



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:16 AM UTC

PDB ID : 1FFX / pdb_00001ffx
Title : TUBULIN:STATHMIN-LIKE DOMAIN COMPLEX
Authors : Gigant, B.; Martin-Barbey, C.; Knossow, M.
Deposited on : 2000-07-26
Resolution : 3.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

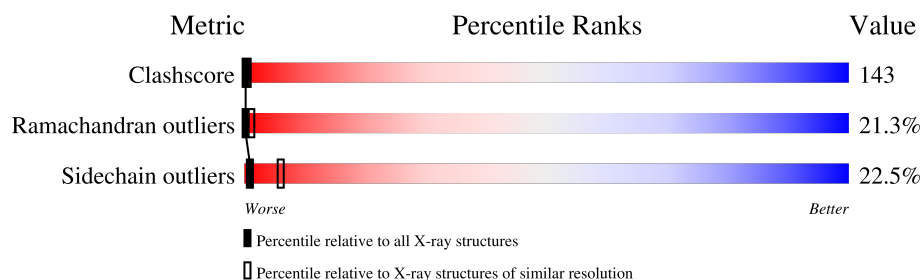
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	91	

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
5	GDP	D	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13568 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 PROTEIN (TUBULIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3295	2082	559	632	22			
1	C	423	Total	C	N	O	S	0	0	0
			3295	2082	559	632	22			

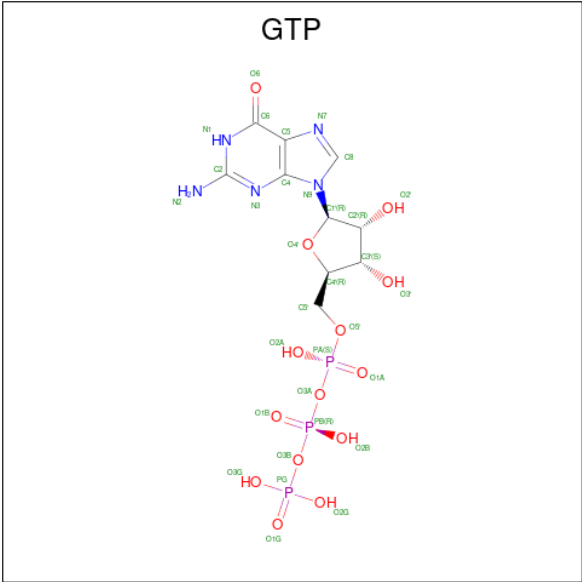
- Molecule 2 is a protein called PROTEIN (TUBULIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	0	0
			3201	2014	550	611	26			
2	D	410	Total	C	N	O	S	0	0	0
			3201	2014	550	611	26			

- Molecule 3 is a protein called PROTEIN (STATHMIN-LIKE DOMAIN OF RB3).

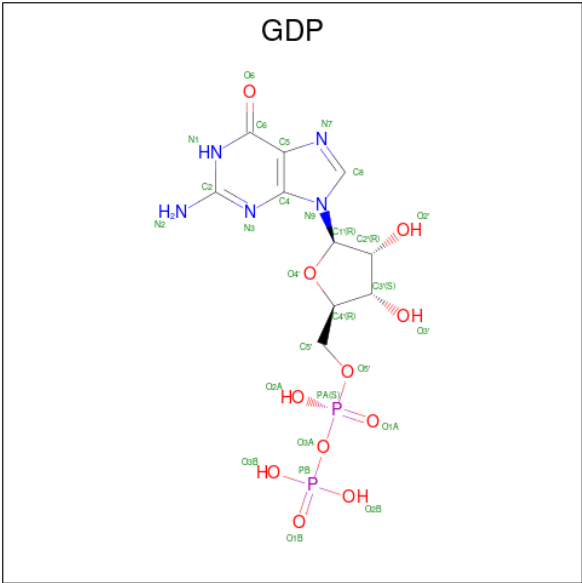
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	91	Total	C	N	O	0	0	0
			456	273	91	92			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



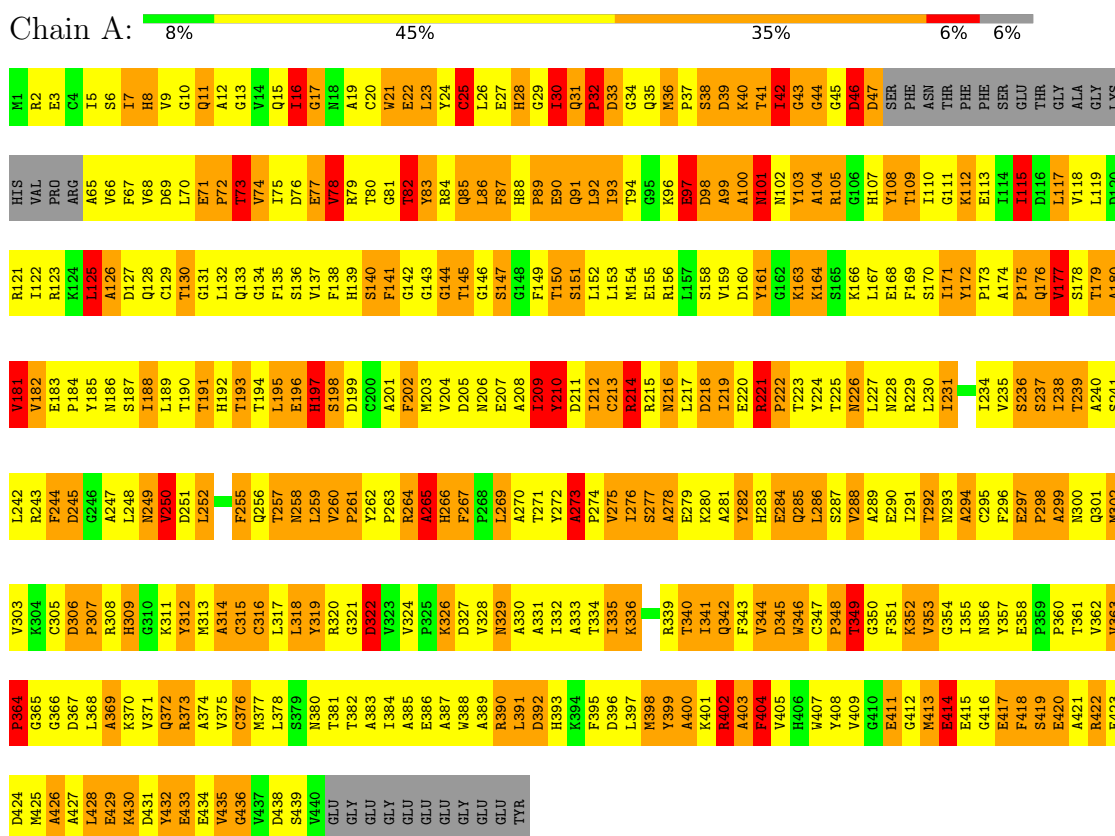
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
5	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

3 Residue-property plots

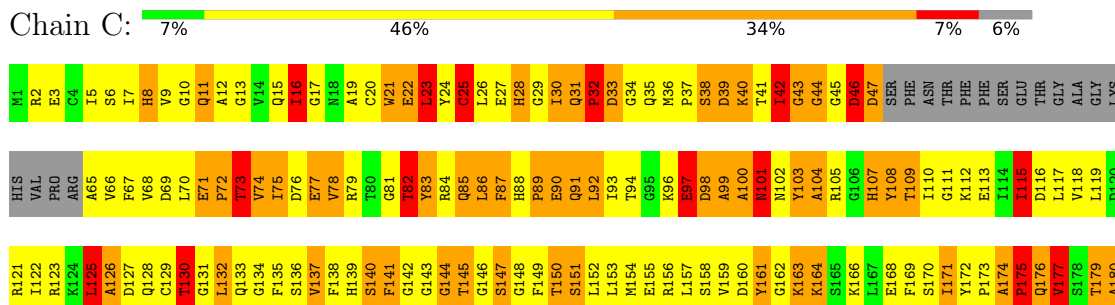
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: PROTEIN (TUBULIN)



• Molecule 1: PROTEIN (TUBULIN)



V181	S241	M302	P364	D424
V182	L242	V303	G365	M425
P183	R243	K304	G366	A426
P184	F244	C305	D367	A427
Y185	L245	D306	L368	L428
M186	G246	P307	A369	E429
S187	A247	R308	K370	K430
L188	L248	H309	V371	D431
L189	N249	G310	Q372	Y432
T190	V250	K311	R373	E433
T191	D251	Y312	A374	E434
H192	T252	K313	V375	V435
T193	T253	A314	Q376	G436
T194	E254	C315	K377	V437
L195	P255	C316	L378	D438
E196	Q256	L317	S379	S439
H197	T257	L318	N380	Y440
S198	N258	Y319	T381	GLY
D199	L259	R320	T382	GLY
G200	V260	G321	A383	GLY
A201	P261	R322	I384	GLY
F202	Y262	K326	A385	GLY
M203	P263	D327	E386	GLY
V204	R264	V328	A387	GLY
D205	A265	N329	A389	GLY
N206	H266	A330	R390	GLY
E207	P267	A331	L391	TYR
A208	L269	I332	D392	
I209	L270	A333	H393	
Y210	A270	T334	K394	
D211		I335	F395	
I212	A273	K336	D396	
C213	P274	L337	L397	
R214	V275	K338	N398	
R215	I276	R339	Y399	
N216	S277	T340	A400	
L217	A278	I341	K401	
D218	E279	Q342	R402	
I219	K280	F343	A403	
E220	A281	V344	P404	
P221	H283	D345	G405	
P222	E284	K346	H406	
T223	Q285	C347	W407	
Y224	L286	P348	Y408	
T225	V287	T349	V409	
N226	V288	F351	G410	
L227	A289	G412	E411	
N228	E290	M413	Y412	
R229	I291	K352	G413	
L230	T292	K353	E414	
I231	N293	L355	E415	
G232	A294	N356	G416	
Q233	C295	Y357	A417	
I234	F296	F358	F418	
V235	E297	P359	S419	
S236	P298	P360	E420	
S237	A299	T361	A421	
I238	N300	V362	V122	
T239	P301			
A240				

• Molecule 2: PROTEIN (TUBULIN)

Chain B: . 52% 29% 8% 8%

K1	R64	K124	P184	F244	A304	K372	Y432
R2	A65	E125	Y185	P245	C305	M373	Q433
E3	I66	E126	N186	Q246	D306	M374	Q434
I4	L67	E127	A187	Q247	P307	A375	Y435
V5	V68	S128	T188	G248	H309	T376	Q436
H6	D69	C129	L189	N249	G310	F377	D437
I7	L70	D130	S190	A250	R311	L378	ALA
Q8	E71	C131	V191	D251	A9	G379	THR
G10	P72	L132	H192	L252	L132	N380	ALA
G11	G73	Q133	Q193	R253	L133	S381	ASP
Q11	T74	G134	L194	K254	T314	T382	GLU
C12	M75	F135	V195	L255	V315	A383	GLN
G13	G76	C136	E196	A256	A316	T384	GLY
N14	S77	L137	N197	V257	K317	Q385	GLY
Q15	V78	T138	T198	M258	V318	E386	PHE
I16	R79	H139	D199	M259	F319	E387	GLU
G17	S80	S140	E200	V260	R320	K388	GLU
A18	G81	L141	T201	P261	G321	F389	GLU
K19	P82	G142	Y202	F262	R322	R390	GLY
F20	F83	G143	G203	P263	H323	I391	GLU
W21	G84	G144	L204	R264	M324	S392	GLU
E22	K85	T145	D205	L265	K325	E393	ASP
V23	L86	G146	N206	H266	K326	Q394	GLU
I24	F87	S147	E207	F267	E327	T395	ASP
S25	R88	G148	A208	F268	V328	T396	ALA
D26	P89	H149	L209	M269	D329	A397	
E27	D90	G150	Y210	G270	E330	K398	
I30	N91	T151	D211	P271	Q331	R399	
P31	F92	L152	T212	G272	M332	F399	
L313	V93	L153	C213	A273	K333	R401	
F94	F94	I154	F214	P274	N334	K402	
G95	G95	S155	R215	L275	V335	A403	
THR	Q96	K156	L216	T276	Q336	F404	
GLY	S97	L157	L217	S277	N337	L405	
SER	S97	R158	K218	R278	K338	H406	
TYR	G98	E159	L219	G279	N339	W407	
HIS	A99	E160	T220	S280	S340	Y408	
GLY	G100	E161	T221	Q281	S341	T409	
ASP	N101	P162	P222	Q282	Y342	G410	
SER	M102	D163	T223	Y283	F343	E411	
ASP	M103	R164	Y224	R284	V344	G412	
LEU	A104	I165	G225	A285	E345	M413	
GLN	K105	M166	D226	L286	V346	D414	
LEU	G106	N167	L227	T287	E415	E415	
GLU	H107	Y108	N228	V288	M416		
ARG	Y108	F169	H229	P289	E417		
ILE	T109	S170	L230	E290	F418		
ASN	G110	V171	V231	L291	T419		
Y51	G111	V172	S232	T292	E420		
Y52	A112	P173	A233	Q293	M421		
Y53	E113	S174	T234	Q294	E422		
N54	L114	P175	M235	F295	S423		
E55	V115	K176	G236	D297	M424		
A56	D116	V177	G237	S177	N425		
A57	S117	F178	V238	G58	M426		
G58	V118	D179	T239	K299	D427		
N59	L119	T180	T240	K300	L428		
K60	D120	V181	C241	M301	V429		
Y61	V121	V182	M302	S430			
V62	V122	E183	R243				
P63	R123						

• Molecule 2: PROTEIN (TUBULIN)

Chain D: . 52% 29% 7% 8%

M1	R64	K124	P184	F244	A304	K372	Y432
R2	A65	E125	Y185	P245	C305	M373	Q433
I3	I66	E126	N186	Q246	D306	M374	Q434
I4	L67	E127	A187	Q247	P307	A375	Y435
V5	V68	S128	T188	G248	H309	T376	Q436
H6	D69	C129	L189	N249	G310	F377	D437
I7	L70	D130	S190	A250	R311	L378	ALA
Q8	E71	C131	V191	D251	A9	G379	THR
A9	P72	L132	H192	L252	L132	N380	ALA
G10	G73	Q133	Q193	R253	L133	S381	ASP
T74	T74	G134	L194	K254	T314	T382	GLU
C12	M75	F135	V195	L255	V315	A383	GLN
G13	G76	C136	E196	A256	A316	T384	GLY
N14	S77	L137	N197	V257	K317	Q385	GLY
Q15	V78	T138	T198	M258	V318	E386	PHE
R79	R79	H139	D199	M259	F319	E387	GLU
G17	S80	S140	E200	V260	R320	K388	GLU
A18	G81	L141	T201	P261	G321	F389	GLU
K19	P82	G142	Y202	F262	R322	R390	GLY
F20	F83	G143	G203	P263	H323	I391	GLU
W21	G84	G144	L204	R264	M324	S392	GLU
E22	K85	T145	D205	L265	K325	E393	ASP
V23	L86	G146	N206	H266	K326	Q394	GLU
I24	F87	S147	E207	F267	E327	T395	ASP
S25	R88	G148	A208	F268	V328	T396	ALA
D26	P89	H149	L209	M269	D329	A397	
E27	D90	G150	Y210	G270	E330	K398	
I30	N91	T151	D211	P271	Q331	R399	
P31	F92	L152	T212	G272	M332	F399	
L313	V93	L153	C213	A273	K333	R401	
F94	F94	I154	F214	P274	N334	K402	
G95	G95	S155	R215	L275	V335	A403	
THR	Q96	K156	L216	T276	Q336	F404	
GLY	S97	L157	L217	S277	N337	L405	
SER	S97	R158	K218	R278	K338	H406	
TYR	G98	E159	L219	G279	N339	W407	
HIS	A99	E160	T220	S280	S340	Y408	
GLY	G100	E161	T221	Q281	S341	T409	
ASP	N101	P162	P222	Q282	Y342	G410	
SER	M102	D163	T223	Y283	F343	E411	
ASP	M103	R164	Y224	R284	V344	G412	
LEU	A104	I165	G225	A285	E345	M413	
GLN	K105	M166	D226	L286	V346	D414	
LEU	G106	N167	L227	T287	E415	E415	
GLU	H107	Y108	N228	V288	M416		
ARG	Y108	F169	H229	P289	E417		
ILE	T109	S170	L230	E290	F418		
ASN	G110	V171	V231	L291	T419		
Y51	G111	V172	S232	T292	E420		
Y52	A112	P173	A233	Q293	M421		
Y53	E113	S174	T234	Q294	E422		
N54	L114	P175	M235	F295	S423		
E55	V115	K176	G236	D297	M424		
A56	D116	V177	G237	S177	N425		
A57	S117	F178	V238	G58	M426		
G58	V118	D179	T239	K299	D427		
N59	L119	T180	T240	K300	L428		
K60	D120	V181	C241	M301	V429		
Y61	V121	V182	M302	S430			
V62	V122	E183	R243				
P63	R123						

