG22	2.07	0.54
1:A:283:LEU:CD1	1:A:311:LEU:HD21	2.36	0.54
1:A:339:ALA:N	1:A:369:LEU:HD21	2.22	0.54
1:A:381:ARG:HH11	1:A:381:ARG:CG	2.21	0.54
1:B:348:VAL:HG13	1:B:350:LEU:H	1.72	0.54
1:C:147:LEU:HD23	1:C:217:PHE:HB3	1.88	0.54
1:C:236:ARG:O	1:C:238:ARG:N	2.39	0.54
1:C:334:ILE:HD13	2:C:1001:ADP:N1	2.23	0.54
1:C:381:ARG:HH11	1:C:381:ARG:CG	2.20	0.54
1:C:506:THR:HA	1:C:519:TYR:HD1	1.72	0.54
1:C:516:PRO:HB2	1:D:494:PHE:CE1	2.42	0.54
1:D:193:LEU:C	1:D:194:LEU:HD12	2.28	0.54
1:D:203:THR:HG23	1:D:253:PHE:CZ	2.41	0.54
1:D:222:GLY:N	1:D:255:ASP:O	2.37	0.54
1:D:391:GLU:O	1:D:394:ASP:OD1	2.26	0.54
1:E:194:LEU:HA	1:E:321:ILE:O	2.08	0.54
1:F:257:ILE:O	1:F:260:VAL:HG13	2.07	0.54
1:A:189:PRO:O	1:A:190:LYS:HG2	2.07	0.54
1:A:215:VAL:CG2	1:A:216:PRO:N	2.70	0.54
1:A:263:LYS:HD2	1:A:276:GLU:CG	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:TYR:O	1:A:533:ARG:CG	2.56	0.54
1:B:190:LYS:NZ	1:B:289:PHE:CZ	2.73	0.54
1:C:194:LEU:HA	1:C:321:ILE:O	2.08	0.54
1:C:236:ARG:NH1	1:C:236:ARG:CG	2.60	0.54
1:D:180:ARG:O	1:D:184:MET:HB3	2.06	0.54
1:D:207:ARG:HB2	1:D:217:PHE:CE2	2.41	0.54
1:D:391:GLU:O	1:D:395:ARG:HB3	2.06	0.54
1:E:174:PHE:CZ	1:E:294:ALA:HB1	2.41	0.54
1:E:189:PRO:HD3	1:E:319:ARG:NH1	2.23	0.54
1:E:234:ALA:HB1	1:E:281:GLN:CD	2.27	0.54
1:E:283:LEU:O	1:E:286:MET:HB2	2.07	0.54
1:F:311:LEU:HD12	1:F:311:LEU:O	2.07	0.54
1:A:174:PHE:CZ	1:A:294:ALA:HB1	2.42	0.54
1:A:353:LEU:O	1:A:357:THR:HG22	2.06	0.54
1:B:192:VAL:C	1:B:317:PHE:CE2	2.80	0.54
1:B:433:ASP:N	1:B:433:ASP:OD1	2.41	0.54
1:C:353:LEU:O	1:C:357:THR:HG22	2.08	0.54
1:D:165:LYS:CD	1:D:168:LEU:CD2	2.77	0.54
1:D:238:ARG:CB	1:D:281:GLN:HE22	2.20	0.54
1:D:283:LEU:HD12	1:D:316:ARG:NH2	2.20	0.54
1:E:333:GLN:HG3	1:E:336:ARG:HH12	1.71	0.54
1:E:519:TYR:O	1:E:533:ARG:CG	2.56	0.54
1:A:149:GLU:O	1:A:150:ALA:CB	2.53	0.54
1:A:179:SER:C	1:A:181:PHE:H	2.10	0.54
1:A:583:THR:HG22	1:A:586:GLU:OE1	2.07	0.54
1:B:311:LEU:N	1:B:316:ARG:HH12	2.04	0.54
1:C:196:GLY:C	1:C:443:ARG:NH2	2.61	0.54
1:C:218:ILE:HG12	1:C:251:ILE:O	2.08	0.54
1:D:166:GLU:O	1:D:169:LYS:HG2	2.07	0.54
1:D:180:ARG:NH1	1:D:184:MET:HE1	2.22	0.54
1:D:190:LYS:NZ	1:D:289:PHE:CZ	2.73	0.54
1:D:512:PRO:HB2	1:D:514:PHE:CD2	2.43	0.54
1:E:339:ALA:N	1:E:369:LEU:HD21	2.23	0.54
1:E:401:ALA:HB3	1:E:405:LEU:HD21	1.89	0.54
1:F:190:LYS:HD2	1:F:289:PHE:HZ	1.71	0.54
1:F:237:VAL:C	1:F:240:LEU:HB3	2.28	0.54
1:A:236:ARG:NH1	1:A:236:ARG:CB	2.70	0.54
1:A:588:GLN:HA	1:A:591:VAL:HG23	1.89	0.54
1:B:163:GLU:O	1:B:167:GLU:HB3	2.07	0.54
1:B:192:VAL:O	1:B:317:PHE:CE2	2.60	0.54
1:B:277:GLN:HA	1:B:280:ASN:HD21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:GLY:H	2:D:2001:ADP:PB	2.29	0.54
1:E:211:GLY:O	1:E:214:ARG:CD	2.53	0.54
1:E:263:LYS:HD2	1:E:276:GLU:CG	2.38	0.54
1:E:305:ASP:O	1:E:307:LEU:N	2.41	0.54
1:E:338:HIS:ND1	1:E:366:GLU:HG3	2.22	0.54
1:E:449:PHE:N	1:E:449:PHE:HD2	2.04	0.54
1:F:165:LYS:CE	1:F:205:LEU:CG	2.86	0.54
1:F:203:THR:HG23	1:F:253:PHE:CZ	2.42	0.54
1:F:234:ALA:O	1:F:237:VAL:HG13	2.07	0.54
1:A:325:ALA:N	1:A:326:PRO:CD	2.71	0.54
1:A:342:LYS:CE	1:F:184:MET:SD	2.95	0.54
1:A:374:LEU:CD1	1:F:186:ALA:HB1	2.38	0.54
1:A:541:LYS:HA	1:F:536:SER:OG	2.07	0.54
1:B:210:ALA:O	1:B:214:ARG:N	2.41	0.54
1:B:319:ARG:CG	1:B:319:ARG:NH1	2.67	0.54
1:B:418:HIS:NE2	1:B:479:GLU:OE1	2.40	0.54
1:D:201:GLY:N	2:D:2001:ADP:O1A	2.34	0.54
1:D:207:ARG:CB	1:D:217:PHE:CZ	2.91	0.54
1:E:179:SER:O	1:E:182:HIS:CD2	2.60	0.54
1:E:438:VAL:HG23	1:E:439:THR:N	2.23	0.54
1:E:512:PRO:HB2	1:E:514:PHE:HD2	1.72	0.54
1:F:216:PRO:HB2	1:F:218:ILE:HD11	1.90	0.54
1:A:563:LEU:HD12	1:A:564:GLU:N	2.22	0.54
1:A:585:GLU:OE2	1:A:589:ARG:CD	2.56	0.54
1:B:241:PHE:CE2	1:B:285:GLU:CG	2.91	0.54
1:B:313:ARG:HG3	1:B:314:PRO:CG	2.38	0.54
1:B:344:LEU:HG	1:B:346:GLU:OE1	2.08	0.54
1:C:319:ARG:C	1:C:320:GLN:NE2	2.61	0.54
1:D:237:VAL:CG2	1:D:281:GLN:CG	2.86	0.54
1:D:313:ARG:CG	1:D:314:PRO:N	2.70	0.54
1:D:503:ARG:HH12	1:D:522:ARG:NH2	2.05	0.54
1:E:202:LYS:CD	1:E:300:ALA:HB1	2.36	0.54
1:E:305:ASP:OD1	1:E:305:ASP:N	2.26	0.54
1:E:334:ILE:O	1:E:335:LEU:C	2.47	0.54
1:E:589:ARG:HH22	1:E:596:LEU:HB2	1.38	0.54
1:F:238:ARG:CB	1:F:281:GLN:HE22	2.18	0.54
1:F:417:TYR:CE1	1:F:482:VAL:HG21	2.42	0.54
1:A:219:THR:HA	1:A:253:PHE:O	2.08	0.54
1:B:170:GLU:CB	1:C:378:ARG:HH22	2.20	0.54
1:B:236:ARG:O	1:B:239:ASP:OD1	2.26	0.54
1:D:285:GLU:O	1:D:288:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:LEU:HD13	1:E:393:ALA:CA	2.37	0.54
1:F:238:ARG:NH1	1:F:239:ASP:HB3	2.15	0.54
1:F:375:LEU:CD1	1:F:388:ASP:HB3	2.36	0.54
1:F:454:ARG:NH2	1:F:528:GLY:C	2.61	0.54
1:F:511:HIS:C	1:F:512:PRO:O	2.45	0.54
1:A:196:GLY:O	1:A:302:ASN:OD1	2.25	0.53
1:A:367:ASN:O	1:A:371:GLU:HB3	2.07	0.53
1:B:334:ILE:O	1:B:337:ILE:HG22	2.09	0.53
1:C:551:ILE:O	1:C:552:GLU:C	2.46	0.53
1:D:319:ARG:CG	1:D:319:ARG:NH1	2.62	0.53
1:D:334:ILE:O	1:D:337:ILE:HG22	2.08	0.53
1:D:522:ARG:HD2	1:D:530:TYR:CA	2.32	0.53
1:F:177:ASN:O	1:F:180:ARG:HB3	2.07	0.53
1:F:261:GLY:O	1:F:308:ASP:N	2.35	0.53
1:F:285:GLU:O	1:F:288:GLY:N	2.41	0.53
1:F:289:PHE:CD2	1:F:290:GLU:N	2.75	0.53
1:F:327:ASP:O	1:F:331:ARG:NH2	2.41	0.53
1:A:166:GLU:C	1:A:169:LYS:HG2	2.28	0.53
1:A:218:ILE:HG12	1:A:251:ILE:O	2.08	0.53
1:A:311:LEU:HB3	1:A:316:ARG:HH22	1.73	0.53
1:A:336:ARG:CG	1:A:337:ILE:N	2.72	0.53
1:B:165:LYS:CD	1:B:168:LEU:CD2	2.76	0.53
1:B:328:VAL:HG21	1:B:355:LYS:HE3	1.88	0.53
1:D:152:LYS:HB2	1:D:207:ARG:NH1	2.23	0.53
1:D:257:ILE:O	1:D:260:VAL:HG13	2.08	0.53
1:D:480:GLU:OE1	1:D:555:TYR:OH	2.26	0.53
1:D:517:VAL:HG11	1:D:519:TYR:CZ	2.43	0.53
1:E:179:SER:HA	1:E:182:HIS:NE2	2.24	0.53
1:E:367:ASN:O	1:E:371:GLU:HB3	2.09	0.53
1:F:166:GLU:O	1:F:169:LYS:HG2	2.08	0.53
1:A:240:LEU:O	1:A:243:THR:OG1	2.20	0.53
1:A:292:ASP:OD1	1:A:293:THR:N	2.41	0.53
1:A:334:ILE:CD1	2:A:1001:ADP:C6	2.91	0.53
1:B:216:PRO:HG2	1:B:250:CYS:CB	2.39	0.53
1:B:253:PHE:C	1:B:253:PHE:CD2	2.82	0.53
1:B:522:ARG:HD2	1:B:530:TYR:CA	2.31	0.53
1:C:305:ASP:O	1:C:307:LEU:N	2.41	0.53
1:C:368:LEU:HD13	1:C:393:ALA:HA	1.89	0.53
1:C:461:SER:HA	1:D:487:THR:O	2.08	0.53
1:D:467:ASP:O	1:D:470:ALA:HB3	2.08	0.53
1:E:177:ASN:ND2	1:E:180:ARG:HD3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:GLU:HG3	1:E:381:ARG:HB2	1.91	0.53
1:E:467:ASP:O	1:E:471:VAL:HG23	2.08	0.53
1:F:376:ALA:CA	1:F:381:ARG:NH1	2.71	0.53
1:F:417:TYR:CD2	1:F:483:PHE:HE2	2.26	0.53
1:A:313:ARG:NH1	1:A:526:TYR:HA	2.24	0.53
1:A:448:GLY:O	1:A:449:PHE:C	2.46	0.53
1:A:465:LEU:CD2	1:A:508:TRP:CZ3	2.92	0.53
1:A:493:ASP:N	1:A:493:ASP:OD1	2.41	0.53
1:A:525:THR:OG1	1:A:528:GLY:HA3	2.08	0.53
1:B:592:GLU:O	1:B:594:LEU:N	2.41	0.53
1:C:202:LYS:CD	1:C:300:ALA:HB1	2.36	0.53
1:C:410:ARG:HG3	1:C:411:ASP:H	1.73	0.53
1:D:165:LYS:HZ1	1:D:205:LEU:HB3	1.73	0.53
1:D:202:LYS:HD3	2:D:2001:ADP:O2B	2.08	0.53
1:E:196:GLY:C	1:E:443:ARG:NH2	2.61	0.53
1:A:552:GLU:O	1:A:555:TYR:HB3	2.09	0.53
1:A:586:GLU:CB	1:A:589:ARG:CZ	2.72	0.53
1:A:587:PHE:CD2	1:A:588:GLN:N	2.76	0.53
1:B:177:ASN:O	1:B:180:ARG:HB3	2.08	0.53
1:C:507:GLU:CD	1:C:522:ARG:HE	2.12	0.53
1:C:563:LEU:HD12	1:C:564:GLU:N	2.23	0.53
1:C:594:LEU:HG	1:C:594:LEU:O	2.09	0.53
1:E:334:ILE:CD1	2:E:1001:ADP:N6	2.71	0.53
1:F:163:GLU:O	1:F:167:GLU:HB3	2.08	0.53
1:F:212:GLU:O	1:F:214:ARG:HG2	2.09	0.53
1:A:319:ARG:O	1:A:320:GLN:NE2	2.42	0.53
1:A:349:ASP:OD1	1:A:349:ASP:O	2.26	0.53
1:A:585:GLU:CD	1:A:586:GLU:N	2.62	0.53
1:B:201:GLY:N	2:B:2001:ADP:O1A	2.39	0.53
1:C:368:LEU:HD13	1:C:393:ALA:CA	2.39	0.53
1:D:441:VAL:O	1:D:443:ARG:N	2.42	0.53
1:E:169:LYS:HA	1:E:172:VAL:CG1	2.38	0.53
1:F:194:LEU:HD23	1:F:323:ILE:HD11	1.90	0.53
1:F:467:ASP:OD1	1:F:557:ARG:NH2	2.42	0.53
1:F:477:ALA:O	1:F:481:ILE:HG13	2.09	0.53
1:A:334:ILE:O	1:A:335:LEU:C	2.46	0.53
1:A:368:LEU:HD13	1:A:393:ALA:HA	1.91	0.53
1:A:537:GLU:N	1:B:537:GLU:OE2	2.41	0.53
1:B:366:GLU:O	1:B:369:LEU:HB2	2.08	0.53
1:B:397:MET:O	1:B:400:PRO:HG2	2.09	0.53
1:B:447:LEU:O	1:B:449:PHE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:HG23	1:D:172:VAL:N	2.23	0.53
1:D:517:VAL:HG13	1:D:519:TYR:CZ	2.44	0.53
1:E:525:THR:O	1:E:528:GLY:N	2.42	0.53
1:E:539:THR:O	1:E:543:ILE:HG13	2.08	0.53
1:E:585:GLU:CD	1:E:586:GLU:N	2.62	0.53
1:F:155:PHE:CE2	1:F:212:GLU:OE2	2.61	0.53
1:F:318:ASP:OD1	1:F:318:ASP:N	2.21	0.53
1:F:451:MET:HB3	1:F:452:PRO:CD	2.38	0.53
1:A:401:ALA:HB3	1:A:405:LEU:HD21	1.91	0.53
1:B:181:PHE:O	1:B:185:GLY:N	2.42	0.53
1:B:216:PRO:HB2	1:B:218:ILE:HD11	1.89	0.53
1:C:193:LEU:HD12	1:C:299:ALA:O	2.09	0.53
1:D:417:TYR:CE1	1:D:482:VAL:HG21	2.44	0.53
1:D:463:LYS:HE3	1:E:486:VAL:HG21	1.91	0.53
1:E:200:VAL:CG1	1:E:323:ILE:HG13	2.39	0.53
1:E:336:ARG:CG	1:E:337:ILE:N	2.71	0.53
1:F:210:ALA:O	1:F:214:ARG:CA	2.57	0.53
1:F:253:PHE:C	1:F:253:PHE:CD2	2.82	0.53
1:F:331:ARG:HD2	1:F:354:ALA:O	2.09	0.53
1:F:494:PHE:O	1:F:495:ARG:C	2.45	0.53
1:A:155:PHE:CZ	1:A:209:VAL:HG22	2.44	0.53
1:A:264:ARG:HD2	1:A:266:SER:OG	2.09	0.53
1:A:382:ARG:HG3	1:A:383:LYS:HB2	1.91	0.53
1:A:424:LEU:HD22	1:A:569:LEU:HA	1.90	0.53
1:B:158:VAL:CG1	1:B:205:LEU:HD11	2.38	0.53
1:B:262:ARG:CG	1:B:263:LYS:H	2.18	0.53
1:D:277:GLN:HA	1:D:280:ASN:HD21	1.74	0.53
1:D:592:GLU:O	1:D:594:LEU:N	2.42	0.53
1:E:319:ARG:O	1:E:320:GLN:NE2	2.41	0.53
1:E:343:PRO:C	1:E:344:LEU:HD13	2.28	0.53
1:E:349:ASP:O	1:E:349:ASP:OD1	2.26	0.53
1:E:514:PHE:N	1:E:514:PHE:CD2	2.77	0.53
1:F:391:GLU:O	1:F:395:ARG:HB3	2.08	0.53
1:F:514:PHE:HB3	1:F:519:TYR:HE1	1.74	0.53
1:A:214:ARG:NH1	1:A:214:ARG:HG2	2.23	0.53
1:A:227:GLU:HG3	1:F:263:LYS:HZ1	1.68	0.53
1:A:521:VAL:HG12	1:B:495:ARG:HD2	1.90	0.53
1:B:165:LYS:O	1:B:168:LEU:CB	2.57	0.53
1:C:169:LYS:HA	1:C:172:VAL:CG1	2.38	0.53
1:C:196:GLY:HA2	1:C:443:ARG:NH2	2.24	0.53
1:C:262:ARG:CG	1:C:275:ARG:HH22	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ASP:O	1:C:319:ARG:HG3	2.09	0.53
1:C:345:ALA:O	1:C:348:VAL:HB	2.09	0.53
1:D:181:PHE:O	1:D:185:GLY:N	2.42	0.53
1:D:181:PHE:HA	1:D:184:MET:HG2	1.89	0.53
1:D:387:LYS:HG3	1:D:388:ASP:N	2.21	0.53
1:D:585:GLU:HA	1:D:588:GLN:OE1	2.09	0.53
1:E:168:LEU:O	1:E:169:LYS:C	2.47	0.53
1:E:461:SER:HA	1:F:487:THR:O	2.09	0.53
1:F:186:ALA:O	1:F:187:ARG:HB3	2.08	0.53
1:B:181:PHE:HA	1:B:184:MET:HG2	1.90	0.52
1:B:319:ARG:O	1:B:320:GLN:HB3	2.09	0.52
1:B:479:GLU:OE2	1:B:488:THR:HG23	2.10	0.52
1:C:189:PRO:O	1:C:190:LYS:HG2	2.08	0.52
1:C:343:PRO:C	1:C:344:LEU:HD13	2.30	0.52
1:D:421:GLY:HA2	1:D:562:LEU:HD11	1.90	0.52
1:D:459:HIS:O	1:D:459:HIS:CG	2.56	0.52
1:E:179:SER:C	1:E:181:PHE:H	2.13	0.52
1:F:165:LYS:HZ1	1:F:205:LEU:CB	2.21	0.52
1:F:479:GLU:OE2	1:F:488:THR:HG23	2.09	0.52
1:F:526:TYR:CD2	1:F:526:TYR:N	2.76	0.52
1:A:172:VAL:CB	1:A:213:ALA:HB2	2.39	0.52
1:B:158:VAL:HG11	1:B:205:LEU:HD11	1.91	0.52
1:C:460:TRP:HB3	1:C:465:LEU:HD11	1.91	0.52
1:D:263:LYS:HE2	1:E:228:MET:HE1	1.91	0.52
1:D:335:LEU:HD21	1:D:365:LEU:HB3	1.90	0.52
1:E:240:LEU:O	1:E:243:THR:OG1	2.22	0.52
1:E:521:VAL:HG12	1:F:495:ARG:HD2	1.92	0.52
1:F:376:ALA:O	1:F:381:ARG:CG	2.57	0.52
1:A:179:SER:HA	1:A:182:HIS:NE2	2.24	0.52
1:B:521:VAL:HG23	1:B:532:VAL:CG1	2.37	0.52
1:C:354:ALA:O	1:C:357:THR:CG2	2.57	0.52
1:C:510:MET:O	1:C:512:PRO:CD	2.57	0.52
1:C:525:THR:O	1:C:528:GLY:N	2.42	0.52
1:D:187:ARG:O	1:E:374:LEU:HD21	2.08	0.52
1:E:177:ASN:HD22	1:E:180:ARG:CD	2.22	0.52
1:E:178:PRO:O	1:E:182:HIS:CD2	2.62	0.52
1:E:190:LYS:HD2	1:E:289:PHE:HE1	1.70	0.52
1:E:212:GLU:O	1:E:214:ARG:HD3	2.10	0.52
1:E:568:VAL:O	1:E:572:VAL:HG23	2.10	0.52
1:F:277:GLN:HA	1:F:280:ASN:HD21	1.74	0.52
1:F:356:ARG:O	1:F:358:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD13	1:A:393:ALA:CA	2.39	0.52
1:A:436:HIS:HB3	1:A:584:ALA:HB1	1.90	0.52
1:A:503:ARG:NH2	1:A:522:ARG:NH1	2.57	0.52
1:B:463:LYS:HE3	1:C:486:VAL:HG21	1.90	0.52
1:C:451:MET:HB2	1:C:452:PRO:HD3	1.92	0.52
1:D:243:THR:HG22	1:D:244:ALA:N	2.25	0.52
1:D:348:VAL:HG11	1:D:386:MET:SD	2.49	0.52
1:D:554:GLN:O	1:D:557:ARG:HB3	2.09	0.52
1:E:442:PRO:HG2	1:E:443:ARG:H	1.74	0.52
1:F:165:LYS:CD	1:F:168:LEU:CD2	2.79	0.52
1:F:235:ALA:HA	1:F:238:ARG:HD3	1.91	0.52
1:A:273:ASP:CG	1:A:274:GLU:N	2.63	0.52
1:A:374:LEU:CD1	1:F:187:ARG:H	2.11	0.52
1:B:171:ILE:HG23	1:B:172:VAL:N	2.23	0.52
1:B:180:ARG:NH1	1:B:184:MET:HE1	2.24	0.52
1:B:571:ARG:HH12	1:B:593:GLY:H	1.57	0.52
1:C:463:LYS:HD2	1:D:486:VAL:HG22	1.90	0.52
1:D:216:PRO:HG2	1:D:250:CYS:CB	2.39	0.52
1:D:331:ARG:HH22	1:D:580:GLU:CD	2.10	0.52
1:D:376:ALA:C	1:D:381:ARG:CB	2.77	0.52
1:D:417:TYR:CD2	1:D:483:PHE:HE2	2.28	0.52
1:D:507:GLU:HG3	1:D:520:ALA:O	2.10	0.52
1:E:241:PHE:O	1:E:244:ALA:N	2.42	0.52
1:E:354:ALA:HA	1:E:357:THR:CG2	2.39	0.52
1:A:343:PRO:C	1:A:344:LEU:HD13	2.29	0.52
1:A:451:MET:HB2	1:A:452:PRO:HD3	1.92	0.52
1:A:574:GLU:C	1:A:574:GLU:OE1	2.48	0.52
1:A:583:THR:N	1:A:586:GLU:OE2	2.36	0.52
1:C:470:ALA:HB1	1:C:558:VAL:CG2	2.36	0.52
1:C:568:VAL:O	1:C:572:VAL:HG23	2.09	0.52
1:D:350:LEU:HA	1:D:353:LEU:HB3	1.91	0.52
1:F:174:PHE:HZ	1:F:294:ALA:CA	2.22	0.52
1:F:348:VAL:HG13	1:F:350:LEU:H	1.73	0.52
1:A:374:LEU:HA	1:A:377:ALA:HB3	1.92	0.52
1:B:281:GLN:O	1:B:285:GLU:OE1	2.28	0.52
1:C:207:ARG:NH2	1:C:217:PHE:CD2	2.76	0.52
1:C:379:GLU:HG3	1:C:381:ARG:HB2	1.92	0.52
1:D:174:PHE:HZ	1:D:294:ALA:CA	2.23	0.52
1:D:194:LEU:HD23	1:D:323:ILE:HD11	1.92	0.52
1:E:236:ARG:HG3	1:E:237:VAL:CA	2.37	0.52
1:F:350:LEU:HA	1:F:353:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:381:ARG:CZ	1:F:388:ASP:OD2	2.57	0.52
1:A:241:PHE:O	1:A:244:ALA:N	2.43	0.52
1:A:286:MET:HE3	1:A:297:VAL:HG21	1.90	0.52
1:B:190:LYS:HD2	1:B:289:PHE:HZ	1.73	0.52
1:B:297:VAL:HG13	1:B:317:PHE:HZ	1.75	0.52
1:B:398:MET:O	1:B:401:ALA:HB3	2.09	0.52
1:B:505:ILE:HD13	1:B:547:VAL:HG23	1.90	0.52
1:C:179:SER:C	1:C:181:PHE:H	2.13	0.52
1:C:218:ILE:CG1	1:C:251:ILE:O	2.57	0.52
1:C:325:ALA:N	1:C:326:PRO:CD	2.72	0.52
1:C:574:GLU:OE1	1:C:575:THR:N	2.43	0.52
1:D:338:HIS:HB3	1:D:369:LEU:CD1	2.40	0.52
1:D:378:ARG:C	1:D:380:GLY:N	2.51	0.52
1:D:398:MET:O	1:D:401:ALA:HB3	2.10	0.52
1:D:503:ARG:HG2	1:D:508:TRP:CZ2	2.44	0.52
1:E:462:ARG:HB2	1:E:510:MET:SD	2.50	0.52
1:F:165:LYS:CE	1:F:205:LEU:HG	2.39	0.52
1:B:180:ARG:HH12	1:B:184:MET:HE1	1.75	0.52
1:C:219:THR:HB	1:C:253:PHE:CD2	2.38	0.52
1:C:225:PHE:CE1	1:C:233:GLY:HA3	2.43	0.52
1:C:334:ILE:CD1	2:C:1001:ADP:N6	2.73	0.52
1:C:449:PHE:N	1:C:449:PHE:HD2	2.08	0.52
1:D:245:LYS:HG3	1:D:246:ARG:N	2.24	0.52
1:D:281:GLN:O	1:D:285:GLU:OE1	2.28	0.52
1:D:319:ARG:O	1:D:320:GLN:HB3	2.10	0.52
1:D:355:LYS:NZ	1:D:578:GLU:O	2.43	0.52
1:E:331:ARG:CZ	1:E:358:PRO:HD3	2.39	0.52
1:E:353:LEU:O	1:E:357:THR:HG22	2.09	0.52
1:E:378:ARG:HG2	1:E:379:GLU:N	2.23	0.52
1:E:436:HIS:HB3	1:E:584:ALA:HB1	1.92	0.52
1:E:447:LEU:CB	1:E:496:GLN:HE22	2.23	0.52
1:F:557:ARG:O	1:F:560:ALA:HB3	2.10	0.52
1:A:331:ARG:HD2	1:A:357:THR:CG2	2.40	0.52
1:B:202:LYS:HD3	2:B:2001:ADP:O2B	2.10	0.52
1:B:350:LEU:HA	1:B:353:LEU:HB3	1.91	0.52
1:C:241:PHE:O	1:C:244:ALA:N	2.43	0.52
1:C:539:THR:OG1	1:D:544:ASP:OD2	2.25	0.52
1:D:180:ARG:HH12	1:D:184:MET:HE1	1.73	0.52
1:D:190:LYS:CE	1:D:289:PHE:HZ	2.13	0.52
1:D:260:VAL:HG23	1:D:279:LEU:CD1	2.40	0.52
1:D:455:GLU:O	1:D:457:MET:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ALA:O	1:D:474:ALA:HB2	2.10	0.52
1:F:237:VAL:CG2	1:F:281:GLN:CG	2.88	0.52
1:F:453:ARG:HA	1:F:456:ASP:OD2	2.10	0.52
1:A:206:ALA:HB1	1:A:217:PHE:HZ	1.75	0.51
1:A:238:ARG:O	1:A:241:PHE:N	2.43	0.51
1:A:334:ILE:HD13	2:A:1001:ADP:N1	2.26	0.51
1:A:346:GLU:OE1	1:A:347:ASP:OD1	2.28	0.51
1:B:173:GLU:OE1	1:C:378:ARG:HA	2.10	0.51
1:B:174:PHE:HZ	1:B:294:ALA:HA	1.76	0.51
1:B:376:ALA:C	1:B:381:ARG:CD	2.61	0.51
1:B:417:TYR:CD2	1:B:483:PHE:HE2	2.26	0.51
1:B:526:TYR:O	1:B:528:GLY:N	2.42	0.51
1:C:175:LEU:O	1:C:249:PRO:HG3	2.10	0.51
1:C:200:VAL:CG1	1:C:323:ILE:HG13	2.39	0.51
1:D:366:GLU:O	1:D:369:LEU:HB2	2.09	0.51
1:E:345:ALA:O	1:E:348:VAL:HB	2.10	0.51
1:F:180:ARG:NH1	1:F:184:MET:CE	2.73	0.51
1:A:172:VAL:O	1:A:213:ALA:HB1	2.10	0.51
1:A:594:LEU:HG	1:A:594:LEU:O	2.11	0.51
1:B:159:ALA:H	2:B:2001:ADP:HN62	1.57	0.51
1:B:166:GLU:O	1:B:169:LYS:HG2	2.10	0.51
1:B:467:ASP:OD1	1:B:557:ARG:NH2	2.43	0.51
1:B:583:THR:O	1:B:584:ALA:C	2.48	0.51
1:C:174:PHE:HB2	1:C:181:PHE:CE2	2.46	0.51
1:C:368:LEU:HG	1:C:369:LEU:N	2.25	0.51
1:D:192:VAL:O	1:D:317:PHE:CE2	2.64	0.51
1:D:338:HIS:CE1	1:D:366:GLU:HG3	2.44	0.51
1:D:352:LEU:O	1:D:353:LEU:C	2.48	0.51
1:D:376:ALA:O	1:D:381:ARG:HG2	2.10	0.51
1:E:193:LEU:HD12	1:E:299:ALA:O	2.09	0.51
1:F:158:VAL:CG1	1:F:205:LEU:HD11	2.40	0.51
1:F:376:ALA:HA	1:F:381:ARG:HH11	1.74	0.51
1:A:379:GLU:HG3	1:A:381:ARG:HB2	1.92	0.51
1:B:175:LEU:HB3	1:B:213:ALA:HB1	1.93	0.51
1:B:215:VAL:HG22	1:B:250:CYS:HB3	1.92	0.51
1:B:356:ARG:O	1:B:358:PRO:HD3	2.11	0.51
1:B:455:GLU:O	1:B:457:MET:N	2.43	0.51
1:B:523:GLU:OE1	1:C:264:ARG:NH2	2.43	0.51
1:C:154:THR:OG1	1:C:155:PHE:N	2.43	0.51
1:C:179:SER:O	1:C:182:HIS:CD2	2.61	0.51
1:C:240:LEU:O	1:C:243:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:PHE:O	1:C:242:GLU:C	2.49	0.51
1:C:334:ILE:O	1:C:335:LEU:C	2.48	0.51
1:C:397:MET:SD	1:C:406:VAL:CG1	2.98	0.51
1:C:525:THR:OG1	1:C:528:GLY:HA3	2.11	0.51
1:D:331:ARG:HD2	1:D:354:ALA:O	2.11	0.51
1:E:594:LEU:HG	1:E:594:LEU:O	2.10	0.51
1:A:313:ARG:NH1	1:A:526:TYR:CA	2.73	0.51
1:A:354:ALA:HA	1:A:357:THR:CG2	2.40	0.51
1:C:338:HIS:ND1	1:C:366:GLU:HG3	2.25	0.51
1:D:175:LEU:O	1:D:249:PRO:CB	2.58	0.51
1:E:196:GLY:H	1:E:202:LYS:HZ1	1.55	0.51
1:E:206:ALA:HB1	1:E:217:PHE:HZ	1.75	0.51
1:F:174:PHE:HZ	1:F:294:ALA:HA	1.75	0.51
1:A:169:LYS:O	1:A:172:VAL:CG1	2.58	0.51
1:A:236:ARG:HG3	1:A:237:VAL:CA	2.36	0.51
1:A:464:ARG:HH11	1:A:464:ARG:CG	2.23	0.51
1:B:175:LEU:O	1:B:249:PRO:CB	2.58	0.51
1:B:355:LYS:HZ3	1:B:578:GLU:HG3	1.74	0.51
1:B:452:PRO:O	1:B:456:ASP:N	2.43	0.51
1:B:557:ARG:O	1:B:560:ALA:HB3	2.11	0.51
1:C:236:ARG:NH1	1:C:236:ARG:CB	2.73	0.51
1:D:210:ALA:O	1:D:214:ARG:N	2.41	0.51
1:D:447:LEU:O	1:D:449:PHE:N	2.43	0.51
1:D:452:PRO:O	1:D:456:ASP:N	2.43	0.51
1:E:218:ILE:CG1	1:E:251:ILE:O	2.59	0.51
1:E:313:ARG:HH12	1:E:526:TYR:CA	2.23	0.51
1:F:171:ILE:HG23	1:F:172:VAL:N	2.25	0.51
1:F:222:GLY:N	1:F:255:ASP:O	2.40	0.51
1:F:281:GLN:O	1:F:285:GLU:OE1	2.29	0.51
1:F:318:ASP:O	1:F:319:ARG:CB	2.35	0.51
1:F:428:PHE:CE1	1:F:432:ALA:C	2.84	0.51
1:B:461:SER:O	1:B:464:ARG:HB3	2.10	0.51
1:C:236:ARG:HG3	1:C:237:VAL:CA	2.36	0.51
1:C:292:ASP:OD1	1:C:293:THR:N	2.43	0.51
1:D:327:ASP:O	1:D:331:ARG:NH2	2.43	0.51
1:D:514:PHE:HB3	1:D:519:TYR:HE1	1.74	0.51
1:E:563:LEU:HD12	1:E:564:GLU:N	2.25	0.51
1:F:193:LEU:HB3	1:F:317:PHE:HD2	1.76	0.51
1:F:567:GLU:O	1:F:570:GLU:CB	2.58	0.51
1:A:334:ILE:O	1:A:337:ILE:HG13	2.10	0.51
1:B:180:ARG:NH1	1:B:184:MET:CE	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ALA:O	1:B:187:ARG:HB3	2.09	0.51
1:B:454:ARG:HH21	1:B:526:TYR:CA	2.24	0.51
1:C:174:PHE:CE1	1:C:188:ILE:CD1	2.70	0.51
1:C:181:PHE:HA	1:C:184:MET:HE2	1.91	0.51
1:C:554:GLN:O	1:C:557:ARG:HB3	2.11	0.51
1:D:563:LEU:O	1:D:566:ARG:HB3	2.11	0.51
1:E:175:LEU:O	1:E:249:PRO:HG3	2.10	0.51
1:E:313:ARG:NH1	1:E:526:TYR:CA	2.74	0.51
1:F:286:MET:O	1:F:289:PHE:CD1	2.64	0.51
1:A:169:LYS:O	1:A:172:VAL:N	2.44	0.51
1:A:218:ILE:CG1	1:A:251:ILE:O	2.58	0.51
1:B:459:HIS:O	1:B:459:HIS:CG	2.60	0.51
1:B:592:GLU:O	1:B:594:LEU:CB	2.59	0.51
1:C:313:ARG:NH1	1:C:526:TYR:HA	2.26	0.51
1:C:459:HIS:HE1	1:D:411:ASP:HB3	1.76	0.51
1:D:191:GLY:HA3	1:D:297:VAL:HG12	1.92	0.51
1:D:319:ARG:HG2	1:D:319:ARG:NH1	2.06	0.51
1:D:521:VAL:HG12	1:E:495:ARG:HD2	1.93	0.51
1:E:166:GLU:HB2	1:E:169:LYS:HZ1	1.75	0.51
1:E:513:GLU:O	1:F:548:ARG:NH2	2.44	0.51
1:E:566:ARG:O	1:E:569:LEU:N	2.44	0.51
1:E:583:THR:HG22	1:E:586:GLU:CD	2.31	0.51
1:F:215:VAL:HG22	1:F:250:CYS:HB3	1.93	0.51
1:F:375:LEU:HD11	1:F:388:ASP:CB	2.38	0.51
1:A:397:MET:SD	1:A:406:VAL:CG1	2.99	0.51
1:A:416:ALA:HB2	1:A:577:LEU:CD2	2.06	0.51
1:A:470:ALA:O	1:A:558:VAL:HG21	2.10	0.51
1:B:286:MET:SD	1:B:316:ARG:HG2	2.51	0.51
1:B:480:GLU:OE1	1:B:555:TYR:OH	2.27	0.51
1:C:450:MET:HG3	1:C:451:MET:H	1.76	0.51
1:D:225:PHE:HA	1:D:236:ARG:CZ	2.41	0.51
1:D:290:GLU:HG3	1:D:292:ASP:HB3	1.93	0.51
1:E:292:ASP:OD1	1:E:293:THR:N	2.43	0.51
1:E:346:GLU:OE1	1:E:347:ASP:OD1	2.28	0.51
1:E:524:ASP:N	1:E:524:ASP:OD1	2.43	0.51
1:E:589:ARG:HH21	1:E:596:LEU:CB	1.74	0.51
1:F:190:LYS:NZ	1:F:289:PHE:CZ	2.77	0.51
1:F:243:THR:HG22	1:F:244:ALA:N	2.25	0.51
1:F:410:ARG:HA	1:F:413:ARG:HG2	1.93	0.51
1:F:505:ILE:HD13	1:F:547:VAL:HG23	1.91	0.51
1:F:572:VAL:O	1:F:576:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:O	1:A:242:GLU:C	2.48	0.51
1:A:316:ARG:O	1:A:317:PHE:C	2.50	0.51
1:A:331:ARG:CZ	1:A:358:PRO:HD3	2.40	0.51
1:A:586:GLU:HG2	1:A:587:PHE:N	2.26	0.51
1:B:536:SER:OG	1:C:541:LYS:HA	2.11	0.51
1:B:585:GLU:O	1:B:587:PHE:N	2.44	0.51
1:C:331:ARG:HD2	1:C:357:THR:CG2	2.40	0.51
1:C:374:LEU:HA	1:C:377:ALA:HB3	1.93	0.51
1:C:503:ARG:NH2	1:C:522:ARG:NH1	2.58	0.51
1:D:503:ARG:HH22	1:D:522:ARG:CZ	2.23	0.51
1:D:572:VAL:O	1:D:576:LEU:HB2	2.11	0.51
1:E:191:GLY:CA	1:E:297:VAL:HG22	2.41	0.51
1:E:354:ALA:O	1:E:357:THR:CG2	2.56	0.51
1:E:371:GLU:OE2	1:E:395:ARG:HD2	2.10	0.51
1:F:175:LEU:HB3	1:F:213:ALA:HB1	1.93	0.51
1:F:241:PHE:CD2	1:F:285:GLU:HG2	2.46	0.51
1:F:331:ARG:HH22	1:F:580:GLU:CD	2.13	0.51
1:F:332:GLU:HB2	1:F:354:ALA:HB2	1.93	0.51
1:F:381:ARG:HH22	1:F:388:ASP:CG	2.15	0.51
1:F:469:ILE:HG22	1:F:473:LEU:HD12	1.92	0.51
1:F:522:ARG:HD2	1:F:530:TYR:CA	2.33	0.51
1:A:414:ILE:HG22	1:A:415:THR:H	1.75	0.50
1:A:512:PRO:HB2	1:A:514:PHE:CD2	2.46	0.50
1:B:286:MET:O	1:B:289:PHE:CG	2.63	0.50
1:B:417:TYR:CE1	1:B:482:VAL:HG21	2.45	0.50
1:D:397:MET:O	1:D:400:PRO:HG2	2.11	0.50
1:D:428:PHE:CE1	1:D:432:ALA:C	2.85	0.50
1:D:538:GLU:O	1:D:541:LYS:N	2.44	0.50
1:A:345:ALA:HB1	1:A:347:ASP:OD1	2.12	0.50
1:A:519:TYR:HA	1:A:533:ARG:NH2	2.27	0.50
1:B:155:PHE:CE2	1:B:212:GLU:OE2	2.64	0.50
1:B:237:VAL:CG2	1:B:281:GLN:CG	2.87	0.50
1:B:297:VAL:HG13	1:B:317:PHE:CZ	2.47	0.50
1:C:178:PRO:O	1:C:182:HIS:CD2	2.65	0.50
1:C:188:ILE:O	1:C:190:LYS:NZ	2.38	0.50
1:C:215:VAL:CG2	1:C:216:PRO:N	2.75	0.50
1:D:355:LYS:NZ	1:D:578:GLU:HG3	2.26	0.50
1:D:454:ARG:HH21	1:D:526:TYR:CA	2.23	0.50
1:E:329:LYS:O	1:E:332:GLU:HB3	2.11	0.50
1:F:335:LEU:HB3	1:F:350:LEU:HD13	1.92	0.50
1:F:345:ALA:CB	1:F:383:LYS:HE3	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:592:GLU:O	1:F:594:LEU:CB	2.60	0.50
1:B:243:THR:HG22	1:B:244:ALA:N	2.26	0.50
1:B:335:LEU:HD21	1:B:365:LEU:HB3	1.92	0.50
1:B:451:MET:HB3	1:B:452:PRO:CD	2.37	0.50
1:C:198:PRO:HD3	1:C:302:ASN:ND2	2.27	0.50
1:C:331:ARG:CZ	1:C:358:PRO:HD3	2.41	0.50
1:C:346:GLU:OE1	1:C:347:ASP:OD1	2.29	0.50
1:C:378:ARG:HG3	1:C:379:GLU:N	2.21	0.50
1:D:236:ARG:NH1	1:D:237:VAL:HG12	2.27	0.50
1:D:262:ARG:CG	1:D:263:LYS:H	2.19	0.50
1:D:325:ALA:CB	1:D:326:PRO:HD3	2.37	0.50
1:D:508:TRP:CD1	1:E:491:GLU:HG2	2.45	0.50
1:E:300:ALA:O	1:E:301:THR:HG22	2.11	0.50
1:F:260:VAL:HG23	1:F:279:LEU:CD1	2.41	0.50
1:F:352:LEU:O	1:F:355:LYS:HB2	2.10	0.50
1:F:441:VAL:O	1:F:443:ARG:N	2.44	0.50
1:F:454:ARG:NH2	1:F:526:TYR:HA	2.26	0.50
1:F:595:PRO:O	1:F:596:LEU:HD12	2.11	0.50
1:A:313:ARG:HH12	1:A:526:TYR:CA	2.25	0.50
1:A:357:THR:OG1	1:A:360:PHE:HB2	2.12	0.50
1:A:479:GLU:OE2	1:A:488:THR:N	2.45	0.50
1:B:174:PHE:HZ	1:B:294:ALA:CA	2.24	0.50
1:B:538:GLU:HB2	1:C:541:LYS:NZ	2.26	0.50
1:C:168:LEU:O	1:C:169:LYS:C	2.47	0.50
1:C:382:ARG:HG2	1:C:383:LYS:H	1.75	0.50
1:C:447:LEU:HB2	1:C:496:GLN:HE22	1.77	0.50
1:C:469:ILE:O	1:C:473:LEU:HD12	2.11	0.50
1:D:451:MET:HB3	1:D:452:PRO:CD	2.38	0.50
1:D:479:GLU:OE2	1:D:488:THR:HG23	2.11	0.50
1:E:368:LEU:HG	1:E:369:LEU:N	2.25	0.50
1:E:381:ARG:HH11	1:E:381:ARG:CG	2.21	0.50
1:E:389:LEU:O	1:E:392:ALA:HB3	2.11	0.50
1:E:479:GLU:OE2	1:E:488:THR:N	2.45	0.50
1:F:564:GLU:C	1:F:566:ARG:N	2.65	0.50
1:B:175:LEU:HD12	1:B:215:VAL:CG1	2.36	0.50
1:B:193:LEU:HB3	1:B:317:PHE:HD2	1.77	0.50
1:C:282:LEU:O	1:C:286:MET:HG2	2.11	0.50
1:C:357:THR:OG1	1:C:360:PHE:HB2	2.11	0.50
1:C:574:GLU:OE1	1:C:574:GLU:C	2.49	0.50
1:D:278:THR:O	1:D:281:GLN:HB3	2.12	0.50
1:D:285:GLU:C	1:D:288:GLY:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:LYS:O	1:D:332:GLU:HB3	2.12	0.50
1:E:302:ASN:HB3	1:E:443:ARG:HH12	1.76	0.50
1:E:325:ALA:N	1:E:326:PRO:CD	2.74	0.50
1:E:334:ILE:O	1:E:337:ILE:HG13	2.10	0.50
1:E:397:MET:SD	1:E:406:VAL:CG1	2.99	0.50
1:E:507:GLU:HB2	1:E:520:ALA:HB3	1.92	0.50
1:E:536:SER:O	1:E:537:GLU:C	2.49	0.50
1:F:207:ARG:O	1:F:210:ALA:N	2.45	0.50
1:F:225:PHE:HA	1:F:236:ARG:CZ	2.42	0.50
1:F:549:ARG:O	1:F:550:LEU:C	2.49	0.50
1:A:279:LEU:O	1:A:282:LEU:N	2.45	0.50
1:A:325:ALA:N	1:A:326:PRO:HD2	2.27	0.50
1:A:580:GLU:O	1:A:580:GLU:CG	2.59	0.50
1:B:158:VAL:HG22	1:B:204:HIS:ND1	2.26	0.50
1:B:260:VAL:HG23	1:B:279:LEU:CD1	2.42	0.50
1:C:279:LEU:O	1:C:282:LEU:N	2.44	0.50
1:C:325:ALA:N	1:C:326:PRO:HD2	2.27	0.50
1:C:408:SER:C	1:C:410:ARG:H	2.14	0.50
1:C:450:MET:O	1:C:454:ARG:HB3	2.12	0.50
1:E:218:ILE:HG12	1:E:251:ILE:O	2.11	0.50
1:E:319:ARG:C	1:E:320:GLN:NE2	2.65	0.50
1:F:297:VAL:HG13	1:F:317:PHE:HZ	1.77	0.50
1:F:398:MET:O	1:F:401:ALA:HB3	2.11	0.50
1:F:449:PHE:CZ	1:F:496:GLN:OE1	2.64	0.50
1:A:196:GLY:H	1:A:202:LYS:HZ1	1.58	0.50
1:A:445:ARG:O	1:A:447:LEU:N	2.45	0.50
1:B:238:ARG:HA	1:B:241:PHE:CE2	2.47	0.50
1:B:285:GLU:C	1:B:288:GLY:H	2.15	0.50
1:B:345:ALA:CB	1:B:383:LYS:HE3	2.37	0.50
1:C:313:ARG:NH1	1:C:526:TYR:CA	2.75	0.50
1:C:449:PHE:HE2	1:C:496:GLN:NE2	2.10	0.50
1:C:493:ASP:N	1:C:493:ASP:OD1	2.44	0.50
1:C:524:ASP:OD1	1:C:524:ASP:N	2.44	0.50
1:D:158:VAL:HG22	1:D:204:HIS:ND1	2.26	0.50
1:D:239:ASP:O	1:D:242:GLU:OE2	2.30	0.50
1:D:567:GLU:O	1:D:570:GLU:CB	2.59	0.50
1:E:241:PHE:O	1:E:242:GLU:C	2.49	0.50
1:E:313:ARG:NH1	1:E:526:TYR:HA	2.27	0.50
1:E:583:THR:HG22	1:E:586:GLU:OE1	2.10	0.50
1:F:334:ILE:O	1:F:337:ILE:HG22	2.12	0.50
1:F:387:LYS:HG3	1:F:388:ASP:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:554:GLN:O	1:F:557:ARG:HB3	2.11	0.50
1:A:286:MET:HB3	1:A:316:ARG:HB2	1.94	0.50
1:A:345:ALA:O	1:A:348:VAL:HB	2.12	0.50
1:B:301:THR:HG22	1:B:303:ARG:H	1.77	0.50
1:B:585:GLU:O	1:B:586:GLU:C	2.50	0.50
1:C:365:LEU:O	1:C:368:LEU:HB3	2.11	0.50
1:C:382:ARG:HG3	1:C:383:LYS:HB2	1.93	0.50
1:C:566:ARG:O	1:C:569:LEU:N	2.45	0.50
1:D:389:LEU:O	1:D:390:GLU:C	2.50	0.50
1:D:447:LEU:O	1:D:450:MET:HG3	2.11	0.50
1:E:210:ALA:HA	1:E:251:ILE:HD11	1.94	0.50
1:E:448:GLY:O	1:E:449:PHE:C	2.51	0.50
1:A:211:GLY:HA2	1:A:214:ARG:NE	2.25	0.50
1:A:319:ARG:C	1:A:320:GLN:NE2	2.65	0.50
1:A:450:MET:HG3	1:A:451:MET:H	1.77	0.50
1:B:441:VAL:O	1:B:443:ARG:N	2.45	0.50
1:C:334:ILE:O	1:C:337:ILE:HG13	2.11	0.50
1:C:463:LYS:HB2	1:D:486:VAL:HG11	1.94	0.50
1:D:238:ARG:NH1	1:D:239:ASP:HB3	2.16	0.50
1:D:313:ARG:HG3	1:D:314:PRO:HG2	1.94	0.50
1:D:313:ARG:O	1:D:316:ARG:HB3	2.12	0.50
1:E:282:LEU:O	1:E:286:MET:HG2	2.12	0.50
1:E:503:ARG:NH2	1:E:522:ARG:NH1	2.60	0.50
1:E:525:THR:OG1	1:E:528:GLY:HA3	2.11	0.50
1:F:510:MET:O	1:F:512:PRO:HD2	2.12	0.50
1:A:179:SER:O	1:A:182:HIS:CD2	2.62	0.49
1:A:428:PHE:HE1	1:A:432:ALA:HA	1.66	0.49
1:A:588:GLN:HA	1:A:591:VAL:HG21	1.92	0.49
1:B:449:PHE:CZ	1:B:496:GLN:OE1	2.65	0.49
1:C:354:ALA:HA	1:C:357:THR:CG2	2.42	0.49
1:D:512:PRO:HB2	1:D:514:PHE:HD2	1.76	0.49
1:E:447:LEU:HA	1:E:496:GLN:HE21	1.76	0.49
1:F:181:PHE:O	1:F:185:GLY:N	2.44	0.49
1:A:175:LEU:O	1:A:249:PRO:HG3	2.12	0.49
1:A:178:PRO:O	1:A:182:HIS:CD2	2.64	0.49
1:A:365:LEU:O	1:A:368:LEU:HB3	2.12	0.49
1:A:514:PHE:HB3	1:A:519:TYR:HE1	1.73	0.49
1:B:376:ALA:O	1:B:381:ARG:CG	2.60	0.49
1:B:529:GLY:O	1:B:530:TYR:CB	2.55	0.49
1:B:554:GLN:O	1:B:557:ARG:HB3	2.11	0.49
1:C:171:ILE:HD12	1:C:172:VAL:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:HIS:HB3	1:C:584:ALA:CB	2.42	0.49
1:C:531:ASP:C	1:C:531:ASP:OD1	2.51	0.49
1:D:174:PHE:HZ	1:D:294:ALA:HA	1.76	0.49
1:D:336:ARG:O	1:D:339:ALA:N	2.27	0.49
1:D:563:LEU:O	1:D:566:ARG:CB	2.61	0.49
1:E:174:PHE:HB2	1:E:181:PHE:CE2	2.47	0.49
1:E:215:VAL:CG2	1:E:216:PRO:N	2.74	0.49
1:F:197:PRO:HD2	1:F:200:VAL:HG11	1.94	0.49
1:F:225:PHE:CD2	1:F:225:PHE:N	2.80	0.49
1:F:236:ARG:NH1	1:F:237:VAL:HG12	2.26	0.49
1:A:150:ALA:CB	1:A:214:ARG:NH1	2.75	0.49
1:A:225:PHE:CE1	1:A:233:GLY:HA3	2.47	0.49
1:A:264:ARG:CD	1:A:266:SER:CB	2.87	0.49
1:B:242:GLU:CA	1:B:245:LYS:HB3	2.41	0.49
1:B:311:LEU:HA	1:B:316:ARG:CZ	2.39	0.49
1:C:206:ALA:HB1	1:C:217:PHE:HZ	1.77	0.49
1:C:302:ASN:HB3	1:C:443:ARG:HH12	1.76	0.49
1:C:357:THR:N	1:C:358:PRO:CD	2.74	0.49
1:C:448:GLY:O	1:C:449:PHE:C	2.50	0.49
1:C:539:THR:O	1:C:543:ILE:HG13	2.13	0.49
1:C:594:LEU:HD12	1:C:595:PRO:O	2.12	0.49
1:D:186:ALA:O	1:D:187:ARG:HB3	2.12	0.49
1:D:241:PHE:HE2	1:D:285:GLU:OE2	1.91	0.49
1:E:460:TRP:HD1	1:E:464:ARG:NH1	2.08	0.49
1:E:537:GLU:N	1:F:537:GLU:OE2	2.41	0.49
1:F:193:LEU:C	1:F:194:LEU:HD12	2.33	0.49
1:F:338:HIS:CE1	1:F:366:GLU:HG3	2.47	0.49
1:F:443:ARG:O	1:F:445:ARG:N	2.45	0.49
1:F:454:ARG:HH21	1:F:526:TYR:CA	2.25	0.49
1:A:147:LEU:HD23	1:A:217:PHE:HB3	1.93	0.49
1:A:449:PHE:CE2	1:A:496:GLN:NE2	2.79	0.49
1:A:453:ARG:HH21	1:A:464:ARG:HH22	1.55	0.49
1:B:336:ARG:C	1:B:338:HIS:N	2.62	0.49
1:C:313:ARG:HH12	1:C:526:TYR:CA	2.25	0.49
1:C:519:TYR:HB3	1:C:535:TYR:HD2	1.76	0.49
1:D:454:ARG:NH2	1:D:528:GLY:C	2.66	0.49
1:D:564:GLU:C	1:D:566:ARG:N	2.64	0.49
1:E:195:VAL:HG22	1:E:301:THR:O	2.12	0.49
1:F:313:ARG:HG3	1:F:314:PRO:CG	2.41	0.49
1:A:354:ALA:O	1:A:357:THR:CG2	2.55	0.49
1:A:389:LEU:O	1:A:392:ALA:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASP:OD1	1:B:310:ALA:N	2.43	0.49
1:B:454:ARG:NH2	1:B:528:GLY:C	2.66	0.49
1:C:191:GLY:CA	1:C:297:VAL:HG22	2.43	0.49
1:C:370:ASN:OD1	1:C:374:LEU:HD13	2.12	0.49
1:D:209:VAL:CG1	1:D:210:ALA:H	2.20	0.49
1:E:154:THR:OG1	1:E:155:PHE:N	2.44	0.49
1:E:470:ALA:C	1:E:558:VAL:HG21	2.32	0.49
1:F:241:PHE:HE2	1:F:285:GLU:OE2	1.90	0.49
1:F:334:ILE:HG21	1:F:365:LEU:HD12	1.93	0.49
1:A:273:ASP:OD1	1:A:274:GLU:N	2.46	0.49
1:C:237:VAL:HG11	1:C:281:GLN:CB	2.26	0.49
1:D:566:ARG:O	1:D:569:LEU:HB3	2.13	0.49
1:E:580:GLU:O	1:E:580:GLU:CG	2.60	0.49
1:F:239:ASP:O	1:F:242:GLU:OE2	2.30	0.49
1:A:219:THR:HB	1:A:253:PHE:CD2	2.40	0.49
2:A:1001:ADP:N3	2:A:1001:ADP:H2'	2.27	0.49
1:B:174:PHE:C	1:B:174:PHE:CD2	2.86	0.49
1:B:261:GLY:O	1:B:308:ASP:N	2.38	0.49
1:B:376:ALA:O	1:B:381:ARG:HG3	2.12	0.49
1:C:172:VAL:CB	1:C:213:ALA:HB2	2.41	0.49
1:D:183:GLU:OE1	1:D:184:MET:HB3	2.13	0.49
1:D:453:ARG:HA	1:D:456:ASP:OD2	2.13	0.49
1:E:279:LEU:O	1:E:282:LEU:N	2.45	0.49
1:F:165:LYS:O	1:F:168:LEU:CB	2.60	0.49
1:F:191:GLY:HA3	1:F:297:VAL:HG12	1.94	0.49
1:A:378:ARG:NH1	1:F:170:GLU:HB2	2.28	0.49
1:B:334:ILE:HG21	1:B:365:LEU:HD12	1.94	0.49
1:B:567:GLU:O	1:B:570:GLU:CB	2.61	0.49
1:C:155:PHE:CZ	1:C:209:VAL:HG22	2.47	0.49
1:C:583:THR:HG22	1:C:586:GLU:CD	2.32	0.49
2:C:1001:ADP:H2'	2:C:1001:ADP:N3	2.28	0.49
1:D:409:PRO:O	1:D:413:ARG:HD3	2.13	0.49
1:E:169:LYS:O	1:E:172:VAL:CG1	2.60	0.49
1:F:175:LEU:O	1:F:249:PRO:CB	2.61	0.49
1:F:319:ARG:O	1:F:320:GLN:HB3	2.11	0.49
1:F:335:LEU:HD13	1:F:365:LEU:HB3	1.93	0.49
1:F:336:ARG:C	1:F:338:HIS:N	2.64	0.49
1:F:352:LEU:O	1:F:353:LEU:C	2.49	0.49
1:F:360:PHE:HE1	1:F:364:ASP:HB3	1.77	0.49
1:B:278:THR:O	1:B:281:GLN:HB3	2.13	0.49
1:C:329:LYS:O	1:C:332:GLU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:PRO:HG2	1:C:443:ARG:H	1.78	0.49
1:C:503:ARG:CG	1:C:508:TRP:CE3	2.95	0.49
1:D:174:PHE:CD2	1:D:174:PHE:C	2.85	0.49
1:D:525:THR:HG22	1:D:526:TYR:H	1.77	0.49
1:E:220:ALA:O	1:E:254:ILE:HA	2.13	0.49
1:E:236:ARG:HG2	1:E:236:ARG:NH1	2.11	0.49
1:E:260:VAL:HG23	1:E:261:GLY:H	1.78	0.49
1:E:357:THR:OG1	1:E:360:PHE:HB2	2.11	0.49
1:E:374:LEU:HA	1:E:377:ALA:HB3	1.93	0.49
1:F:564:GLU:O	1:F:566:ARG:N	2.45	0.49
1:A:203:THR:OG1	2:A:1001:ADP:O2A	2.20	0.49
1:A:260:VAL:HG23	1:A:261:GLY:H	1.76	0.49
1:A:408:SER:C	1:A:410:ARG:H	2.15	0.49
1:A:447:LEU:CB	1:A:496:GLN:HE22	2.25	0.49
1:B:191:GLY:HA3	1:B:297:VAL:HG12	1.94	0.49
1:B:589:ARG:NE	1:B:596:LEU:CD2	2.76	0.49
1:C:447:LEU:CA	1:C:496:GLN:NE2	2.75	0.49
1:C:507:GLU:HB2	1:C:520:ALA:HB3	1.94	0.49
1:D:238:ARG:HH11	1:D:238:ARG:CB	2.26	0.49
1:D:360:PHE:HE1	1:D:364:ASP:HB3	1.77	0.49
1:D:469:ILE:HG22	1:D:473:LEU:HD12	1.95	0.49
1:E:198:PRO:HD3	1:E:302:ASN:ND2	2.27	0.49
1:E:373:ALA:HA	1:E:384:ILE:CD1	2.42	0.49
1:F:159:ALA:H	2:F:2001:ADP:HN62	1.61	0.49
1:F:174:PHE:CZ	1:F:294:ALA:CB	2.95	0.49
1:F:286:MET:O	1:F:289:PHE:CG	2.65	0.49
1:B:369:LEU:O	1:B:370:ASN:C	2.51	0.48
1:C:220:ALA:O	1:C:254:ILE:HA	2.13	0.48
1:C:359:GLY:HA3	1:C:360:PHE:CG	2.48	0.48
1:C:389:LEU:O	1:C:392:ALA:HB3	2.12	0.48
1:D:215:VAL:HG22	1:D:250:CYS:HB3	1.94	0.48
1:D:334:ILE:HG21	1:D:365:LEU:HD12	1.94	0.48
1:E:574:GLU:C	1:E:574:GLU:OE1	2.52	0.48
1:F:199:GLY:H	2:F:2001:ADP:PB	2.34	0.48
1:F:238:ARG:HH11	1:F:238:ARG:CB	2.26	0.48
1:F:503:ARG:NH2	1:F:522:ARG:NH2	2.59	0.48
1:A:198:PRO:HD3	1:A:302:ASN:ND2	2.28	0.48
1:A:210:ALA:HB2	1:A:251:ILE:CD1	2.42	0.48
1:B:241:PHE:CD2	1:B:285:GLU:HG2	2.48	0.48
1:B:360:PHE:HE1	1:B:364:ASP:HB3	1.79	0.48
1:B:454:ARG:NH2	1:B:526:TYR:HA	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:SER:HB2	1:C:409:PRO:CD	2.43	0.48
1:C:416:ALA:HB2	1:C:440:ILE:HD11	1.94	0.48
1:C:447:LEU:CB	1:C:496:GLN:NE2	2.77	0.48
1:C:580:GLU:O	1:C:580:GLU:CG	2.61	0.48
1:D:159:ALA:H	2:D:2001:ADP:HN62	1.61	0.48
1:D:175:LEU:O	1:D:249:PRO:HG2	2.13	0.48
1:D:225:PHE:CD2	1:D:225:PHE:N	2.80	0.48
1:D:312:LEU:HD23	1:D:312:LEU:O	2.13	0.48
1:D:336:ARG:C	1:D:338:HIS:N	2.61	0.48
1:D:548:ARG:NH1	1:D:548:ARG:HG2	2.28	0.48
1:E:181:PHE:HA	1:E:184:MET:HE2	1.95	0.48
1:E:196:GLY:O	1:E:302:ASN:OD1	2.30	0.48
1:E:262:ARG:HG2	1:E:275:ARG:NH2	2.08	0.48
1:E:483:PHE:C	1:E:485:ASP:H	2.17	0.48
1:E:594:LEU:HD12	1:E:595:PRO:O	2.13	0.48
1:F:190:LYS:HG3	1:F:190:LYS:O	2.12	0.48
1:F:348:VAL:HG11	1:F:386:MET:SD	2.53	0.48
1:A:519:TYR:HA	1:A:533:ARG:CZ	2.43	0.48
1:B:212:GLU:O	1:B:214:ARG:HG3	2.13	0.48
1:B:447:LEU:O	1:B:450:MET:HG3	2.12	0.48
1:C:260:VAL:HG23	1:C:261:GLY:H	1.78	0.48
1:C:273:ASP:CG	1:C:274:GLU:H	2.17	0.48
1:E:236:ARG:HH11	1:E:236:ARG:CB	2.26	0.48
1:E:357:THR:N	1:E:358:PRO:CD	2.76	0.48
1:E:520:ALA:HA	1:E:533:ARG:CG	2.43	0.48
1:F:548:ARG:NH1	1:F:548:ARG:HG2	2.28	0.48
1:F:566:ARG:O	1:F:569:LEU:HB3	2.13	0.48
1:A:233:GLY:O	1:A:236:ARG:CG	2.58	0.48
1:A:453:ARG:NH2	1:A:464:ARG:CZ	2.76	0.48
1:A:576:LEU:O	1:A:580:GLU:N	2.32	0.48
1:B:193:LEU:C	1:B:194:LEU:HD12	2.34	0.48
1:B:207:ARG:O	1:B:210:ALA:N	2.47	0.48
1:B:238:ARG:HA	1:B:241:PHE:HE2	1.78	0.48
1:B:274:GLU:HA	1:B:277:GLN:HE21	1.78	0.48
1:B:313:ARG:HG3	1:B:314:PRO:HG2	1.96	0.48
1:B:511:HIS:O	1:B:512:PRO:O	2.31	0.48
1:C:196:GLY:O	1:C:302:ASN:OD1	2.31	0.48
1:C:249:PRO:HB3	1:C:294:ALA:HB3	1.95	0.48
1:C:328:VAL:HG12	1:C:329:LYS:N	2.27	0.48
1:D:157:ASP:O	1:D:204:HIS:HE1	1.96	0.48
1:D:175:LEU:HD12	1:D:215:VAL:CG1	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LEU:HB2	1:D:384:ILE:O	2.13	0.48
1:E:147:LEU:HD23	1:E:217:PHE:CB	2.43	0.48
1:E:212:GLU:N	1:E:214:ARG:CG	2.76	0.48
1:E:397:MET:HG3	1:E:406:VAL:CG1	2.43	0.48
1:E:443:ARG:O	1:E:443:ARG:HG2	2.14	0.48
1:F:311:LEU:C	1:F:316:ARG:NH1	2.66	0.48
1:F:517:VAL:CG1	1:F:519:TYR:OH	2.60	0.48
1:A:380:GLY:C	1:F:180:ARG:NH2	2.66	0.48
1:A:554:GLN:O	1:A:557:ARG:HB3	2.14	0.48
1:B:225:PHE:CD2	1:B:236:ARG:NE	2.81	0.48
1:B:313:ARG:CG	1:B:314:PRO:N	2.74	0.48
1:B:394:ASP:HA	1:B:397:MET:HE3	1.94	0.48
1:C:520:ALA:HA	1:C:533:ARG:CG	2.43	0.48
1:D:165:LYS:CE	1:D:205:LEU:HG	2.43	0.48
1:D:180:ARG:NH1	1:D:184:MET:CE	2.76	0.48
1:D:242:GLU:CA	1:D:245:LYS:HB3	2.42	0.48
1:E:462:ARG:CG	1:E:463:LYS:N	2.76	0.48
1:F:183:GLU:OE1	1:F:184:MET:HB3	2.14	0.48
1:F:376:ALA:HB1	1:F:381:ARG:CD	2.42	0.48
1:F:454:ARG:HH21	1:F:526:TYR:HA	1.78	0.48
1:A:200:VAL:HG11	1:A:323:ILE:HG13	1.96	0.48
1:A:302:ASN:HB3	1:A:443:ARG:HH12	1.78	0.48
1:A:447:LEU:HA	1:A:496:GLN:HE21	1.77	0.48
1:B:157:ASP:HB3	1:B:337:ILE:CD1	2.44	0.48
1:B:190:LYS:HG3	1:B:190:LYS:O	2.14	0.48
1:C:228:MET:CG	1:C:236:ARG:HH22	2.27	0.48
1:C:373:ALA:HA	1:C:384:ILE:CD1	2.43	0.48
1:C:445:ARG:O	1:C:447:LEU:N	2.47	0.48
1:D:174:PHE:CZ	1:D:294:ALA:CB	2.96	0.48
1:E:147:LEU:HB3	1:E:217:PHE:O	2.12	0.48
1:F:397:MET:HA	1:F:400:PRO:HG2	1.95	0.48
1:F:563:LEU:O	1:F:566:ARG:CB	2.61	0.48
1:A:174:PHE:HB2	1:A:181:PHE:CE2	2.48	0.48
1:A:179:SER:C	1:A:181:PHE:N	2.65	0.48
1:A:311:LEU:CG	1:A:316:ARG:HH22	2.25	0.48
1:B:564:GLU:O	1:B:566:ARG:N	2.47	0.48
1:C:280:ASN:O	1:C:281:GLN:C	2.52	0.48
1:C:467:ASP:O	1:C:471:VAL:HG23	2.13	0.48
1:D:228:MET:SD	1:D:232:VAL:CG1	3.01	0.48
1:D:286:MET:O	1:D:289:PHE:CD1	2.67	0.48
1:D:369:LEU:O	1:D:370:ASN:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ARG:O	1:E:239:ASP:C	2.51	0.48
1:E:300:ALA:O	1:E:301:THR:CG2	2.62	0.48
1:E:414:ILE:HG22	1:E:415:THR:H	1.78	0.48
1:E:519:TYR:C	1:E:533:ARG:NE	2.67	0.48
1:F:285:GLU:C	1:F:288:GLY:H	2.16	0.48
1:F:336:ARG:HD3	1:F:336:ARG:HA	1.50	0.48
1:F:388:ASP:OD1	1:F:388:ASP:N	2.46	0.48
1:F:400:PRO:HB2	1:F:404:SER:OG	2.14	0.48
1:F:476:ARG:NH1	1:F:487:THR:HG21	2.29	0.48
1:F:505:ILE:HG23	1:F:514:PHE:CD2	2.48	0.48
1:A:177:ASN:HD22	1:A:180:ARG:CD	2.25	0.48
1:A:280:ASN:O	1:A:281:GLN:C	2.50	0.48
1:B:222:GLY:N	1:B:255:ASP:O	2.43	0.48
1:B:311:LEU:HD12	1:B:311:LEU:O	2.13	0.48
1:B:468:GLN:O	1:B:471:VAL:N	2.45	0.48
1:C:179:SER:C	1:C:181:PHE:N	2.67	0.48
1:C:274:GLU:HB3	1:C:275:ARG:H	1.43	0.48
1:D:302:ASN:ND2	1:D:443:ARG:NH2	2.55	0.48
1:D:397:MET:HA	1:D:400:PRO:HG2	1.95	0.48
1:D:410:ARG:O	1:D:413:ARG:CB	2.61	0.48
1:D:592:GLU:O	1:D:594:LEU:CB	2.61	0.48
1:E:215:VAL:HG21	1:E:250:CYS:CB	2.43	0.48
1:E:328:VAL:HG12	1:E:329:LYS:N	2.29	0.48
1:E:531:ASP:OD1	1:E:531:ASP:C	2.52	0.48
1:F:159:ALA:HB1	1:F:333:GLN:HG3	1.96	0.48
1:F:175:LEU:O	1:F:249:PRO:HG2	2.14	0.48
1:F:470:ALA:O	1:F:474:ALA:HB2	2.14	0.48
1:A:460:TRP:HD1	1:A:464:ARG:NH1	2.10	0.48
1:A:470:ALA:HB1	1:A:558:VAL:CG2	2.40	0.48
1:A:562:LEU:O	1:A:565:LYS:N	2.47	0.48
1:B:336:ARG:HA	1:B:336:ARG:HD3	1.47	0.48
1:B:428:PHE:CE1	1:B:432:ALA:C	2.87	0.48
1:B:453:ARG:HA	1:B:456:ASP:OD2	2.14	0.48
1:C:410:ARG:HA	1:C:413:ARG:HB3	1.96	0.48
1:C:449:PHE:HB3	1:C:468:GLN:HE22	1.72	0.48
1:C:479:GLU:OE2	1:C:488:THR:N	2.47	0.48
1:C:528:GLY:HA2	1:C:530:TYR:CE2	2.49	0.48
1:C:575:THR:HA	1:C:578:GLU:OE1	2.13	0.48
1:D:356:ARG:O	1:D:358:PRO:HD3	2.13	0.48
1:D:374:LEU:C	1:D:374:LEU:HD23	2.34	0.48
1:E:179:SER:C	1:E:181:PHE:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:ALA:N	1:E:326:PRO:HD2	2.29	0.48
1:E:506:THR:CG2	1:E:543:ILE:HD13	2.44	0.48
1:F:159:ALA:HA	1:F:333:GLN:HE21	1.79	0.48
1:F:237:VAL:HG21	1:F:281:GLN:HG3	1.96	0.48
1:F:302:ASN:ND2	1:F:443:ARG:HH22	1.89	0.48
1:B:199:GLY:H	2:B:2001:ADP:PB	2.34	0.48
1:B:233:GLY:CA	1:B:236:ARG:NH2	2.59	0.48
1:B:286:MET:HE2	1:B:315:GLY:O	2.14	0.48
1:B:314:PRO:C	1:B:316:ARG:H	2.16	0.48
1:B:387:LYS:HG3	1:B:388:ASP:N	2.26	0.48
1:B:488:THR:O	1:B:490:ALA:N	2.47	0.48
1:B:564:GLU:C	1:B:566:ARG:N	2.64	0.48
1:C:169:LYS:O	1:C:172:VAL:N	2.47	0.48
1:C:576:LEU:O	1:C:580:GLU:N	2.35	0.48
1:D:154:THR:OG1	1:D:212:GLU:OE2	2.32	0.48
1:D:158:VAL:CG1	1:D:205:LEU:HD11	2.44	0.48
1:D:159:ALA:HB1	1:D:333:GLN:HG3	1.96	0.48
1:E:169:LYS:O	1:E:172:VAL:N	2.46	0.48
1:F:238:ARG:HA	1:F:241:PHE:CE2	2.49	0.48
1:F:242:GLU:CA	1:F:245:LYS:HB3	2.43	0.48
1:F:338:HIS:CB	1:F:369:LEU:HD11	2.43	0.48
1:A:400:PRO:HG2	1:A:405:LEU:CD1	2.44	0.47
1:A:594:LEU:HD12	1:A:595:PRO:O	2.13	0.47
1:B:170:GLU:CB	1:C:378:ARG:NH2	2.77	0.47
1:B:196:GLY:O	1:B:302:ASN:HA	2.14	0.47
1:B:338:HIS:CB	1:B:369:LEU:HD11	2.44	0.47
1:B:571:ARG:HH12	1:B:593:GLY:N	2.11	0.47
1:C:345:ALA:HB1	1:C:347:ASP:OD1	2.13	0.47
1:C:470:ALA:C	1:C:558:VAL:HG21	2.35	0.47
1:D:564:GLU:O	1:D:566:ARG:N	2.46	0.47
1:F:154:THR:CG2	1:F:156:LYS:HB3	2.44	0.47
1:F:157:ASP:O	1:F:204:HIS:CE1	2.67	0.47
1:F:261:GLY:O	1:F:308:ASP:HB3	2.14	0.47
1:F:297:VAL:HG13	1:F:317:PHE:CZ	2.48	0.47
1:F:449:PHE:CE2	1:F:453:ARG:CZ	2.97	0.47
1:A:182:HIS:CD2	1:A:182:HIS:H	2.30	0.47
1:A:207:ARG:HH21	1:A:217:PHE:HD2	1.62	0.47
1:A:357:THR:HG1	1:A:360:PHE:CB	2.27	0.47
1:A:387:LYS:CA	1:A:390:GLU:HB2	2.42	0.47
1:A:520:ALA:HA	1:A:533:ARG:CG	2.44	0.47
1:B:225:PHE:HA	1:B:236:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:TRP:CD1	1:B:464:ARG:HG2	2.49	0.47
1:B:517:VAL:CG2	1:B:518:ALA:N	2.76	0.47
1:C:357:THR:C	1:C:360:PHE:HD1	2.17	0.47
1:C:536:SER:O	1:C:537:GLU:C	2.51	0.47
1:D:199:GLY:O	1:D:361:VAL:HG22	2.13	0.47
1:D:344:LEU:CD2	1:D:346:GLU:OE1	2.61	0.47
1:D:517:VAL:CG1	1:D:519:TYR:OH	2.63	0.47
1:E:182:HIS:CD2	1:E:182:HIS:H	2.30	0.47
1:F:157:ASP:O	1:F:204:HIS:HE1	1.96	0.47
1:F:203:THR:OG1	2:F:2001:ADP:O1B	2.32	0.47
1:F:393:ALA:O	1:F:397:MET:HB3	2.15	0.47
1:F:452:PRO:O	1:F:456:ASP:CG	2.53	0.47
1:F:563:LEU:O	1:F:566:ARG:HB3	2.14	0.47
1:A:191:GLY:CA	1:A:297:VAL:HG22	2.44	0.47
1:A:462:ARG:HH12	1:A:511:HIS:H	1.62	0.47
1:A:506:THR:HA	1:A:519:TYR:HD1	1.79	0.47
1:B:162:GLU:HA	1:B:162:GLU:OE1	2.15	0.47
1:B:241:PHE:HE2	1:B:285:GLU:OE2	1.90	0.47
1:D:263:LYS:HE2	1:E:228:MET:CE	2.43	0.47
1:D:388:ASP:OD1	1:D:388:ASP:N	2.42	0.47
1:D:438:VAL:CG2	1:D:439:THR:N	2.76	0.47
1:E:210:ALA:HB2	1:E:251:ILE:CD1	2.38	0.47
1:F:436:HIS:O	1:F:437:LYS:CG	2.61	0.47
1:A:357:THR:N	1:A:358:PRO:CD	2.77	0.47
1:B:201:GLY:O	1:B:204:HIS:HB3	2.13	0.47
1:B:409:PRO:O	1:B:413:ARG:HD3	2.14	0.47
1:C:195:VAL:HG22	1:C:301:THR:O	2.13	0.47
1:C:331:ARG:O	1:C:335:LEU:HG	2.14	0.47
1:C:479:GLU:OE2	1:C:487:THR:HA	2.15	0.47
1:D:157:ASP:O	1:D:204:HIS:CE1	2.67	0.47
1:D:225:PHE:CD2	1:D:236:ARG:CD	2.95	0.47
1:E:519:TYR:HB3	1:E:535:TYR:HD2	1.78	0.47
1:F:290:GLU:CG	1:F:293:THR:HG23	2.29	0.47
1:F:589:ARG:CD	1:F:596:LEU:HD11	2.44	0.47
1:A:238:ARG:O	1:A:239:ASP:C	2.51	0.47
1:B:186:ALA:HB1	1:C:374:LEU:CD1	2.44	0.47
1:B:376:ALA:HB1	1:B:381:ARG:HD3	1.95	0.47
1:B:384:ILE:HG22	1:B:385:THR:N	2.30	0.47
1:C:548:ARG:NH2	1:C:552:GLU:OE1	2.43	0.47
1:C:589:ARG:HB3	1:C:589:ARG:HH11	1.73	0.47
1:D:169:LYS:O	1:D:172:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:HIS:O	1:D:249:PRO:O	2.33	0.47
1:D:571:ARG:HH12	1:D:593:GLY:H	1.61	0.47
1:E:159:ALA:HB1	1:E:333:GLN:HB3	1.96	0.47
1:E:172:VAL:CB	1:E:213:ALA:HB2	2.44	0.47
1:E:449:PHE:HE2	1:E:496:GLN:HE21	1.63	0.47
1:E:462:ARG:HH12	1:E:511:HIS:H	1.62	0.47
1:E:523:GLU:O	1:E:529:GLY:HA2	2.14	0.47
1:F:168:LEU:O	1:F:171:ILE:N	2.48	0.47
1:F:175:LEU:HD12	1:F:215:VAL:CG1	2.38	0.47
1:F:302:ASN:ND2	1:F:443:ARG:NH2	2.52	0.47
1:F:571:ARG:HH12	1:F:593:GLY:H	1.63	0.47
1:A:311:LEU:HD22	1:A:316:ARG:NH1	2.28	0.47
1:A:436:HIS:HB3	1:A:584:ALA:CB	2.45	0.47
1:B:165:LYS:HZ2	1:B:168:LEU:CD2	2.27	0.47
1:C:357:THR:HG1	1:C:360:PHE:CB	2.28	0.47
1:D:165:LYS:CE	1:D:205:LEU:CG	2.93	0.47
1:D:274:GLU:HA	1:D:277:GLN:HE21	1.80	0.47
1:F:169:LYS:O	1:F:172:VAL:HG22	2.15	0.47
1:F:235:ALA:O	1:F:238:ARG:NH1	2.48	0.47
1:F:262:ARG:CG	1:F:263:LYS:H	2.20	0.47
1:A:329:LYS:O	1:A:332:GLU:HB3	2.15	0.47
1:A:331:ARG:O	1:A:335:LEU:HG	2.14	0.47
1:B:159:ALA:CB	1:B:334:ILE:HG13	2.36	0.47
1:B:332:GLU:HB2	1:B:354:ALA:HB2	1.95	0.47
1:B:397:MET:HA	1:B:400:PRO:HG2	1.95	0.47
1:B:455:GLU:O	1:B:456:ASP:C	2.53	0.47
1:C:169:LYS:O	1:C:172:VAL:CG1	2.61	0.47
1:C:192:VAL:N	1:C:297:VAL:O	2.39	0.47
1:C:210:ALA:HA	1:C:251:ILE:HD11	1.96	0.47
1:D:336:ARG:O	1:D:338:HIS:N	2.47	0.47
1:D:381:ARG:NH2	1:D:388:ASP:CG	2.47	0.47
1:D:454:ARG:NH2	1:D:526:TYR:HA	2.29	0.47
1:D:505:ILE:HD13	1:D:547:VAL:HG23	1.95	0.47
1:D:510:MET:O	1:D:512:PRO:CD	2.61	0.47
1:E:188:ILE:CG2	1:E:189:PRO:HD2	2.45	0.47
1:E:191:GLY:CA	1:E:297:VAL:CG2	2.93	0.47
1:E:192:VAL:O	1:E:298:MET:HA	2.14	0.47
1:E:207:ARG:HH21	1:E:217:PHE:HD2	1.61	0.47
1:E:331:ARG:O	1:E:335:LEU:HG	2.15	0.47
1:E:382:ARG:CG	1:E:383:LYS:N	2.75	0.47
1:E:589:ARG:HH22	1:E:596:LEU:N	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:VAL:HG22	1:F:204:HIS:ND1	2.29	0.47
1:F:301:THR:HG22	1:F:303:ARG:H	1.79	0.47
1:F:449:PHE:CZ	1:F:453:ARG:NH2	2.81	0.47
1:F:494:PHE:O	1:F:496:GLN:N	2.47	0.47
1:A:316:ARG:HG2	1:A:317:PHE:CD2	2.49	0.47
1:A:348:VAL:O	1:A:348:VAL:HG12	2.14	0.47
1:A:449:PHE:HZ	1:A:496:GLN:HG2	1.60	0.47
1:A:524:ASP:OD1	1:A:524:ASP:N	2.47	0.47
1:B:159:ALA:HA	1:B:333:GLN:HE21	1.79	0.47
1:B:331:ARG:HH22	1:B:580:GLU:CD	2.14	0.47
1:B:338:HIS:CE1	1:B:366:GLU:HG3	2.50	0.47
1:B:410:ARG:O	1:B:411:ASP:C	2.53	0.47
1:B:563:LEU:O	1:B:566:ARG:CB	2.62	0.47
1:C:277:GLN:HG3	1:C:278:THR:N	2.28	0.47
1:D:400:PRO:O	1:D:403:LYS:N	2.48	0.47
1:D:536:SER:OG	1:E:541:LYS:HA	2.15	0.47
1:E:206:ALA:CB	1:E:217:PHE:HZ	2.28	0.47
1:E:345:ALA:HB1	1:E:347:ASP:OD1	2.14	0.47
1:E:408:SER:C	1:E:410:ARG:H	2.17	0.47
1:E:576:LEU:O	1:E:580:GLU:N	2.39	0.47
1:F:314:PRO:C	1:F:316:ARG:H	2.18	0.47
1:F:428:PHE:CZ	1:F:433:ASP:N	2.83	0.47
1:F:533:ARG:NH1	1:F:535:TYR:CD1	2.83	0.47
1:A:225:PHE:CE1	1:A:236:ARG:HG2	2.50	0.47
1:C:272:ASN:C	1:C:272:ASN:OD1	2.53	0.47
1:C:371:GLU:OE2	1:C:395:ARG:HD2	2.14	0.47
1:D:175:LEU:HB3	1:D:213:ALA:HB1	1.97	0.47
1:D:237:VAL:HG21	1:D:281:GLN:HG3	1.95	0.47
1:D:238:ARG:HA	1:D:241:PHE:CE2	2.50	0.47
1:D:559:LYS:O	1:D:563:LEU:HB2	2.15	0.47
1:E:168:LEU:O	1:E:171:ILE:HG13	2.14	0.47
1:E:172:VAL:O	1:E:213:ALA:HB1	2.15	0.47
1:E:365:LEU:O	1:E:368:LEU:HB3	2.14	0.47
1:E:413:ARG:HA	1:E:577:LEU:HD21	1.91	0.47
1:E:528:GLY:HA2	1:E:530:TYR:CE2	2.50	0.47
1:F:369:LEU:O	1:F:370:ASN:C	2.53	0.47
1:A:361:VAL:CG1	1:A:364:ASP:HB2	2.45	0.47
1:B:154:THR:OG1	1:B:212:GLU:OE2	2.33	0.47
1:B:194:LEU:HD23	1:B:323:ILE:CD1	2.45	0.47
1:C:172:VAL:O	1:C:213:ALA:HB1	2.15	0.47
1:C:189:PRO:HG3	1:C:319:ARG:NH1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:MET:HG3	1:C:236:ARG:HH22	1.80	0.47
1:C:506:THR:CG2	1:C:543:ILE:HD13	2.45	0.47
1:C:514:PHE:HD2	1:C:514:PHE:H	1.62	0.47
1:D:199:GLY:O	1:D:361:VAL:CG2	2.63	0.47
1:D:308:ASP:OD1	1:D:310:ALA:N	2.46	0.47
1:D:344:LEU:HA	1:D:383:LYS:CG	2.44	0.47
1:E:428:PHE:HE1	1:E:432:ALA:HA	1.67	0.47
1:F:319:ARG:CG	1:F:319:ARG:NH1	2.66	0.47
1:A:359:GLY:HA3	1:A:360:PHE:CG	2.50	0.46
1:A:450:MET:O	1:A:454:ARG:HB3	2.15	0.46
1:A:596:LEU:HG	1:A:597:GLU:H	1.80	0.46
1:B:225:PHE:CD2	1:B:225:PHE:N	2.81	0.46
1:C:147:LEU:C	1:C:147:LEU:HD12	2.36	0.46
1:C:300:ALA:O	1:C:301:THR:HG22	2.15	0.46
1:C:387:LYS:CA	1:C:390:GLU:HB2	2.44	0.46
1:C:387:LYS:C	1:C:390:GLU:HB2	2.35	0.46
1:D:458:LEU:HD11	1:D:460:TRP:HB3	1.96	0.46
1:E:147:LEU:C	1:E:147:LEU:HD12	2.35	0.46
1:E:410:ARG:HA	1:E:413:ARG:HB3	1.97	0.46
1:E:449:PHE:CE2	1:E:496:GLN:NE2	2.83	0.46
1:A:292:ASP:OD2	1:B:227:GLU:OE1	2.33	0.46
1:A:377:ALA:HB1	1:F:181:PHE:CD1	2.50	0.46
1:B:157:ASP:HB3	1:B:337:ILE:CG1	2.45	0.46
1:B:263:LYS:HA	1:B:263:LYS:HD2	1.39	0.46
1:B:336:ARG:O	1:B:339:ALA:N	2.23	0.46
1:B:469:ILE:HG23	1:B:497:ALA:HB1	1.98	0.46
1:B:505:ILE:HG23	1:B:514:PHE:CD2	2.50	0.46
1:B:506:THR:OG1	1:B:520:ALA:HB3	2.15	0.46
1:C:147:LEU:HD23	1:C:217:PHE:CB	2.44	0.46
1:C:182:HIS:CD2	1:C:182:HIS:H	2.32	0.46
1:C:210:ALA:O	1:C:214:ARG:HA	2.15	0.46
1:C:238:ARG:O	1:C:239:ASP:C	2.52	0.46
1:C:316:ARG:O	1:C:317:PHE:C	2.54	0.46
1:C:352:LEU:HD11	1:C:356:ARG:HH21	1.76	0.46
1:C:583:THR:HG22	1:C:586:GLU:OE1	2.15	0.46
1:D:345:ALA:CB	1:D:383:LYS:HE3	2.36	0.46
1:D:379:GLU:OE1	1:D:381:ARG:NE	2.48	0.46
1:D:455:GLU:O	1:D:456:ASP:C	2.54	0.46
1:E:348:VAL:O	1:E:348:VAL:HG12	2.14	0.46
1:E:357:THR:HG1	1:E:360:PHE:CB	2.28	0.46
1:F:154:THR:HG23	1:F:156:LYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:ARG:O	1:F:411:ASP:C	2.53	0.46
1:F:455:GLU:O	1:F:457:MET:N	2.48	0.46
1:A:171:ILE:HG22	1:A:188:ILE:CG2	2.44	0.46
1:A:249:PRO:HB3	1:A:294:ALA:HB3	1.96	0.46
1:B:336:ARG:O	1:B:338:HIS:N	2.48	0.46
1:B:563:LEU:O	1:B:566:ARG:HB3	2.15	0.46
1:C:168:LEU:O	1:C:171:ILE:HG13	2.15	0.46
1:C:210:ALA:HB2	1:C:251:ILE:CD1	2.43	0.46
1:C:361:VAL:O	1:C:365:LEU:HG	2.16	0.46
1:C:570:GLU:O	1:C:571:ARG:C	2.54	0.46
1:D:200:VAL:HG12	1:D:325:ALA:HB2	1.98	0.46
1:D:311:LEU:HA	1:D:316:ARG:CZ	2.45	0.46
1:D:352:LEU:O	1:D:355:LYS:HB2	2.16	0.46
1:D:517:VAL:CG2	1:D:518:ALA:N	2.78	0.46
1:D:572:VAL:HG11	1:D:587:PHE:HE1	1.81	0.46
1:E:312:LEU:HD21	1:E:320:GLN:OE1	2.16	0.46
1:F:452:PRO:O	1:F:456:ASP:N	2.48	0.46
1:F:503:ARG:HG2	1:F:508:TRP:CZ2	2.49	0.46
1:F:572:VAL:HG11	1:F:587:PHE:HE1	1.80	0.46
1:A:282:LEU:O	1:A:286:MET:HG2	2.15	0.46
1:A:378:ARG:HH12	1:F:170:GLU:HB2	1.80	0.46
1:A:507:GLU:HB2	1:A:520:ALA:HB3	1.98	0.46
1:B:297:VAL:CG1	1:B:317:PHE:CE1	2.98	0.46
1:B:469:ILE:HG22	1:B:473:LEU:HD12	1.96	0.46
1:C:282:LEU:HG	1:C:283:LEU:HD12	1.97	0.46
1:D:159:ALA:HA	1:D:333:GLN:HE21	1.80	0.46
1:D:411:ASP:O	1:D:414:ILE:HG13	2.16	0.46
1:D:571:ARG:HH12	1:D:593:GLY:N	2.13	0.46
1:E:249:PRO:HB3	1:E:294:ALA:HB3	1.98	0.46
1:E:436:HIS:HB3	1:E:584:ALA:CB	2.45	0.46
1:F:467:ASP:O	1:F:471:VAL:HG13	2.16	0.46
1:A:212:GLU:C	1:A:214:ARG:HB2	2.34	0.46
1:A:253:PHE:HA	1:A:298:MET:O	2.16	0.46
1:A:373:ALA:HA	1:A:384:ILE:CD1	2.46	0.46
1:A:551:ILE:O	1:A:552:GLU:C	2.52	0.46
1:B:384:ILE:CG2	1:B:385:THR:N	2.79	0.46
1:C:190:LYS:CD	1:C:289:PHE:CE1	2.87	0.46
1:C:361:VAL:CG1	1:C:364:ASP:HB2	2.45	0.46
1:D:399:LEU:O	1:D:402:LYS:HB3	2.16	0.46
1:D:476:ARG:NH1	1:D:487:THR:HG21	2.30	0.46
1:E:155:PHE:CZ	1:E:209:VAL:HG22	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:VAL:CG1	1:E:364:ASP:HB2	2.46	0.46
1:F:204:HIS:CD2	2:F:2001:ADP:H2'	2.50	0.46
1:F:256:GLU:O	1:F:256:GLU:CG	2.62	0.46
1:A:191:GLY:CA	1:A:297:VAL:CG2	2.93	0.46
1:A:198:PRO:HD3	1:A:302:ASN:HD21	1.81	0.46
1:A:305:ASP:C	1:A:307:LEU:N	2.68	0.46
1:A:449:PHE:HE2	1:A:496:GLN:HE21	1.60	0.46
1:A:481:ILE:HG22	1:A:482:VAL:N	2.31	0.46
1:B:228:MET:SD	1:B:232:VAL:CG1	3.04	0.46
1:B:494:PHE:O	1:B:496:GLN:N	2.48	0.46
1:C:218:ILE:HG12	1:C:218:ILE:H	1.64	0.46
1:C:407:LEU:HA	1:C:411:ASP:HB2	1.97	0.46
1:D:201:GLY:O	1:D:204:HIS:HB3	2.16	0.46
1:D:241:PHE:CZ	1:D:285:GLU:OE2	2.67	0.46
1:D:242:GLU:HA	1:D:245:LYS:CB	2.43	0.46
1:D:329:LYS:CG	1:D:330:GLY:N	2.78	0.46
1:D:454:ARG:HH21	1:D:526:TYR:HA	1.80	0.46
1:E:225:PHE:CE1	1:E:236:ARG:HG2	2.51	0.46
1:F:174:PHE:C	1:F:174:PHE:CD2	2.89	0.46
1:F:242:GLU:HA	1:F:245:LYS:CB	2.45	0.46
1:F:374:LEU:HD23	1:F:374:LEU:C	2.36	0.46
1:F:438:VAL:CG2	1:F:439:THR:N	2.79	0.46
1:F:454:ARG:HH11	1:F:454:ARG:HA	1.80	0.46
1:A:215:VAL:HG22	1:A:216:PRO:N	2.30	0.46
1:A:408:SER:HB2	1:A:409:PRO:CD	2.41	0.46
1:A:503:ARG:CG	1:A:508:TRP:CE3	2.99	0.46
1:B:149:GLU:O	1:B:150:ALA:C	2.54	0.46
1:B:328:VAL:HG22	1:B:355:LYS:CE	2.38	0.46
1:B:336:ARG:O	1:B:337:ILE:C	2.54	0.46
1:B:400:PRO:O	1:B:403:LYS:N	2.49	0.46
1:C:308:ASP:OD1	1:C:310:ALA:CB	2.64	0.46
1:C:464:ARG:CG	1:C:464:ARG:HH11	2.29	0.46
1:C:520:ALA:HA	1:C:533:ARG:HG2	1.96	0.46
1:D:164:ALA:C	1:D:168:LEU:HD13	2.35	0.46
1:D:202:LYS:N	2:D:2001:ADP:O1A	2.49	0.46
1:D:455:GLU:O	1:D:455:GLU:HG2	2.16	0.46
1:D:521:VAL:HG23	1:D:532:VAL:CG1	2.42	0.46
1:E:311:LEU:HD23	1:E:311:LEU:HA	1.68	0.46
1:E:316:ARG:O	1:E:317:PHE:C	2.51	0.46
1:A:272:ASN:C	1:A:272:ASN:OD1	2.54	0.46
1:A:312:LEU:HD21	1:A:320:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ARG:CG	1:A:411:ASP:N	2.77	0.46
1:A:523:GLU:O	1:A:529:GLY:HA2	2.16	0.46
1:B:314:PRO:HA	1:B:318:ASP:OD2	2.16	0.46
1:B:329:LYS:CG	1:B:330:GLY:N	2.78	0.46
1:B:443:ARG:O	1:B:445:ARG:N	2.49	0.46
1:C:340:ARG:C	1:C:342:LYS:N	2.59	0.46
1:D:192:VAL:C	1:D:317:PHE:CE2	2.89	0.46
1:D:207:ARG:O	1:D:210:ALA:N	2.49	0.46
1:D:286:MET:HE3	1:D:286:MET:HB2	1.82	0.46
1:D:585:GLU:O	1:D:587:PHE:N	2.49	0.46
1:E:238:ARG:O	1:E:241:PHE:N	2.48	0.46
1:E:280:ASN:O	1:E:281:GLN:C	2.54	0.46
1:E:469:ILE:HD11	1:E:500:LEU:HB3	1.98	0.46
1:F:199:GLY:O	1:F:361:VAL:HG22	2.14	0.46
1:F:238:ARG:HH12	1:F:239:ASP:H	1.43	0.46
1:F:488:THR:O	1:F:490:ALA:N	2.48	0.46
1:F:517:VAL:HG11	1:F:519:TYR:CZ	2.51	0.46
1:F:571:ARG:O	1:F:575:THR:HG23	2.16	0.46
1:A:159:ALA:HB1	1:A:333:GLN:HB3	1.97	0.46
1:A:503:ARG:HG2	1:A:508:TRP:CE3	2.51	0.46
1:B:242:GLU:HA	1:B:245:LYS:CB	2.42	0.46
1:B:389:LEU:O	1:B:390:GLU:C	2.54	0.46
1:B:454:ARG:HA	1:B:454:ARG:HH11	1.81	0.46
1:C:192:VAL:O	1:C:298:MET:HA	2.16	0.46
1:C:262:ARG:HG2	1:C:275:ARG:NH2	2.09	0.46
1:C:462:ARG:HG3	1:C:466:LEU:HD11	1.97	0.46
1:D:165:LYS:NZ	1:D:168:LEU:CD2	2.79	0.46
1:D:286:MET:O	1:D:289:PHE:CG	2.69	0.46
1:D:297:VAL:HG13	1:D:317:PHE:CZ	2.51	0.46
1:D:469:ILE:HG23	1:D:497:ALA:HB1	1.98	0.46
1:D:501:ALA:CB	1:D:550:LEU:HD23	2.45	0.46
1:E:207:ARG:CZ	1:E:207:ARG:CB	2.91	0.46
1:E:370:ASN:C	1:E:370:ASN:OD1	2.55	0.46
1:E:520:ALA:HA	1:E:533:ARG:HG2	1.96	0.46
1:F:537:GLU:O	1:F:540:ALA:HB3	2.16	0.46
1:F:538:GLU:O	1:F:541:LYS:N	2.49	0.46
1:B:228:MET:HE3	1:B:236:ARG:HD3	1.98	0.46
1:B:301:THR:HG23	1:B:303:ARG:H	1.81	0.46
1:C:305:ASP:C	1:C:307:LEU:N	2.69	0.46
1:C:356:ARG:C	1:C:358:PRO:HD2	2.37	0.46
1:D:297:VAL:HG13	1:D:317:PHE:HZ	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:PRO:HA	1:D:318:ASP:OD2	2.16	0.46
1:E:173:GLU:CA	1:E:176:LYS:HG3	2.36	0.46
1:E:441:VAL:O	1:E:441:VAL:CG1	2.61	0.46
1:F:329:LYS:CG	1:F:330:GLY:N	2.79	0.46
1:F:447:LEU:O	1:F:449:PHE:N	2.49	0.46
1:A:155:PHE:HZ	1:A:209:VAL:CG2	2.29	0.45
1:A:174:PHE:O	1:A:177:ASN:C	2.55	0.45
1:A:192:VAL:N	1:A:297:VAL:O	2.43	0.45
1:A:206:ALA:CB	1:A:217:PHE:HZ	2.29	0.45
1:A:237:VAL:O	1:A:240:LEU:HB3	2.16	0.45
1:A:410:ARG:O	1:A:411:ASP:C	2.54	0.45
1:A:520:ALA:HA	1:A:533:ARG:HG2	1.98	0.45
1:B:352:LEU:O	1:B:353:LEU:C	2.53	0.45
1:C:228:MET:HG3	1:C:236:ARG:NH2	2.31	0.45
1:C:450:MET:HE2	1:C:451:MET:SD	2.56	0.45
1:C:459:HIS:CE1	1:D:411:ASP:HB3	2.51	0.45
1:C:503:ARG:CD	1:C:508:TRP:CE2	2.95	0.45
1:D:428:PHE:HE1	1:D:432:ALA:C	2.19	0.45
1:D:476:ARG:CZ	1:D:487:THR:HG21	2.46	0.45
1:D:537:GLU:O	1:D:540:ALA:HB3	2.16	0.45
1:E:168:LEU:C	1:E:168:LEU:HD12	2.36	0.45
1:E:462:ARG:HG3	1:E:466:LEU:HD11	1.98	0.45
1:E:506:THR:HA	1:E:519:TYR:HD1	1.80	0.45
1:E:534:GLN:N	1:E:534:GLN:CD	2.70	0.45
1:F:238:ARG:HA	1:F:241:PHE:HE2	1.81	0.45
1:A:328:VAL:HG12	1:A:329:LYS:N	2.30	0.45
1:B:175:LEU:O	1:B:249:PRO:HG2	2.15	0.45
1:B:523:GLU:OE2	1:C:264:ARG:NH2	2.50	0.45
1:D:354:ALA:O	1:D:357:THR:HG23	2.15	0.45
1:D:410:ARG:O	1:D:411:ASP:C	2.54	0.45
1:E:147:LEU:O	1:E:216:PRO:HB3	2.17	0.45
1:E:274:GLU:O	1:E:277:GLN:CB	2.54	0.45
1:F:313:ARG:CG	1:F:314:PRO:N	2.76	0.45
1:F:329:LYS:O	1:F:332:GLU:HB3	2.16	0.45
1:F:384:ILE:HG22	1:F:385:THR:N	2.30	0.45
1:F:428:PHE:CD1	1:F:432:ALA:HB3	2.50	0.45
1:F:571:ARG:HH12	1:F:593:GLY:N	2.14	0.45
1:A:182:HIS:HD1	1:A:291:LYS:HB2	1.81	0.45
1:A:274:GLU:C	1:A:277:GLN:HB3	2.37	0.45
1:A:443:ARG:O	1:A:443:ARG:HG2	2.16	0.45
1:A:503:ARG:HG3	1:A:504:MET:N	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:THR:CG2	1:A:543:ILE:HD13	2.46	0.45
1:B:470:ALA:O	1:B:474:ALA:HB2	2.16	0.45
1:C:300:ALA:O	1:C:301:THR:CG2	2.64	0.45
1:C:372:ALA:CB	1:C:389:LEU:HD23	2.47	0.45
1:D:336:ARG:O	1:D:337:ILE:C	2.53	0.45
1:D:379:GLU:OE1	1:D:381:ARG:CD	2.65	0.45
1:E:359:GLY:HA3	1:E:360:PHE:CG	2.51	0.45
1:E:408:SER:HB2	1:E:409:PRO:CD	2.44	0.45
1:E:410:ARG:CG	1:E:411:ASP:N	2.77	0.45
1:E:469:ILE:HG13	1:E:500:LEU:HD23	1.97	0.45
1:E:517:VAL:HG23	1:F:498:THR:OG1	2.16	0.45
1:E:552:GLU:O	1:E:555:TYR:HB3	2.16	0.45
1:F:274:GLU:HA	1:F:277:GLN:HE21	1.80	0.45
1:F:357:THR:HB	1:F:360:PHE:CD2	2.52	0.45
1:F:511:HIS:O	1:F:512:PRO:O	2.34	0.45
1:A:277:GLN:HG3	1:A:278:THR:N	2.32	0.45
1:A:361:VAL:O	1:A:365:LEU:HG	2.17	0.45
1:B:589:ARG:CZ	1:B:596:LEU:HD22	2.46	0.45
1:C:198:PRO:HD3	1:C:302:ASN:HD21	1.81	0.45
1:C:222:GLY:O	1:C:225:PHE:HB2	2.17	0.45
1:C:438:VAL:HG22	1:C:582:LEU:HB2	1.99	0.45
1:D:261:GLY:O	1:D:308:ASP:HB3	2.16	0.45
1:D:449:PHE:CZ	1:D:496:GLN:OE1	2.69	0.45
1:D:527:LEU:HD11	1:E:226:VAL:HG12	1.97	0.45
1:E:308:ASP:OD1	1:E:310:ALA:CB	2.65	0.45
1:E:487:THR:OG1	1:E:488:THR:N	2.49	0.45
1:F:162:GLU:OE1	1:F:162:GLU:HA	2.16	0.45
1:F:165:LYS:O	1:F:167:GLU:N	2.50	0.45
1:F:165:LYS:NZ	1:F:205:LEU:CB	2.68	0.45
1:F:384:ILE:CG2	1:F:385:THR:N	2.79	0.45
1:A:218:ILE:HG12	1:A:218:ILE:H	1.65	0.45
1:A:449:PHE:N	1:A:449:PHE:HD2	2.11	0.45
1:A:528:GLY:HA2	1:A:530:TYR:CE2	2.52	0.45
1:B:184:MET:O	1:C:342:LYS:CD	2.63	0.45
1:B:241:PHE:CZ	1:B:285:GLU:OE2	2.69	0.45
1:B:329:LYS:O	1:B:332:GLU:HB3	2.16	0.45
1:B:410:ARG:O	1:B:413:ARG:CB	2.65	0.45
1:B:503:ARG:HG2	1:B:508:TRP:CZ2	2.51	0.45
1:C:381:ARG:CG	1:C:381:ARG:NH1	2.79	0.45
1:C:459:HIS:HE1	1:D:411:ASP:CB	2.29	0.45
1:C:519:TYR:CA	1:C:533:ARG:CZ	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:PRO:HD3	1:E:319:ARG:HH11	1.82	0.45
1:F:381:ARG:NH2	1:F:388:ASP:OD2	2.50	0.45
1:A:286:MET:CE	1:A:297:VAL:HG21	2.46	0.45
1:A:574:GLU:OE1	1:A:575:THR:N	2.49	0.45
1:B:175:LEU:O	1:B:249:PRO:HB2	2.17	0.45
1:B:454:ARG:HH21	1:B:526:TYR:HA	1.81	0.45
1:C:345:ALA:HA	1:C:383:LYS:HD3	1.97	0.45
1:D:350:LEU:O	1:D:353:LEU:N	2.50	0.45
1:D:583:THR:O	1:D:584:ALA:C	2.55	0.45
1:E:200:VAL:N	2:E:1001:ADP:O1A	2.50	0.45
1:F:162:GLU:OE1	1:F:162:GLU:CA	2.64	0.45
1:F:247:HIS:O	1:F:249:PRO:O	2.34	0.45
1:F:278:THR:O	1:F:281:GLN:HB3	2.16	0.45
1:F:352:LEU:HD12	1:F:353:LEU:N	2.30	0.45
1:F:449:PHE:HZ	1:F:496:GLN:OE1	2.00	0.45
1:F:460:TRP:CD1	1:F:464:ARG:HG2	2.52	0.45
1:F:523:GLU:O	1:F:530:TYR:N	2.43	0.45
1:F:582:LEU:CD2	1:F:590:VAL:HG21	2.42	0.45
1:A:196:GLY:C	1:A:202:LYS:HZ1	2.18	0.45
1:A:212:GLU:O	1:A:214:ARG:CB	2.65	0.45
1:A:381:ARG:CG	1:A:381:ARG:NH1	2.80	0.45
1:A:387:LYS:C	1:A:390:GLU:HB2	2.37	0.45
1:A:464:ARG:NH1	1:A:464:ARG:HG2	2.32	0.45
1:A:483:PHE:C	1:A:485:ASP:H	2.20	0.45
1:A:519:TYR:C	1:A:533:ARG:NE	2.68	0.45
1:B:342:LYS:HA	1:B:342:LYS:HD2	1.60	0.45
1:B:510:MET:O	1:B:512:PRO:CD	2.63	0.45
1:C:236:ARG:HG2	1:C:236:ARG:NH1	2.12	0.45
1:C:274:GLU:C	1:C:277:GLN:HB3	2.34	0.45
1:C:346:GLU:OE1	1:C:347:ASP:N	2.45	0.45
1:C:361:VAL:HG12	1:C:364:ASP:HB2	1.99	0.45
1:D:175:LEU:O	1:D:249:PRO:HB2	2.17	0.45
1:D:301:THR:HG23	1:D:303:ARG:H	1.80	0.45
1:D:302:ASN:ND2	1:D:443:ARG:HH22	1.91	0.45
1:D:336:ARG:HD3	1:D:336:ARG:HA	1.51	0.45
1:D:393:ALA:O	1:D:397:MET:HB3	2.17	0.45
1:D:443:ARG:O	1:D:445:ARG:N	2.50	0.45
1:D:503:ARG:NH2	1:D:522:ARG:CZ	2.80	0.45
1:E:286:MET:CG	1:E:316:ARG:HG2	2.45	0.45
1:E:453:ARG:NH2	1:E:464:ARG:CZ	2.79	0.45
1:E:470:ALA:HB1	1:E:558:VAL:CG2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:LEU:HD11	1:F:386:MET:CE	2.40	0.45
1:A:236:ARG:HH11	1:A:236:ARG:CB	2.29	0.45
1:A:361:VAL:HG12	1:A:364:ASP:HB2	1.99	0.45
1:A:519:TYR:HB3	1:A:535:TYR:HD2	1.82	0.45
1:B:312:LEU:HD23	1:B:312:LEU:O	2.16	0.45
1:C:462:ARG:HH12	1:C:511:HIS:H	1.64	0.45
1:E:334:ILE:HD11	2:E:1001:ADP:N6	2.32	0.45
1:E:424:LEU:HD22	1:E:569:LEU:HA	1.99	0.45
1:E:447:LEU:HB2	1:E:496:GLN:HE22	1.82	0.45
1:F:202:LYS:CD	2:F:2001:ADP:O2B	2.65	0.45
1:F:255:ASP:OD1	1:F:256:GLU:N	2.49	0.45
1:F:428:PHE:CE1	1:F:433:ASP:N	2.84	0.45
1:A:168:LEU:C	1:A:168:LEU:HD12	2.38	0.45
1:A:352:LEU:HD11	1:A:356:ARG:HH21	1.74	0.45
1:B:286:MET:HE3	1:B:286:MET:HB2	1.87	0.45
1:B:438:VAL:CG2	1:B:439:THR:N	2.80	0.45
1:B:536:SER:HB2	1:C:537:GLU:OE2	2.17	0.45
1:C:159:ALA:HB1	1:C:333:GLN:HB3	1.99	0.45
1:C:191:GLY:CA	1:C:297:VAL:CG2	2.94	0.45
1:C:233:GLY:O	1:C:236:ARG:CG	2.62	0.45
1:C:236:ARG:CG	1:C:237:VAL:H	2.18	0.45
1:C:238:ARG:O	1:C:241:PHE:N	2.50	0.45
1:D:157:ASP:O	1:D:158:VAL:HG23	2.16	0.45
1:E:305:ASP:C	1:E:307:LEU:N	2.70	0.45
1:E:372:ALA:CB	1:E:389:LEU:HD23	2.47	0.45
1:E:407:LEU:H	1:E:407:LEU:HG	1.57	0.45
1:E:548:ARG:NH2	1:E:552:GLU:OE1	2.46	0.45
1:A:204:HIS:CD2	2:A:1001:ADP:C2	3.04	0.45
1:A:442:PRO:HG2	1:A:443:ARG:H	1.81	0.45
1:A:527:LEU:HD12	1:A:527:LEU:O	2.16	0.45
1:B:153:VAL:O	1:B:154:THR:HB	2.17	0.45
1:B:344:LEU:HA	1:B:383:LYS:CG	2.46	0.45
1:B:517:VAL:HG13	1:B:519:TYR:CZ	2.52	0.45
1:C:271:GLY:O	1:C:275:ARG:NE	2.50	0.45
1:C:397:MET:HG3	1:C:406:VAL:CG1	2.46	0.45
1:C:451:MET:HB2	1:C:452:PRO:CD	2.47	0.45
1:D:197:PRO:HD2	1:D:200:VAL:CG1	2.45	0.45
1:D:505:ILE:HG23	1:D:514:PHE:CD2	2.52	0.45
1:E:286:MET:CG	1:E:316:ARG:CG	2.94	0.45
1:F:201:GLY:O	1:F:204:HIS:HB3	2.17	0.45
1:F:313:ARG:HG3	1:F:314:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:468:GLN:O	1:F:471:VAL:N	2.49	0.45
1:F:508:TRP:O	1:F:510:MET:HG3	2.17	0.45
1:A:447:LEU:HB2	1:A:496:GLN:HE22	1.80	0.44
1:A:465:LEU:O	1:A:469:ILE:HG13	2.17	0.44
1:A:582:LEU:CD2	1:A:587:PHE:HA	2.34	0.44
1:B:150:ALA:HA	1:B:151:PRO:HD2	1.84	0.44
1:B:207:ARG:CB	1:B:217:PHE:CZ	2.96	0.44
1:B:354:ALA:O	1:B:357:THR:HG23	2.17	0.44
1:C:337:ILE:CD1	1:C:338:HIS:CD2	3.00	0.44
1:D:175:LEU:O	1:D:249:PRO:CG	2.65	0.44
1:D:279:LEU:O	1:D:283:LEU:HB2	2.17	0.44
1:D:307:LEU:CD1	1:D:307:LEU:H	2.31	0.44
1:D:332:GLU:HB2	1:D:354:ALA:HB2	1.98	0.44
1:E:153:VAL:HG13	1:E:157:ASP:CB	2.47	0.44
1:E:225:PHE:HZ	1:E:278:THR:HB	1.66	0.44
1:E:228:MET:HG3	1:E:236:ARG:NH2	2.31	0.44
1:E:236:ARG:O	1:E:239:ASP:N	2.51	0.44
1:E:237:VAL:HG11	1:E:281:GLN:CB	2.27	0.44
1:E:263:LYS:CG	1:E:264:ARG:H	2.28	0.44
1:E:586:GLU:HG2	1:E:587:PHE:N	2.30	0.44
1:E:589:ARG:HB3	1:E:589:ARG:HH11	1.74	0.44
1:F:158:VAL:HG11	1:F:205:LEU:HD11	1.98	0.44
1:F:200:VAL:HA	1:F:361:VAL:HG23	1.99	0.44
1:F:314:PRO:HA	1:F:318:ASP:OD2	2.16	0.44
1:F:338:HIS:HB3	1:F:369:LEU:HD12	1.99	0.44
1:F:344:LEU:HA	1:F:383:LYS:CG	2.47	0.44
1:A:220:ALA:O	1:A:254:ILE:HA	2.16	0.44
1:A:280:ASN:HA	1:A:283:LEU:HB2	1.99	0.44
1:A:327:ASP:OD1	1:A:329:LYS:N	2.50	0.44
1:A:382:ARG:CG	1:A:383:LYS:H	2.29	0.44
1:A:438:VAL:HG22	1:A:582:LEU:HB2	2.00	0.44
1:A:467:ASP:HA	1:A:557:ARG:NH2	2.32	0.44
1:B:566:ARG:O	1:B:569:LEU:HB3	2.17	0.44
1:C:147:LEU:HB3	1:C:217:PHE:O	2.17	0.44
1:C:312:LEU:HD21	1:C:320:GLN:OE1	2.16	0.44
1:C:370:ASN:OD1	1:C:370:ASN:C	2.55	0.44
1:D:193:LEU:HB3	1:D:317:PHE:HD2	1.82	0.44
1:D:338:HIS:CB	1:D:369:LEU:HD11	2.47	0.44
1:D:525:THR:HG22	1:D:526:TYR:CD2	2.52	0.44
1:E:192:VAL:N	1:E:297:VAL:O	2.38	0.44
1:E:211:GLY:C	1:E:214:ARG:HG2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:GLY:O	1:E:236:ARG:CG	2.61	0.44
1:E:277:GLN:HG3	1:E:278:THR:N	2.31	0.44
1:E:387:LYS:CA	1:E:390:GLU:HB2	2.44	0.44
1:E:454:ARG:HG3	1:E:455:GLU:N	2.32	0.44
1:F:149:GLU:O	1:F:150:ALA:C	2.56	0.44
1:F:238:ARG:HH11	1:F:238:ARG:CG	2.30	0.44
1:F:376:ALA:C	1:F:381:ARG:CB	2.84	0.44
1:F:583:THR:O	1:F:584:ALA:C	2.56	0.44
1:A:147:LEU:HD23	1:A:217:PHE:CB	2.47	0.44
1:A:263:LYS:CG	1:A:264:ARG:H	2.27	0.44
1:A:305:ASP:OD2	1:A:447:LEU:HD13	2.16	0.44
1:B:343:PRO:HG2	1:B:383:LYS:CA	2.40	0.44
1:D:170:GLU:HG2	1:D:171:ILE:N	2.32	0.44
1:D:428:PHE:CZ	1:D:433:ASP:N	2.85	0.44
1:D:428:PHE:CD1	1:D:432:ALA:HB3	2.52	0.44
1:D:452:PRO:O	1:D:456:ASP:CA	2.65	0.44
1:E:266:SER:C	1:E:268:VAL:N	2.71	0.44
1:E:587:PHE:CD2	1:E:588:GLN:N	2.85	0.44
1:F:225:PHE:CD2	1:F:236:ARG:CD	2.99	0.44
1:F:308:ASP:OD1	1:F:310:ALA:N	2.45	0.44
1:F:312:LEU:O	1:F:312:LEU:HD23	2.17	0.44
1:A:182:HIS:CB	1:A:291:LYS:HD2	2.20	0.44
1:A:291:LYS:O	1:A:292:ASP:C	2.56	0.44
1:A:451:MET:HB2	1:A:452:PRO:CD	2.47	0.44
1:B:231:GLY:H	1:B:277:GLN:HE22	1.65	0.44
1:B:353:LEU:O	1:B:357:THR:CG2	2.65	0.44
1:B:361:VAL:HG13	1:B:364:ASP:CG	2.38	0.44
1:B:548:ARG:NH1	1:B:548:ARG:HG2	2.32	0.44
1:C:454:ARG:HB2	1:C:460:TRP:HH2	1.82	0.44
1:C:503:ARG:HG2	1:C:508:TRP:CE3	2.51	0.44
1:C:533:ARG:HD2	1:C:533:ARG:HA	1.91	0.44
1:D:168:LEU:O	1:D:171:ILE:N	2.51	0.44
1:D:454:ARG:HA	1:D:454:ARG:HH11	1.83	0.44
1:D:533:ARG:HG3	1:D:533:ARG:NH1	2.21	0.44
1:E:198:PRO:HD3	1:E:302:ASN:HD21	1.82	0.44
1:E:273:ASP:CG	1:E:274:GLU:H	2.20	0.44
1:E:387:LYS:C	1:E:390:GLU:HB2	2.38	0.44
1:E:471:VAL:O	1:E:474:ALA:HB3	2.17	0.44
1:E:519:TYR:O	1:E:533:ARG:HG2	2.17	0.44
1:F:382:ARG:HD2	1:F:382:ARG:HA	1.08	0.44
1:F:503:ARG:CG	1:F:508:TRP:CZ2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:THR:CG2	1:F:526:TYR:CD2	2.98	0.44
1:A:215:VAL:CG2	1:A:216:PRO:CD	2.93	0.44
1:A:266:SER:C	1:A:268:VAL:N	2.70	0.44
1:A:318:ASP:O	1:A:319:ARG:HG3	2.18	0.44
1:A:548:ARG:NH1	1:F:513:GLU:O	2.50	0.44
1:B:238:ARG:NH1	1:B:239:ASP:CA	2.67	0.44
1:B:538:GLU:O	1:B:541:LYS:N	2.50	0.44
1:C:168:LEU:C	1:C:168:LEU:HD12	2.38	0.44
1:C:327:ASP:C	1:C:327:ASP:OD1	2.56	0.44
1:C:509:GLY:O	1:D:476:ARG:NH2	2.36	0.44
1:C:519:TYR:C	1:C:533:ARG:CZ	2.86	0.44
1:D:215:VAL:O	1:D:216:PRO:C	2.56	0.44
1:D:353:LEU:O	1:D:357:THR:CG2	2.65	0.44
1:E:225:PHE:CE1	1:E:233:GLY:HA3	2.48	0.44
1:E:464:ARG:O	1:E:465:LEU:C	2.56	0.44
1:F:147:LEU:HD13	1:F:149:GLU:OE1	2.18	0.44
1:F:154:THR:OG1	1:F:212:GLU:OE2	2.35	0.44
1:F:231:GLY:H	1:F:277:GLN:HE22	1.65	0.44
1:F:476:ARG:CZ	1:F:487:THR:HG21	2.47	0.44
1:A:236:ARG:O	1:A:239:ASP:N	2.51	0.44
1:A:370:ASN:OD1	1:A:370:ASN:C	2.55	0.44
1:A:503:ARG:CD	1:A:508:TRP:CE2	2.98	0.44
1:B:572:VAL:O	1:B:576:LEU:HB2	2.18	0.44
1:B:592:GLU:O	1:B:594:LEU:HB3	2.18	0.44
1:C:206:ALA:CB	1:C:217:PHE:HZ	2.31	0.44
1:C:382:ARG:HH11	1:C:383:LYS:HB2	1.83	0.44
1:C:465:LEU:CD2	1:C:508:TRP:CZ3	2.99	0.44
1:C:586:GLU:HG2	1:C:587:PHE:N	2.32	0.44
1:D:231:GLY:H	1:D:277:GLN:HE22	1.65	0.44
1:D:257:ILE:HG22	1:D:261:GLY:H	1.83	0.44
1:D:260:VAL:O	1:D:262:ARG:N	2.46	0.44
1:D:526:TYR:O	1:D:528:GLY:CA	2.65	0.44
1:E:171:ILE:HD12	1:E:172:VAL:H	1.81	0.44
1:E:352:LEU:HD11	1:E:356:ARG:HH21	1.80	0.44
1:E:399:LEU:N	1:E:400:PRO:CD	2.81	0.44
1:E:481:ILE:HG22	1:E:482:VAL:N	2.31	0.44
1:E:511:HIS:O	1:E:512:PRO:O	2.36	0.44
1:E:588:GLN:O	1:E:591:VAL:CB	2.55	0.44
1:F:373:ALA:CA	1:F:384:ILE:HD11	2.45	0.44
1:F:526:TYR:O	1:F:528:GLY:CA	2.66	0.44
1:A:237:VAL:HG13	1:A:238:ARG:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ARG:HG2	1:A:379:GLU:N	2.22	0.44
1:A:410:ARG:HA	1:A:413:ARG:HB3	2.00	0.44
1:B:175:LEU:O	1:B:249:PRO:CG	2.66	0.44
1:B:238:ARG:N	1:B:281:GLN:HE21	2.16	0.44
1:C:203:THR:HG23	2:C:1001:ADP:O2A	2.18	0.44
1:C:400:PRO:HG2	1:C:405:LEU:CD1	2.46	0.44
1:D:301:THR:HG22	1:D:303:ARG:H	1.82	0.44
1:D:374:LEU:HD23	1:D:375:LEU:N	2.33	0.44
1:D:506:THR:OG1	1:D:520:ALA:HB3	2.17	0.44
1:D:585:GLU:O	1:D:586:GLU:C	2.56	0.44
1:E:413:ARG:O	1:E:577:LEU:HD21	2.18	0.44
1:E:551:ILE:O	1:E:552:GLU:C	2.56	0.44
1:F:153:VAL:O	1:F:154:THR:HB	2.17	0.44
1:F:209:VAL:CG1	1:F:210:ALA:H	2.21	0.44
1:F:525:THR:HG22	1:F:526:TYR:N	2.33	0.44
1:A:381:ARG:C	1:F:180:ARG:HH22	2.18	0.44
1:B:161:ALA:O	1:B:164:ALA:HB3	2.18	0.44
1:B:162:GLU:OE1	1:B:162:GLU:CA	2.66	0.44
1:B:355:LYS:NZ	1:B:578:GLU:O	2.51	0.44
1:B:355:LYS:HZ1	1:B:578:GLU:HG3	1.83	0.44
1:B:476:ARG:O	1:B:479:GLU:N	2.51	0.44
1:B:585:GLU:C	1:B:587:PHE:N	2.71	0.44
1:C:147:LEU:HD21	1:C:151:PRO:CG	2.46	0.44
1:C:218:ILE:CD1	1:C:250:CYS:SG	2.91	0.44
1:C:266:SER:C	1:C:268:VAL:N	2.70	0.44
1:C:290:GLU:CD	1:D:226:VAL:HG11	2.37	0.44
1:E:272:ASN:C	1:E:272:ASN:OD1	2.55	0.44
1:F:178:PRO:O	1:F:182:HIS:CE1	2.71	0.44
1:F:355:LYS:NZ	1:F:578:GLU:O	2.51	0.44
1:F:589:ARG:CZ	1:F:596:LEU:HD11	2.45	0.44
1:A:192:VAL:O	1:A:298:MET:HA	2.18	0.44
1:A:378:ARG:NH2	1:F:170:GLU:HB2	2.28	0.44
1:A:397:MET:SD	1:A:406:VAL:HG11	2.58	0.44
1:A:467:ASP:O	1:A:471:VAL:HG23	2.18	0.44
1:A:493:ASP:O	1:A:496:GLN:CB	2.65	0.44
1:B:187:ARG:N	1:C:374:LEU:HD11	2.27	0.44
1:B:307:LEU:HD12	1:B:307:LEU:N	2.33	0.44
1:C:518:ALA:HB2	1:D:495:ARG:HA	2.00	0.44
1:C:518:ALA:HB3	1:D:495:ARG:HA	2.00	0.44
1:D:165:LYS:HZ2	1:D:168:LEU:HD23	1.83	0.44
1:D:286:MET:HG3	1:D:287:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:PHE:O	1:D:495:ARG:C	2.56	0.44
1:E:282:LEU:HG	1:E:283:LEU:HD12	2.00	0.44
1:E:450:MET:HG3	1:E:451:MET:H	1.83	0.44
1:F:159:ALA:CA	1:F:333:GLN:HE21	2.31	0.44
1:F:274:GLU:HB2	1:F:275:ARG:H	1.65	0.44
1:F:301:THR:HG23	1:F:303:ARG:H	1.81	0.44
1:A:228:MET:CG	1:A:236:ARG:HH22	2.31	0.43
1:A:282:LEU:HG	1:A:283:LEU:HD12	2.00	0.43
1:A:462:ARG:HG3	1:A:466:LEU:HD11	1.99	0.43
1:A:566:ARG:O	1:A:569:LEU:N	2.51	0.43
1:B:174:PHE:CZ	1:B:294:ALA:CB	3.00	0.43
1:B:297:VAL:CG1	1:B:317:PHE:CZ	3.01	0.43
1:B:357:THR:HB	1:B:360:PHE:CD2	2.53	0.43
1:B:367:ASN:O	1:B:371:GLU:HG2	2.17	0.43
1:B:517:VAL:CG1	1:B:519:TYR:CZ	3.01	0.43
1:B:582:LEU:CD2	1:B:590:VAL:HG21	2.43	0.43
1:C:252:VAL:O	1:C:297:VAL:HA	2.18	0.43
1:C:311:LEU:HA	1:C:311:LEU:HD23	1.68	0.43
1:C:462:ARG:O	1:C:465:LEU:N	2.51	0.43
1:C:527:LEU:HD12	1:C:527:LEU:O	2.18	0.43
1:D:210:ALA:O	1:D:214:ARG:HA	2.18	0.43
1:D:414:ILE:H	1:D:414:ILE:HG12	1.65	0.43
1:D:558:VAL:HG12	1:D:559:LYS:N	2.32	0.43
1:E:370:ASN:OD1	1:E:374:LEU:HD13	2.18	0.43
1:E:449:PHE:CB	1:E:468:GLN:HE21	2.28	0.43
1:F:343:PRO:HG2	1:F:383:LYS:CA	2.43	0.43
1:F:411:ASP:O	1:F:414:ILE:HG13	2.18	0.43
1:F:428:PHE:HE1	1:F:432:ALA:C	2.20	0.43