K124	P184	R245	C305	M373	Q433
E125	Y185	G246	D306	S374	Q434
S126	N186	Q247	P307	A375	Y435
E127	A187	L248	R308	T376	Q436
S128	T188	N249	H309	F377	D437
G129	G189	A250	G310	I378	ALA
D130	S190	D251	R311	G379	THR
C131	V191	L252	Y312	N380	ALA
L132	H192	R253	L313	S381	ASP
Q133	Q193	K254	T314	T382	GLU
G134	L194	L255	V315	A383	GLN
F135	V195	A256	I384	I384	GLY
E136	E196	Q257	A316	Q385	GLY
L137	N197	N258	A317	E386	PHE
T138	T198	M259	V318	L387	GLU
H139	D199	V260	F319	F388	GLU
S140	E200	P261	R320	F389	GLU
L141	T201	F262	G321	K389	GLY
G142	Y202	P263	R322	R390	GLY
G143	C203	R264	M323	I391	GLU
G144	L204	L265	S324	S392	GLU
T145	D205	H266	N325	E393	ASP
G146	N206	F267	K326	Q394	ALA
S147	E207	F268	E327	F395	
G148	A208	M269	V328	T396	
R149	L209	F270	D329	A397	
G150	Y210	G271	E330	K388	
L151	T211	F272	Q331	F399	
L152	L212	A273	N332	R400	
L153	C213	P274	L333	R401	
I154	F214	L275	N334	K402	
S155	R215	T276	Q335	A403	
K156	T216	S277	Q336	F404	
I157	L217	R278	N337	L405	
E158	K218	G279	K338	H406	
E159	L219	S280	N339	Y407	
E160		Q281	S341	Y408	
Y161	P222	Q282	Y342	T409	
P162	T223	Y283	F343	G410	
D163	Y224	R284	V344	E411	
R164	G225	A285	E345	G412	
I165	D226	L286	D414	M413	
M166	L227	T287	I347	D414	
N167	N228	V288	P348	E415	
T168	H229	P289	N348	M416	
F169	L230	E290	N350	E417	
S170	V231	L291	V351	F418	
V171	S232	T292	K352	T419	
V172	A233	Q293	T353	E420	
P173	T234	Q294	A354	E422	
S174	M235	M295	V355	S423	
P175	S236	F296	C356	M424	
K176	G237	D297	D357	M425	
V177	V238	A298	I358	M426	
S178	T239	K299	P359	D427	
D179	T240	M300	P360	L428	
T180	C241	M301	R369	V429	
V181	L242	M302	G370	S430	
V182	R243	A303	L371	E431	
E183	F244	A304	K372	Y432	

● Molecule 3: PROTEIN (STATHMIN-LIKE DOMAIN OF RB3)

Chain E: 32% 68%

X1	X10	X24	X42
X2	X11	X25	X43
X3	X12	X26	X44
X4	X13	X27	X45
X5	X14	X28	X46
X6	X15	X29	X47
X7	X16	X30	X48
X8	X17	X31	X49
X9	X18	X32	X50
X10	X19	X33	X51
X11	X20	X34	X52
X12	X21	X35	X53
X13		X36	X54
X14		X37	X55
X15		X38	X56
X16		X39	X57
X17			X58
X18			X59
X19			X60
X20			X61
X21			X62
X22			X63
X23			X64
X24			
X25			
X26			
X27			
X28			
X29			
X30			
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X81			
X82			
X83			
X84			
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X86			
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X88			
X89			
X90			
X91			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	328.50Å 328.50Å 54.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 3.95	Depositor
% Data completeness (in resolution range)	94.3 (7.00-3.95)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.267 , 0.367	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13568	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

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: GTP, GDP

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	0.78	5/3367 (0.1%)	1.35	60/4570 (1.3%)
1	C	0.71	1/3367 (0.0%)	1.33	65/4570 (1.4%)
2	B	0.69	0/3270	1.26	51/4428 (1.2%)
2	D	0.72	1/3270 (0.0%)	1.27	48/4428 (1.1%)
All	All	0.73	7/13274 (0.1%)	1.31	224/17996 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
2	B	0	1
2	D	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	ILE	CA-CB	-6.30	1.45	1.54
1	A	78	VAL	CA-CB	5.80	1.62	1.54
1	A	250	VAL	CA-CB	5.65	1.59	1.55
2	D	86	ILE	CA-CB	5.30	1.61	1.54
1	C	16	ILE	CA-CB	5.11	1.61	1.54
1	A	36	MET	SD-CE	5.08	1.92	1.79
1	A	80	THR	CA-CB	5.08	1.59	1.52

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	417	GLU	N-CA-C	-14.39	94.99	112.54
1	A	417	GLU	N-CA-C	-14.03	95.43	112.54
1	A	294	ALA	N-CA-C	-13.67	96.46	111.36
1	C	294	ALA	N-CA-C	-13.53	96.61	111.36
1	A	117	LEU	N-CA-C	-12.32	98.72	113.88
1	C	81	GLY	N-CA-C	-11.56	100.27	113.79
1	A	81	GLY	N-CA-C	-11.37	100.49	113.79
1	C	117	LEU	N-CA-C	-11.36	99.90	113.88
2	B	180	THR	N-CA-C	-11.30	99.74	113.19
1	A	176	GLN	N-CA-C	-10.89	98.35	113.37
2	D	180	THR	N-CA-C	-10.75	100.39	113.19
1	C	176	GLN	N-CA-C	-10.73	98.56	113.37
1	C	43	GLY	N-CA-C	-10.65	100.47	114.85
2	B	356	CYS	N-CA-C	10.48	125.05	110.06
2	B	420	GLU	N-CA-C	-10.04	101.03	113.18
1	A	43	GLY	N-CA-C	-9.98	100.88	114.95
2	D	22	GLU	N-CA-C	-9.39	99.39	112.45
2	D	420	GLU	N-CA-C	-9.31	101.34	112.89
2	D	356	CYS	N-CA-C	9.06	123.02	110.06
2	B	22	GLU	N-CA-C	-9.02	99.91	112.45
1	C	396	ASP	N-CA-C	-8.92	101.49	112.38
1	C	231	ILE	N-CA-C	-8.86	100.18	112.50
2	B	394	GLN	N-CA-C	-8.62	104.79	114.62
1	A	396	ASP	N-CA-C	-8.57	102.59	112.87
1	C	390	ARG	N-CA-C	-8.52	101.93	111.82
2	D	191	VAL	N-CA-C	-8.42	104.82	112.90
1	A	231	ILE	N-CA-C	-8.40	100.65	113.16
1	A	426	ALA	N-CA-C	-8.38	102.98	113.55
2	B	77	SER	N-CA-C	-8.35	102.65	113.17
2	D	403	ALA	N-CA-C	8.31	119.60	107.88
1	C	372	GLN	N-CA-C	-8.12	102.97	113.12
1	C	180	ALA	N-CA-C	-7.96	98.14	110.17
1	C	25	CYS	N-CA-C	-7.90	103.20	112.92
2	D	77	SER	N-CA-C	-7.85	103.28	113.17
2	D	20	PHE	N-CA-C	-7.79	100.83	112.04
2	B	191	VAL	N-CA-C	-7.75	105.46	112.90
2	D	347	ILE	CA-C-N	7.72	129.49	119.84
2	D	347	ILE	C-N-CA	7.72	129.49	119.84
2	D	244	PHE	CA-C-N	7.62	129.37	119.84
2	D	244	PHE	C-N-CA	7.62	129.37	119.84
2	B	244	PHE	CA-C-N	7.56	129.29	119.84
2	B	244	PHE	C-N-CA	7.56	129.29	119.84
1	A	390	ARG	N-CA-C	-7.55	103.06	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	ALA	N-CA-C	-7.55	103.06	112.72
2	D	224	TYR	N-CA-C	-7.50	103.87	112.87
2	B	20	PHE	N-CA-C	-7.49	101.26	112.04
1	A	180	ALA	N-CA-C	-7.41	98.99	110.17
1	A	434	GLU	N-CA-C	-7.39	104.71	113.21
1	C	21	TRP	N-CA-C	-7.39	104.40	113.19
1	A	372	GLN	N-CA-C	-7.34	103.94	113.12
2	D	157	ILE	N-CA-C	-7.32	102.03	112.35
1	A	422	ARG	N-CA-C	-7.32	105.53	114.75
1	C	434	GLU	N-CA-C	-7.27	104.50	113.15
2	D	178	SER	N-CA-C	-7.25	98.50	110.17
1	A	21	TRP	N-CA-C	-7.19	104.63	113.19
2	D	113	GLU	N-CA-C	-7.11	101.80	112.04
2	D	254	LYS	N-CA-C	-7.11	103.70	112.38
2	B	113	GLU	N-CA-C	-7.10	102.08	111.24
1	A	392	ASP	N-CA-C	-7.09	104.78	113.50
2	B	347	ILE	CA-C-N	7.09	128.70	119.84
2	B	347	ILE	C-N-CA	7.09	128.70	119.84
2	D	149	MET	N-CA-C	-7.01	102.85	111.40
2	B	120	ASP	N-CA-C	-7.00	106.65	114.62
2	D	54	ASN	N-CA-C	7.00	120.14	110.35
2	B	178	SER	N-CA-C	-6.99	98.92	110.17
2	D	336	GLN	N-CA-C	-6.89	104.13	112.54
1	C	422	ARG	N-CA-C	-6.86	106.11	114.75
1	A	400	ALA	N-CA-C	-6.83	106.14	114.75
2	D	122	VAL	N-CA-C	-6.83	103.56	111.00
2	D	396	THR	N-CA-C	-6.80	104.09	112.38
1	C	400	ALA	N-CA-C	-6.79	106.19	114.75
2	B	122	VAL	N-CA-C	-6.79	103.60	111.00
1	A	236	SER	N-CA-C	-6.78	103.50	111.03
2	D	421	ALA	N-CA-C	-6.78	104.82	113.23
1	C	33	ASP	N-CA-C	-6.71	105.00	113.72
2	B	403	ALA	N-CA-C	6.69	117.32	107.88
2	B	242	LEU	N-CA-C	-6.67	104.20	112.47
2	B	254	LYS	N-CA-C	-6.64	104.28	112.38
2	B	336	GLN	N-CA-C	-6.60	104.48	112.54
1	C	209	ILE	N-CA-C	6.60	116.75	110.42
1	A	438	ASP	N-CA-C	6.59	118.97	109.14
2	B	241	CYS	N-CA-C	-6.59	101.25	110.35
2	D	242	LEU	N-CA-C	-6.57	104.33	112.47
1	C	429	GLU	N-CA-C	-6.56	105.14	113.01
1	A	42	ILE	N-CA-C	6.53	122.93	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	422	GLU	N-CA-C	-6.52	105.14	113.23
2	B	157	ILE	N-CA-C	-6.50	103.18	112.35
1	A	85	GLN	N-CA-C	6.48	118.17	107.73
2	D	120	ASP	N-CA-C	-6.47	107.24	114.62
2	B	54	ASN	N-CA-C	6.46	119.39	110.35
1	C	363	VAL	CA-C-N	6.44	127.89	119.84
1	C	363	VAL	C-N-CA	6.44	127.89	119.84
2	B	224	TYR	N-CA-C	-6.44	105.15	112.87
1	C	22	GLU	N-CA-C	-6.40	104.51	112.90
1	A	429	GLU	N-CA-C	-6.37	105.37	113.01
1	C	236	SER	N-CA-C	-6.34	104.05	110.97
2	D	223	THR	N-CA-C	-6.32	101.59	110.50
1	A	22	GLU	N-CA-C	-6.29	104.67	112.90
1	A	25	CYS	N-CA-C	-6.28	105.26	113.17
2	B	421	ALA	N-CA-C	-6.28	105.45	113.23
2	B	378	ILE	CA-C-N	-6.27	117.86	122.18
2	B	378	ILE	C-N-CA	-6.27	117.86	122.18
1	A	151	SER	N-CA-C	-6.26	104.74	112.38
1	C	137	VAL	CB-CA-C	-6.21	105.22	111.80
1	C	151	SER	N-CA-C	-6.20	104.81	112.38
2	B	422	GLU	N-CA-C	-6.18	105.57	113.23
1	C	183	GLU	CA-C-N	6.17	127.56	119.84
1	C	183	GLU	C-N-CA	6.17	127.56	119.84
2	B	223	THR	N-CA-C	-6.17	101.80	110.50
2	B	262	PHE	N-CA-C	6.16	119.81	109.09
1	A	33	ASP	N-CA-C	-6.10	105.79	113.72
1	A	209	ILE	N-CA-C	6.10	116.27	110.42
2	D	333	LEU	N-CA-C	-6.09	104.20	111.69
2	D	435	TYR	N-CA-C	-6.07	106.86	114.56
1	C	23	LEU	N-CA-C	-6.05	104.60	112.23
1	C	107	HIS	N-CA-C	-6.04	106.44	113.88
2	D	241	CYS	N-CA-C	-6.04	102.02	110.35
1	C	255	PHE	N-CA-C	-6.03	106.47	113.88
2	D	329	ASP	N-CA-C	-6.01	105.78	113.23
2	B	329	ASP	N-CA-C	-5.98	105.81	113.23
2	D	164	ARG	N-CA-C	5.95	118.69	110.35
1	C	85	GLN	N-CA-C	5.92	117.26	107.73
1	A	226	ASN	N-CA-C	-5.91	104.84	111.28
2	B	299	LYS	N-CA-C	-5.91	105.92	113.01
1	A	430	LYS	N-CA-C	-5.90	103.62	111.24
1	A	31	GLN	CA-C-N	5.90	127.22	119.84
1	A	31	GLN	C-N-CA	5.90	127.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	N-CA-C	-5.90	107.07	114.56
1	C	104	ALA	N-CA-C	-5.90	104.03	111.11
2	B	283	TYR	N-CA-C	-5.89	98.24	110.80
1	A	218	ASP	CB-CA-C	-5.89	109.76	116.54
1	A	265	ALA	N-CA-C	5.88	123.33	110.80
2	B	333	LEU	N-CA-C	-5.88	104.45	111.69
2	B	201	THR	N-CA-C	5.85	117.66	107.49
1	C	42	ILE	N-CA-C	5.84	121.49	109.34
2	B	396	THR	N-CA-C	-5.84	105.26	112.38
2	B	203	CYS	N-CA-C	5.83	117.56	107.93
2	D	262	PHE	N-CA-C	5.83	119.24	109.09
2	D	61	TYR	N-CA-C	5.82	123.20	110.80
1	C	273	ALA	N-CA-C	5.82	122.67	109.81
1	A	273	ALA	N-CA-C	5.82	122.66	109.81
1	C	265	ALA	N-CA-C	5.82	123.19	110.80
1	A	391	LEU	N-CA-C	-5.81	106.17	113.20
2	B	418	PHE	N-CA-C	-5.80	105.98	114.39
1	C	438	ASP	N-CA-C	5.78	117.76	109.14
2	B	346	TRP	N-CA-C	-5.78	103.97	113.50
1	A	221	ARG	CA-C-N	5.77	127.05	119.84
1	A	221	ARG	C-N-CA	5.77	127.05	119.84
2	D	284	ARG	N-CA-C	-5.75	106.65	113.38
2	B	149	MET	N-CA-C	-5.74	104.39	111.40
2	B	291	LEU	N-CA-C	-5.72	104.41	111.33
1	C	199	ASP	N-CA-C	-5.70	106.45	113.41
1	C	290	GLU	N-CA-C	-5.67	105.62	112.54
1	C	391	LEU	N-CA-C	-5.66	106.36	113.20
1	C	248	LEU	N-CA-C	-5.64	102.05	110.23
1	A	255	PHE	N-CA-C	-5.64	106.94	113.88
2	D	346	TRP	N-CA-C	-5.64	104.19	113.50
1	A	147	SER	N-CA-C	-5.61	107.08	114.04
2	D	183	GLU	CA-C-N	-5.61	112.83	119.84
2	D	183	GLU	C-N-CA	-5.61	112.83	119.84
1	A	249	ASN	N-CA-C	5.58	118.97	108.65
1	C	392	ASP	N-CA-C	-5.57	106.65	113.50
1	A	74	VAL	N-CA-C	-5.55	104.11	111.05
2	B	248	LEU	CB-CA-C	-5.55	110.16	116.54
1	A	104	ALA	N-CA-C	-5.54	102.23	111.37
1	C	75	ILE	N-CA-C	-5.53	106.99	111.91
1	C	126	ALA	N-CA-C	-5.51	106.64	113.19
1	C	214	ARG	N-CA-C	-5.48	107.24	114.31
1	C	31	GLN	CA-C-N	5.48	126.69	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	GLN	C-N-CA	5.48	126.69	119.84
1	A	44	GLY	N-CA-C	-5.46	100.23	113.18
1	A	202	PHE	N-CA-C	5.45	118.22	107.98
1	C	82	THR	CB-CA-C	-5.44	108.71	115.89
2	B	61	TYR	N-CA-C	5.43	122.38	110.80
1	C	425	MET	N-CA-C	-5.39	106.74	113.15
1	C	331	ALA	N-CA-C	-5.38	106.76	113.55
2	D	147	SER	N-CA-C	-5.36	104.16	111.56
1	A	363	VAL	CA-C-N	5.36	126.54	119.84
1	A	363	VAL	C-N-CA	5.36	126.54	119.84
1	C	147	SER	N-CA-C	-5.33	107.42	114.04
1	C	295	CYS	N-CA-C	-5.33	106.47	112.87
2	B	188	THR	N-CA-C	-5.29	106.05	112.88
2	B	21	TRP	N-CA-C	-5.24	106.96	113.19
2	B	384	ILE	N-CA-C	-5.24	106.11	112.76
2	D	299	LYS	N-CA-C	-5.23	106.73	113.01
2	D	342	TYR	N-CA-C	5.22	116.71	110.44
2	D	59	ASN	N-CA-C	5.22	116.22	108.86
1	C	281	ALA	N-CA-C	5.21	117.22	109.25
2	D	400	ARG	N-CA-C	-5.21	106.25	113.18
2	B	124	LYS	N-CA-C	-5.20	106.12	113.20
1	C	218	ASP	CB-CA-C	-5.20	110.56	116.54
1	C	430	LYS	N-CA-C	-5.19	104.55	111.24
1	A	82	THR	CB-CA-C	-5.19	109.04	115.89
1	A	126	ALA	N-CA-C	-5.18	107.03	113.19
1	A	260	VAL	CA-C-N	5.18	126.31	119.84
1	A	260	VAL	C-N-CA	5.18	126.31	119.84
2	D	328	VAL	N-CA-C	5.16	117.50	111.05
1	A	36	MET	CA-C-N	5.15	124.65	119.19
1	A	36	MET	C-N-CA	5.15	124.65	119.19
1	C	226	ASN	N-CA-C	-5.14	105.67	111.28
2	D	291	LEU	N-CA-C	-5.14	105.11	111.33
2	B	410	GLY	N-CA-C	-5.14	106.42	112.64
2	B	92	PHE	N-CA-C	5.13	117.85	109.59
1	C	384	ILE	N-CA-C	-5.12	104.69	111.09
1	A	193	THR	N-CA-C	-5.10	107.57	112.97
1	A	281	ALA	N-CA-C	5.09	117.04	109.25
2	D	151	THR	N-CA-C	-5.09	106.17	112.38
1	C	221	ARG	CA-C-N	5.08	126.18	119.84
1	C	221	ARG	C-N-CA	5.08	126.18	119.84
2	D	188	THR	N-CA-C	-5.08	106.33	112.88
1	A	172	TYR	CA-C-N	5.07	126.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	C-N-CA	5.07	126.18	119.84
1	C	44	GLY	N-CA-C	-5.07	101.16	113.18
1	A	322	ASP	N-CA-C	5.07	121.60	110.80
2	D	201	THR	N-CA-C	5.06	116.83	108.13
1	A	319	TYR	N-CA-C	-5.05	102.30	110.32
1	A	41	THR	N-CA-C	5.04	117.01	110.65
2	B	183	GLU	CA-C-N	-5.04	113.53	119.84
2	B	183	GLU	C-N-CA	-5.04	113.53	119.84
1	C	282	TYR	N-CA-C	-5.03	106.40	112.54
1	C	353	VAL	N-CA-C	5.02	119.79	109.34
1	C	174	ALA	CA-C-N	5.02	126.11	119.84
1	C	174	ALA	C-N-CA	5.02	126.11	119.84
1	C	74	VAL	N-CA-C	-5.00	104.80	111.05