1:A:180:ARG:O	1:A:184:MET:HE2	2.18	0.43
1:B:159:ALA:HB1	1:B:333:GLN:HG3	1.98	0.43
1:B:348:VAL:HG21	1:B:386:MET:HE2	2.00	0.43
1:B:563:LEU:CD1	1:B:563:LEU:C	2.87	0.43
1:C:153:VAL:HG13	1:C:157:ASP:CB	2.48	0.43
1:D:158:VAL:HG11	1:D:205:LEU:HD11	2.00	0.43
1:D:196:GLY:O	1:D:302:ASN:HA	2.17	0.43
1:D:297:VAL:CG1	1:D:317:PHE:CZ	3.01	0.43
1:D:538:GLU:HB2	1:E:541:LYS:NZ	2.34	0.43
1:E:357:THR:C	1:E:360:PHE:HD1	2.21	0.43
1:E:503:ARG:CD	1:E:508:TRP:CE2	3.00	0.43
1:E:574:GLU:OE1	1:E:575:THR:N	2.51	0.43
1:F:361:VAL:HG13	1:F:364:ASP:CG	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:LEU:O	1:F:390:GLU:C	2.56	0.43
1:F:453:ARG:HH12	1:F:495:ARG:NH2	2.08	0.43
1:A:397:MET:HG3	1:A:406:VAL:CG1	2.47	0.43
1:A:445:ARG:O	1:A:448:GLY:N	2.51	0.43
1:A:454:ARG:HB2	1:A:460:TRP:HH2	1.84	0.43
1:A:541:LYS:HD3	1:F:538:GLU:CB	2.48	0.43
1:A:587:PHE:HD2	1:A:588:GLN:N	2.15	0.43
1:B:237:VAL:HG21	1:B:281:GLN:HG3	1.98	0.43
1:B:261:GLY:O	1:B:308:ASP:HB3	2.18	0.43
1:B:393:ALA:O	1:B:397:MET:HB3	2.18	0.43
1:C:174:PHE:HB2	1:C:181:PHE:CZ	2.53	0.43
1:C:200:VAL:HG11	1:C:323:ILE:HG13	2.00	0.43
1:C:238:ARG:HG2	1:C:242:GLU:OE2	2.18	0.43
1:C:261:GLY:O	1:C:262:ARG:HB2	2.18	0.43
1:C:408:SER:O	1:C:410:ARG:N	2.45	0.43
1:D:194:LEU:HD23	1:D:323:ILE:CD1	2.49	0.43
1:D:307:LEU:HD12	1:D:307:LEU:N	2.32	0.43
1:D:589:ARG:C	1:D:591:VAL:N	2.70	0.43
1:D:595:PRO:C	1:D:596:LEU:HD12	2.38	0.43
1:E:346:GLU:CD	1:E:347:ASP:N	2.71	0.43
1:E:511:HIS:C	1:E:512:PRO:O	2.56	0.43
1:F:194:LEU:HD23	1:F:323:ILE:CD1	2.48	0.43
1:F:360:PHE:CE1	1:F:364:ASP:HB3	2.54	0.43
1:A:371:GLU:OE2	1:A:395:ARG:HD2	2.17	0.43
1:A:425:ALA:C	1:A:427:HIS:N	2.72	0.43
1:A:453:ARG:NH1	1:A:460:TRP:NE1	2.66	0.43
1:B:173:GLU:O	1:B:176:LYS:N	2.52	0.43
1:B:176:LYS:HE2	1:B:176:LYS:HB3	1.83	0.43
1:B:210:ALA:O	1:B:214:ARG:CA	2.67	0.43
1:B:235:ALA:HA	1:B:238:ARG:NE	2.33	0.43
1:B:428:PHE:C	1:B:428:PHE:HD1	2.21	0.43
1:B:436:HIS:O	1:B:437:LYS:CG	2.64	0.43
1:B:452:PRO:O	1:B:456:ASP:CA	2.67	0.43
1:C:411:ASP:O	1:C:415:THR:OG1	2.28	0.43
1:C:443:ARG:O	1:C:443:ARG:HG2	2.18	0.43
1:C:585:GLU:O	1:C:588:GLN:N	2.51	0.43
1:C:586:GLU:HA	1:C:589:ARG:CB	2.49	0.43
1:D:204:HIS:CD2	2:D:2001:ADP:H2'	2.53	0.43
1:D:468:GLN:O	1:D:471:VAL:N	2.51	0.43
1:D:589:ARG:CD	1:D:596:LEU:HD11	2.48	0.43
1:E:408:SER:O	1:E:410:ARG:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:ASP:O	1:E:496:GLN:CB	2.65	0.43
1:E:516:PRO:HB2	1:F:494:PHE:CE1	2.53	0.43
1:F:175:LEU:O	1:F:249:PRO:CG	2.66	0.43
1:F:179:SER:HA	1:F:182:HIS:NE2	2.33	0.43
1:F:297:VAL:CG1	1:F:317:PHE:CE1	3.02	0.43
1:F:325:ALA:CB	1:F:326:PRO:HD3	2.42	0.43
1:F:397:MET:O	1:F:400:PRO:CD	2.66	0.43
1:A:147:LEU:O	1:A:216:PRO:HB3	2.19	0.43
1:A:346:GLU:CD	1:A:347:ASP:N	2.71	0.43
1:B:183:GLU:OE1	1:B:184:MET:HB3	2.17	0.43
1:B:200:VAL:HA	1:B:361:VAL:HG23	2.00	0.43
1:B:248:ALA:HB1	1:B:294:ALA:HB3	1.99	0.43
1:B:375:LEU:HD21	1:B:388:ASP:O	2.18	0.43
1:B:428:PHE:CZ	1:B:433:ASP:N	2.87	0.43
1:B:455:GLU:O	1:B:455:GLU:HG2	2.19	0.43
1:C:145:ARG:CB	1:C:145:ARG:HH11	2.30	0.43
1:C:327:ASP:OD1	1:C:329:LYS:N	2.51	0.43
1:C:358:PRO:CA	1:C:359:GLY:C	2.84	0.43
1:C:382:ARG:HG3	1:C:383:LYS:CA	2.48	0.43
1:D:149:GLU:O	1:D:150:ALA:C	2.57	0.43
1:D:248:ALA:HB1	1:D:294:ALA:HB3	2.00	0.43
1:D:428:PHE:CE1	1:D:433:ASP:N	2.87	0.43
1:E:228:MET:CG	1:E:236:ARG:HH22	2.31	0.43
1:E:327:ASP:OD1	1:E:329:LYS:N	2.51	0.43
1:E:336:ARG:O	1:E:337:ILE:C	2.55	0.43
1:F:342:LYS:HA	1:F:342:LYS:HD2	1.66	0.43
1:F:559:LYS:O	1:F:563:LEU:HB2	2.18	0.43
1:F:568:VAL:HG13	1:F:591:VAL:HA	2.00	0.43
1:A:227:GLU:CG	1:F:263:LYS:NZ	2.67	0.43
1:A:346:GLU:OE1	1:A:347:ASP:N	2.44	0.43
1:A:574:GLU:O	1:A:575:THR:C	2.57	0.43
1:B:170:GLU:HG2	1:B:171:ILE:N	2.33	0.43
1:B:247:HIS:O	1:B:249:PRO:O	2.36	0.43
1:B:391:GLU:O	1:B:395:ARG:CB	2.66	0.43
1:B:478:ALA:O	1:B:479:GLU:C	2.57	0.43
1:B:559:LYS:O	1:B:563:LEU:HB2	2.18	0.43
1:C:188:ILE:HG22	1:C:190:LYS:H	1.84	0.43
1:C:344:LEU:HB3	1:C:348:VAL:HG11	2.00	0.43
1:C:357:THR:O	1:C:360:PHE:CD1	2.72	0.43
1:C:596:LEU:HG	1:C:597:GLU:N	2.34	0.43
1:D:177:ASN:OD1	1:D:180:ARG:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:VAL:HA	1:D:361:VAL:HG23	2.01	0.43
1:D:428:PHE:C	1:D:428:PHE:HD1	2.22	0.43
1:E:361:VAL:HG12	1:E:364:ASP:HB2	1.99	0.43
1:E:361:VAL:O	1:E:365:LEU:HG	2.18	0.43
1:E:570:GLU:O	1:E:571:ARG:C	2.57	0.43
1:A:145:ARG:CB	1:A:145:ARG:HH11	2.32	0.43
1:A:225:PHE:CE1	1:A:233:GLY:O	2.72	0.43
1:A:228:MET:SD	1:A:236:ARG:NH2	2.89	0.43
1:A:286:MET:HA	1:A:289:PHE:CE2	2.54	0.43
1:B:374:LEU:HD23	1:B:374:LEU:C	2.38	0.43
1:B:399:LEU:O	1:B:402:LYS:HB3	2.19	0.43
1:C:462:ARG:HH11	1:C:510:MET:HB3	1.84	0.43
1:D:241:PHE:C	1:D:243:THR:N	2.71	0.43
1:D:428:PHE:CE1	1:D:432:ALA:HB3	2.52	0.43
1:E:261:GLY:O	1:E:262:ARG:HB2	2.19	0.43
1:E:451:MET:HB2	1:E:452:PRO:CD	2.47	0.43
1:E:454:ARG:HB2	1:E:460:TRP:HH2	1.84	0.43
1:E:512:PRO:HB2	1:E:514:PHE:CD2	2.54	0.43
1:F:202:LYS:N	2:F:2001:ADP:O1A	2.52	0.43
1:F:225:PHE:CG	1:F:236:ARG:NH1	2.86	0.43
1:F:228:MET:SD	1:F:232:VAL:CG1	3.04	0.43
1:F:297:VAL:CG1	1:F:317:PHE:CZ	3.01	0.43
1:F:355:LYS:HD2	1:F:355:LYS:HA	1.46	0.43
1:A:287:ASP:N	1:A:287:ASP:OD1	2.51	0.43
1:A:332:GLU:O	1:A:335:LEU:HB2	2.19	0.43
1:A:408:SER:O	1:A:410:ARG:N	2.47	0.43
1:A:449:PHE:CE2	1:A:496:GLN:CD	2.92	0.43
1:A:471:VAL:O	1:A:474:ALA:HB3	2.19	0.43
1:A:480:GLU:OE1	1:A:555:TYR:OH	2.30	0.43
1:A:587:PHE:CD2	1:A:587:PHE:C	2.92	0.43
1:B:257:ILE:HG22	1:B:261:GLY:H	1.83	0.43
1:B:597:GLU:O	1:B:599:PRO:CD	2.66	0.43
1:C:503:ARG:HD2	1:C:508:TRP:CD2	2.52	0.43
1:D:342:LYS:HA	1:D:342:LYS:HD2	1.66	0.43
1:D:394:ASP:HA	1:D:397:MET:HE2	1.98	0.43
1:D:417:TYR:CZ	1:D:482:VAL:HG21	2.54	0.43
1:D:428:PHE:CD1	1:D:428:PHE:C	2.92	0.43
1:D:583:THR:HG22	1:D:586:GLU:OE1	2.19	0.43
1:E:177:ASN:HA	1:E:178:PRO:HD2	1.91	0.43
1:E:327:ASP:OD1	1:E:327:ASP:C	2.57	0.43
1:E:372:ALA:O	1:E:375:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:ARG:CG	1:E:508:TRP:CE3	3.02	0.43
1:F:503:ARG:HA	1:F:503:ARG:HD3	1.58	0.43
1:A:200:VAL:HG13	1:A:323:ILE:HG13	2.00	0.43
1:A:378:ARG:NH2	1:F:170:GLU:CA	2.80	0.43
1:B:164:ALA:C	1:B:168:LEU:HD13	2.37	0.43
1:B:165:LYS:CE	1:B:205:LEU:HG	2.48	0.43
1:B:178:PRO:O	1:B:182:HIS:CE1	2.72	0.43
1:B:225:PHE:CB	1:B:236:ARG:NH1	2.79	0.43
1:B:307:LEU:CD1	1:B:307:LEU:H	2.31	0.43
1:B:338:HIS:HB3	1:B:369:LEU:HD12	2.00	0.43
1:B:449:PHE:HZ	1:B:496:GLN:OE1	2.01	0.43
1:B:523:GLU:O	1:B:530:TYR:N	2.43	0.43
1:C:203:THR:OG1	1:C:204:HIS:N	2.52	0.43
1:C:204:HIS:CD2	2:C:1001:ADP:C2	3.07	0.43
1:C:371:GLU:CG	1:C:392:ALA:HB1	2.40	0.43
1:C:399:LEU:N	1:C:400:PRO:CD	2.81	0.43
1:C:448:GLY:O	1:C:452:PRO:CD	2.52	0.43
1:C:483:PHE:C	1:C:485:ASP:H	2.23	0.43
1:D:235:ALA:HA	1:D:238:ARG:HD3	2.00	0.43
1:D:255:ASP:OD1	1:D:256:GLU:N	2.52	0.43
1:D:355:LYS:HA	1:D:355:LYS:HD2	1.44	0.43
1:D:568:VAL:HG11	1:D:591:VAL:HG13	2.00	0.43
1:E:234:ALA:HB1	1:E:281:GLN:HG2	2.01	0.43
1:E:252:VAL:O	1:E:297:VAL:HA	2.19	0.43
1:E:274:GLU:C	1:E:277:GLN:HB3	2.36	0.43
1:E:344:LEU:HB3	1:E:348:VAL:HG11	1.99	0.43
1:E:438:VAL:HG22	1:E:582:LEU:HB2	2.01	0.43
1:E:445:ARG:O	1:E:447:LEU:N	2.52	0.43
1:F:458:LEU:HD11	1:F:460:TRP:HB3	2.01	0.43
1:F:585:GLU:O	1:F:586:GLU:C	2.55	0.43
1:F:585:GLU:O	1:F:587:PHE:N	2.52	0.43
1:F:594:LEU:C	1:F:594:LEU:HD23	2.39	0.43
1:A:337:ILE:CD1	1:A:338:HIS:CD2	3.01	0.43
1:A:372:ALA:CB	1:A:389:LEU:HD23	2.48	0.43
1:A:411:ASP:O	1:A:415:THR:OG1	2.29	0.43
1:A:453:ARG:NH1	1:A:460:TRP:HE1	2.16	0.43
1:B:169:LYS:O	1:B:172:VAL:HG22	2.19	0.43
1:B:215:VAL:CG2	1:B:216:PRO:CD	2.87	0.43
1:B:238:ARG:HH11	1:B:238:ARG:CB	2.32	0.43
1:B:382:ARG:HA	1:B:382:ARG:HD2	1.08	0.43
1:B:539:THR:O	1:B:543:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:VAL:O	1:C:348:VAL:HG12	2.18	0.43
1:C:460:TRP:HD1	1:C:464:ARG:NH1	2.13	0.43
1:C:480:GLU:OE1	1:C:555:TYR:OH	2.31	0.43
1:C:500:LEU:O	1:C:504:MET:HG2	2.19	0.43
1:D:203:THR:HG23	1:D:253:PHE:CE1	2.53	0.43
1:D:422:HIS:CD2	1:D:475:GLY:CA	3.02	0.43
1:D:471:VAL:O	1:D:474:ALA:CB	2.58	0.43
1:D:533:ARG:NH1	1:D:535:TYR:CD1	2.86	0.43
1:E:400:PRO:HG2	1:E:405:LEU:CD1	2.44	0.43
1:E:479:GLU:OE2	1:E:487:THR:HA	2.19	0.43
1:F:160:GLY:N	1:F:333:GLN:NE2	2.66	0.43
1:F:367:ASN:O	1:F:371:GLU:HG2	2.19	0.43
1:A:308:ASP:OD1	1:A:310:ALA:CB	2.67	0.42
1:A:399:LEU:N	1:A:400:PRO:CD	2.83	0.42
1:A:453:ARG:HH11	1:A:460:TRP:HZ2	1.57	0.42
1:A:462:ARG:CG	1:A:463:LYS:N	2.81	0.42
1:B:188:ILE:HD13	1:B:188:ILE:HA	1.80	0.42
1:B:411:ASP:O	1:B:414:ILE:HG13	2.18	0.42
1:B:428:PHE:CE1	1:B:433:ASP:N	2.87	0.42
1:B:449:PHE:CE2	1:B:453:ARG:CZ	3.01	0.42
1:B:554:GLN:OE1	1:B:554:GLN:HA	2.19	0.42
1:C:263:LYS:CG	1:C:264:ARG:H	2.29	0.42
1:C:264:ARG:HD2	1:C:266:SER:CB	2.49	0.42
1:C:297:VAL:HG23	1:C:317:PHE:CE1	2.54	0.42
1:C:350:LEU:H	1:C:350:LEU:HG	1.48	0.42
1:D:173:GLU:O	1:D:176:LYS:N	2.51	0.42
1:D:253:PHE:HA	1:D:298:MET:CB	2.46	0.42
1:D:518:ALA:CB	1:E:495:ARG:HA	2.48	0.42
1:E:147:LEU:HD21	1:E:151:PRO:CG	2.45	0.42
1:E:188:ILE:O	1:E:190:LYS:NZ	2.42	0.42
1:E:346:GLU:OE1	1:E:347:ASP:N	2.45	0.42
1:E:355:LYS:HA	1:E:355:LYS:HD3	1.88	0.42
1:E:493:ASP:N	1:E:493:ASP:OD1	2.50	0.42
1:E:527:LEU:O	1:E:530:TYR:OH	2.30	0.42
1:E:574:GLU:O	1:E:575:THR:C	2.57	0.42
1:F:190:LYS:CD	1:F:289:PHE:CZ	3.02	0.42
1:F:301:THR:HG23	1:F:302:ASN:N	2.34	0.42
1:F:353:LEU:O	1:F:357:THR:CG2	2.66	0.42
1:A:153:VAL:HG13	1:A:157:ASP:CB	2.48	0.42
1:A:336:ARG:O	1:A:337:ILE:C	2.58	0.42
1:B:147:LEU:HD13	1:B:149:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:PRO:HG3	1:B:247:HIS:CE1	2.53	0.42
1:B:253:PHE:HA	1:B:298:MET:CB	2.47	0.42
1:B:321:ILE:HD12	1:B:321:ILE:HA	1.82	0.42
1:B:538:GLU:C	1:B:540:ALA:N	2.72	0.42
1:C:172:VAL:HG22	1:C:173:GLU:N	2.34	0.42
1:C:236:ARG:O	1:C:239:ASP:N	2.52	0.42
1:C:334:ILE:HD11	2:C:1001:ADP:N6	2.34	0.42
1:C:410:ARG:CG	1:C:411:ASP:N	2.79	0.42
1:C:508:TRP:HD1	1:D:491:GLU:HG2	1.84	0.42
1:D:159:ALA:CA	1:D:333:GLN:HE21	2.32	0.42
1:D:187:ARG:H	1:E:374:LEU:HD11	1.82	0.42
1:D:352:LEU:HD11	1:D:356:ARG:NH1	2.33	0.42
1:D:376:ALA:HA	1:D:381:ARG:NH1	2.34	0.42
1:E:480:GLU:OE1	1:E:555:TYR:OH	2.29	0.42
1:F:175:LEU:O	1:F:249:PRO:HB2	2.19	0.42
1:F:257:ILE:HG22	1:F:261:GLY:H	1.84	0.42
1:F:455:GLU:O	1:F:455:GLU:HG2	2.19	0.42
1:F:536:SER:O	1:F:538:GLU:N	2.51	0.42
1:B:215:VAL:HG21	1:B:249:PRO:C	2.38	0.42
1:B:397:MET:O	1:B:400:PRO:CD	2.68	0.42
1:C:157:ASP:OD1	1:C:157:ASP:N	2.51	0.42
1:C:234:ALA:HB1	1:C:281:GLN:HG2	2.01	0.42
1:C:237:VAL:HG13	1:C:238:ARG:N	2.34	0.42
1:D:488:THR:O	1:D:490:ALA:N	2.53	0.42
1:E:157:ASP:N	1:E:157:ASP:OD1	2.51	0.42
1:E:168:LEU:O	1:E:171:ILE:CG1	2.67	0.42
1:E:234:ALA:O	1:E:237:VAL:CG1	2.65	0.42
1:E:316:ARG:O	1:E:318:ASP:N	2.51	0.42
1:E:416:ALA:HB2	1:E:577:LEU:CD2	2.11	0.42
1:E:424:LEU:HD12	1:E:424:LEU:HA	1.83	0.42
1:E:462:ARG:HG3	1:E:463:LYS:N	2.28	0.42
1:F:193:LEU:HB3	1:F:317:PHE:CD2	2.54	0.42
1:F:205:LEU:HA	1:F:208:ALA:HB3	2.02	0.42
1:F:238:ARG:O	1:F:239:ASP:C	2.56	0.42
1:F:286:MET:SD	1:F:316:ARG:HG3	2.59	0.42
1:F:506:THR:OG1	1:F:520:ALA:HB3	2.19	0.42
1:F:532:VAL:HG13	1:F:532:VAL:O	2.19	0.42
1:A:147:LEU:HB3	1:A:217:PHE:O	2.19	0.42
1:A:169:LYS:HA	1:A:172:VAL:HG13	2.01	0.42
1:A:215:VAL:HG21	1:A:250:CYS:CB	2.49	0.42
1:A:236:ARG:CG	1:A:237:VAL:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:C	1:A:238:ARG:N	2.71	0.42
1:A:372:ALA:O	1:A:375:LEU:HB3	2.20	0.42
1:A:458:LEU:C	1:A:458:LEU:HD12	2.39	0.42
1:B:159:ALA:CA	1:B:333:GLN:HE21	2.32	0.42
1:B:228:MET:O	1:B:229:PHE:HB2	2.20	0.42
1:B:256:GLU:CG	1:B:256:GLU:O	2.67	0.42
1:B:417:TYR:CZ	1:B:482:VAL:HG21	2.55	0.42
1:C:471:VAL:O	1:C:474:ALA:HB3	2.20	0.42
1:D:225:PHE:CG	1:D:236:ARG:NH1	2.88	0.42
1:D:328:VAL:HG21	1:D:579:ARG:HA	2.01	0.42
1:E:200:VAL:HG11	1:E:323:ILE:HG13	2.01	0.42
1:E:236:ARG:CG	1:E:237:VAL:H	2.19	0.42
1:E:237:VAL:HG13	1:E:238:ARG:N	2.35	0.42
1:F:215:VAL:O	1:F:216:PRO:C	2.56	0.42
1:F:319:ARG:NH1	1:F:319:ARG:HB3	2.35	0.42
1:F:348:VAL:CG2	1:F:352:LEU:CD1	2.98	0.42
1:F:563:LEU:C	1:F:563:LEU:CD1	2.88	0.42
1:A:344:LEU:HB3	1:A:348:VAL:HG11	2.01	0.42
1:A:350:LEU:H	1:A:350:LEU:HG	1.47	0.42
1:A:445:ARG:C	1:A:447:LEU:N	2.73	0.42
1:A:454:ARG:HD3	1:A:454:ARG:C	2.39	0.42
1:A:463:LYS:HB2	1:B:486:VAL:HG11	2.00	0.42
1:B:458:LEU:HG	1:B:460:TRP:CE3	2.55	0.42
1:B:464:ARG:O	1:B:467:ASP:N	2.51	0.42
1:B:558:VAL:HG12	1:B:559:LYS:N	2.33	0.42
1:C:225:PHE:CE1	1:C:236:ARG:NH1	2.87	0.42
1:C:274:GLU:O	1:C:277:GLN:CB	2.54	0.42
1:C:336:ARG:O	1:C:337:ILE:C	2.57	0.42
1:C:425:ALA:C	1:C:427:HIS:N	2.71	0.42
1:C:527:LEU:O	1:C:530:TYR:OH	2.31	0.42
1:C:581:THR:O	1:C:582:LEU:CD1	2.66	0.42
1:C:587:PHE:CD2	1:C:588:GLN:N	2.88	0.42
1:D:147:LEU:HD13	1:D:149:GLU:OE1	2.19	0.42
1:D:178:PRO:O	1:D:182:HIS:CE1	2.72	0.42
1:D:311:LEU:C	1:D:316:ARG:HG2	2.31	0.42
1:D:373:ALA:CA	1:D:384:ILE:HD11	2.49	0.42
1:E:174:PHE:O	1:E:177:ASN:C	2.58	0.42
1:E:264:ARG:HB3	1:E:265:GLY:H	1.50	0.42
1:E:302:ASN:HB3	1:E:443:ARG:NH1	2.35	0.42
1:E:582:LEU:HA	1:E:586:GLU:OE2	2.20	0.42
2:E:1001:ADP:N3	2:E:1001:ADP:H2'	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:THR:HG23	1:F:253:PHE:CE1	2.54	0.42
1:F:216:PRO:HG3	1:F:247:HIS:CE1	2.53	0.42
1:F:233:GLY:O	1:F:236:ARG:NH2	2.53	0.42
1:F:328:VAL:HG22	1:F:355:LYS:CD	2.49	0.42
1:F:399:LEU:O	1:F:402:LYS:HB3	2.20	0.42
1:A:188:ILE:CG2	1:A:189:PRO:HD2	2.50	0.42
1:B:155:PHE:O	1:B:156:LYS:C	2.57	0.42
1:B:193:LEU:HB3	1:B:317:PHE:CD2	2.54	0.42
1:B:199:GLY:O	1:B:361:VAL:HG22	2.19	0.42
1:B:215:VAL:O	1:B:216:PRO:C	2.55	0.42
1:B:476:ARG:HD3	1:B:494:PHE:HZ	1.85	0.42
1:B:477:ALA:O	1:B:478:ALA:C	2.55	0.42
1:C:273:ASP:OD1	1:C:273:ASP:C	2.58	0.42
1:D:414:ILE:O	1:D:415:THR:C	2.57	0.42
1:E:586:GLU:CA	1:E:589:ARG:HG3	2.41	0.42
1:F:215:VAL:HG21	1:F:249:PRO:C	2.38	0.42
1:F:344:LEU:CG	1:F:346:GLU:OE1	2.67	0.42
1:F:357:THR:HG1	1:F:360:PHE:HD2	1.65	0.42
1:F:455:GLU:O	1:F:456:ASP:C	2.58	0.42
1:F:464:ARG:O	1:F:467:ASP:N	2.53	0.42
1:F:517:VAL:CG2	1:F:518:ALA:N	2.81	0.42
1:A:251:ILE:HG23	1:A:296:VAL:HG23	2.01	0.42
1:A:271:GLY:O	1:A:275:ARG:NE	2.50	0.42
1:A:327:ASP:OD1	1:A:327:ASP:C	2.57	0.42
1:A:338:HIS:ND1	1:A:366:GLU:HB2	2.35	0.42
1:A:408:SER:CB	1:A:409:PRO:HD2	2.45	0.42
1:A:462:ARG:O	1:A:466:LEU:HD12	2.19	0.42
1:A:470:ALA:C	1:A:558:VAL:HG21	2.39	0.42
1:A:561:LEU:O	1:A:564:GLU:HB3	2.19	0.42
1:B:165:LYS:CE	1:B:205:LEU:CG	2.98	0.42
1:B:205:LEU:HA	1:B:208:ALA:HB3	2.02	0.42
1:B:428:PHE:C	1:B:428:PHE:CD1	2.92	0.42
1:C:155:PHE:HZ	1:C:209:VAL:CG2	2.31	0.42
1:D:155:PHE:HB2	1:D:158:VAL:HB	2.01	0.42
1:D:361:VAL:HG13	1:D:364:ASP:CG	2.40	0.42
1:E:449:PHE:CD1	1:E:468:GLN:NE2	2.87	0.42
1:F:529:GLY:O	1:F:530:TYR:CB	2.58	0.42
1:A:155:PHE:CZ	1:A:209:VAL:CG2	3.03	0.42
1:A:381:ARG:CG	1:A:382:ARG:N	2.81	0.42
1:A:582:LEU:HA	1:A:586:GLU:OE2	2.19	0.42
1:B:197:PRO:HD2	1:B:200:VAL:CG1	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:VAL:HG23	1:B:580:GLU:CG	2.47	0.42
1:B:373:ALA:CA	1:B:384:ILE:HD11	2.49	0.42
1:C:194:LEU:H	1:C:194:LEU:HD12	1.85	0.42
1:C:361:VAL:HG22	1:C:362:GLY:N	2.35	0.42
1:C:589:ARG:HH22	1:C:596:LEU:N	2.17	0.42
1:D:307:LEU:H	1:D:307:LEU:HD12	1.85	0.42
1:D:355:LYS:HZ3	1:D:578:GLU:HG3	1.85	0.42
1:D:563:LEU:C	1:D:563:LEU:CD1	2.87	0.42
1:E:145:ARG:CB	1:E:145:ARG:HH11	2.32	0.42
1:E:147:LEU:HD12	1:E:148:THR:N	2.35	0.42
1:E:222:GLY:O	1:E:225:PHE:HB2	2.20	0.42
1:F:164:ALA:C	1:F:168:LEU:HD13	2.36	0.42
1:F:236:ARG:O	1:F:237:VAL:C	2.58	0.42
1:F:417:TYR:CZ	1:F:482:VAL:HG21	2.55	0.42
1:A:180:ARG:H	1:A:180:ARG:HG2	1.50	0.42
1:A:252:VAL:HB	1:A:297:VAL:HA	2.01	0.42
1:A:356:ARG:C	1:A:358:PRO:HD2	2.40	0.42
1:A:407:LEU:HA	1:A:411:ASP:HB2	2.02	0.42
1:B:157:ASP:O	1:B:204:HIS:CE1	2.73	0.42
1:B:376:ALA:C	1:B:381:ARG:CB	2.84	0.42
1:B:533:ARG:HG3	1:B:533:ARG:NH1	2.31	0.42
1:C:216:PRO:HG2	1:C:247:HIS:CD2	2.55	0.42
1:C:325:ALA:O	1:C:327:ASP:N	2.53	0.42
1:C:332:GLU:HA	1:C:335:LEU:HD12	2.02	0.42
1:C:453:ARG:NH2	1:C:464:ARG:CZ	2.82	0.42
1:D:162:GLU:OE1	1:D:162:GLU:CA	2.68	0.42
1:D:200:VAL:HG12	1:D:325:ALA:CB	2.50	0.42
1:D:238:ARG:NH1	1:D:239:ASP:CA	2.69	0.42
1:D:238:ARG:HA	1:D:241:PHE:HE2	1.84	0.42
1:D:360:PHE:CE1	1:D:364:ASP:HB3	2.53	0.42
1:D:375:LEU:HD21	1:D:388:ASP:O	2.19	0.42
1:D:449:PHE:CZ	1:D:453:ARG:NH2	2.88	0.42
1:D:478:ALA:O	1:D:482:VAL:HG12	2.20	0.42
1:E:163:GLU:H	1:E:163:GLU:CD	2.08	0.42
1:E:175:LEU:O	1:E:175:LEU:HD12	2.20	0.42
1:E:204:HIS:CD2	2:E:1001:ADP:C2	3.07	0.42
1:E:253:PHE:HA	1:E:298:MET:O	2.20	0.42
1:F:172:VAL:O	1:F:175:LEU:HB2	2.20	0.42
1:F:173:GLU:O	1:F:176:LYS:N	2.50	0.42
1:F:253:PHE:HA	1:F:298:MET:CB	2.45	0.42
1:F:307:LEU:N	1:F:307:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:PRO:O	1:F:403:LYS:N	2.52	0.42
1:F:567:GLU:O	1:F:568:VAL:C	2.59	0.42
1:A:277:GLN:CG	1:A:278:THR:N	2.83	0.42
1:A:311:LEU:HD23	1:A:316:ARG:HH21	1.75	0.42
1:B:157:ASP:O	1:B:204:HIS:HE1	2.03	0.42
1:B:168:LEU:O	1:B:171:ILE:N	2.52	0.42
1:B:388:ASP:OD1	1:B:388:ASP:N	2.48	0.42
1:B:589:ARG:CZ	1:B:596:LEU:CD2	2.97	0.42
1:C:215:VAL:HG21	1:C:250:CYS:CB	2.49	0.42
1:C:250:CYS:HB3	1:C:295:ILE:HG13	2.01	0.42
1:C:252:VAL:HB	1:C:297:VAL:HA	2.02	0.42
1:C:264:ARG:HD2	1:C:266:SER:HB2	2.00	0.42
1:C:333:GLN:HA	1:C:336:ARG:NH2	2.35	0.42
1:D:154:THR:HG23	1:D:156:LYS:N	2.35	0.42
1:D:214:ARG:CB	1:D:214:ARG:NH1	2.80	0.42
1:D:233:GLY:O	1:D:236:ARG:NH2	2.52	0.42
1:D:449:PHE:HZ	1:D:496:GLN:OE1	2.03	0.42
1:D:452:PRO:O	1:D:456:ASP:CG	2.59	0.42
1:D:453:ARG:CZ	1:D:495:ARG:NH2	2.57	0.42
1:E:174:PHE:HZ	1:E:294:ALA:HB1	1.85	0.42
1:E:180:ARG:H	1:E:180:ARG:HG2	1.51	0.42
1:E:180:ARG:O	1:E:184:MET:HE2	2.19	0.42
1:E:461:SER:OG	1:F:486:VAL:HG11	2.19	0.42
1:E:571:ARG:O	1:E:575:THR:HG23	2.20	0.42
1:F:333:GLN:O	1:F:336:ARG:CB	2.65	0.42
1:A:172:VAL:HG22	1:A:173:GLU:N	2.35	0.41
1:A:174:PHE:CG	1:A:175:LEU:N	2.85	0.41
1:A:203:THR:OG1	1:A:204:HIS:N	2.52	0.41
1:A:222:GLY:O	1:A:225:PHE:HB2	2.19	0.41
1:A:361:VAL:HG22	1:A:362:GLY:N	2.35	0.41
1:A:382:ARG:HG2	1:A:383:LYS:H	1.84	0.41
1:A:464:ARG:NH1	1:A:464:ARG:CG	2.80	0.41
1:B:255:ASP:OD1	1:B:256:GLU:N	2.53	0.41
1:B:355:LYS:HA	1:B:355:LYS:HD3	1.68	0.41
1:B:536:SER:O	1:B:538:GLU:N	2.53	0.41
1:C:332:GLU:O	1:C:335:LEU:HB2	2.20	0.41
1:C:442:PRO:HB3	1:C:445:ARG:NH2	2.34	0.41
1:C:447:LEU:CB	1:C:496:GLN:HE22	2.33	0.41
1:C:586:GLU:HA	1:C:589:ARG:HB2	2.02	0.41
1:D:206:ALA:O	1:D:209:VAL:CG1	2.67	0.41
1:D:477:ALA:O	1:D:478:ALA:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:PHE:HB2	1:E:181:PHE:CZ	2.55	0.41
1:E:228:MET:HG3	1:E:236:ARG:HH22	1.85	0.41
1:E:356:ARG:C	1:E:358:PRO:HD2	2.39	0.41
1:E:468:GLN:O	1:E:471:VAL:HB	2.20	0.41
1:F:241:PHE:CZ	1:F:285:GLU:OE2	2.73	0.41
1:F:350:LEU:O	1:F:353:LEU:N	2.53	0.41
1:B:301:THR:HG23	1:B:302:ASN:N	2.35	0.41
1:B:332:GLU:CD	1:B:351:ALA:HA	2.41	0.41
1:B:500:LEU:O	1:B:503:ARG:CB	2.68	0.41
1:B:508:TRP:O	1:B:509:GLY:C	2.58	0.41
1:C:236:ARG:HH11	1:C:236:ARG:CB	2.32	0.41
1:C:313:ARG:NH1	1:C:526:TYR:C	2.66	0.41
1:C:462:ARG:O	1:C:466:LEU:HD12	2.20	0.41
1:C:566:ARG:O	1:C:567:GLU:C	2.56	0.41
1:D:153:VAL:O	1:D:154:THR:HB	2.20	0.41
1:D:202:LYS:CD	2:D:2001:ADP:O2B	2.68	0.41
1:D:235:ALA:O	1:D:238:ARG:NH1	2.53	0.41
1:D:319:ARG:NH1	1:D:319:ARG:HB3	2.36	0.41
1:D:349:ASP:C	1:D:350:LEU:HG	2.40	0.41
1:D:525:THR:HG22	1:D:526:TYR:HD2	1.84	0.41
1:E:200:VAL:HG13	1:E:323:ILE:HG13	2.01	0.41
1:E:442:PRO:CG	1:E:443:ARG:H	2.33	0.41
1:E:589:ARG:HH22	1:E:596:LEU:CA	2.30	0.41
1:F:158:VAL:HG13	1:F:205:LEU:HD11	2.02	0.41
1:F:307:LEU:CD1	1:F:307:LEU:H	2.32	0.41
1:F:344:LEU:CD1	1:F:346:GLU:OE1	2.68	0.41
1:F:412:ARG:O	1:F:413:ARG:C	2.59	0.41
1:F:500:LEU:O	1:F:503:ARG:CB	2.67	0.41
1:A:345:ALA:CB	1:A:347:ASP:OD1	2.69	0.41
1:A:495:ARG:HD2	1:F:521:VAL:CG1	2.50	0.41
1:A:517:VAL:HG21	1:B:547:VAL:HG12	2.02	0.41
1:B:235:ALA:O	1:B:238:ARG:NH1	2.53	0.41
1:B:236:ARG:O	1:B:237:VAL:C	2.59	0.41
1:C:210:ALA:CB	1:C:217:PHE:CD1	3.04	0.41
1:C:234:ALA:O	1:C:237:VAL:CG1	2.65	0.41
1:C:391:GLU:O	1:C:391:GLU:HG3	2.21	0.41
1:C:512:PRO:HB2	1:C:514:PHE:CD2	2.52	0.41
1:D:205:LEU:HA	1:D:208:ALA:HB3	2.01	0.41
1:D:215:VAL:CG2	1:D:216:PRO:CD	2.86	0.41
1:D:238:ARG:HH11	1:D:238:ARG:CG	2.32	0.41
1:D:346:GLU:OE2	1:D:348:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:VAL:HG22	1:E:274:GLU:HG2	2.03	0.41
1:E:381:ARG:CG	1:E:381:ARG:NH1	2.80	0.41
1:E:407:LEU:HA	1:E:411:ASP:HB2	2.01	0.41
1:E:423:ALA:HB1	1:E:587:PHE:CE1	2.55	0.41
1:F:228:MET:O	1:F:229:PHE:HB2	2.20	0.41
1:F:336:ARG:O	1:F:338:HIS:N	2.53	0.41
1:A:174:PHE:HB2	1:A:181:PHE:CZ	2.56	0.41
1:A:203:THR:HG22	1:A:253:PHE:CZ	2.55	0.41
1:A:279:LEU:HD11	1:A:311:LEU:HD11	2.02	0.41
1:A:448:GLY:O	1:A:452:PRO:CD	2.51	0.41
1:B:154:THR:HG23	1:B:156:LYS:N	2.33	0.41
1:B:190:LYS:CD	1:B:289:PHE:CZ	3.04	0.41
1:B:353:LEU:O	1:B:357:THR:HG23	2.20	0.41
1:B:405:LEU:O	1:B:405:LEU:HD12	2.20	0.41
1:B:538:GLU:O	1:B:540:ALA:N	2.53	0.41
1:C:196:GLY:C	1:C:202:LYS:HZ1	2.19	0.41
1:C:253:PHE:HA	1:C:298:MET:O	2.19	0.41
1:C:305:ASP:OD2	1:C:447:LEU:HD13	2.20	0.41
1:C:445:ARG:O	1:C:448:GLY:N	2.51	0.41
1:C:462:ARG:CG	1:C:463:LYS:N	2.83	0.41
1:C:566:ARG:HG2	1:C:567:GLU:N	2.35	0.41
1:D:155:PHE:O	1:D:156:LYS:C	2.59	0.41
1:D:172:VAL:CG2	1:D:173:GLU:N	2.82	0.41
1:D:249:PRO:O	1:D:250:CYS:HB3	2.20	0.41
1:D:460:TRP:CD1	1:D:464:ARG:HG2	2.54	0.41
1:D:517:VAL:HG13	1:D:519:TYR:CE1	2.55	0.41
1:E:188:ILE:HG22	1:E:189:PRO:CD	2.50	0.41
1:F:280:ASN:O	1:F:283:LEU:HB3	2.19	0.41
1:A:357:THR:C	1:A:360:PHE:HD1	2.24	0.41
1:B:206:ALA:O	1:B:209:VAL:CG1	2.69	0.41
1:B:400:PRO:HB2	1:B:404:SER:OG	2.21	0.41
1:B:402:LYS:HE3	1:B:403:LYS:HG3	2.03	0.41
1:B:453:ARG:HH12	1:B:495:ARG:NH2	2.12	0.41
1:B:508:TRP:O	1:B:510:MET:HG3	2.20	0.41
1:C:277:GLN:CG	1:C:278:THR:N	2.81	0.41
1:C:286:MET:HA	1:C:289:PHE:CE2	2.54	0.41
1:C:491:GLU:O	1:C:492:ASN:C	2.58	0.41
1:C:519:TYR:O	1:C:533:ARG:HG2	2.19	0.41
1:C:549:ARG:O	1:C:550:LEU:C	2.58	0.41
1:D:179:SER:HA	1:D:182:HIS:NE2	2.35	0.41
1:D:237:VAL:HG13	1:D:281:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:THR:HG23	1:D:302:ASN:N	2.36	0.41
1:D:529:GLY:O	1:D:530:TYR:CB	2.55	0.41
1:E:575:THR:HA	1:E:578:GLU:OE1	2.20	0.41
1:F:176:LYS:HB3	1:F:176:LYS:HE2	1.83	0.41
1:A:261:GLY:O	1:A:262:ARG:HB2	2.20	0.41
1:A:328:VAL:HG22	1:A:331:ARG:HH12	1.86	0.41
1:A:331:ARG:NH2	1:A:358:PRO:HG3	2.35	0.41
1:A:519:TYR:O	1:A:533:ARG:HG2	2.20	0.41
1:B:165:LYS:O	1:B:167:GLU:N	2.53	0.41
1:B:206:ALA:HB1	1:B:298:MET:HG2	2.02	0.41
1:B:345:ALA:HB2	1:B:383:LYS:NZ	2.35	0.41
1:B:428:PHE:CD1	1:B:432:ALA:HB3	2.56	0.41
1:C:181:PHE:HA	1:C:184:MET:CE	2.51	0.41
1:C:236:ARG:C	1:C:238:ARG:N	2.71	0.41
1:C:264:ARG:HG2	1:C:267:GLY:H	1.85	0.41
1:C:302:ASN:HB3	1:C:443:ARG:NH1	2.35	0.41
1:C:396:VAL:CG1	1:C:397:MET:N	2.83	0.41
1:C:424:LEU:HD22	1:C:569:LEU:HA	2.02	0.41
1:C:468:GLN:O	1:C:471:VAL:HB	2.20	0.41
1:C:523:GLU:O	1:C:529:GLY:HA2	2.21	0.41
1:D:162:GLU:OE1	1:D:162:GLU:HA	2.19	0.41
1:D:283:LEU:HD13	1:D:316:ARG:HH21	1.82	0.41
1:D:500:LEU:O	1:D:503:ARG:CB	2.69	0.41
1:E:596:LEU:HG	1:E:597:GLU:N	2.36	0.41
1:F:243:THR:CA	1:F:246:ARG:HH21	2.26	0.41
1:F:286:MET:HE2	1:F:315:GLY:O	2.21	0.41
1:F:301:THR:CG2	1:F:302:ASN:N	2.83	0.41
1:F:428:PHE:CE1	1:F:432:ALA:HB3	2.52	0.41
1:A:147:LEU:C	1:A:147:LEU:HD12	2.40	0.41
1:A:168:LEU:HA	1:A:171:ILE:HD12	2.02	0.41
1:A:234:ALA:HB1	1:A:281:GLN:HG2	2.02	0.41
1:B:202:LYS:CD	2:B:2001:ADP:O2B	2.68	0.41
1:B:241:PHE:C	1:B:243:THR:N	2.71	0.41
1:B:327:ASP:HB3	1:B:330:GLY:H	1.86	0.41
1:B:335:LEU:HD23	1:B:365:LEU:HB3	2.00	0.41
1:B:338:HIS:HB3	1:B:369:LEU:HD11	2.03	0.41
1:B:343:PRO:O	1:B:344:LEU:CB	2.68	0.41
1:B:508:TRP:HD1	1:C:491:GLU:HG2	1.85	0.41
1:C:168:LEU:O	1:C:171:ILE:CG1	2.68	0.41
1:C:191:GLY:O	1:C:317:PHE:HA	2.21	0.41
1:C:372:ALA:O	1:C:375:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:MET:SD	1:E:342:LYS:CE	3.08	0.41
1:D:349:ASP:O	1:D:350:LEU:CG	2.68	0.41
1:D:376:ALA:HB2	1:D:381:ARG:HH11	1.79	0.41
1:D:597:GLU:O	1:D:599:PRO:CD	2.66	0.41
1:E:172:VAL:HG22	1:E:173:GLU:N	2.34	0.41
1:E:271:GLY:O	1:E:275:ARG:NE	2.54	0.41
1:E:277:GLN:CG	1:E:278:THR:N	2.83	0.41
1:E:297:VAL:HG23	1:E:317:PHE:CE1	2.56	0.41
1:E:503:ARG:CZ	1:E:522:ARG:CZ	2.99	0.41
1:E:538:GLU:O	1:E:539:THR:C	2.59	0.41
1:E:570:GLU:O	1:E:573:ALA:HB3	2.21	0.41
1:F:150:ALA:HA	1:F:151:PRO:HD2	1.85	0.41
1:F:172:VAL:CG2	1:F:173:GLU:N	2.84	0.41
1:F:241:PHE:C	1:F:243:THR:N	2.72	0.41
1:F:248:ALA:HB1	1:F:294:ALA:HB3	2.02	0.41
1:F:249:PRO:O	1:F:250:CYS:HB3	2.21	0.41
1:F:428:PHE:C	1:F:428:PHE:HD1	2.24	0.41
1:F:452:PRO:O	1:F:456:ASP:CA	2.68	0.41
1:F:551:ILE:HG22	1:F:552:GLU:N	2.35	0.41
1:A:214:ARG:NH1	1:A:214:ARG:CG	2.78	0.41
1:A:218:ILE:CD1	1:A:250:CYS:SG	2.92	0.41
1:A:570:GLU:O	1:A:571:ARG:C	2.58	0.41
1:B:172:VAL:CG2	1:B:173:GLU:N	2.84	0.41
1:B:202:LYS:N	2:B:2001:ADP:O1A	2.52	0.41
1:B:422:HIS:CD2	1:B:475:GLY:CA	3.04	0.41
1:C:180:ARG:O	1:C:184:MET:HE2	2.21	0.41
1:C:200:VAL:HG13	1:C:323:ILE:HG13	2.03	0.41
1:C:212:GLU:C	1:C:214:ARG:HB2	2.41	0.41
1:C:346:GLU:CD	1:C:347:ASP:N	2.72	0.41
1:C:423:ALA:HB1	1:C:436:HIS:HE1	1.85	0.41
1:D:387:LYS:O	1:D:390:GLU:HB3	2.20	0.41
1:D:422:HIS:CD2	1:D:475:GLY:HA3	2.56	0.41
1:D:589:ARG:O	1:D:590:VAL:C	2.58	0.41
1:E:274:GLU:HB3	1:E:275:ARG:H	1.56	0.41
1:E:328:VAL:HG22	1:E:331:ARG:HH12	1.86	0.41
1:E:331:ARG:NH2	1:E:358:PRO:HG3	2.36	0.41
1:E:447:LEU:CA	1:E:496:GLN:NE2	2.82	0.41
1:F:161:ALA:O	1:F:164:ALA:HB3	2.21	0.41
1:F:352:LEU:HD12	1:F:353:LEU:H	1.86	0.41
1:A:157:ASP:OD1	1:A:157:ASP:N	2.53	0.41
1:A:163:GLU:O	1:A:164:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:HG2	1:A:167:GLU:N	2.34	0.41
1:B:307:LEU:HD12	1:B:307:LEU:H	1.86	0.41
1:B:327:ASP:O	1:B:331:ARG:NH2	2.54	0.41
1:B:468:GLN:O	1:B:469:ILE:C	2.59	0.41
1:B:521:VAL:HG12	1:C:495:ARG:HD2	2.03	0.41
1:B:567:GLU:O	1:B:568:VAL:C	2.59	0.41
1:B:572:VAL:HG11	1:B:587:PHE:HE1	1.86	0.41
1:B:589:ARG:CD	1:B:596:LEU:HD21	2.50	0.41
1:C:163:GLU:O	1:C:164:ALA:C	2.59	0.41
1:C:180:ARG:H	1:C:180:ARG:HG2	1.53	0.41
1:C:215:VAL:CG2	1:C:216:PRO:CD	2.97	0.41
1:C:286:MET:CE	1:C:297:VAL:HG21	2.50	0.41
1:C:291:LYS:O	1:C:292:ASP:C	2.59	0.41
1:C:463:LYS:H	1:D:486:VAL:CG1	2.34	0.41
1:C:509:GLY:C	1:D:476:ARG:NH2	2.61	0.41
1:C:513:GLU:O	1:D:548:ARG:CZ	2.69	0.41
1:D:212:GLU:O	1:D:214:ARG:HG3	2.21	0.41
1:D:228:MET:O	1:D:229:PHE:HB2	2.20	0.41
1:D:257:ILE:HD11	1:D:299:ALA:HB1	2.03	0.41
1:D:280:ASN:HA	1:D:283:LEU:CD2	2.51	0.41
1:D:357:THR:HB	1:D:360:PHE:CD2	2.56	0.41
1:D:376:ALA:CA	1:D:381:ARG:CG	2.80	0.41
1:D:381:ARG:NH1	1:D:384:ILE:HA	2.35	0.41
1:D:417:TYR:O	1:D:420:ALA:HB3	2.21	0.41
1:D:458:LEU:HG	1:D:460:TRP:CE3	2.56	0.41
1:D:527:LEU:HD11	1:E:226:VAL:CG1	2.51	0.41
1:D:594:LEU:HD23	1:D:594:LEU:C	2.41	0.41
1:E:153:VAL:CG1	1:E:157:ASP:HB2	2.51	0.41
1:E:177:ASN:OD1	1:E:177:ASN:N	2.54	0.41
1:E:196:GLY:CA	1:E:202:LYS:NZ	2.84	0.41
1:E:210:ALA:HB2	1:E:217:PHE:CD1	2.56	0.41
1:E:236:ARG:C	1:E:238:ARG:N	2.70	0.41
1:E:337:ILE:CD1	1:E:338:HIS:CD2	3.03	0.41
1:E:408:SER:CB	1:E:409:PRO:HD2	2.49	0.41
1:E:451:MET:CB	1:E:452:PRO:HD3	2.51	0.41
1:E:576:LEU:O	1:E:577:LEU:C	2.59	0.41
1:F:155:PHE:C	1:F:157:ASP:N	2.71	0.41
1:F:207:ARG:CB	1:F:217:PHE:CZ	2.95	0.41
1:F:274:GLU:O	1:F:275:ARG:C	2.59	0.41
1:F:286:MET:HE3	1:F:286:MET:HB2	1.91	0.41
1:F:311:LEU:C	1:F:311:LEU:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:LEU:O	1:F:357:THR:HG23	2.21	0.41
1:F:354:ALA:O	1:F:357:THR:HG23	2.20	0.41
1:F:391:GLU:O	1:F:395:ARG:CB	2.69	0.41
1:F:424:LEU:O	1:F:425:ALA:C	2.60	0.41
1:F:441:VAL:O	1:F:442:PRO:C	2.58	0.41
1:F:509:GLY:O	1:F:510:MET:HG2	2.21	0.41
1:A:182:HIS:CD2	1:A:182:HIS:N	2.89	0.41
1:A:225:PHE:HB3	1:A:226:VAL:H	1.77	0.41
1:A:352:LEU:CD1	1:A:356:ARG:NH2	2.72	0.41
1:A:378:ARG:HA	1:F:173:GLU:OE2	2.20	0.41
1:A:513:GLU:O	1:B:548:ARG:CZ	2.68	0.41
1:B:179:SER:HA	1:B:182:HIS:NE2	2.36	0.41
1:B:412:ARG:NH2	1:B:440:ILE:HB	2.28	0.41
1:B:428:PHE:HE1	1:B:432:ALA:C	2.23	0.41
1:B:467:ASP:O	1:B:471:VAL:HG13	2.20	0.41
1:B:492:ASN:O	1:B:493:ASP:C	2.59	0.41
1:C:226:VAL:HG22	1:C:274:GLU:HG2	2.02	0.41
1:C:372:ALA:HB3	1:C:389:LEU:HD23	2.03	0.41
1:C:373:ALA:HA	1:C:384:ILE:HD11	2.02	0.41
1:D:180:ARG:NH2	1:E:377:ALA:HA	2.36	0.41
1:D:215:VAL:HG21	1:D:249:PRO:C	2.41	0.41
1:D:376:ALA:HB1	1:D:381:ARG:CB	2.51	0.41
1:D:468:GLN:O	1:D:469:ILE:C	2.58	0.41
1:D:594:LEU:HD23	1:D:594:LEU:O	2.20	0.41
1:E:199:GLY:HA2	2:E:1001:ADP:PA	2.61	0.41
1:E:203:THR:HG22	1:E:253:PHE:CZ	2.56	0.41
1:E:250:CYS:HB3	1:E:295:ILE:HG13	2.02	0.41
1:F:199:GLY:O	1:F:361:VAL:CG2	2.69	0.41
1:F:336:ARG:O	1:F:337:ILE:C	2.58	0.41
1:A:248:ALA:HA	1:A:249:PRO:HA	1.92	0.40
1:A:252:VAL:O	1:A:297:VAL:HA	2.21	0.40
1:A:423:ALA:HB1	1:A:587:PHE:CE1	2.57	0.40
1:A:571:ARG:O	1:A:575:THR:HG23	2.20	0.40
1:B:230:VAL:C	1:B:232:VAL:H	2.24	0.40
1:B:459:HIS:HD1	1:B:459:HIS:C	2.15	0.40
1:B:483:PHE:C	1:B:485:ASP:H	2.24	0.40
1:B:568:VAL:HG13	1:B:591:VAL:HA	2.02	0.40
1:C:147:LEU:HD12	1:C:148:THR:N	2.36	0.40
1:C:171:ILE:O	1:C:172:VAL:C	2.59	0.40
1:C:210:ALA:HB2	1:C:217:PHE:CD1	2.56	0.40
1:C:410:ARG:O	1:C:411:ASP:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ARG:C	1:C:447:LEU:N	2.74	0.40
1:C:514:PHE:HB3	1:C:519:TYR:OH	2.20	0.40
1:E:561:LEU:O	1:E:564:GLU:HB3	2.21	0.40
1:F:160:GLY:H	1:F:333:GLN:HE22	1.68	0.40
1:F:260:VAL:O	1:F:262:ARG:N	2.48	0.40
1:A:382:ARG:HG3	1:A:383:LYS:CA	2.51	0.40
1:A:407:LEU:H	1:A:407:LEU:HG	1.57	0.40
1:A:413:ARG:O	1:A:577:LEU:HD21	2.21	0.40
1:B:360:PHE:CE1	1:B:364:ASP:HB3	2.55	0.40
1:C:316:ARG:O	1:C:318:ASP:N	2.54	0.40
1:C:331:ARG:NH2	1:C:358:PRO:HG3	2.36	0.40
1:C:381:ARG:CG	1:C:382:ARG:N	2.81	0.40
1:D:216:PRO:HG3	1:D:247:HIS:CE1	2.56	0.40
1:D:256:GLU:CG	1:D:256:GLU:O	2.69	0.40
1:D:441:VAL:O	1:D:442:PRO:C	2.59	0.40
1:E:238:ARG:HG2	1:E:242:GLU:OE2	2.21	0.40
1:E:286:MET:HA	1:E:289:PHE:CE2	2.57	0.40
1:E:396:VAL:CG1	1:E:397:MET:N	2.84	0.40
1:E:411:ASP:O	1:E:415:THR:OG1	2.31	0.40
1:E:461:SER:O	1:E:462:ARG:C	2.60	0.40
1:F:155:PHE:HB2	1:F:158:VAL:HB	2.03	0.40
1:F:192:VAL:O	1:F:317:PHE:HE2	2.04	0.40
1:F:238:ARG:N	1:F:281:GLN:HE21	2.20	0.40
1:F:260:VAL:C	1:F:279:LEU:HD11	2.38	0.40
1:F:303:ARG:HA	1:F:304:PRO:HD2	1.90	0.40
1:F:307:LEU:HD12	1:F:307:LEU:H	1.86	0.40
1:F:538:GLU:O	1:F:540:ALA:N	2.54	0.40
1:A:422:HIS:O	1:A:423:ALA:C	2.59	0.40
1:B:188:ILE:HD12	1:B:189:PRO:HD3	2.03	0.40
1:B:235:ALA:O	1:B:238:ARG:NE	2.51	0.40
1:B:329:LYS:HG2	1:B:330:GLY:N	2.36	0.40
1:B:344:LEU:CD1	1:B:346:GLU:OE1	2.70	0.40
1:B:452:PRO:O	1:B:456:ASP:CG	2.60	0.40
1:B:460:TRP:HD1	1:B:464:ARG:HG2	1.86	0.40
1:B:531:ASP:OD1	1:B:531:ASP:N	2.55	0.40
1:B:567:GLU:O	1:B:570:GLU:HB3	2.21	0.40
1:C:153:VAL:CG1	1:C:157:ASP:HB2	2.51	0.40
1:C:176:LYS:HG2	1:C:176:LYS:H	1.76	0.40
1:C:464:ARG:O	1:C:465:LEU:C	2.57	0.40
1:C:484:ASP:C	1:C:486:VAL:H	2.23	0.40
1:D:155:PHE:C	1:D:157:ASP:N	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ILE:O	1:D:258:ASP:C	2.60	0.40
1:D:367:ASN:O	1:D:371:GLU:HG2	2.22	0.40
1:D:377:ALA:N	1:D:381:ARG:HB2	2.35	0.40
1:D:508:TRP:O	1:D:510:MET:HG3	2.22	0.40
1:D:536:SER:HB2	1:E:537:GLU:OE2	2.20	0.40
1:E:450:MET:O	1:E:454:ARG:HB3	2.21	0.40
1:E:582:LEU:HD21	1:E:590:VAL:HG11	2.02	0.40
1:F:349:ASP:C	1:F:350:LEU:HG	2.41	0.40
1:F:538:GLU:C	1:F:540:ALA:N	2.72	0.40
1:A:166:GLU:HB2	1:A:169:LYS:HZ1	1.82	0.40
1:A:173:GLU:CA	1:A:176:LYS:HG3	2.43	0.40
1:A:263:LYS:CG	1:A:264:ARG:N	2.83	0.40
1:A:314:PRO:HA	1:A:318:ASP:HB3	2.04	0.40
1:A:355:LYS:HA	1:A:355:LYS:HD3	1.90	0.40
1:B:313:ARG:O	1:B:316:ARG:HB2	2.21	0.40
1:B:346:GLU:OE2	1:B:348:VAL:HG12	2.22	0.40
1:B:417:TYR:O	1:B:420:ALA:HB3	2.21	0.40
1:B:422:HIS:CD2	1:B:475:GLY:HA3	2.57	0.40
1:D:193:LEU:HD12	1:D:194:LEU:H	1.86	0.40
1:D:464:ARG:O	1:D:467:ASP:N	2.55	0.40
1:D:478:ALA:O	1:D:479:GLU:C	2.58	0.40
1:D:505:ILE:HG21	1:D:543:ILE:HG12	2.04	0.40
1:D:518:ALA:HB3	1:E:495:ARG:HA	2.03	0.40
1:D:568:VAL:HG13	1:D:591:VAL:HA	2.02	0.40
1:E:173:GLU:HG2	1:E:174:PHE:N	2.37	0.40
1:E:182:HIS:CD2	1:E:182:HIS:N	2.90	0.40
1:E:226:VAL:CG2	1:E:274:GLU:HG2	2.51	0.40
1:F:180:ARG:HH12	1:F:184:MET:CE	2.31	0.40
1:F:241:PHE:O	1:F:243:THR:N	2.54	0.40
1:F:263:LYS:HD2	1:F:263:LYS:HA	1.38	0.40
1:F:469:ILE:HG23	1:F:497:ALA:HB1	2.02	0.40
1:F:478:ALA:O	1:F:482:VAL:HG12	2.21	0.40
1:F:597:GLU:O	1:F:599:PRO:CD	2.68	0.40
1:A:194:LEU:HD12	1:A:194:LEU:H	1.87	0.40
1:A:316:ARG:O	1:A:318:ASP:N	2.55	0.40
1:A:333:GLN:HA	1:A:336:ARG:NH2	2.36	0.40
1:B:249:PRO:O	1:B:250:CYS:HB3	2.21	0.40
1:B:260:VAL:O	1:B:262:ARG:N	2.47	0.40
1:B:349:ASP:C	1:B:350:LEU:HG	2.41	0.40
1:B:387:LYS:O	1:B:390:GLU:HB3	2.21	0.40
1:B:525:THR:HG22	1:B:526:TYR:N	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PHE:HB3	1:C:226:VAL:H	1.73	0.40
1:D:161:ALA:O	1:D:164:ALA:HB3	2.21	0.40
1:D:173:GLU:OE1	1:E:378:ARG:HA	2.21	0.40
1:D:332:GLU:CD	1:D:351:ALA:HA	2.42	0.40
1:D:424:LEU:O	1:D:425:ALA:C	2.60	0.40
1:D:467:ASP:O	1:D:471:VAL:HG13	2.21	0.40
1:D:514:PHE:HB3	1:D:519:TYR:CE1	2.56	0.40
1:E:174:PHE:CG	1:E:175:LEU:N	2.85	0.40
1:E:182:HIS:HD1	1:E:291:LYS:HB2	1.86	0.40
1:E:252:VAL:HB	1:E:297:VAL:HA	2.03	0.40
1:E:397:MET:SD	1:E:406:VAL:HG11	2.62	0.40
1:E:572:VAL:O	1:E:573:ALA:C	2.60	0.40
1:F:183:GLU:OE1	1:F:184:MET:N	2.55	0.40
1:F:216:PRO:O	1:F:250:CYS:HB2	2.22	0.40
1:F:345:ALA:HB2	1:F:383:LYS:NZ	2.37	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLU:CG	1:D:382:ARG:NH2[3_564]	1.61	0.59
1:A:417:TYR:OH	1:D:382:ARG:NE[3_564]	1.74	0.46
1:A:177:ASN:OD1	1:E:214:ARG:NH2[6_665]	1.85	0.35
1:B:238:ARG:NE	1:F:378:ARG:NH2[6_665]	1.91	0.29
1:A:570:GLU:CB	1:D:382:ARG:NH2[3_564]	2.08	0.12
1:A:176:LYS:O	1:E:214:ARG:NH1[6_665]	2.11	0.09
1:B:224:ASP:OD2	1:E:180:ARG:NH2[6_665]	2.17	0.03
1:B:238:ARG:CZ	1:F:378:ARG:NH2[6_665]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/508 (90%)	323 (71%)	111 (24%)	22 (5%)	2	24
1	B	442/508 (87%)	289 (65%)	125 (28%)	28 (6%)	1	19
1	C	456/508 (90%)	323 (71%)	112 (25%)	21 (5%)	2	25
1	D	442/508 (87%)	288 (65%)	121 (27%)	33 (8%)	1	16
1	E	456/508 (90%)	324 (71%)	110 (24%)	22 (5%)	2	24
1	F	442/508 (87%)	288 (65%)	120 (27%)	34 (8%)	1	16
All	All	2694/3048 (88%)	1835 (68%)	699 (26%)	160 (6%)	1	20