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	TYR	Sidechain
2	B	61	TYR	Sidechain
1	C	108	TYR	Sidechain
1	C	210	TYR	Sidechain
2	D	312	TYR	Sidechain

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	3295	0	3202	916	0
1	C	3295	0	3202	966	0
2	B	3201	0	3091	964	0
2	D	3201	0	3091	924	0
3	E	456	0	103	79	0
4	A	32	0	12	4	0
4	C	32	0	12	8	0
5	B	28	0	12	5	0
5	D	28	0	12	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13568	0	12737	3761	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 143.

All (3761) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:PRO:HD2	2:B:207:GLU:HB2	1.23	1.16
2:D:158:ARG:HD3	2:D:197:ASN:ND2	1.63	1.14
1:A:214:ARG:HH21	1:A:220:GLU:HA	1.04	1.14
2:B:179:ASP:HA	1:C:352:LYS:HE2	1.20	1.12
1:C:222:PRO:HB2	1:C:227:LEU:HD11	1.31	1.12
2:D:311:ARG:HH21	2:D:437:ASP:HB2	1.03	1.13
1:C:175:PRO:HD2	1:C:207:GLU:HB2	1.16	1.12
1:C:214:ARG:HH21	1:C:220:GLU:HA	0.99	1.12
2:D:175:PRO:HD2	2:D:207:GLU:HB2	1.26	1.12
2:B:92:PHE:HE1	2:B:118:VAL:HA	0.96	1.12
1:C:419:SER:HA	1:C:422:ARG:HD3	1.22	1.12
2:D:278:ARG:HA	2:D:278:ARG:HH11	0.96	1.12
1:A:222:PRO:HB2	1:A:227:LEU:HD11	1.31	1.11
1:A:102:ASN:HB2	1:A:105:ARG:HB2	1.31	1.11
1:A:70:LEU:HD12	1:A:145:THR:HA	1.26	1.11
2:B:92:PHE:CE1	2:B:118:VAL:HA	1.85	1.10
2:D:92:PHE:HE1	2:D:118:VAL:HA	0.98	1.10
1:A:419:SER:HA	1:A:422:ARG:HD3	1.20	1.09
1:A:175:PRO:HD2	1:A:207:GLU:HB2	1.09	1.08
1:C:70:LEU:HD12	1:C:145:THR:HA	1.22	1.08
2:B:311:ARG:HH21	2:B:437:ASP:HB2	1.04	1.08
1:C:306:ASP:OD1	1:C:308:ARG:HB3	1.54	1.08
2:D:92:PHE:CE1	2:D:118:VAL:HA	1.88	1.08
1:C:102:ASN:HB2	1:C:105:ARG:HB2	1.33	1.08
2:B:206:ASN:HD22	2:B:227:LEU:HD21	1.19	1.07
2:B:213:CYS:HB3	2:B:219:LEU:HD12	1.32	1.07
2:B:2:ARG:HG3	2:B:133:GLN:NE2	1.70	1.06
1:C:316:CYS:HB2	1:C:352:LYS:HB3	1.33	1.06
2:D:192:HIS:HA	2:D:195:VAL:HG22	1.34	1.06
1:A:133:GLN:H	1:A:164:LYS:HD3	1.12	1.06
2:D:240:THR:O	2:D:243:ARG:HB2	1.56	1.06
1:A:383:ALA:O	1:A:386:GLU:HG2	1.55	1.05
2:B:190:SER:HB2	2:B:425:MET:HG3	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:VAL:HG21	2:B:421:ALA:HB1	1.38	1.05
2:D:158:ARG:HG3	2:D:159:GLU:H	1.16	1.05
2:D:213:CYS:HB3	2:D:219:LEU:HD12	1.37	1.04
1:A:306:ASP:OD1	1:A:308:ARG:HB3	1.57	1.04
1:A:7:ILE:HG22	1:A:66:VAL:HB	1.37	1.04
2:B:178:SER:O	2:B:182:VAL:HB	1.57	1.04
2:B:192:HIS:HA	2:B:195:VAL:HG22	1.36	1.04
2:B:278:ARG:HA	2:B:278:ARG:NH1	1.72	1.04
1:C:7:ILE:HG22	1:C:66:VAL:HB	1.33	1.04
2:B:278:ARG:HA	2:B:278:ARG:HH11	0.91	1.03
2:D:2:ARG:HG3	2:D:133:GLN:NE2	1.73	1.03
2:B:158:ARG:HD3	2:B:197:ASN:ND2	1.74	1.03
1:A:409:VAL:HA	1:A:414:GLU:OE1	1.57	1.02
2:D:178:SER:O	2:D:182:VAL:HB	1.56	1.02
1:A:141:PHE:HE2	1:A:172:TYR:HA	1.23	1.02
2:B:264:ARG:HH21	2:B:428:LEU:HD12	1.22	1.02
2:B:158:ARG:HG3	2:B:159:GLU:H	1.22	1.01
1:C:133:GLN:H	1:C:164:LYS:HD3	1.19	1.01
1:A:88:HIS:HB3	1:A:91:GLN:NE2	1.75	1.01
1:C:9:VAL:HG12	1:C:68:VAL:HG13	1.43	1.01
1:A:413:MET:SD	3:E:15:UNK:HA	2.01	1.00
1:A:9:VAL:HG12	1:A:68:VAL:HG13	1.44	1.00
2:B:240:THR:O	2:B:243:ARG:HB2	1.62	1.00
1:C:93:ILE:HD13	1:C:118:VAL:HG22	1.43	0.99
1:A:242:LEU:HD21	1:A:318:LEU:HD21	1.43	0.99
2:B:322:ARG:HG2	2:B:357:ASP:HA	1.45	0.99
2:D:278:ARG:HA	2:D:278:ARG:NH1	1.76	0.99
2:D:264:ARG:HH21	2:D:428:LEU:HD12	1.25	0.99
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.45	0.98
2:D:191:VAL:HG21	2:D:421:ALA:HB1	1.42	0.98
2:D:206:ASN:HD22	2:D:227:LEU:HD21	1.26	0.98
1:A:316:CYS:HB2	1:A:352:LYS:HB3	1.41	0.98
2:B:220:THR:HB	1:C:326:LYS:HD2	1.43	0.98
1:A:387:ALA:HA	1:A:390:ARG:HD3	1.45	0.98
2:D:190:SER:HB2	2:D:425:MET:HG3	1.44	0.98
2:B:196:GLU:O	2:B:198:THR:HG22	1.64	0.97
1:C:387:ALA:HA	1:C:390:ARG:HD3	1.46	0.97
2:B:77:SER:HA	2:B:80:SER:HB3	1.46	0.97
1:A:102:ASN:HB2	1:A:105:ARG:CB	1.95	0.97
1:A:115:ILE:HD11	1:A:156:ARG:HG3	1.47	0.97
1:C:141:PHE:HE2	1:C:172:TYR:HA	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.45	0.97
2:D:263:PRO:C	2:D:265:LEU:H	1.68	0.97
1:C:88:HIS:HB3	1:C:91:GLN:NE2	1.80	0.97
1:C:115:ILE:HD11	1:C:156:ARG:HG3	1.47	0.96
2:D:158:ARG:HB2	2:D:197:ASN:HB2	1.47	0.96
1:A:69:ASP:HB3	1:A:75:ILE:HG21	1.46	0.96
2:B:132:LEU:HB3	2:B:164:ARG:NH2	1.80	0.96
1:A:322:ASP:H	1:A:357:TYR:HA	1.30	0.96
1:C:166:LYS:HE3	1:C:198:SER:H	1.31	0.96
1:C:409:VAL:HA	1:C:414:GLU:OE1	1.64	0.96
2:D:91:ASN:HD22	2:D:91:ASN:H	1.10	0.96
1:A:237:SER:HA	1:A:241:SER:HB2	1.48	0.96
2:B:278:ARG:HH11	2:B:278:ARG:CA	1.79	0.95
1:C:214:ARG:NH2	1:C:220:GLU:HA	1.80	0.95
2:B:91:ASN:H	2:B:91:ASN:HD22	1.05	0.95
1:C:185:TYR:HA	1:C:188:ILE:HD11	1.48	0.95
2:B:223:THR:HG22	2:B:226:ASP:OD2	1.66	0.95
1:C:386:GLU:HG3	1:C:387:ALA:H	1.32	0.95
2:D:8:GLN:HG2	2:D:14:ASN:HD22	1.30	0.95
1:C:102:ASN:HB2	1:C:105:ARG:CB	1.97	0.95
1:A:214:ARG:NH2	1:A:220:GLU:HA	1.81	0.94
1:C:362:VAL:HG13	1:C:367:ASP:HB2	1.49	0.94
1:A:311:LYS:HD3	1:A:344:VAL:HG13	1.48	0.94
2:D:322:ARG:HG2	2:D:357:ASP:HA	1.45	0.94
2:D:77:SER:HA	2:D:80:SER:HB3	1.48	0.94
2:D:196:GLU:O	2:D:198:THR:HG22	1.66	0.94
1:A:93:ILE:HD13	1:A:118:VAL:HG22	1.48	0.94
2:B:115:VAL:HG11	2:B:156:LYS:HZ2	1.29	0.94
2:B:407:TRP:HZ2	1:C:256:GLN:HB2	1.30	0.94
1:A:79:ARG:HD3	1:A:89:PRO:HB3	1.50	0.93
2:D:218:LYS:HZ3	2:D:278:ARG:N	1.65	0.93
1:A:175:PRO:CD	1:A:207:GLU:HB2	1.97	0.93
1:C:322:ASP:H	1:C:357:TYR:HA	1.32	0.93
1:A:409:VAL:HG22	1:A:414:GLU:HG3	1.51	0.93
2:B:263:PRO:C	2:B:265:LEU:H	1.64	0.93
1:C:102:ASN:HD21	2:D:257:VAL:HG11	1.33	0.93
1:A:398:MET:SD	2:B:348:PRO:HD2	2.09	0.93
2:D:19:LYS:HZ1	2:D:82:PRO:HG3	1.32	0.93
2:B:218:LYS:HZ3	2:B:278:ARG:H	0.96	0.92
1:C:175:PRO:C	1:C:177:VAL:H	1.65	0.92
1:A:322:ASP:N	1:A:357:TYR:HA	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PHE:HE2	1:C:92:LEU:HD21	1.34	0.92
1:C:383:ALA:O	1:C:386:GLU:HG2	1.68	0.92
1:C:322:ASP:N	1:C:357:TYR:HA	1.84	0.92
2:B:158:ARG:HB2	2:B:197:ASN:HB2	1.51	0.92
1:A:102:ASN:HD21	2:B:257:VAL:HG11	1.31	0.92
1:A:386:GLU:HG3	1:A:387:ALA:H	1.33	0.92
1:C:409:VAL:HG22	1:C:414:GLU:CG	2.00	0.92
2:D:311:ARG:NH2	2:D:437:ASP:HB2	1.83	0.92
1:A:287:SER:H	1:A:290:GLU:CD	1.77	0.92
2:D:132:LEU:HB3	2:D:164:ARG:NH2	1.84	0.91
1:C:237:SER:HA	1:C:241:SER:HB2	1.49	0.91
2:D:218:LYS:HZ3	2:D:278:ARG:H	0.91	0.91
1:A:362:VAL:HG13	1:A:367:ASP:HB2	1.50	0.91
1:C:409:VAL:HG22	1:C:414:GLU:HG3	1.50	0.91
2:D:284:ARG:O	2:D:287:THR:HG23	1.71	0.91
2:B:194:LEU:HD23	2:B:195:VAL:HG13	1.52	0.91
1:A:409:VAL:HG22	1:A:414:GLU:CG	2.01	0.91
2:B:8:GLN:HG2	2:B:14:ASN:HD22	1.32	0.91
1:A:398:MET:HG3	1:A:399:TYR:HD1	1.33	0.91
1:C:335:ILE:HG13	1:C:336:LYS:H	1.32	0.91
2:B:223:THR:HG22	2:B:226:ASP:CG	1.97	0.90
1:A:175:PRO:C	1:A:177:VAL:H	1.70	0.90
2:D:194:LEU:HD23	2:D:195:VAL:HG13	1.50	0.90
2:B:218:LYS:HZ3	2:B:278:ARG:N	1.70	0.90
1:A:166:LYS:HE3	1:A:198:SER:H	1.35	0.90
2:D:262:PHE:HB3	2:D:263:PRO:HD2	1.53	0.90
1:A:223:THR:HB	1:A:226:ASN:OD1	1.71	0.90
2:B:2:ARG:NE	2:B:243:ARG:HD2	1.86	0.90
2:D:278:ARG:N	2:D:278:ARG:HD2	1.84	0.90
1:A:402:ARG:HD2	2:B:346:TRP:CZ3	2.07	0.90
2:B:59:ASN:HB2	2:B:64:ARG:NE	1.86	0.90
2:B:286:LEU:HD12	2:B:373:MET:HB2	1.54	0.90
1:C:398:MET:SD	2:D:348:PRO:HD2	2.11	0.90
2:B:278:ARG:N	2:B:278:ARG:HD2	1.83	0.90
2:D:70:LEU:HG	2:D:99:ALA:HB3	1.53	0.89
2:D:121:VAL:HA	2:D:124:LYS:HG2	1.54	0.89
2:B:96:GLN:HE22	1:C:130:THR:HG22	1.35	0.89
2:B:311:ARG:NH2	2:B:437:ASP:HB2	1.88	0.89
1:A:335:ILE:HG13	1:A:336:LYS:H	1.36	0.89
1:A:243:ARG:HH12	1:A:250:VAL:HG13	1.38	0.88
2:B:19:LYS:HZ1	2:B:82:PRO:HG3	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ARG:NH2	1:C:133:GLN:HE22	1.70	0.88
2:B:321:GLY:HA2	2:B:359:PRO:HB3	1.53	0.88
2:D:58:GLY:C	2:D:64:ARG:HE	1.81	0.88
1:A:9:VAL:HG12	1:A:68:VAL:CG1	2.03	0.88
1:A:166:LYS:NZ	1:A:197:HIS:HB2	1.88	0.88
1:C:79:ARG:HD3	1:C:89:PRO:HB3	1.55	0.88
1:A:16:ILE:HG22	1:A:17:GLY:N	1.87	0.88
1:A:418:PHE:HD2	1:A:418:PHE:N	1.72	0.88
1:C:242:LEU:HD21	1:C:318:LEU:HD21	1.52	0.88
2:D:51:VAL:HG23	2:D:53:TYR:H	1.38	0.88
1:C:31:GLN:HB3	1:C:32:PRO:HD2	1.56	0.88
1:C:69:ASP:OD1	1:C:70:LEU:N	2.05	0.88
2:B:133:GLN:NE2	2:B:252:LEU:HB3	1.87	0.88
1:C:261:PRO:HG2	1:C:380:ASN:HD21	1.39	0.88
1:A:107:HIS:HD1	1:A:151:SER:HB2	1.37	0.88
2:D:278:ARG:HH11	2:D:278:ARG:CA	1.84	0.88
2:B:192:HIS:C	2:B:194:LEU:H	1.82	0.87
2:B:284:ARG:O	2:B:287:THR:HG23	1.73	0.87
1:A:186:ASN:ND2	1:A:391:LEU:HD11	1.90	0.87
1:C:175:PRO:CD	1:C:207:GLU:HB2	2.04	0.87
2:D:339:ASN:HB3	2:D:342:TYR:HD1	1.37	0.87
1:C:186:ASN:ND2	1:C:391:LEU:HD11	1.90	0.87
1:A:350:GLY:C	1:A:351:PHE:HD1	1.82	0.87
1:C:36:MET:HA	1:C:36:MET:HE3	1.57	0.87
1:C:206:ASN:HB3	1:C:210:TYR:CE2	2.10	0.87
1:C:398:MET:HG3	1:C:399:TYR:HD1	1.38	0.87
1:A:216:ASN:HD22	1:A:275:VAL:HG12	1.38	0.87
1:A:409:VAL:HG13	1:A:414:GLU:OE2	1.75	0.87
1:A:339:ARG:HD2	1:A:339:ARG:C	1.98	0.87
2:B:189:LEU:C	2:B:191:VAL:H	1.83	0.87
1:A:144:GLY:N	1:A:147:SER:HB3	1.89	0.87
1:A:261:PRO:HG2	1:A:380:ASN:HD21	1.38	0.87
1:A:320:ARG:HB3	1:A:374:ALA:HB3	1.56	0.87
2:B:176:LYS:HD2	2:B:210:TYR:CZ	2.10	0.87
1:C:27:GLU:HG3	1:C:28:HIS:H	1.40	0.86
1:C:243:ARG:HH12	1:C:250:VAL:HG13	1.39	0.86
2:D:189:LEU:C	2:D:191:VAL:H	1.83	0.86
2:D:115:VAL:HG11	2:D:156:LYS:HZ2	1.39	0.86
2:B:396:THR:HG23	2:B:400:ARG:HD3	1.54	0.86
1:C:287:SER:H	1:C:290:GLU:CD	1.82	0.86
2:D:396:THR:HG23	2:D:400:ARG:HD3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:HZ2	1:A:164:LYS:N	1.72	0.86
2:D:88:ARG:HB2	2:D:89:PRO:HD3	1.56	0.86
2:D:223:THR:HG22	2:D:226:ASP:OD2	1.76	0.86
1:A:322:ASP:H	1:A:357:TYR:CA	1.88	0.86
2:B:88:ARG:HB2	2:B:89:PRO:HD3	1.55	0.86
2:B:311:ARG:HB2	2:B:344:VAL:H	1.40	0.86
2:B:339:ASN:HB3	2:B:342:TYR:HD1	1.40	0.86
1:A:166:LYS:HZ2	1:A:197:HIS:HB2	1.38	0.86
2:D:358:ILE:H	2:D:358:ILE:HD12	1.40	0.86
1:C:87:PHE:CE2	1:C:92:LEU:HD21	2.10	0.86
2:D:321:GLY:HA2	2:D:359:PRO:HB3	1.58	0.86
1:C:418:PHE:HD2	1:C:418:PHE:N	1.73	0.86
1:C:362:VAL:HG21	1:C:370:LYS:HA	1.57	0.85
2:D:142:GLY:HA2	2:D:185:TYR:HB3	1.57	0.85
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.58	0.85
1:C:409:VAL:HG13	1:C:414:GLU:OE2	1.75	0.85
2:D:149:MET:HA	2:D:149:MET:HE3	1.57	0.85
1:C:223:THR:HB	1:C:226:ASN:OD1	1.76	0.85
1:C:322:ASP:H	1:C:357:TYR:CA	1.88	0.85
1:A:138:PHE:HZ	1:A:235:VAL:HG11	1.37	0.85
1:C:190:THR:HA	1:C:193:THR:HG22	1.58	0.85
2:D:408:TYR:HB3	2:D:413:MET:HE3	1.58	0.85
2:B:149:MET:HA	2:B:149:MET:HE3	1.59	0.85
1:A:332:ILE:HD11	1:A:353:VAL:HG21	1.58	0.85
1:C:102:ASN:O	1:C:104:ALA:N	2.09	0.85
1:C:344:VAL:HG11	1:C:346:TRP:NE1	1.91	0.85
2:D:103:TRP:HE1	2:D:189:LEU:HD21	1.40	0.85
2:D:344:VAL:HB	2:D:346:TRP:NE1	1.91	0.85
2:D:59:ASN:HB2	2:D:64:ARG:NE	1.90	0.85
3:E:35:UNK:C	3:E:37:UNK:N	2.35	0.85
2:B:58:GLY:C	2:B:64:ARG:HE	1.83	0.85
2:D:158:ARG:HG3	2:D:159:GLU:N	1.91	0.85
2:B:91:ASN:HD22	2:B:91:ASN:N	1.75	0.84
2:B:141:LEU:HB3	2:B:186:ASN:HB3	1.57	0.84
1:A:413:MET:HE2	1:A:413:MET:H	1.40	0.84
2:B:132:LEU:HB3	2:B:164:ARG:HH21	1.35	0.84
1:C:214:ARG:HA	1:C:218:ASP:O	1.77	0.84
2:D:286:LEU:HD12	2:D:373:MET:HB2	1.58	0.84
1:A:362:VAL:HB	1:A:370:LYS:HG2	1.59	0.84
1:C:206:ASN:HD22	1:C:210:TYR:HE2	1.21	0.84
1:C:386:GLU:HG3	1:C:387:ALA:N	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:PHE:N	1:C:418:PHE:CD2	2.45	0.84
2:D:176:LYS:HD2	2:D:210:TYR:CZ	2.13	0.84
2:B:51:VAL:HG23	2:B:53:TYR:H	1.42	0.84
2:B:133:GLN:HE21	2:B:252:LEU:HB3	1.41	0.84
1:C:166:LYS:NZ	1:C:197:HIS:HB2	1.91	0.84
2:D:13:GLY:O	2:D:16:ILE:HG23	1.76	0.84
1:A:2:ARG:NH2	1:A:133:GLN:HE22	1.76	0.84
1:C:216:ASN:HD22	1:C:275:VAL:HG12	1.42	0.84
1:C:409:VAL:HG13	1:C:414:GLU:CD	2.01	0.84
1:C:320:ARG:HB3	1:C:374:ALA:HB3	1.60	0.84
1:A:206:ASN:HB3	1:A:210:TYR:CE2	2.11	0.84
1:A:362:VAL:HG21	1:A:370:LYS:HA	1.59	0.84
1:C:138:PHE:HZ	1:C:235:VAL:HG11	1.41	0.84
2:D:12:CYS:HB3	5:D:503:GDP:C8	2.12	0.84
1:C:339:ARG:HD2	1:C:339:ARG:C	2.03	0.84
1:C:362:VAL:HB	1:C:370:LYS:HG2	1.58	0.84
2:D:213:CYS:HA	2:D:217:LEU:HD23	1.58	0.84
2:B:103:TRP:HE1	2:B:189:LEU:HD21	1.42	0.83
1:C:241:SER:HA	1:C:320:ARG:NH2	1.92	0.83
1:C:284:GLU:HG2	1:C:285:GLN:HE21	1.41	0.83
1:C:295:CYS:SG	1:C:377:MET:HE2	2.17	0.83
2:B:121:VAL:HA	2:B:124:LYS:HG2	1.57	0.83
2:D:141:LEU:HB3	2:D:186:ASN:HB3	1.61	0.83
1:A:402:ARG:HG2	1:A:403:ALA:H	1.43	0.83
1:C:69:ASP:HB3	1:C:75:ILE:HG21	1.60	0.83
1:A:27:GLU:HG3	1:A:28:HIS:H	1.43	0.83
2:B:109:THR:HG21	2:B:411:GLU:HG2	1.61	0.83
2:B:264:ARG:HH21	2:B:428:LEU:CD1	1.92	0.83
2:D:2:ARG:NE	2:D:243:ARG:HD2	1.93	0.83
2:D:259:MET:HE2	2:D:316:ALA:HB2	1.58	0.83
2:D:3:GLU:OE2	2:D:130:ASP:HB3	1.79	0.83
2:D:92:PHE:HE1	2:D:118:VAL:CA	1.88	0.83
1:A:92:LEU:N	1:A:92:LEU:HD12	1.94	0.82
1:A:100:ALA:HB1	1:A:105:ARG:O	1.78	0.82
1:A:180:ALA:C	1:A:182:VAL:H	1.86	0.82
2:D:132:LEU:HB3	2:D:164:ARG:HH21	1.42	0.82
2:D:223:THR:HG22	2:D:226:ASP:CG	2.03	0.82
2:D:311:ARG:HB2	2:D:344:VAL:H	1.43	0.82
2:D:311:ARG:HG3	2:D:344:VAL:HA	1.61	0.82
1:A:284:GLU:HG2	1:A:285:GLN:HE21	1.42	0.82
2:B:398:MET:O	2:B:400:ARG:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:HG12	1:C:68:VAL:CG1	2.08	0.82
3:E:42:UNK:C	3:E:44:UNK:N	2.41	0.82
1:A:88:HIS:HB3	1:A:91:GLN:HE22	1.45	0.82
2:B:175:PRO:HD2	2:B:207:GLU:CB	2.09	0.82
1:A:102:ASN:O	1:A:104:ALA:N	2.12	0.82
1:A:190:THR:HA	1:A:193:THR:HG22	1.60	0.82
1:A:212:ILE:HG13	1:A:213:CYS:N	1.94	0.82
1:A:373:ARG:HB3	1:A:373:ARG:HH11	1.45	0.82
1:C:208:ALA:O	1:C:211:ASP:HB2	1.80	0.82
2:D:19:LYS:NZ	2:D:82:PRO:HG3	1.93	0.82
2:D:109:THR:O	2:D:111:GLY:N	2.13	0.82
2:D:313:LEU:HA	2:D:344:VAL:HG11	1.60	0.82
1:A:206:ASN:HD22	1:A:210:TYR:HE2	1.26	0.82
1:A:295:CYS:SG	1:A:377:MET:HE2	2.19	0.82
2:B:358:ILE:H	2:B:358:ILE:HD12	1.44	0.82
2:D:59:ASN:HA	2:D:64:ARG:HH21	1.45	0.82
2:D:183:GLU:C	2:D:185:TYR:H	1.88	0.81
2:D:287:THR:HB	2:D:289:PRO:HD2	1.61	0.81
1:A:418:PHE:N	1:A:418:PHE:CD2	2.45	0.81
2:B:19:LYS:NZ	2:B:82:PRO:HG3	1.96	0.81
2:B:96:GLN:HE22	1:C:130:THR:CG2	1.94	0.81
2:B:102:ASN:HD22	2:B:105:LYS:HG3	1.45	0.81
1:C:417:GLU:HB3	1:C:418:PHE:CD2	2.14	0.81
2:D:103:TRP:NE1	2:D:189:LEU:HD21	1.95	0.81
2:D:175:PRO:HD2	2:D:207:GLU:CB	2.10	0.81
1:C:258:ASN:HD22	1:C:258:ASN:N	1.78	0.81
2:D:143:GLY:O	2:D:145:THR:N	2.11	0.81
1:A:115:ILE:O	1:A:115:ILE:HD13	1.80	0.81
1:A:386:GLU:HG3	1:A:387:ALA:N	1.93	0.81
1:C:175:PRO:C	1:C:177:VAL:N	2.36	0.81
1:C:115:ILE:O	1:C:115:ILE:HD13	1.81	0.81
1:C:388:TRP:CH2	1:C:428:LEU:HD13	2.15	0.81
2:D:19:LYS:HA	2:D:22:GLU:CD	2.06	0.81
2:D:109:THR:HG21	2:D:411:GLU:HG2	1.63	0.81
1:A:107:HIS:ND1	1:A:151:SER:HB2	1.96	0.81
2:B:179:ASP:HA	1:C:352:LYS:CE	2.09	0.81
2:D:218:LYS:NZ	2:D:278:ARG:H	1.77	0.81
3:E:48:UNK:O	3:E:50:UNK:N	2.13	0.81
1:C:180:ALA:C	1:C:182:VAL:H	1.84	0.81
1:C:402:ARG:HD2	2:D:346:TRP:CZ3	2.15	0.81
2:B:287:THR:HB	2:B:289:PRO:HD2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:VAL:HG13	1:A:414:GLU:CD	2.06	0.80
1:A:417:GLU:HB3	1:A:418:PHE:CD2	2.16	0.80
2:B:109:THR:O	2:B:111:GLY:N	2.14	0.80
2:D:184:PRO:HB2	2:D:399:PHE:CE1	2.17	0.80
2:D:311:ARG:HH21	2:D:437:ASP:CB	1.91	0.80
2:D:390:ARG:O	2:D:392:SER:N	2.13	0.80
3:E:61:UNK:O	3:E:63:UNK:N	2.14	0.80
2:B:262:PHE:HB3	2:B:263:PRO:HD2	1.61	0.80
1:C:373:ARG:HB3	1:C:373:ARG:HH11	1.46	0.80
2:D:264:ARG:HH11	2:D:264:ARG:HG3	1.47	0.80
2:D:390:ARG:C	2:D:392:SER:H	1.88	0.80
1:A:104:ALA:HA	1:A:108:TYR:HD2	1.46	0.80
1:A:174:ALA:O	1:A:177:VAL:N	2.15	0.80
2:D:168:THR:OG1	2:D:201:THR:HB	1.82	0.80
2:B:401:ARG:NH1	1:C:440:VAL:HA	1.95	0.80
2:D:335:VAL:HA	2:D:338:LYS:CB	2.12	0.80
1:A:388:TRP:CH2	1:A:428:LEU:HD13	2.16	0.80
2:B:286:LEU:HG	2:B:286:LEU:O	1.79	0.80
1:C:291:ILE:HD12	1:C:373:ARG:HG3	1.63	0.80
2:D:133:GLN:NE2	2:D:252:LEU:HB3	1.97	0.80