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	VAL
1	A	511	HIS
1	B	153	VAL
1	B	274	GLU
1	B	379	GLU
1	B	511	HIS
1	B	580	GLU
1	C	153	VAL
1	D	153	VAL
1	D	274	GLU
1	D	319	ARG
1	D	379	GLU
1	D	511	HIS
1	D	580	GLU
1	E	153	VAL
1	E	511	HIS
1	F	153	VAL
1	F	274	GLU
1	F	379	GLU
1	F	511	HIS
1	F	580	GLU
1	A	169	LYS
1	A	224	ASP
1	A	390	GLU
1	A	449	PHE
1	A	457	MET
1	A	489	GLY
1	A	492	ASN
1	A	512	PRO
1	B	180	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	319	ARG
1	B	376	ALA
1	B	435	VAL
1	B	456	ASP
1	B	489	GLY
1	B	512	PRO
1	B	530	TYR
1	B	593	GLY
1	C	224	ASP
1	C	341	GLY
1	C	390	GLU
1	C	457	MET
1	C	489	GLY
1	C	492	ASN
1	C	512	PRO
1	D	180	ARG
1	D	292	ASP
1	D	305	ASP
1	D	376	ALA
1	D	435	VAL
1	D	489	GLY
1	D	512	PRO
1	D	530	TYR
1	D	593	GLY
1	E	224	ASP
1	E	449	PHE
1	E	457	MET
1	E	489	GLY
1	E	492	ASN
1	E	512	PRO
1	F	180	ARG
1	F	319	ARG
1	F	376	ALA
1	F	435	VAL
1	F	489	GLY
1	F	512	PRO
1	F	530	TYR
1	F	593	GLY
1	A	172	VAL
1	A	262	ARG
1	A	264	ARG
1	A	341	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	442	PRO
1	B	305	ASP
1	B	565	LYS
1	C	169	LYS
1	C	172	VAL
1	C	262	ARG
1	C	264	ARG
1	C	442	PRO
1	C	449	PHE
1	C	458	LEU
1	C	511	HIS
1	D	162	GLU
1	D	383	LYS
1	D	413	ARG
1	D	442	PRO
1	D	456	ASP
1	D	565	LYS
1	E	262	ARG
1	E	264	ARG
1	E	341	GLY
1	E	390	GLU
1	E	442	PRO
1	E	464	ARG
1	F	162	GLU
1	F	305	ASP
1	F	456	ASP
1	F	565	LYS
1	A	458	LEU
1	B	162	GLU
1	B	448	GLY
1	B	570	GLU
1	C	150	ALA
1	D	570	GLU
1	E	150	ALA
1	E	169	LYS
1	E	172	VAL
1	E	458	LEU
1	F	283	LEU
1	F	442	PRO
1	F	570	GLU
1	A	150	ALA
1	A	410	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	258	ASP
1	B	283	LEU
1	B	442	PRO
1	C	214	ARG
1	C	274	GLU
1	C	410	ARG
1	D	258	ASP
1	D	283	LEU
1	D	369	LEU
1	D	567	GLU
1	E	410	ARG
1	F	165	LYS
1	F	258	ASP
1	F	527	LEU
1	A	202	LYS
1	A	484	ASP
1	B	228	MET
1	B	359	GLY
1	D	228	MET
1	D	261	GLY
1	D	448	GLY
1	D	527	LEU
1	E	202	LYS
1	F	164	ALA
1	F	228	MET
1	F	292	ASP
1	F	383	LYS
1	F	444	GLY
1	F	448	GLY
1	B	261	GLY
1	D	326	PRO
1	F	359	GLY
1	D	359	GLY
1	F	261	GLY
1	F	326	PRO
1	B	209	VAL
1	B	326	PRO
1	B	444	GLY
1	D	209	VAL
1	F	209	VAL
1	A	261	GLY
1	F	197	PRO