2:D:192:HIS:C	2:D:194:LEU:H	1.89	0.80
1:A:36:MET:HA	1:A:36:MET:HE3	1.60	0.80
2:B:142:GLY:HA2	2:B:185:TYR:HB3	1.61	0.80
2:D:12:CYS:HB2	5:D:503:GDP:O2A	1.81	0.80
3:E:21:UNK:O	3:E:24:UNK:N	2.15	0.80
1:A:346:TRP:CD1	1:A:346:TRP:H	1.99	0.80
2:D:285:ALA:O	2:D:286:LEU:HD23	1.82	0.80
2:D:387:LEU:O	2:D:387:LEU:HD23	1.81	0.80
1:A:133:GLN:N	1:A:164:LYS:HD3	1.94	0.79
2:B:103:TRP:NE1	2:B:189:LEU:HD21	1.96	0.79
2:D:218:LYS:HZ1	2:D:278:ARG:HB2	1.46	0.79
2:D:391:ILE:H	2:D:391:ILE:HD12	1.47	0.79
2:B:335:VAL:HA	2:B:338:LYS:HB3	1.63	0.79
1:C:16:ILE:HG22	1:C:17:GLY:N	1.96	0.79
3:E:31:UNK:HA	3:E:34:UNK:CB	2.13	0.79
2:B:59:ASN:HA	2:B:64:ARG:HH21	1.47	0.79
1:A:154:MET:HE3	1:A:197:HIS:NE2	1.97	0.79
1:C:212:ILE:HG13	1:C:213:CYS:N	1.95	0.79
1:A:419:SER:HA	1:A:422:ARG:CD	2.10	0.79
2:B:335:VAL:HA	2:B:338:LYS:CB	2.13	0.79
1:C:311:LYS:HD3	1:C:344:VAL:HG13	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:ASN:HD22	2:D:105:LYS:HG3	1.47	0.79
2:D:353:THR:HG22	2:D:354:ALA:N	1.96	0.79
1:A:39:ASP:CG	1:A:40:LYS:H	1.88	0.79
2:B:102:ASN:ND2	2:B:105:LYS:HG3	1.98	0.79
1:C:350:GLY:C	1:C:351:PHE:HD1	1.90	0.79
2:D:179:ASP:HB3	2:D:181:VAL:HG12	1.63	0.79
2:B:70:LEU:HG	2:B:99:ALA:HB3	1.62	0.79
1:C:335:ILE:HG13	1:C:336:LYS:N	1.97	0.79
1:A:417:GLU:HB3	1:A:418:PHE:CE2	2.18	0.79
2:B:179:ASP:HB3	2:B:181:VAL:HG12	1.65	0.79
2:B:182:VAL:O	2:B:182:VAL:HG12	1.81	0.79
1:C:92:LEU:N	1:C:92:LEU:HD12	1.97	0.79
1:C:417:GLU:HB3	1:C:418:PHE:CE2	2.17	0.79
1:A:388:TRP:HH2	1:A:428:LEU:HD13	1.47	0.79
2:D:80:SER:C	2:D:82:PRO:HD2	2.07	0.79
2:D:274:PRO:HB2	2:D:371:LEU:HD12	1.65	0.78
2:D:322:ARG:HE	2:D:357:ASP:HB3	1.46	0.78
1:A:185:TYR:HA	1:A:188:ILE:HD11	1.63	0.78
1:A:196:GLU:O	1:A:197:HIS:HB3	1.82	0.78
1:A:344:VAL:HG11	1:A:346:TRP:NE1	1.98	0.78
2:D:205:ASP:HB2	2:D:387:LEU:HD11	1.62	0.78
1:C:227:LEU:O	1:C:231:ILE:HG12	1.84	0.78
2:D:91:ASN:HD22	2:D:91:ASN:N	1.77	0.78
2:D:179:ASP:C	2:D:181:VAL:H	1.90	0.78
2:B:217:LEU:HG	2:B:218:LYS:N	1.98	0.78
1:C:107:HIS:HD1	1:C:151:SER:HB2	1.49	0.78
1:A:209:ILE:C	1:A:211:ASP:H	1.90	0.78
2:B:179:ASP:C	2:B:181:VAL:H	1.88	0.78
1:C:362:VAL:HG13	1:C:367:ASP:CB	2.13	0.78
1:C:371:VAL:HG12	1:C:373:ARG:H	1.48	0.78
2:D:2:ARG:HG3	2:D:133:GLN:HE21	1.48	0.78
3:E:31:UNK:O	3:E:34:UNK:N	2.17	0.78
1:C:144:GLY:N	1:C:147:SER:HB3	1.99	0.78
1:A:33:ASP:HA	1:A:36:MET:HB3	1.66	0.78
2:B:285:ALA:O	2:B:286:LEU:HD23	1.84	0.78
1:A:30:ILE:HG13	1:A:31:GLN:N	1.97	0.78
1:C:234:ILE:HD13	1:C:302:MET:SD	2.24	0.78
1:C:282:TYR:N	1:C:282:TYR:CD2	2.50	0.78
2:D:292:THR:HG21	2:D:331:GLN:HB3	1.66	0.78
2:B:179:ASP:HB2	2:B:182:VAL:HG23	1.63	0.78
2:B:390:ARG:C	2:B:392:SER:H	1.92	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:TRP:HH2	1:C:428:LEU:HD13	1.49	0.78
1:C:402:ARG:HG2	1:C:403:ALA:H	1.46	0.78
2:D:102:ASN:ND2	2:D:105:LYS:HG3	1.99	0.78
2:D:244:PHE:HB2	2:D:245:PRO:HD2	1.66	0.78
2:B:87:PHE:O	2:B:87:PHE:HD1	1.67	0.77
2:B:158:ARG:HG3	2:B:159:GLU:N	1.98	0.77
1:C:104:ALA:HA	1:C:108:TYR:HD2	1.48	0.77
1:C:212:ILE:HD11	1:C:230:LEU:HD21	1.65	0.77
2:D:288:VAL:HG11	2:D:327:GLU:OE1	1.84	0.77
2:D:339:ASN:HB3	2:D:342:TYR:CD1	2.19	0.77
3:E:35:UNK:O	3:E:37:UNK:N	2.18	0.77
2:B:402:LYS:HE3	1:C:440:VAL:HB	1.65	0.77
2:B:213:CYS:HA	2:B:217:LEU:HD23	1.67	0.77
1:C:413:MET:HG3	3:E:66:UNK:CB	2.14	0.77
2:D:18:ALA:C	2:D:20:PHE:H	1.92	0.77
2:D:274:PRO:HB2	2:D:371:LEU:CD1	2.15	0.77
1:C:298:PRO:O	1:C:301:GLN:HG3	1.85	0.77
1:C:322:ASP:H	1:C:357:TYR:C	1.92	0.77
2:D:179:ASP:CB	2:D:182:VAL:H	1.98	0.77
1:A:413:MET:H	1:A:413:MET:CE	1.97	0.77
1:C:133:GLN:N	1:C:164:LYS:HD3	1.99	0.77
1:C:322:ASP:CA	1:C:357:TYR:HA	2.15	0.77
1:A:69:ASP:OD1	1:A:70:LEU:N	2.17	0.77
2:B:4:ILE:O	2:B:58:GLY:HA2	1.84	0.77
2:D:305:CYS:SG	2:D:387:LEU:HB2	2.24	0.77
3:E:73:UNK:O	3:E:75:UNK:N	2.17	0.77
1:A:102:ASN:CB	1:A:105:ARG:HB2	2.14	0.77
2:B:344:VAL:HB	2:B:346:TRP:NE1	2.00	0.77
2:D:286:LEU:HG	2:D:373:MET:HE3	1.67	0.77
1:A:258:ASN:HD22	1:A:258:ASN:N	1.82	0.77
2:B:172:VAL:HG13	2:B:173:PRO:HD2	1.67	0.77
2:B:313:LEU:HA	2:B:344:VAL:HG11	1.66	0.77
1:C:419:SER:HA	1:C:422:ARG:CD	2.11	0.77
2:D:230:LEU:H	2:D:230:LEU:HD12	1.48	0.77
1:C:322:ASP:HA	1:C:357:TYR:HD1	1.49	0.77
2:B:286:LEU:HG	2:B:373:MET:HE3	1.67	0.76
1:A:402:ARG:CG	1:A:403:ALA:H	1.98	0.76
2:B:175:PRO:CD	2:B:207:GLU:HB2	2.12	0.76
2:B:266:HIS:ND1	2:B:432:TYR:CZ	2.53	0.76
2:B:311:ARG:HG3	2:B:344:VAL:HA	1.65	0.76
1:C:33:ASP:HA	1:C:36:MET:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:SER:HB3	1:C:192:HIS:CE1	2.20	0.76
2:B:264:ARG:NH2	2:B:428:LEU:HD12	1.99	0.76
2:D:264:ARG:HH21	2:D:428:LEU:CD1	1.98	0.76
1:A:414:GLU:HG2	1:A:415:GLU:H	1.50	0.76
2:B:184:PRO:HB2	2:B:399:PHE:CE1	2.20	0.76
2:B:262:PHE:O	2:B:265:LEU:HA	1.85	0.76
3:E:42:UNK:O	3:E:44:UNK:N	2.18	0.76
1:A:371:VAL:HG12	1:A:373:ARG:H	1.50	0.76
1:C:388:TRP:CZ3	1:C:428:LEU:HD22	2.21	0.76
2:D:180:THR:HB	2:D:404:PHE:CE1	2.19	0.76
2:B:407:TRP:CZ2	1:C:256:GLN:HB2	2.19	0.76
2:D:303:ALA:HB1	2:D:387:LEU:CD1	2.14	0.76
1:A:227:LEU:O	1:A:231:ILE:HG12	1.86	0.76
1:A:243:ARG:HH12	1:A:250:VAL:CG1	1.99	0.76
2:B:91:ASN:H	2:B:91:ASN:ND2	1.82	0.76
1:C:88:HIS:HB3	1:C:91:GLN:HE22	1.48	0.76
1:C:311:LYS:HD2	1:C:436:GLY:HA2	1.66	0.76
2:D:175:PRO:CD	2:D:207:GLU:HB2	2.12	0.76
2:D:194:LEU:CD2	2:D:195:VAL:HG13	2.16	0.76
2:D:202:TYR:CE1	2:D:378:ILE:HD12	2.20	0.76
1:A:98:ASP:OD1	2:B:1:MET:HB3	1.85	0.76
2:B:398:MET:C	2:B:400:ARG:H	1.94	0.76
2:B:401:ARG:HH11	1:C:440:VAL:HA	1.48	0.76
2:B:408:TYR:HB3	2:B:413:MET:HE3	1.68	0.76
1:C:269:LEU:HD12	1:C:270:ALA:N	2.00	0.76
2:D:94:PHE:HB2	2:D:114:LEU:HD13	1.68	0.76
1:A:398:MET:HG3	1:A:399:TYR:CD1	2.21	0.76
1:C:39:ASP:CG	1:C:40:LYS:H	1.91	0.76
1:C:97:GLU:O	1:C:99:ALA:N	2.17	0.76
2:D:286:LEU:HA	2:D:290:GLU:OE2	1.84	0.76
2:D:335:VAL:HA	2:D:338:LYS:HB3	1.67	0.76
1:A:398:MET:HB3	2:B:346:TRP:O	1.85	0.76
2:B:385:GLN:HE21	2:B:433:GLN:HE21	1.31	0.76
2:B:390:ARG:O	2:B:392:SER:N	2.17	0.76
1:C:89:PRO:O	1:C:90:GLU:HB2	1.85	0.76
1:C:174:ALA:O	1:C:177:VAL:N	2.19	0.76
1:C:256:GLN:HB3	1:C:260:VAL:HB	1.68	0.76
2:D:115:VAL:HG11	2:D:156:LYS:NZ	2.00	0.76
1:A:115:ILE:HG13	1:A:152:LEU:CD2	2.16	0.75
2:D:344:VAL:HB	2:D:346:TRP:CE2	2.21	0.75
2:B:179:ASP:CB	2:B:182:VAL:H	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:PHE:HB2	2:B:245:PRO:HD2	1.65	0.75
2:B:273:ALA:HB2	2:B:295:MET:HB2	1.67	0.75
2:D:70:LEU:HG	2:D:99:ALA:CB	2.15	0.75
2:D:87:PHE:O	2:D:87:PHE:HD1	1.67	0.75
1:A:151:SER:HB3	1:A:192:HIS:CE1	2.22	0.75
2:B:115:VAL:HG11	2:B:156:LYS:NZ	2.01	0.75
2:B:205:ASP:HB2	2:B:387:LEU:HD11	1.69	0.75
2:B:407:TRP:CE3	2:B:407:TRP:HA	2.20	0.75
2:D:158:ARG:CG	2:D:159:GLU:H	1.98	0.75
3:E:63:UNK:C	3:E:65:UNK:H	1.94	0.75
2:B:100:GLY:HA3	1:C:254:GLU:OE1	1.86	0.75
1:C:44:GLY:C	1:C:46:ASP:H	1.92	0.75
1:C:340:THR:OG1	1:C:341:ILE:HD12	1.86	0.75
1:C:398:MET:HB3	2:D:346:TRP:O	1.87	0.75
1:C:413:MET:H	1:C:413:MET:HE2	1.49	0.75
3:E:54:UNK:C	3:E:56:UNK:N	2.48	0.75
1:A:234:ILE:HD13	1:A:302:MET:SD	2.25	0.75
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.22	0.75
1:A:208:ALA:O	1:A:211:ASP:HB2	1.87	0.75
2:B:218:LYS:HZ1	2:B:278:ARG:HB2	1.50	0.75
2:D:174:SER:OG	2:D:176:LYS:HG3	1.87	0.75
2:D:196:GLU:HA	2:D:196:GLU:OE2	1.86	0.75
1:A:145:THR:O	1:A:149:PHE:HB3	1.87	0.75
1:A:348:PRO:O	1:A:350:GLY:N	2.19	0.75
1:A:141:PHE:CE2	1:A:172:TYR:HA	2.15	0.75
1:A:175:PRO:C	1:A:177:VAL:N	2.39	0.75
2:B:292:THR:HG21	2:B:331:GLN:HB3	1.69	0.75
2:D:263:PRO:C	2:D:265:LEU:N	2.42	0.75
1:A:322:ASP:CA	1:A:357:TYR:HA	2.17	0.74
2:B:8:GLN:HG2	2:B:14:ASN:ND2	2.02	0.74
2:B:92:PHE:HE1	2:B:118:VAL:CA	1.89	0.74
2:B:179:ASP:CA	1:C:352:LYS:HE2	2.11	0.74
1:C:276:ILE:HG12	1:C:282:TYR:CD2	2.22	0.74
1:A:184:PRO:HG3	1:A:399:TYR:CZ	2.22	0.74
2:B:143:GLY:O	2:B:145:THR:N	2.18	0.74
2:B:220:THR:HB	1:C:326:LYS:CD	2.17	0.74
1:C:107:HIS:ND1	1:C:151:SER:HB2	2.01	0.74
2:B:274:PRO:HB2	2:B:371:LEU:CD1	2.16	0.74
2:B:387:LEU:O	2:B:387:LEU:HD23	1.86	0.74
1:C:78:VAL:C	1:C:82:THR:HA	2.13	0.74
2:D:241:CYS:O	2:D:243:ARG:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:GLN:HE21	2:D:433:GLN:HE21	1.35	0.74
1:A:322:ASP:H	1:A:357:TYR:C	1.94	0.74
1:C:172:TYR:HB3	1:C:205:ASP:CA	2.18	0.74
1:C:177:VAL:HB	2:D:349:ASN:ND2	2.02	0.74
1:C:289:ALA:HA	1:C:292:THR:CG2	2.17	0.74
1:A:269:LEU:HD12	1:A:270:ALA:N	2.03	0.74
1:A:282:TYR:CD2	1:A:282:TYR:N	2.51	0.74
2:B:385:GLN:HE21	2:B:433:GLN:NE2	1.85	0.74
1:A:214:ARG:HA	1:A:218:ASP:O	1.86	0.74
1:A:77:GLU:HB3	1:A:83:TYR:CD2	2.23	0.74
1:C:10:GLY:O	1:C:13:GLY:N	2.19	0.74
1:C:196:GLU:O	1:C:197:HIS:HB3	1.84	0.74
1:C:209:ILE:HG23	1:C:213:CYS:HB2	1.70	0.74
2:D:182:VAL:O	2:D:182:VAL:HG12	1.85	0.74
2:B:163:ASP:OD2	2:B:164:ARG:HD3	1.87	0.74
2:B:176:LYS:HD2	2:B:210:TYR:CE2	2.22	0.74
2:B:322:ARG:HE	2:B:357:ASP:HB3	1.53	0.74
2:B:407:TRP:HZ2	1:C:256:GLN:CB	2.01	0.74
2:D:70:LEU:HD11	2:D:110:GLU:O	1.88	0.74
1:A:291:ILE:HG21	1:A:375:VAL:CG2	2.18	0.74
1:C:101:ASN:OD1	2:D:254:LYS:HD3	1.86	0.74
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.70	0.74
1:C:183:GLU:N	1:C:184:PRO:HD2	2.03	0.74
2:B:94:PHE:HB2	2:B:114:LEU:HD13	1.69	0.73
2:D:371:LEU:HB3	2:D:373:MET:O	1.86	0.73
2:B:145:THR:HB	5:B:501:GDP:O2B	1.88	0.73
2:B:183:GLU:C	2:B:185:TYR:H	1.95	0.73
2:B:385:GLN:NE2	2:B:433:GLN:HG2	2.03	0.73
1:C:269:LEU:HD12	1:C:269:LEU:C	2.13	0.73
2:D:179:ASP:HB2	2:D:182:VAL:H	1.53	0.73
2:D:416:MET:C	2:D:418:PHE:H	1.95	0.73
2:B:13:GLY:O	2:B:16:ILE:HG23	1.88	0.73
2:B:123:ARG:NH2	2:B:160:GLU:HG3	2.03	0.73
1:C:115:ILE:HG13	1:C:152:LEU:CD2	2.18	0.73
2:D:1:MET:O	2:D:3:GLU:N	2.19	0.73
2:D:59:ASN:CG	2:D:60:LYS:H	1.95	0.73
1:A:190:THR:O	1:A:192:HIS:N	2.22	0.73
1:A:238:ILE:HG22	1:A:239:THR:N	2.03	0.73
1:A:385:ALA:HB2	1:A:432:TYR:HD2	1.53	0.73
2:B:77:SER:HA	2:B:80:SER:CB	2.18	0.73
2:B:339:ASN:HB3	2:B:342:TYR:CD1	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TYR:HB3	1:C:263:PRO:HD2	1.70	0.73
2:D:142:GLY:CA	2:D:185:TYR:HB3	2.18	0.73
2:D:343:PHE:O	2:D:345:GLU:N	2.21	0.73
2:D:394:GLN:O	2:D:398:MET:HB3	1.87	0.73
2:B:168:THR:OG1	2:B:201:THR:HB	1.88	0.73
1:C:132:LEU:HB3	1:C:164:LYS:HD3	1.71	0.73
2:D:407:TRP:HA	2:D:407:TRP:CE3	2.22	0.73
1:C:209:ILE:C	1:C:211:ASP:H	1.95	0.73
2:D:191:VAL:O	2:D:191:VAL:HG12	1.87	0.73
1:A:27:GLU:HG3	1:A:28:HIS:ND1	2.04	0.73
1:A:298:PRO:O	1:A:301:GLN:HG3	1.89	0.73
1:A:414:GLU:HB2	1:A:417:GLU:HB2	1.71	0.73
2:B:206:ASN:HD22	2:B:227:LEU:CD2	2.01	0.73
2:B:288:VAL:HG11	2:B:327:GLU:OE1	1.88	0.73
2:B:416:MET:C	2:B:418:PHE:H	1.96	0.73
2:D:77:SER:HA	2:D:80:SER:CB	2.19	0.73
2:D:179:ASP:HB2	2:D:182:VAL:HG23	1.71	0.73
1:A:267:PHE:N	1:A:267:PHE:CD1	2.57	0.73
1:A:322:ASP:HA	1:A:357:TYR:HD1	1.54	0.73
2:B:402:LYS:HG3	1:C:440:VAL:HG12	1.70	0.73
2:D:77:SER:CA	2:D:80:SER:HB3	2.19	0.73
2:D:385:GLN:NE2	2:D:433:GLN:HG2	2.04	0.73
1:A:115:ILE:HG13	1:A:152:LEU:HD21	1.70	0.72
1:A:194:THR:O	1:A:197:HIS:O	2.06	0.72
2:B:407:TRP:HA	2:B:407:TRP:HE3	1.54	0.72
1:C:194:THR:O	1:C:197:HIS:O	2.07	0.72
1:C:322:ASP:HA	1:C:357:TYR:HA	1.71	0.72
1:A:137:VAL:HG11	1:A:154:MET:HE2	1.71	0.72
2:B:190:SER:CB	2:B:425:MET:HG3	2.16	0.72
2:D:286:LEU:HG	2:D:286:LEU:O	1.89	0.72
3:E:25:UNK:C	3:E:27:UNK:N	2.49	0.72
2:B:111:GLY:C	2:B:113:GLU:H	1.94	0.72
2:B:266:HIS:HA	2:B:432:TYR:OH	1.89	0.72
1:C:70:LEU:HD12	1:C:145:THR:CA	2.12	0.72
1:C:100:ALA:HB1	1:C:105:ARG:HD2	1.70	0.72
1:A:215:ARG:HH22	1:A:300:ASN:ND2	1.87	0.72
2:B:16:ILE:HB	2:B:228:ASN:HD21	1.53	0.72
2:B:163:ASP:CG	2:B:164:ARG:N	2.47	0.72
1:C:267:PHE:N	1:C:267:PHE:CD1	2.55	0.72
1:A:202:PHE:HE1	1:A:378:LEU:HD22	1.55	0.72
1:A:335:ILE:HG13	1:A:336:LYS:N	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HH11	2:B:251:ASP:HA	1.54	0.72
2:B:4:ILE:O	2:B:64:ARG:HD2	1.89	0.72
2:B:158:ARG:CG	2:B:159:GLU:H	1.99	0.72
2:D:18:ALA:O	2:D:20:PHE:N	2.21	0.72
2:D:91:ASN:H	2:D:91:ASN:ND2	1.84	0.72
1:A:345:ASP:O	1:A:347:CYS:N	2.23	0.72
2:B:77:SER:CA	2:B:80:SER:HB3	2.20	0.72
2:B:133:GLN:NE2	2:B:252:LEU:H	1.87	0.72
2:B:263:PRO:C	2:B:265:LEU:N	2.39	0.72
2:B:274:PRO:HB2	2:B:371:LEU:HD12	1.70	0.72
2:D:176:LYS:HD2	2:D:210:TYR:CE2	2.25	0.72
2:D:308:ARG:NH2	2:D:342:TYR:CD1	2.56	0.72
2:B:353:THR:HG22	2:B:354:ALA:N	2.04	0.72
1:C:263:PRO:O	1:C:265:ALA:N	2.22	0.72
2:D:132:LEU:HD22	2:D:164:ARG:HG3	1.72	0.72
2:D:331:GLN:O	2:D:334:ASN:HB3	1.89	0.72
1:A:78:VAL:C	1:A:82:THR:HA	2.15	0.72
2:B:158:ARG:O	2:B:160:GLU:N	2.22	0.72
1:C:285:GLN:OE1	1:C:372:GLN:HG2	1.90	0.72
2:D:158:ARG:CA	2:D:197:ASN:HD22	2.02	0.72
1:A:97:GLU:O	1:A:99:ALA:N	2.22	0.72
1:A:289:ALA:HA	1:A:292:THR:CG2	2.20	0.72
2:B:394:GLN:O	2:B:398:MET:HB3	1.89	0.72
1:C:180:ALA:C	1:C:182:VAL:N	2.48	0.72
2:D:194:LEU:HD11	2:D:428:LEU:HD11	1.72	0.72
2:D:273:ALA:HB2	2:D:295:MET:HB2	1.70	0.72
2:D:353:THR:CG2	2:D:354:ALA:N	2.52	0.72
2:B:138:THR:O	2:B:139:HIS:HB3	1.90	0.72
2:B:194:LEU:CD2	2:B:195:VAL:HG13	2.19	0.72
2:B:286:LEU:HA	2:B:290:GLU:OE2	1.89	0.72
2:B:92:PHE:CE1	2:B:118:VAL:CA	2.70	0.71
1:C:164:LYS:N	1:C:164:LYS:HZ1	1.88	0.71
2:D:16:ILE:HB	2:D:228:ASN:HD21	1.55	0.71
1:A:306:ASP:C	1:A:308:ARG:H	1.98	0.71
1:C:194:THR:O	1:C:197:HIS:N	2.22	0.71
1:C:348:PRO:O	1:C:350:GLY:N	2.23	0.71
2:D:386:GLU:C	2:D:388:PHE:H	1.98	0.71
2:D:396:THR:HG23	2:D:400:ARG:CD	2.19	0.71
1:A:256:GLN:HB3	1:A:260:VAL:HB	1.71	0.71
2:B:422:GLU:O	2:B:426:ASN:HB2	1.90	0.71
1:C:177:VAL:HB	2:D:349:ASN:CG	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HG21	1:A:375:VAL:HG21	1.73	0.71
1:C:139:HIS:HB3	1:C:170:SER:HA	1.72	0.71
1:C:402:ARG:CG	1:C:403:ALA:H	2.03	0.71
3:E:58:UNK:O	3:E:61:UNK:N	2.24	0.71
1:A:109:THR:HG21	1:A:411:GLU:OE2	1.90	0.71
1:A:362:VAL:HG13	1:A:367:ASP:CB	2.19	0.71
1:A:194:THR:O	1:A:197:HIS:N	2.22	0.71
1:A:414:GLU:HG2	1:A:415:GLU:N	2.04	0.71
2:B:196:GLU:HA	2:B:196:GLU:OE2	1.91	0.71
1:C:109:THR:HG21	1:C:411:GLU:OE2	1.90	0.71
2:D:322:ARG:NE	2:D:357:ASP:HB3	2.05	0.71
1:C:70:LEU:CD1	1:C:145:THR:HA	2.13	0.71
1:C:427:ALA:O	1:C:430:LYS:HB3	1.90	0.71
2:D:158:ARG:CB	2:D:197:ASN:HD22	2.02	0.71
2:D:158:ARG:HA	2:D:197:ASN:HD22	1.54	0.71
1:A:31:GLN:O	1:A:33:ASP:N	2.23	0.71
1:A:243:ARG:CZ	1:A:243:ARG:HA	2.21	0.71
2:B:142:GLY:CA	2:B:185:TYR:HB3	2.20	0.71
2:B:343:PHE:O	2:B:345:GLU:N	2.24	0.71
1:A:44:GLY:C	1:A:46:ASP:H	1.97	0.71
2:B:19:LYS:HA	2:B:22:GLU:CD	2.16	0.71
1:C:154:MET:HE3	1:C:197:HIS:NE2	2.06	0.71
1:C:306:ASP:C	1:C:308:ARG:H	1.99	0.71
2:D:22:GLU:OE1	2:D:82:PRO:HB2	1.91	0.71
2:D:266:HIS:HA	2:D:432:TYR:OH	1.91	0.71
1:A:78:VAL:HG11	1:A:87:PHE:HE2	1.54	0.71
2:B:386:GLU:C	2:B:388:PHE:H	1.99	0.71
2:D:4:ILE:O	2:D:58:GLY:HA2	1.91	0.71
2:D:427:ASP:O	2:D:429:VAL:N	2.24	0.71
1:A:215:ARG:HH22	1:A:300:ASN:HD21	1.39	0.70
1:A:414:GLU:CB	1:A:417:GLU:HB2	2.21	0.70
2:B:430:SER:O	2:B:434:GLN:HG3	1.90	0.70
1:C:175:PRO:O	1:C:177:VAL:HG23	1.91	0.70
2:D:163:ASP:OD2	2:D:164:ARG:HD3	1.91	0.70
1:A:26:LEU:HG	1:A:361:THR:CB	2.21	0.70
1:A:322:ASP:HA	1:A:357:TYR:HA	1.73	0.70
2:B:87:PHE:O	2:B:90:ASP:OD1	2.08	0.70
2:B:118:VAL:C	2:B:120:ASP:H	1.97	0.70
1:C:264:ARG:O	1:C:266:HIS:N	2.24	0.70
1:C:284:GLU:HG2	1:C:285:GLN:NE2	2.04	0.70
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:O	1:C:156:ARG:HB2	1.90	0.70
1:C:171:ILE:HD12	1:C:171:ILE:N	2.06	0.70
1:C:418:PHE:O	1:C:420:GLU:N	2.23	0.70
1:A:332:ILE:CD1	1:A:353:VAL:HG21	2.21	0.70
2:B:191:VAL:O	2:B:191:VAL:HG12	1.90	0.70
2:B:206:ASN:ND2	2:B:227:LEU:HD21	2.01	0.70
2:B:405:LEU:HD13	2:B:406:HIS:N	2.06	0.70
1:C:398:MET:HG3	1:C:399:TYR:CD1	2.25	0.70
2:D:118:VAL:C	2:D:120:ASP:H	1.99	0.70
2:D:255:LEU:CD2	2:D:259:MET:HG3	2.21	0.70