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Mol	Chain	Res	Type
1	A	326	PRO
1	C	326	PRO
1	E	261	GLY
1	E	326	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/402 (91%)	240 (66%)	125 (34%)	0	1
1	B	361/402 (90%)	242 (67%)	119 (33%)	0	1
1	C	365/402 (91%)	240 (66%)	125 (34%)	0	1
1	D	361/402 (90%)	241 (67%)	120 (33%)	0	1
1	E	365/402 (91%)	244 (67%)	121 (33%)	0	1
1	F	361/402 (90%)	240 (66%)	121 (34%)	0	1
All	All	2178/2412 (90%)	1447 (66%)	731 (34%)	0	1

All (731) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	ARG
1	A	146	VAL
1	A	147	LEU
1	A	154	THR
1	A	157	ASP
1	A	166	GLU
1	A	171	ILE
1	A	172	VAL
1	A	173	GLU
1	A	174	PHE
1	A	175	LEU
1	A	177	ASN
1	A	179	SER
1	A	181	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	182	HIS
1	A	183	GLU
1	A	188	ILE
1	A	190	LYS
1	A	194	LEU
1	A	200	VAL
1	A	207	ARG
1	A	214	ARG
1	A	215	VAL
1	A	217	PHE
1	A	218	ILE
1	A	219	THR
1	A	221	SER
1	A	223	SER
1	A	225	PHE
1	A	226	VAL
1	A	236	ARG
1	A	242	GLU
1	A	245	LYS
1	A	251	ILE
1	A	262	ARG
1	A	264	ARG
1	A	273	ASP
1	A	275	ARG
1	A	277	GLN
1	A	279	LEU
1	A	281	GLN
1	A	282	LEU
1	A	290	GLU
1	A	292	ASP
1	A	293	THR
1	A	296	VAL
1	A	301	THR
1	A	303	ARG
1	A	305	ASP
1	A	306	ILE
1	A	307	LEU
1	A	308	ASP
1	A	312	LEU
1	A	317	PHE
1	A	318	ASP
1	A	320	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	323	ILE
1	A	327	ASP
1	A	344	LEU
1	A	347	ASP
1	A	349	ASP
1	A	350	LEU
1	A	352	LEU
1	A	355	LYS
1	A	357	THR
1	A	360	PHE
1	A	364	ASP
1	A	368	LEU
1	A	371	GLU
1	A	375	LEU
1	A	378	ARG
1	A	381	ARG
1	A	382	ARG
1	A	383	LYS
1	A	388	ASP
1	A	390	GLU
1	A	391	GLU
1	A	394	ASP
1	A	396	VAL
1	A	397	MET
1	A	402	LYS
1	A	405	LEU
1	A	406	VAL
1	A	407	LEU
1	A	414	ILE
1	A	419	GLU
1	A	433	ASP
1	A	436	HIS
1	A	443	ARG
1	A	449	PHE
1	A	453	ARG
1	A	454	ARG
1	A	459	HIS
1	A	461	SER
1	A	462	ARG
1	A	464	ARG
1	A	465	LEU
1	A	484	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	487	THR
1	A	491	GLU
1	A	493	ASP
1	A	502	ARG
1	A	511	HIS
1	A	514	PHE
1	A	524	ASP
1	A	530	TYR
1	A	532	VAL
1	A	535	TYR
1	A	536	SER
1	A	537	GLU
1	A	539	THR
1	A	541	LYS
1	A	548	ARG
1	A	550	LEU
1	A	558	VAL
1	A	561	LEU
1	A	566	ARG
1	A	569	LEU
1	A	574	GLU
1	A	576	LEU
1	A	578	GLU
1	A	579	ARG
1	A	585	GLU
1	A	594	LEU
1	A	596	LEU
1	B	153	VAL
1	B	157	ASP
1	B	162	GLU
1	B	166	GLU
1	B	167	GLU
1	B	171	ILE
1	B	172	VAL
1	B	174	PHE
1	B	175	LEU
1	B	179	SER
1	B	182	HIS
1	B	183	GLU
1	B	184	MET
1	B	187	ARG
1	B	188	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	192	VAL
1	B	193	LEU
1	B	195	VAL
1	B	202	LYS
1	B	203	THR
1	B	207	ARG
1	B	214	ARG
1	B	217	PHE
1	B	223	SER
1	B	227	GLU
1	B	236	ARG
1	B	237	VAL
1	B	238	ARG
1	B	240	LEU
1	B	242	GLU
1	B	243	THR
1	B	245	LYS
1	B	246	ARG
1	B	252	VAL
1	B	253	PHE
1	B	255	ASP
1	B	256	GLU
1	B	258	ASP
1	B	260	VAL
1	B	263	LYS
1	B	273	ASP
1	B	274	GLU
1	B	284	VAL
1	B	287	ASP
1	B	291	LYS
1	B	295	ILE
1	B	297	VAL
1	B	301	THR
1	B	303	ARG
1	B	308	ASP
1	B	311	LEU
1	B	312	LEU
1	B	318	ASP
1	B	319	ARG
1	B	323	ILE
1	B	332	GLU
1	B	342	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	344	LEU
1	B	347	ASP
1	B	348	VAL
1	B	350	LEU
1	B	352	LEU
1	B	356	ARG
1	B	357	THR
1	B	360	PHE
1	B	367	ASN
1	B	375	LEU
1	B	378	ARG
1	B	382	ARG
1	B	386	MET
1	B	387	LYS
1	B	389	LEU
1	B	395	ARG
1	B	397	MET
1	B	405	LEU
1	B	407	LEU
1	B	413	ARG
1	B	414	ILE
1	B	424	LEU
1	B	428	PHE
1	B	429	LEU
1	B	430	GLU
1	B	433	ASP
1	B	435	VAL
1	B	436	HIS
1	B	450	MET
1	B	453	ARG
1	B	455	GLU
1	B	457	MET
1	B	458	LEU
1	B	459	HIS
1	B	460	TRP
1	B	462	ARG
1	B	463	LYS
1	B	476	ARG
1	B	484	ASP
1	B	485	ASP
1	B	503	ARG
1	B	506	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	517	VAL
1	B	521	VAL
1	B	522	ARG
1	B	527	LEU
1	B	531	ASP
1	B	533	ARG
1	B	535	TYR
1	B	539	THR
1	B	548	ARG
1	B	558	VAL
1	B	563	LEU
1	B	570	GLU
1	B	577	LEU
1	B	578	GLU
1	B	581	THR
1	B	583	THR
1	B	586	GLU
1	B	592	GLU
1	B	596	LEU
1	B	600	GLU
1	C	145	ARG
1	C	146	VAL
1	C	147	LEU
1	C	154	THR
1	C	157	ASP
1	C	166	GLU
1	C	172	VAL
1	C	173	GLU
1	C	174	PHE
1	C	175	LEU
1	C	177	ASN
1	C	179	SER
1	C	181	PHE
1	C	182	HIS
1	C	183	GLU
1	C	190	LYS
1	C	194	LEU
1	C	200	VAL
1	C	207	ARG
1	C	215	VAL
1	C	217	PHE
1	C	218	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	219	THR
1	C	221	SER
1	C	225	PHE
1	C	226	VAL
1	C	236	ARG
1	C	242	GLU
1	C	245	LYS
1	C	251	ILE
1	C	262	ARG
1	C	264	ARG
1	C	273	ASP
1	C	274	GLU
1	C	275	ARG
1	C	277	GLN
1	C	279	LEU
1	C	282	LEU
1	C	287	ASP
1	C	290	GLU
1	C	292	ASP
1	C	293	THR
1	C	296	VAL
1	C	303	ARG
1	C	305	ASP
1	C	306	ILE
1	C	307	LEU
1	C	308	ASP
1	C	312	LEU
1	C	317	PHE
1	C	318	ASP
1	C	320	GLN
1	C	323	ILE
1	C	327	ASP
1	C	334	ILE
1	C	340	ARG
1	C	344	LEU
1	C	347	ASP
1	C	349	ASP
1	C	350	LEU
1	C	352	LEU
1	C	355	LYS
1	C	357	THR
1	C	360	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	364	ASP
1	C	368	LEU
1	C	371	GLU
1	C	375	LEU
1	C	378	ARG
1	C	381	ARG
1	C	382	ARG
1	C	388	ASP
1	C	390	GLU
1	C	391	GLU
1	C	394	ASP
1	C	396	VAL
1	C	397	MET
1	C	402	LYS
1	C	405	LEU
1	C	406	VAL
1	C	407	LEU
1	C	414	ILE
1	C	419	GLU
1	C	433	ASP
1	C	436	HIS
1	C	437	LYS
1	C	443	ARG
1	C	449	PHE
1	C	453	ARG
1	C	454	ARG
1	C	459	HIS
1	C	461	SER
1	C	462	ARG
1	C	464	ARG
1	C	465	LEU
1	C	481	ILE
1	C	482	VAL
1	C	484	ASP
1	C	487	THR
1	C	491	GLU
1	C	493	ASP
1	C	496	GLN
1	C	502	ARG
1	C	511	HIS
1	C	514	PHE
1	C	524	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	530	TYR
1	C	532	VAL
1	C	535	TYR
1	C	536	SER
1	C	537	GLU
1	C	539	THR
1	C	548	ARG
1	C	550	LEU
1	C	558	VAL
1	C	561	LEU
1	C	566	ARG
1	C	569	LEU
1	C	574	GLU
1	C	576	LEU
1	C	577	LEU
1	C	578	GLU
1	C	579	ARG
1	C	585	GLU
1	C	594	LEU
1	D	152	LYS
1	D	153	VAL
1	D	162	GLU
1	D	166	GLU
1	D	167	GLU
1	D	171	ILE
1	D	172	VAL
1	D	174	PHE
1	D	175	LEU
1	D	179	SER
1	D	182	HIS
1	D	183	GLU
1	D	184	MET
1	D	187	ARG
1	D	188	ILE
1	D	190	LYS
1	D	193	LEU
1	D	195	VAL
1	D	202	LYS
1	D	203	THR
1	D	207	ARG
1	D	214	ARG
1	D	217	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	223	SER
1	D	227	GLU
1	D	236	ARG
1	D	237	VAL
1	D	238	ARG
1	D	242	GLU
1	D	243	THR
1	D	245	LYS
1	D	246	ARG
1	D	252	VAL
1	D	253	PHE
1	D	256	GLU
1	D	258	ASP
1	D	260	VAL
1	D	263	LYS
1	D	273	ASP
1	D	274	GLU
1	D	284	VAL
1	D	285	GLU
1	D	287	ASP
1	D	289	PHE
1	D	291	LYS
1	D	295	ILE
1	D	297	VAL
1	D	301	THR
1	D	303	ARG
1	D	308	ASP
1	D	311	LEU
1	D	312	LEU
1	D	316	ARG
1	D	318	ASP
1	D	319	ARG
1	D	323	ILE
1	D	332	GLU
1	D	342	LYS
1	D	344	LEU
1	D	347	ASP
1	D	348	VAL
1	D	350	LEU
1	D	352	LEU
1	D	356	ARG
1	D	357	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	360	PHE
1	D	367	ASN
1	D	375	LEU
1	D	378	ARG
1	D	382	ARG
1	D	385	THR
1	D	386	MET
1	D	387	LYS
1	D	388	ASP
1	D	389	LEU
1	D	395	ARG
1	D	397	MET
1	D	405	LEU
1	D	407	LEU
1	D	413	ARG
1	D	414	ILE
1	D	424	LEU
1	D	428	PHE
1	D	429	LEU
1	D	430	GLU
1	D	433	ASP
1	D	435	VAL
1	D	436	HIS
1	D	450	MET
1	D	453	ARG
1	D	455	GLU
1	D	457	MET
1	D	458	LEU
1	D	459	HIS
1	D	460	TRP
1	D	462	ARG
1	D	463	LYS
1	D	476	ARG
1	D	484	ASP
1	D	485	ASP
1	D	500	LEU
1	D	503	ARG
1	D	506	THR
1	D	517	VAL
1	D	521	VAL
1	D	522	ARG
1	D	531	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	533	ARG
1	D	535	TYR
1	D	539	THR
1	D	548	ARG
1	D	563	LEU
1	D	567	GLU
1	D	570	GLU
1	D	577	LEU
1	D	578	GLU
1	D	581	THR
1	D	583	THR
1	D	592	GLU
1	D	600	GLU
1	E	145	ARG
1	E	146	VAL
1	E	147	LEU
1	E	154	THR
1	E	157	ASP
1	E	166	GLU
1	E	172	VAL
1	E	173	GLU
1	E	174	PHE
1	E	175	LEU
1	E	177	ASN
1	E	179	SER
1	E	181	PHE
1	E	182	HIS
1	E	183	GLU
1	E	194	LEU
1	E	200	VAL
1	E	207	ARG
1	E	215	VAL
1	E	217	PHE
1	E	218	ILE
1	E	219	THR
1	E	221	SER
1	E	223	SER
1	E	225	PHE
1	E	226	VAL
1	E	236	ARG
1	E	242	GLU
1	E	245	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	251	ILE
1	E	262	ARG
1	E	264	ARG
1	E	273	ASP
1	E	274	GLU
1	E	275	ARG
1	E	277	GLN
1	E	279	LEU
1	E	282	LEU
1	E	289	PHE
1	E	290	GLU
1	E	292	ASP
1	E	293	THR
1	E	296	VAL
1	E	303	ARG
1	E	305	ASP
1	E	306	ILE
1	E	307	LEU
1	E	308	ASP
1	E	312	LEU
1	E	317	PHE
1	E	318	ASP
1	E	320	GLN
1	E	323	ILE
1	E	327	ASP
1	E	344	LEU
1	E	347	ASP
1	E	349	ASP
1	E	350	LEU
1	E	352	LEU
1	E	355	LYS
1	E	357	THR
1	E	360	PHE
1	E	364	ASP
1	E	368	LEU
1	E	371	GLU
1	E	375	LEU
1	E	378	ARG
1	E	381	ARG
1	E	382	ARG
1	E	383	LYS
1	E	388	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	390	GLU
1	E	391	GLU
1	E	394	ASP
1	E	396	VAL
1	E	397	MET
1	E	402	LYS
1	E	405	LEU
1	E	406	VAL
1	E	407	LEU
1	E	414	ILE
1	E	419	GLU
1	E	433	ASP
1	E	436	HIS
1	E	439	THR
1	E	443	ARG
1	E	449	PHE
1	E	453	ARG
1	E	454	ARG
1	E	459	HIS
1	E	461	SER
1	E	462	ARG
1	E	464	ARG
1	E	465	LEU
1	E	482	VAL
1	E	484	ASP
1	E	487	THR
1	E	491	GLU
1	E	493	ASP
1	E	502	ARG
1	E	511	HIS
1	E	514	PHE
1	E	524	ASP
1	E	530	TYR
1	E	532	VAL
1	E	535	TYR
1	E	536	SER
1	E	537	GLU
1	E	539	THR
1	E	548	ARG
1	E	550	LEU
1	E	558	VAL
1	E	561	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	566	ARG
1	E	569	LEU
1	E	574	GLU
1	E	576	LEU
1	E	578	GLU
1	E	579	ARG
1	E	585	GLU
1	E	594	LEU
1	F	152	LYS
1	F	153	VAL
1	F	162	GLU
1	F	166	GLU
1	F	167	GLU
1	F	171	ILE
1	F	172	VAL
1	F	174	PHE
1	F	175	LEU
1	F	179	SER
1	F	182	HIS
1	F	183	GLU
1	F	184	MET
1	F	187	ARG
1	F	188	ILE
1	F	193	LEU
1	F	195	VAL
1	F	200	VAL
1	F	202	LYS
1	F	203	THR
1	F	207	ARG
1	F	217	PHE
1	F	223	SER
1	F	224	ASP
1	F	227	GLU
1	F	236	ARG
1	F	237	VAL
1	F	238	ARG
1	F	242	GLU
1	F	243	THR
1	F	245	LYS
1	F	246	ARG
1	F	252	VAL
1	F	253	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	255	ASP
1	F	256	GLU
1	F	258	ASP
1	F	260	VAL
1	F	263	LYS
1	F	273	ASP
1	F	274	GLU
1	F	284	VAL
1	F	287	ASP
1	F	291	LYS
1	F	295	ILE
1	F	297	VAL
1	F	301	THR
1	F	303	ARG
1	F	308	ASP
1	F	311	LEU
1	F	312	LEU
1	F	316	ARG
1	F	318	ASP
1	F	319	ARG
1	F	323	ILE
1	F	332	GLU
1	F	335	LEU
1	F	342	LYS
1	F	344	LEU
1	F	347	ASP
1	F	348	VAL
1	F	350	LEU
1	F	352	LEU
1	F	356	ARG
1	F	357	THR
1	F	360	PHE
1	F	367	ASN
1	F	375	LEU
1	F	378	ARG
1	F	382	ARG
1	F	386	MET
1	F	387	LYS
1	F	388	ASP
1	F	389	LEU
1	F	395	ARG
1	F	397	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	405	LEU
1	F	407	LEU
1	F	414	ILE
1	F	424	LEU
1	F	428	PHE
1	F	429	LEU
1	F	430	GLU
1	F	433	ASP
1	F	435	VAL
1	F	436	HIS
1	F	450	MET
1	F	453	ARG
1	F	455	GLU
1	F	457	MET
1	F	458	LEU
1	F	459	HIS
1	F	460	TRP
1	F	462	ARG
1	F	463	LYS
1	F	476	ARG
1	F	484	ASP
1	F	485	ASP
1	F	500	LEU
1	F	503	ARG
1	F	506	THR
1	F	517	VAL
1	F	521	VAL
1	F	522	ARG
1	F	526	TYR
1	F	527	LEU
1	F	531	ASP
1	F	533	ARG
1	F	535	TYR
1	F	539	THR
1	F	548	ARG
1	F	557	ARG
1	F	558	VAL
1	F	563	LEU
1	F	570	GLU
1	F	577	LEU
1	F	578	GLU
1	F	581	THR