2:D:391:ILE:O	2:D:425:MET:HE1	1.90	0.70
1:A:340:THR:OG1	1:A:341:ILE:HD12	1.90	0.70
1:C:98:ASP:OD1	2:D:1:MET:HB3	1.91	0.70
3:E:19:UNK:O	3:E:21:UNK:N	2.24	0.70
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.73	0.70
2:B:22:GLU:OE1	2:B:82:PRO:HB2	1.90	0.70
2:B:230:LEU:H	2:B:230:LEU:HD12	1.55	0.70
1:C:7:ILE:HD12	1:C:153:LEU:HD21	1.74	0.70
1:A:209:ILE:HG23	1:A:213:CYS:HB2	1.73	0.70
1:A:350:GLY:O	1:A:351:PHE:HD1	1.74	0.70
1:C:5:ILE:HD12	1:C:125:LEU:HD22	1.74	0.70
1:C:102:ASN:CB	1:C:105:ARG:HB2	2.16	0.70
1:C:115:ILE:HG13	1:C:152:LEU:HD21	1.73	0.70
1:C:362:VAL:HG21	1:C:369:ALA:O	1.92	0.70
2:D:51:VAL:HG23	2:D:53:TYR:N	2.07	0.70
2:D:111:GLY:C	2:D:113:GLU:H	1.99	0.70
1:A:177:VAL:HB	2:B:349:ASN:CG	2.17	0.70
1:A:418:PHE:O	1:A:420:GLU:N	2.25	0.70
2:B:18:ALA:C	2:B:20:PHE:H	2.00	0.70
2:B:391:ILE:HD12	2:B:391:ILE:N	2.07	0.70
2:D:71:GLU:HB2	2:D:72:PRO:HD2	1.74	0.70
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.54	0.70
1:A:7:ILE:HG21	1:A:122:ILE:HD11	1.73	0.70
1:A:134:GLY:H	1:A:164:LYS:CG	2.04	0.70
2:B:55:GLU:HB2	2:B:244:PHE:HA	1.73	0.70
2:B:158:ARG:HA	2:B:197:ASN:HD22	1.54	0.70
2:B:241:CYS:O	2:B:243:ARG:HG2	1.92	0.70
3:E:19:UNK:C	3:E:21:UNK:N	2.54	0.70
1:A:177:VAL:HB	2:B:349:ASN:ND2	2.06	0.70
1:C:195:LEU:HB3	1:C:196:GLU:OE2	1.90	0.70
2:D:385:GLN:HE21	2:D:433:GLN:NE2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG21	1:C:122:ILE:HD11	1.74	0.69
1:C:77:GLU:HB3	1:C:83:TYR:CD2	2.26	0.69
1:C:407:TRP:C	1:C:409:VAL:H	1.97	0.69
1:C:184:PRO:HG3	1:C:399:TYR:CZ	2.28	0.69
1:C:190:THR:O	1:C:192:HIS:N	2.25	0.69
1:C:220:GLU:OE2	2:D:326:LYS:HD3	1.92	0.69
2:D:264:ARG:NH2	2:D:428:LEU:HD12	2.03	0.69
2:D:391:ILE:HD12	2:D:391:ILE:N	2.07	0.69
1:A:89:PRO:O	1:A:90:GLU:HB2	1.90	0.69
1:A:280:LYS:O	1:A:282:TYR:CE2	2.45	0.69
1:A:284:GLU:HG2	1:A:285:GLN:NE2	2.07	0.69
1:A:407:TRP:C	1:A:409:VAL:H	2.00	0.69
2:B:139:HIS:C	2:B:139:HIS:CD2	2.69	0.69
2:B:259:MET:HE2	2:B:316:ALA:HB2	1.74	0.69
1:C:291:ILE:HG21	1:C:375:VAL:CG2	2.22	0.69
2:D:163:ASP:CG	2:D:164:ARG:N	2.50	0.69
1:A:11:GLN:HB3	4:A:500:GTP:O2A	1.91	0.69
1:A:205:ASP:OD2	1:A:207:GLU:HB3	1.92	0.69
2:B:51:VAL:C	2:B:53:TYR:H	2.00	0.69
2:B:133:GLN:HE21	2:B:252:LEU:CB	2.05	0.69
2:D:59:ASN:HB2	2:D:64:ARG:CZ	2.22	0.69
2:D:183:GLU:O	2:D:185:TYR:N	2.24	0.69
2:D:218:LYS:NZ	2:D:278:ARG:HB2	2.07	0.69
1:A:78:VAL:O	1:A:82:THR:HG23	1.92	0.69
2:B:111:GLY:C	2:B:113:GLU:N	2.47	0.69
2:B:339:ASN:C	2:B:341:SER:H	2.00	0.69
1:C:414:GLU:HG2	1:C:415:GLU:H	1.58	0.69
2:D:218:LYS:NZ	2:D:278:ARG:N	2.39	0.69
2:D:262:PHE:O	2:D:265:LEU:HA	1.93	0.69
1:A:287:SER:C	1:A:289:ALA:H	1.98	0.69
1:C:346:TRP:CD1	1:C:346:TRP:H	2.10	0.69
2:D:59:ASN:CG	2:D:60:LYS:N	2.50	0.69
2:B:59:ASN:CG	2:B:60:LYS:H	1.99	0.69
2:B:345:GLU:O	2:B:345:GLU:HG2	1.92	0.69
1:C:31:GLN:CB	1:C:32:PRO:HD2	2.23	0.69
2:D:183:GLU:C	2:D:185:TYR:N	2.47	0.69
2:D:396:THR:CG2	2:D:400:ARG:HD3	2.23	0.69
1:A:78:VAL:HG11	1:A:92:LEU:HD21	1.73	0.69
1:A:86:LEU:CD2	1:A:89:PRO:HD3	2.23	0.69
1:A:154:MET:SD	1:A:197:HIS:CD2	2.86	0.69
1:A:276:ILE:HD12	1:A:277:SER:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:LYS:NZ	2:B:278:ARG:H	1.83	0.69
2:B:255:LEU:CD2	2:B:259:MET:HG3	2.22	0.69
1:C:30:ILE:HG13	1:C:31:GLN:N	2.07	0.69
1:C:78:VAL:O	1:C:82:THR:HG23	1.91	0.69
1:C:100:ALA:HB1	1:C:105:ARG:O	1.92	0.69
1:C:202:PHE:HE1	1:C:378:LEU:HD22	1.57	0.69
1:C:205:ASP:OD2	1:C:207:GLU:HB3	1.93	0.69
1:C:287:SER:N	1:C:290:GLU:HB2	2.07	0.69
2:B:274:PRO:HA	2:B:294:GLN:NE2	2.08	0.69
2:D:422:GLU:O	2:D:426:ASN:HB2	1.93	0.69
1:A:191:THR:CB	1:A:421:ALA:HB1	2.23	0.69
2:B:320:ARG:HG2	2:B:320:ARG:HH11	1.58	0.69
1:C:171:ILE:HD12	1:C:171:ILE:H	1.56	0.69
2:D:123:ARG:NH2	2:D:160:GLU:HG3	2.08	0.69
3:E:17:UNK:C	3:E:19:UNK:N	2.48	0.69
1:A:413:MET:O	1:A:414:GLU:HB3	1.92	0.68
2:B:333:LEU:HG	2:B:337:ASN:ND2	2.08	0.68
1:C:286:LEU:HA	1:C:290:GLU:OE1	1.93	0.68
2:D:105:LYS:HA	2:D:109:THR:OG1	1.93	0.68
2:D:138:THR:O	2:D:139:HIS:HB3	1.91	0.68
3:E:71:UNK:O	3:E:73:UNK:N	2.27	0.68
2:B:132:LEU:HD22	2:B:164:ARG:HG3	1.75	0.68
1:C:258:ASN:N	1:C:258:ASN:ND2	2.39	0.68
2:D:92:PHE:CE1	2:D:118:VAL:CA	2.71	0.68
2:D:247:GLN:HB2	2:D:355:VAL:O	1.92	0.68
1:A:259:LEU:HD21	1:A:378:LEU:HB3	1.74	0.68
2:B:296:PHE:HA	2:B:377:PHE:HE2	1.59	0.68
2:B:344:VAL:HB	2:B:346:TRP:CE2	2.28	0.68
1:A:10:GLY:O	1:A:13:GLY:N	2.26	0.68
2:B:80:SER:C	2:B:82:PRO:HD2	2.18	0.68
1:C:414:GLU:CB	1:C:417:GLU:HB2	2.24	0.68
2:D:313:LEU:HA	2:D:344:VAL:CG1	2.23	0.68
2:D:407:TRP:HA	2:D:407:TRP:HE3	1.56	0.68
1:A:330:ALA:O	1:A:334:THR:HG23	1.93	0.68
2:B:175:PRO:O	2:B:177:VAL:HG23	1.93	0.68
1:C:101:ASN:CG	2:D:254:LYS:HD3	2.17	0.68
1:C:287:SER:C	1:C:289:ALA:H	2.00	0.68
2:D:430:SER:O	2:D:434:GLN:HG3	1.93	0.68
1:A:103:TYR:N	1:A:185:TYR:HE1	1.92	0.68
1:A:172:TYR:HB3	1:A:205:ASP:CA	2.24	0.68
1:A:311:LYS:HD3	1:A:344:VAL:HG22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.29	0.68
2:B:391:ILE:HD12	2:B:391:ILE:H	1.57	0.68
2:D:175:PRO:O	2:D:177:VAL:HG23	1.93	0.68
1:A:43:GLY:O	1:A:47:ASP:CG	2.37	0.68
2:B:109:THR:HG21	2:B:411:GLU:CG	2.24	0.68
2:B:102:ASN:HB3	2:B:105:LYS:HD2	1.74	0.68
1:C:433:GLU:HA	1:C:433:GLU:OE1	1.92	0.68
2:D:71:GLU:HB2	2:D:72:PRO:CD	2.24	0.68
2:D:126:SER:OG	2:D:127:GLU:N	2.26	0.68
1:A:134:GLY:H	1:A:164:LYS:HG2	1.58	0.68
1:A:153:LEU:O	1:A:156:ARG:HB2	1.93	0.68
1:A:171:ILE:HD12	1:A:171:ILE:N	2.08	0.68
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.75	0.68
1:A:258:ASN:O	1:A:259:LEU:HB2	1.93	0.68
2:B:51:VAL:HG23	2:B:53:TYR:N	2.08	0.68
1:C:145:THR:O	1:C:149:PHE:HB3	1.93	0.68
1:C:215:ARG:HH22	1:C:300:ASN:ND2	1.91	0.68
2:D:55:GLU:HB2	2:D:244:PHE:HA	1.75	0.68
2:D:339:ASN:C	2:D:341:SER:H	2.01	0.68
1:A:321:GLY:HA2	1:A:357:TYR:O	1.94	0.68
1:C:147:SER:O	1:C:189:LEU:HD23	1.93	0.68
1:C:331:ALA:C	1:C:333:ALA:N	2.51	0.68
2:D:158:ARG:HD3	2:D:197:ASN:CG	2.18	0.68
1:A:104:ALA:HA	1:A:108:TYR:CD2	2.28	0.67
2:B:5:VAL:HB	2:B:135:PHE:CD2	2.29	0.67
1:C:31:GLN:O	1:C:33:ASP:N	2.28	0.67
1:C:414:GLU:HB2	1:C:417:GLU:HB2	1.76	0.67
2:D:16:ILE:HD12	2:D:231:VAL:HG11	1.76	0.67
2:D:405:LEU:HD13	2:D:406:HIS:N	2.09	0.67
3:E:50:UNK:O	3:E:52:UNK:N	2.27	0.67
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.29	0.67
1:A:412:GLY:O	1:A:414:GLU:OE1	2.12	0.67
1:A:427:ALA:O	1:A:430:LYS:HB3	1.93	0.67
2:B:398:MET:N	2:B:401:ARG:HB2	2.09	0.67
2:D:104:ALA:O	2:D:108:TYR:HB2	1.94	0.67
1:A:36:MET:HE3	1:A:37:PRO:HD2	1.77	0.67
2:B:102:ASN:HD21	2:B:104:ALA:HB3	1.58	0.67
2:B:163:ASP:CG	2:B:164:ARG:H	2.03	0.67
2:B:174:SER:OG	2:B:176:LYS:HG3	1.94	0.67
2:B:221:THR:OG1	1:C:326:LYS:HB2	1.94	0.67
1:A:75:ILE:O	1:A:75:ILE:HG12	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:HD2	1:A:436:GLY:HA2	1.76	0.67
2:D:8:GLN:HG2	2:D:14:ASN:ND2	2.06	0.67
2:D:353:THR:CG2	2:D:354:ALA:H	2.08	0.67
2:B:166:MET:HE3	2:B:197:ASN:HB3	1.76	0.67
2:B:237:GLY:O	2:B:376:THR:HG21	1.95	0.67
2:B:331:GLN:O	2:B:334:ASN:HB3	1.95	0.67
1:C:287:SER:OG	1:C:290:GLU:N	2.28	0.67
1:A:8:HIS:N	1:A:8:HIS:HD1	1.93	0.67
2:B:179:ASP:HB2	2:B:182:VAL:H	1.58	0.67
1:C:213:CYS:SG	1:C:217:LEU:HD23	2.34	0.67
2:D:217:LEU:HG	2:D:218:LYS:N	2.08	0.67
2:B:3:GLU:OE2	2:B:130:ASP:HB3	1.93	0.67
1:C:264:ARG:O	1:C:266:HIS:ND1	2.28	0.67
1:C:280:LYS:O	1:C:282:TYR:CE2	2.47	0.67
1:C:404:PHE:H	1:C:404:PHE:HD1	1.42	0.67
1:C:414:GLU:HG2	1:C:415:GLU:N	2.09	0.67
2:D:122:VAL:O	2:D:126:SER:N	2.26	0.67
2:D:174:SER:HB2	2:D:207:GLU:N	2.10	0.67
1:A:287:SER:OG	1:A:290:GLU:HG3	1.94	0.67
2:D:205:ASP:OD2	2:D:207:GLU:HB3	1.95	0.67
2:D:241:CYS:C	2:D:243:ARG:N	2.49	0.67
2:D:266:HIS:HB2	2:D:380:ASN:OD1	1.95	0.67
1:A:88:HIS:CB	1:A:91:GLN:HE22	2.08	0.67
1:A:237:SER:CA	1:A:241:SER:HB2	2.23	0.67
2:B:92:PHE:CD1	2:B:118:VAL:HG22	2.30	0.67