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Mol	Chain	Res	Type
1	F	583	THR
1	F	592	GLU
1	F	600	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	A	204	HIS
1	A	320	GLN
1	A	468	GLN
1	A	496	GLN
1	A	511	HIS
1	B	204	HIS
1	B	277	GLN
1	B	281	GLN
1	B	302	ASN
1	B	333	GLN
1	B	338	HIS
1	B	431	HIS
1	C	177	ASN
1	C	182	HIS
1	C	204	HIS
1	C	468	GLN
1	C	496	GLN
1	D	204	HIS
1	D	277	GLN
1	D	281	GLN
1	D	302	ASN
1	D	333	GLN
1	D	338	HIS
1	D	431	HIS
1	E	182	HIS
1	E	204	HIS
1	E	320	GLN
1	E	468	GLN
1	E	496	GLN
1	F	204	HIS
1	F	277	GLN
1	F	281	GLN
1	F	302	ASN
1	F	333	GLN

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Mol	Chain	Res	Type
1	F	338	HIS
1	F	431	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	A	1001	-	24,29,29	1.10	2 (8%)	29,45,45	1.50	4 (13%)
2	ADP	C	1001	-	24,29,29	1.10	3 (12%)	29,45,45	1.56	4 (13%)
2	ADP	D	2001	-	24,29,29	1.03	3 (12%)	29,45,45	1.45	5 (17%)
2	ADP	B	2001	-	24,29,29	1.05	2 (8%)	29,45,45	1.49	4 (13%)
2	ADP	E	1001	-	24,29,29	1.06	2 (8%)	29,45,45	1.45	4 (13%)
2	ADP	F	2001	-	24,29,29	1.01	1 (4%)	29,45,45	1.52	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	D	2001	-	-	2/12/32/32	0/3/3/3
2	ADP	B	2001	-	-	3/12/32/32	0/3/3/3
2	ADP	E	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	F	2001	-	-	2/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C5-C4	2.78	1.48	1.40
2	F	2001	ADP	C5-C4	2.76	1.48	1.40
2	E	1001	ADP	C5-C4	2.73	1.48	1.40
2	C	1001	ADP	C5-C4	2.62	1.47	1.40
2	B	2001	ADP	C5-C4	2.59	1.47	1.40
2	D	2001	ADP	C5-C4	2.42	1.47	1.40
2	A	1001	ADP	C2-N3	2.24	1.35	1.32
2	E	1001	ADP	C2-N3	2.23	1.35	1.32
2	C	1001	ADP	O4'-C1'	2.19	1.44	1.41
2	C	1001	ADP	C2-N3	2.17	1.35	1.32
2	D	2001	ADP	O4'-C1'	2.08	1.44	1.41
2	B	2001	ADP	O4'-C1'	2.06	1.43	1.41
2	D	2001	ADP	C2-N3	2.05	1.35	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	PA-O3A-PB	-4.26	118.21	132.83
2	C	1001	ADP	PA-O3A-PB	-4.20	118.40	132.83
2	E	1001	ADP	PA-O3A-PB	-4.05	118.92	132.83
2	B	2001	ADP	PA-O3A-PB	-3.99	119.13	132.83
2	C	1001	ADP	N3-C2-N1	-3.72	122.86	128.68
2	F	2001	ADP	PA-O3A-PB	-3.69	120.17	132.83
2	D	2001	ADP	C4-C5-N7	-3.61	105.63	109.40
2	F	2001	ADP	C3'-C2'-C1'	3.54	106.30	100.98
2	B	2001	ADP	C3'-C2'-C1'	3.21	105.81	100.98
2	B	2001	ADP	N3-C2-N1	-3.13	123.78	128.68
2	A	1001	ADP	C3'-C2'-C1'	3.13	105.69	100.98
2	C	1001	ADP	C4-C5-N7	-3.12	106.15	109.40
2	D	2001	ADP	N3-C2-N1	-3.10	123.83	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	N3-C2-N1	-3.06	123.89	128.68
2	F	2001	ADP	N3-C2-N1	-3.04	123.93	128.68
2	F	2001	ADP	C4-C5-N7	-3.01	106.27	109.40
2	E	1001	ADP	C3'-C2'-C1'	2.95	105.42	100.98
2	D	2001	ADP	C3'-C2'-C1'	2.88	105.32	100.98
2	A	1001	ADP	C4-C5-N7	-2.82	106.46	109.40
2	D	2001	ADP	PA-O3A-PB	-2.75	123.39	132.83
2	B	2001	ADP	C4-C5-N7	-2.74	106.54	109.40
2	E	1001	ADP	N3-C2-N1	-2.74	124.39	128.68
2	E	1001	ADP	C4-C5-N7	-2.67	106.61	109.40
2	C	1001	ADP	C3'-C2'-C1'	2.57	104.85	100.98
2	D	2001	ADP	O3B-PB-O2B	2.20	116.03	107.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

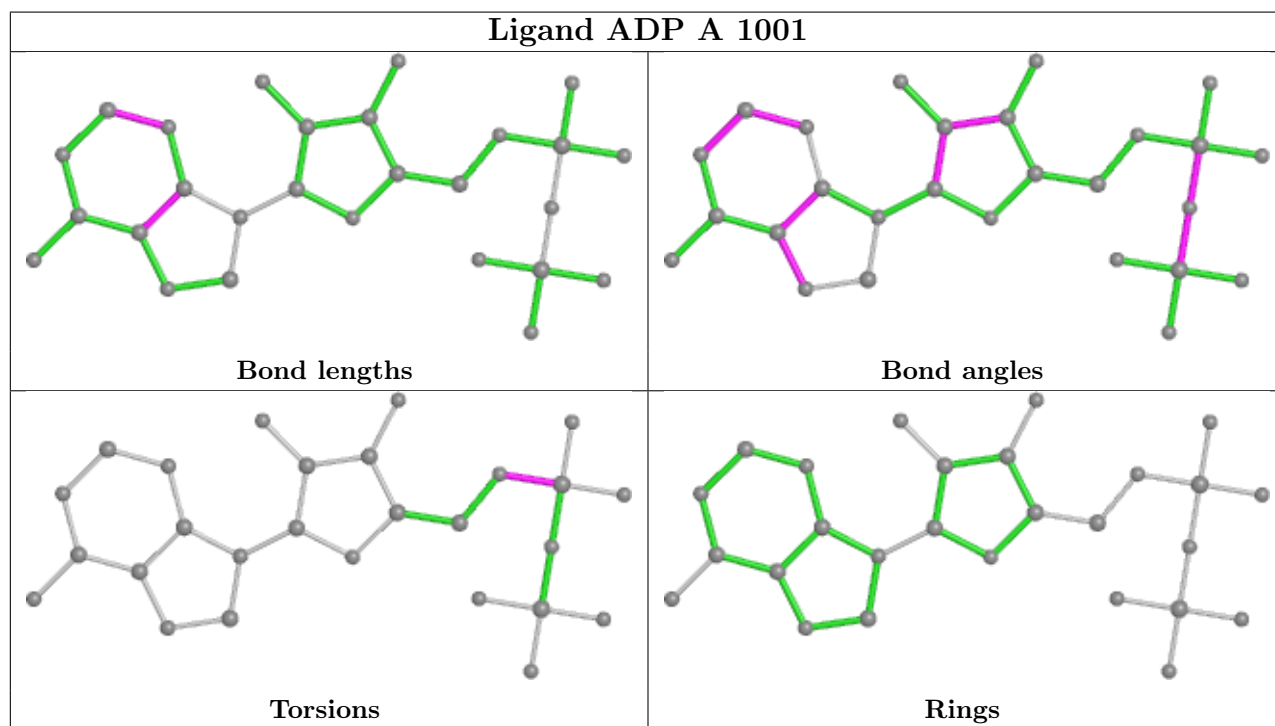
Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C5'-O5'-PA-O3A
2	C	1001	ADP	C5'-O5'-PA-O1A
2	C	1001	ADP	C5'-O5'-PA-O3A
2	D	2001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C5'-O5'-PA-O1A
2	F	2001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C5'-O5'-PA-O3A
2	B	2001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C5'-O5'-PA-O2A
2	D	2001	ADP	C5'-O5'-PA-O1A
2	F	2001	ADP	C5'-O5'-PA-O1A
2	A	1001	ADP	C5'-O5'-PA-O3A