2:B:264:ARG:HH22	2:B:431:GLU:HG3	1.60	0.67
1:C:141:PHE:CE2	1:C:172:TYR:HA	2.19	0.67
1:C:291:ILE:CD1	1:C:373:ARG:HG3	2.24	0.67
1:A:305:CYS:SG	1:A:306:ASP:N	2.65	0.66
1:A:413:MET:SD	1:A:413:MET:N	2.68	0.66
1:C:210:TYR:CE2	1:C:227:LEU:HD23	2.30	0.66
2:D:87:PHE:O	2:D:87:PHE:CD1	2.48	0.66
2:D:255:LEU:HD23	2:D:259:MET:CG	2.25	0.66
1:A:70:LEU:CD1	1:A:145:THR:HA	2.17	0.66
1:A:189:LEU:HD13	1:A:193:THR:HG21	1.77	0.66
2:B:241:CYS:C	2:B:243:ARG:N	2.48	0.66
2:B:305:CYS:SG	2:B:387:LEU:HB2	2.35	0.66
2:D:4:ILE:O	2:D:64:ARG:HD2	1.95	0.66
2:D:62:VAL:O	2:D:62:VAL:HG23	1.94	0.66
1:A:355:ILE:HD12	1:A:355:ILE:N	2.10	0.66
2:B:70:LEU:HG	2:B:99:ALA:CB	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:VAL:HG11	1:C:154:MET:HE2	1.76	0.66
1:A:365:GLY:O	1:A:368:LEU:CD1	2.43	0.66
2:B:87:PHE:O	2:B:87:PHE:CD1	2.48	0.66
1:C:189:LEU:HD13	1:C:193:THR:HG21	1.77	0.66
1:C:386:GLU:CG	1:C:387:ALA:H	2.07	0.66
2:D:350:ASN:HD22	2:D:351:VAL:HG23	1.60	0.66
2:B:58:GLY:C	2:B:64:ARG:NE	2.52	0.66
1:C:273:ALA:HB2	1:C:295:CYS:HB2	1.76	0.66
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.30	0.66
1:A:242:LEU:O	1:A:243:ARG:NH1	2.28	0.66
1:A:287:SER:OG	1:A:290:GLU:N	2.28	0.66
2:B:16:ILE:HD12	2:B:231:VAL:HG11	1.77	0.66
2:B:255:LEU:HD23	2:B:259:MET:HG3	1.78	0.66
2:B:402:LYS:HE3	1:C:440:VAL:CB	2.24	0.66
1:A:8:HIS:N	1:A:8:HIS:ND1	2.43	0.66
2:B:59:ASN:CG	2:B:60:LYS:N	2.54	0.66
2:B:102:ASN:O	2:B:105:LYS:HB2	1.96	0.66
2:B:353:THR:CG2	2:B:354:ALA:N	2.58	0.66
1:C:242:LEU:HB3	1:C:250:VAL:HG11	1.78	0.66
2:D:320:ARG:HG2	2:D:320:ARG:HH11	1.59	0.66
3:E:48:UNK:O	3:E:49:UNK:C	2.44	0.66
1:A:371:VAL:HG12	1:A:372:GLN:N	2.11	0.66
1:C:371:VAL:HG12	1:C:373:ARG:N	2.11	0.66
3:E:25:UNK:O	3:E:29:UNK:N	2.29	0.66
1:A:261:PRO:CG	1:A:380:ASN:HD21	2.09	0.66
1:A:286:LEU:HA	1:A:290:GLU:OE1	1.96	0.66
1:A:295:CYS:HG	1:A:377:MET:HE2	1.59	0.66
2:B:126:SER:OG	2:B:127:GLU:N	2.28	0.66
1:C:7:ILE:HG22	1:C:66:VAL:CB	2.18	0.66
1:C:172:TYR:HB3	1:C:205:ASP:N	2.11	0.66
1:A:195:LEU:HB3	1:A:196:GLU:OE2	1.95	0.66
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.77	0.66
1:A:422:ARG:O	1:A:426:ALA:HB2	1.96	0.66
1:C:206:ASN:ND2	1:C:210:TYR:HE2	1.93	0.66
2:D:51:VAL:C	2:D:53:TYR:H	2.03	0.66
1:A:276:ILE:HG12	1:A:282:TYR:CD2	2.32	0.65
2:B:179:ASP:C	2:B:181:VAL:N	2.45	0.65
1:C:393:HIS:C	1:C:395:PHE:H	2.03	0.65
2:D:163:ASP:CG	2:D:164:ARG:H	2.04	0.65
2:D:203:CYS:SG	2:D:384:ILE:HD11	2.36	0.65
1:A:144:GLY:O	1:A:146:GLY:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:O	2:B:3:GLU:N	2.26	0.65
2:B:189:LEU:C	2:B:191:VAL:N	2.55	0.65
2:B:263:PRO:O	2:B:265:LEU:N	2.27	0.65
1:C:217:LEU:HD11	1:C:368:LEU:HD22	1.79	0.65
1:C:217:LEU:O	1:C:219:ILE:HG13	1.97	0.65
2:D:133:GLN:NE2	2:D:252:LEU:H	1.93	0.65
2:D:296:PHE:HA	2:D:377:PHE:HE2	1.61	0.65
1:A:209:ILE:C	1:A:211:ASP:N	2.51	0.65
1:A:231:ILE:O	1:A:235:VAL:HG23	1.96	0.65
1:A:354:GLY:C	1:A:355:ILE:HD12	2.21	0.65
1:A:363:VAL:HG13	1:A:367:ASP:OD2	1.96	0.65
2:B:58:GLY:O	2:B:64:ARG:NE	2.30	0.65
2:B:75:MET:O	2:B:76:ASP:C	2.39	0.65
2:B:380:ASN:C	2:B:380:ASN:HD22	2.05	0.65
1:C:134:GLY:H	1:C:164:LYS:CG	2.09	0.65
1:C:151:SER:HB3	1:C:192:HIS:NE2	2.12	0.65
1:C:414:GLU:CD	1:C:414:GLU:N	2.54	0.65
1:C:422:ARG:O	1:C:426:ALA:HB2	1.97	0.65
2:D:167:ASN:HA	2:D:200:GLU:O	1.96	0.65
2:D:335:VAL:HA	2:D:338:LYS:HB2	1.79	0.65
1:A:206:ASN:HB3	1:A:210:TYR:HE2	1.58	0.65
2:B:2:ARG:HG3	2:B:133:GLN:CD	2.21	0.65
2:B:311:ARG:HB2	2:B:344:VAL:N	2.10	0.65
1:C:413:MET:O	1:C:414:GLU:HB3	1.96	0.65
2:D:5:VAL:HA	2:D:64:ARG:CD	2.26	0.65
2:D:92:PHE:CD1	2:D:118:VAL:HG22	2.31	0.65
2:D:278:ARG:H	2:D:278:ARG:HD2	1.59	0.65
2:D:303:ALA:HB1	2:D:387:LEU:HD13	1.78	0.65
2:D:307:PRO:C	2:D:309:HIS:H	2.04	0.65
1:A:388:TRP:CZ3	1:A:428:LEU:HD22	2.31	0.65
2:B:218:LYS:NZ	2:B:278:ARG:HB2	2.11	0.65
2:B:255:LEU:HD23	2:B:259:MET:CG	2.27	0.65
1:A:174:ALA:O	1:A:176:GLN:N	2.29	0.65
1:A:186:ASN:ND2	1:A:391:LEU:HD21	2.10	0.65
1:A:286:LEU:O	1:A:373:ARG:HD2	1.97	0.65
2:B:247:GLN:HB2	2:B:355:VAL:O	1.97	0.65
2:B:264:ARG:HH11	2:B:264:ARG:HG3	1.60	0.65
1:C:330:ALA:O	1:C:334:THR:HG23	1.96	0.65
2:D:227:LEU:O	2:D:227:LEU:HD23	1.96	0.65
1:A:247:ALA:O	1:A:249:ASN:ND2	2.30	0.65
2:B:392:SER:HB2	2:B:426:ASN:ND2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ALA:HB3	1:C:140:SER:CB	2.27	0.65
1:C:143:GLY:O	1:C:144:GLY:O	2.13	0.65
1:C:209:ILE:N	1:C:209:ILE:HD12	2.11	0.65
2:D:274:PRO:HA	2:D:294:GLN:NE2	2.11	0.65
1:A:264:ARG:O	1:A:266:HIS:N	2.30	0.65
2:B:169:PHE:CD2	2:B:235:MET:SD	2.90	0.65
1:C:186:ASN:HD22	1:C:391:LEU:HD11	1.60	0.65
1:C:412:GLY:O	1:C:414:GLU:OE1	2.15	0.65
2:D:158:ARG:HB2	2:D:197:ASN:HD22	1.61	0.65
3:E:73:UNK:C	3:E:75:UNK:H	2.10	0.65
1:A:183:GLU:N	1:A:184:PRO:HD2	2.12	0.65
2:B:287:THR:OG1	2:B:290:GLU:HB2	1.97	0.65
2:B:391:ILE:O	2:B:425:MET:HE1	1.96	0.65
2:D:139:HIS:C	2:D:139:HIS:CD2	2.75	0.65
2:D:209:LEU:HB3	2:D:227:LEU:HG	1.79	0.65
2:D:398:MET:N	2:D:401:ARG:HB2	2.12	0.65
1:A:23:LEU:C	1:A:25:CYS:H	2.05	0.65
1:A:133:GLN:HA	1:A:164:LYS:HG3	1.79	0.65
2:B:122:VAL:O	2:B:126:SER:N	2.27	0.65
1:C:144:GLY:O	1:C:146:GLY:N	2.30	0.65
2:D:172:VAL:HG13	2:D:173:PRO:HD2	1.78	0.65
1:A:311:LYS:HD3	1:A:344:VAL:CG1	2.23	0.64
2:B:205:ASP:OD2	2:B:207:GLU:HB3	1.96	0.64
1:C:8:HIS:ND1	1:C:8:HIS:N	2.44	0.64
1:C:133:GLN:HA	1:C:164:LYS:HG3	1.79	0.64
1:C:354:GLY:C	1:C:355:ILE:HD12	2.22	0.64
2:D:111:GLY:C	2:D:113:GLU:N	2.53	0.64
2:D:398:MET:C	2:D:400:ARG:H	2.05	0.64
2:B:123:ARG:C	2:B:125:GLU:H	2.06	0.64
2:B:187:ALA:HA	2:B:425:MET:HE2	1.79	0.64
1:C:362:VAL:CG1	1:C:367:ASP:HB2	2.26	0.64
2:D:5:VAL:HA	2:D:64:ARG:HD2	1.79	0.64
2:D:127:GLU:O	2:D:128:SER:C	2.40	0.64
2:D:137:LEU:HD23	2:D:154:ILE:HD11	1.80	0.64
1:A:277:SER:O	1:A:278:ALA:HB2	1.97	0.64
2:B:96:GLN:NE2	1:C:130:THR:HG22	2.11	0.64
2:B:107:HIS:HD2	2:B:151:THR:HG23	1.62	0.64
2:B:158:ARG:CA	2:B:197:ASN:HD22	2.09	0.64
1:C:100:ALA:CB	1:C:105:ARG:HD2	2.27	0.64
1:C:360:PRO:HB3	1:C:374:ALA:HB2	1.79	0.64
2:D:240:THR:C	2:D:243:ARG:HB2	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:VAL:HG11	1:A:87:PHE:CE2	2.32	0.64
1:A:183:GLU:HB2	1:A:184:PRO:CD	2.27	0.64
2:B:278:ARG:H	2:B:278:ARG:HD2	1.59	0.64
1:C:138:PHE:CZ	1:C:235:VAL:HG11	2.30	0.64
2:D:58:GLY:C	2:D:64:ARG:NE	2.55	0.64
1:A:138:PHE:CZ	1:A:235:VAL:HG11	2.26	0.64
1:A:285:GLN:OE1	1:A:372:GLN:HG2	1.96	0.64
1:A:292:THR:HA	1:A:295:CYS:HB3	1.80	0.64
1:A:433:GLU:OE1	1:A:433:GLU:HA	1.97	0.64
2:B:71:GLU:HB2	2:B:72:PRO:CD	2.27	0.64
2:B:132:LEU:C	2:B:132:LEU:HD23	2.22	0.64
2:B:133:GLN:HE22	2:B:252:LEU:H	1.43	0.64
1:C:203:MET:SD	1:C:388:TRP:CD1	2.91	0.64
1:C:267:PHE:N	1:C:267:PHE:HD1	1.94	0.64
2:D:288:VAL:N	2:D:289:PRO:HD2	2.12	0.64
1:A:16:ILE:HG22	1:A:17:GLY:H	1.62	0.64
1:A:147:SER:O	1:A:189:LEU:HD23	1.97	0.64
1:A:191:THR:HB	1:A:421:ALA:HB1	1.79	0.64
1:A:395:PHE:CD1	1:A:395:PHE:C	2.75	0.64
2:B:2:ARG:HG3	2:B:133:GLN:HE21	1.58	0.64
2:B:192:HIS:O	2:B:194:LEU:N	2.30	0.64
1:C:191:THR:CB	1:C:421:ALA:HB1	2.27	0.64
1:C:395:PHE:CD1	1:C:395:PHE:C	2.75	0.64
2:D:75:MET:O	2:D:76:ASP:C	2.40	0.64
2:D:255:LEU:HD23	2:D:259:MET:HG3	1.80	0.64
2:D:390:ARG:C	2:D:392:SER:N	2.51	0.64
1:A:77:GLU:O	1:A:83:TYR:HB2	1.97	0.64
1:A:86:LEU:HD22	1:A:89:PRO:HD3	1.79	0.64
1:A:287:SER:N	1:A:290:GLU:HB2	2.13	0.64
1:A:350:GLY:O	1:A:351:PHE:CD1	2.50	0.64
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.26	0.64
2:B:339:ASN:O	2:B:341:SER:N	2.30	0.64
1:C:196:GLU:N	1:C:196:GLU:CD	2.55	0.64
1:C:433:GLU:C	1:C:435:VAL:H	2.04	0.64
2:D:380:ASN:C	2:D:380:ASN:HD22	2.05	0.64
2:D:386:GLU:O	2:D:388:PHE:N	2.31	0.64
1:A:87:PHE:HE2	1:A:92:LEU:HD21	1.60	0.64
1:A:111:GLY:O	1:A:113:GLU:N	2.31	0.64
1:A:276:ILE:O	1:A:369:ALA:HB3	1.98	0.64
2:B:307:PRO:C	2:B:309:HIS:H	2.06	0.64
1:C:160:