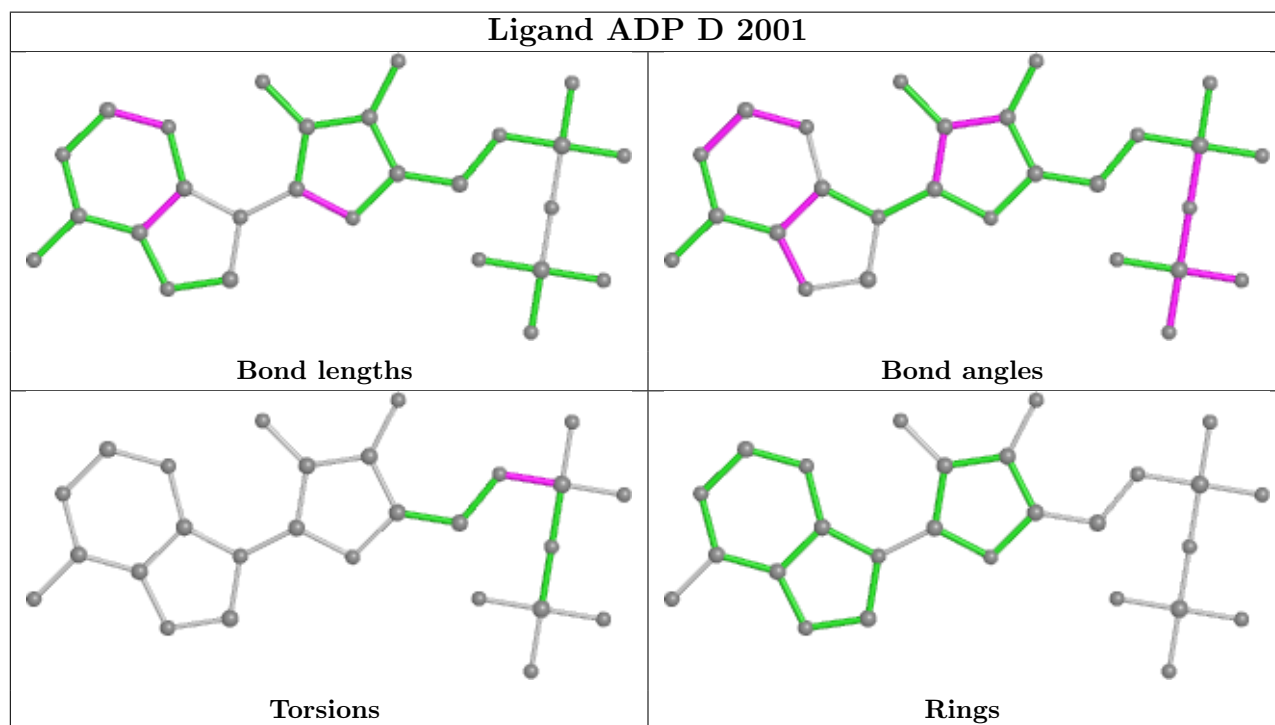
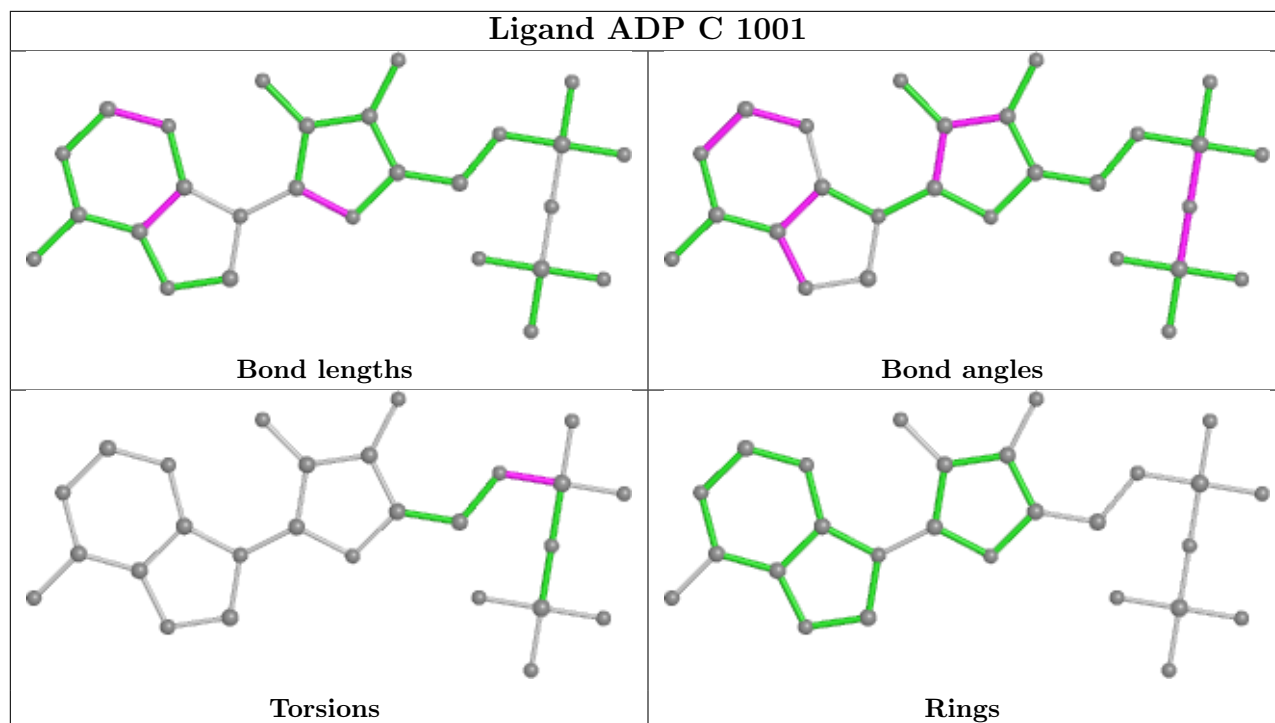
There are no ring outliers.

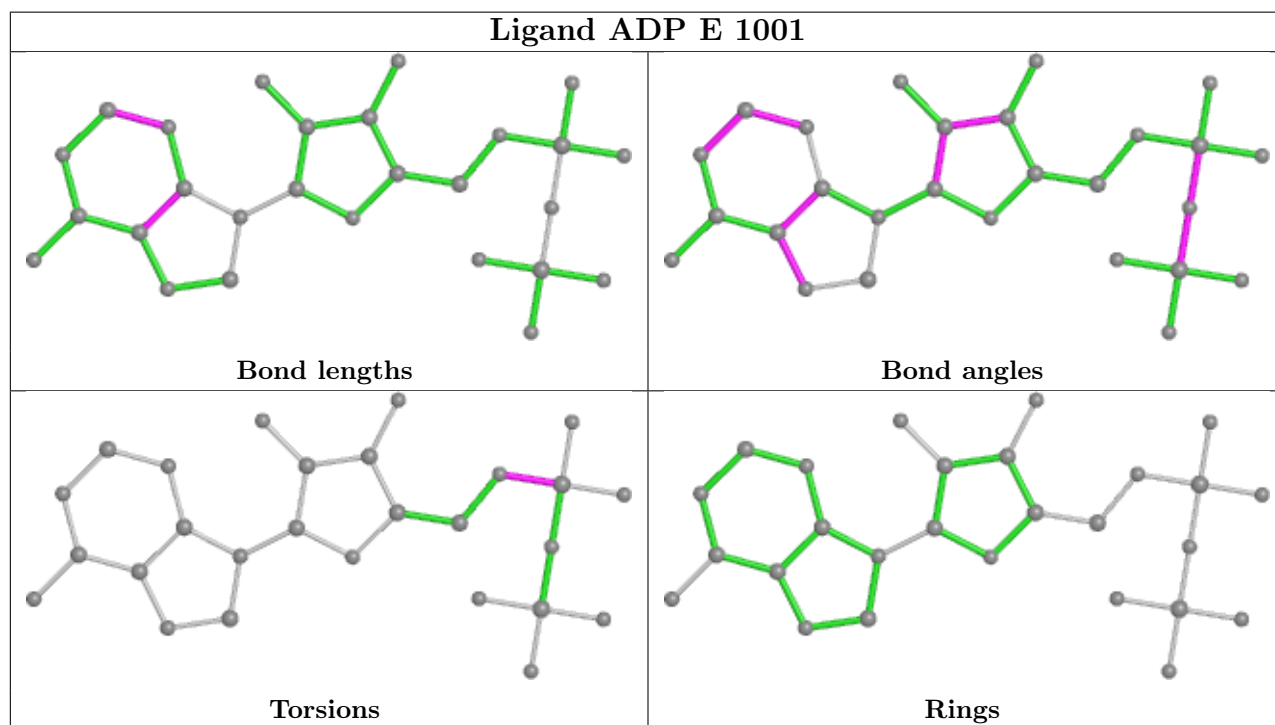
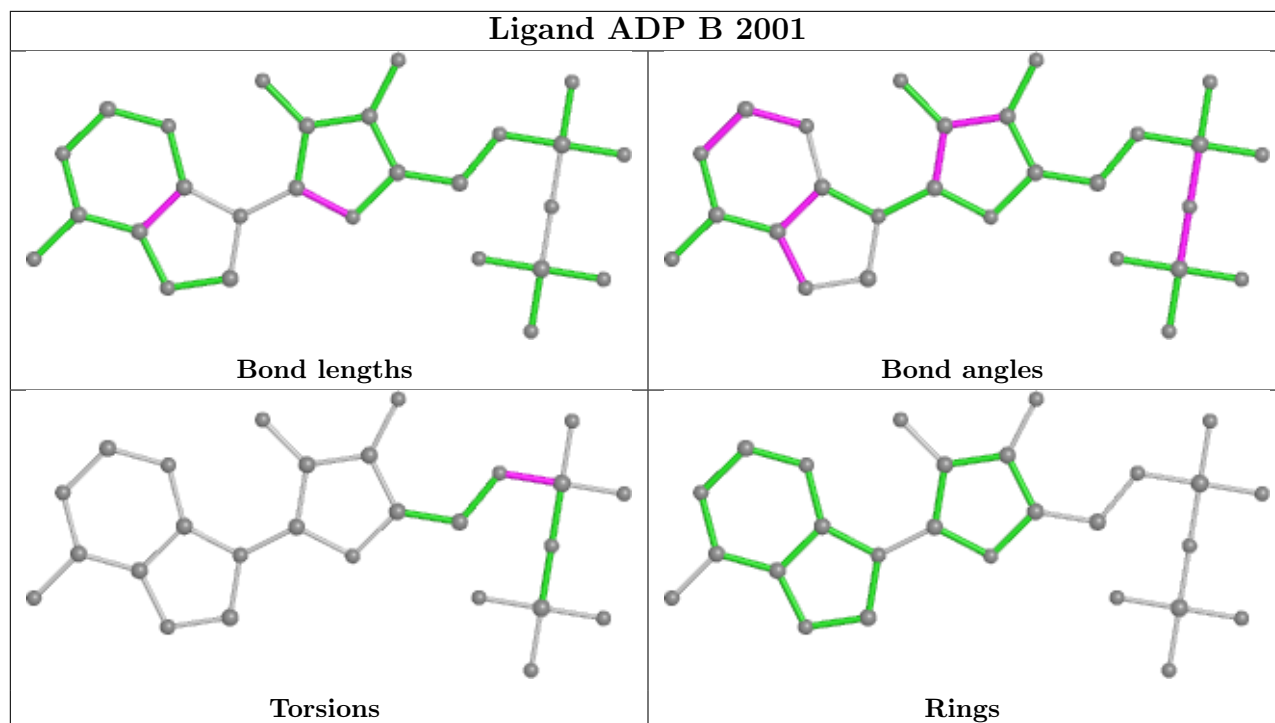
6 monomers are involved in 57 short contacts:

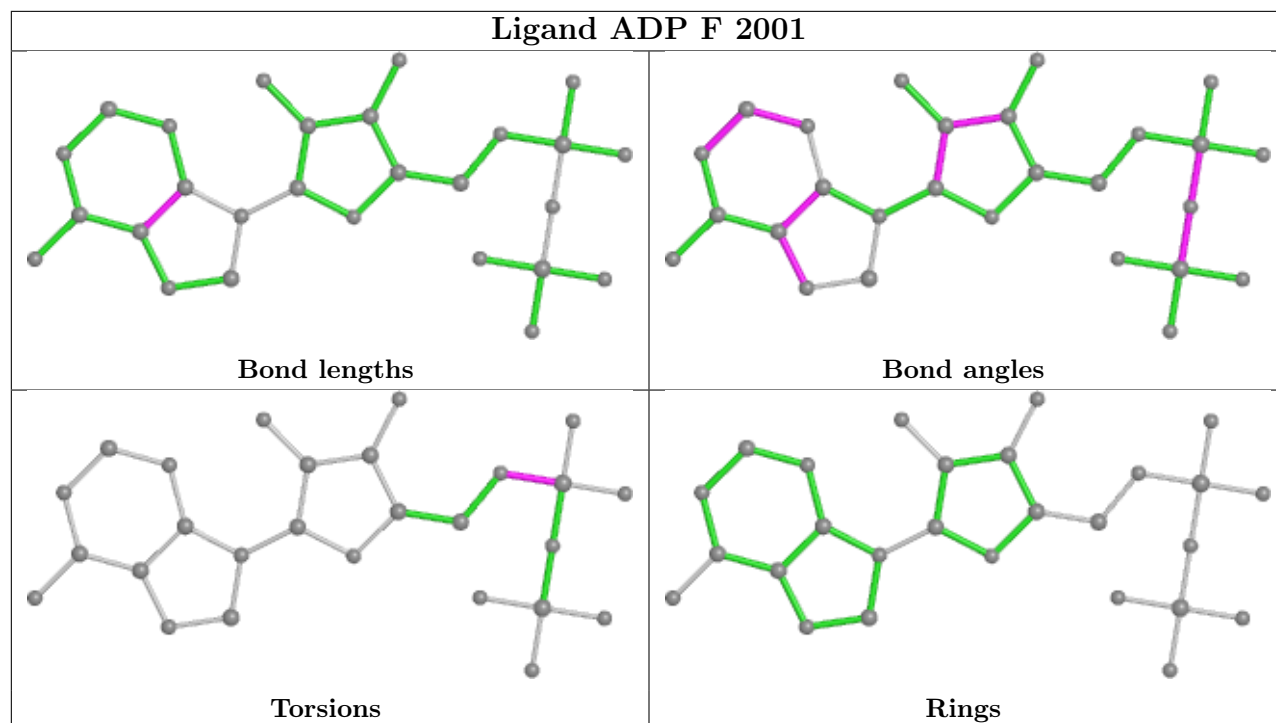
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	8	0
2	C	1001	ADP	10	0
2	D	2001	ADP	9	0
2	B	2001	ADP	9	0
2	E	1001	ADP	11	0
2	F	2001	ADP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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.

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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

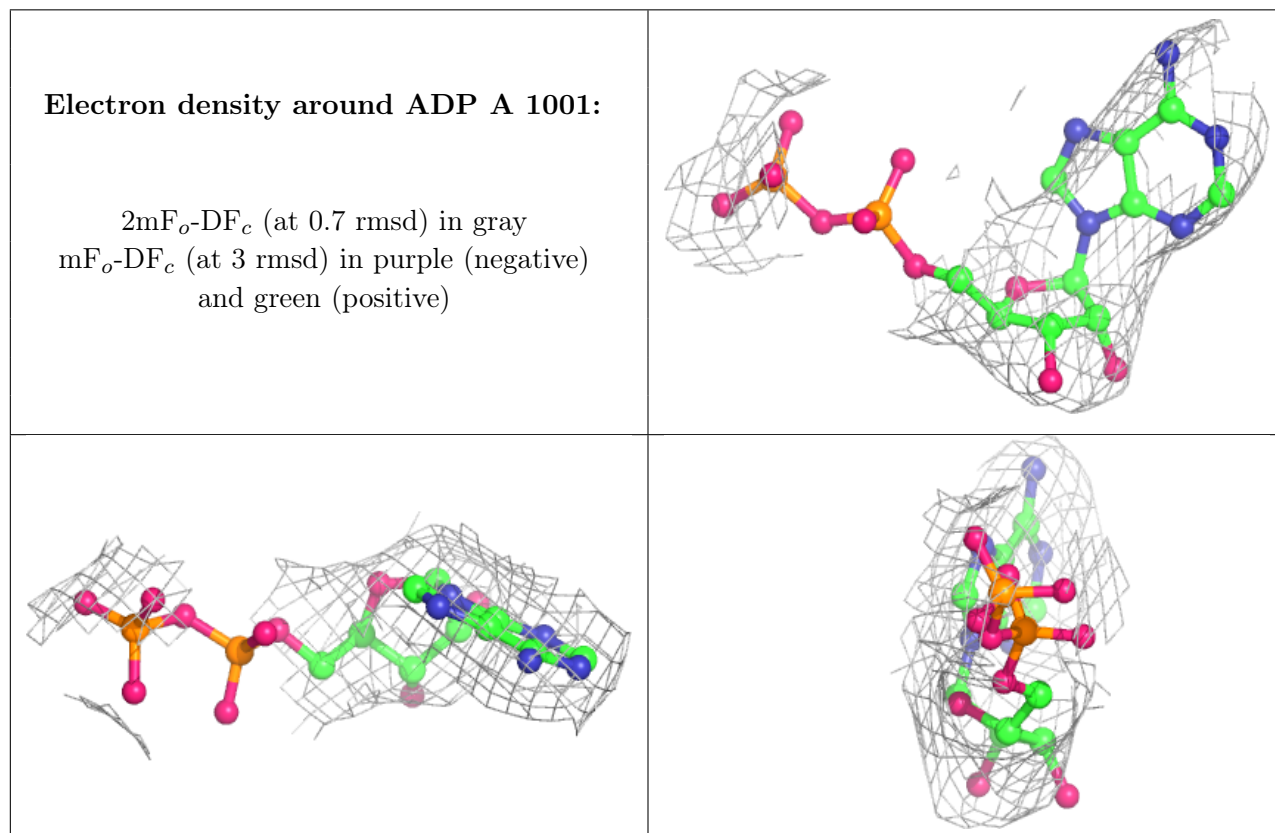
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

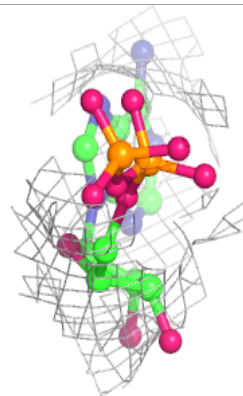
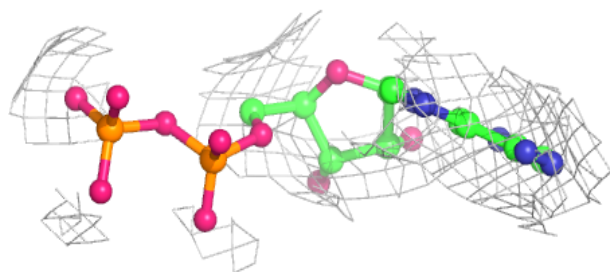
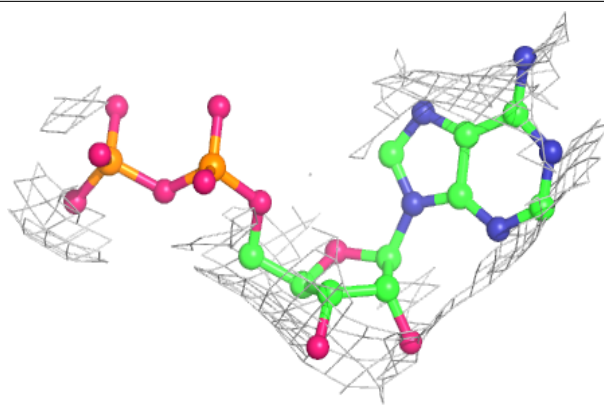
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

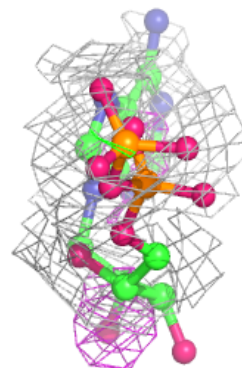
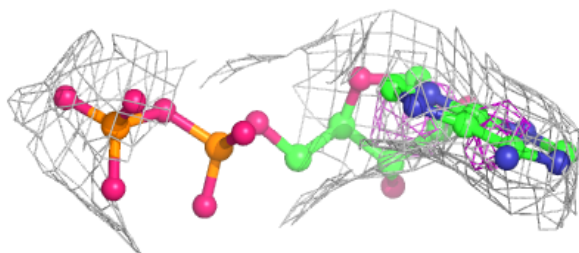
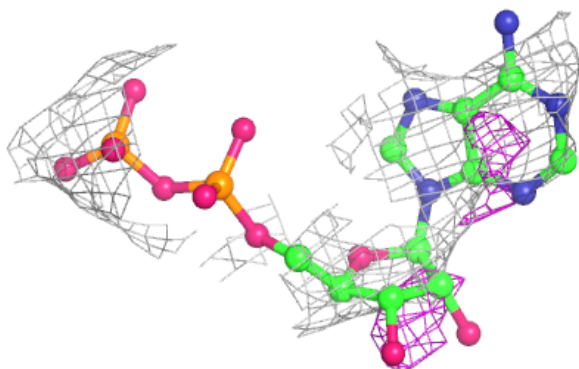


**Electron density around ADP B 2001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP C 1001:**

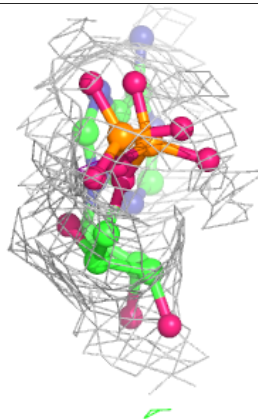
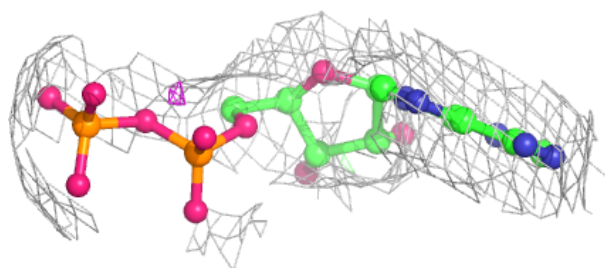
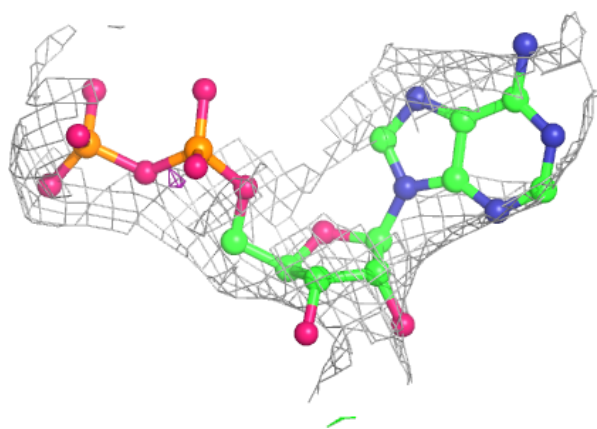
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



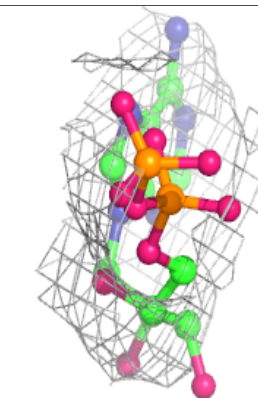
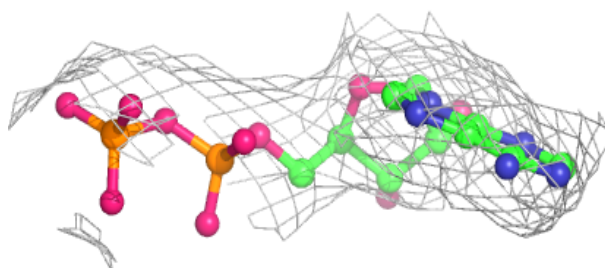
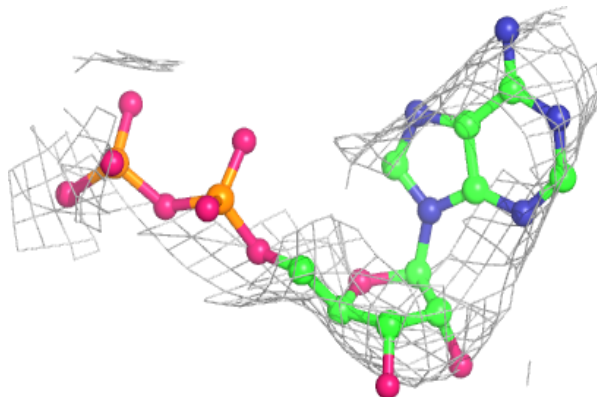


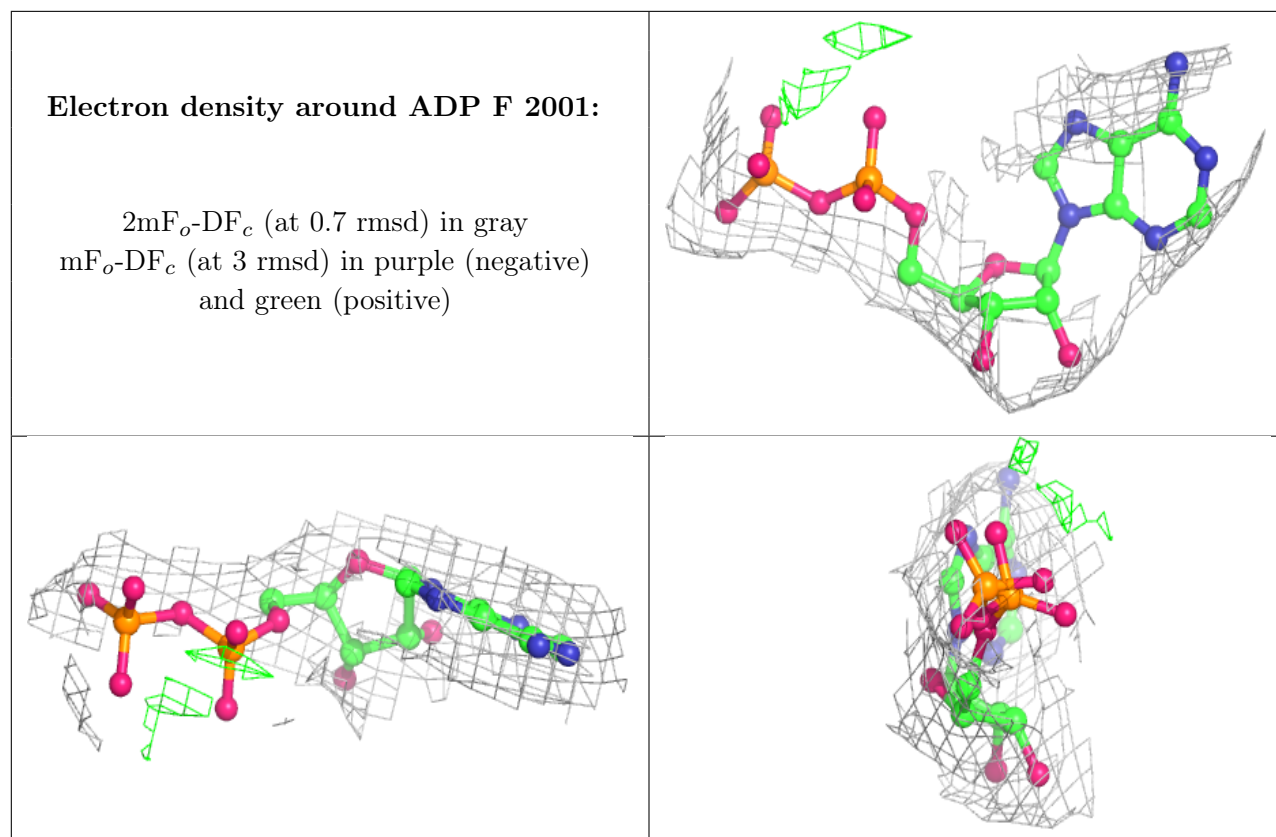
**Electron density around ADP D 2001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP E 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.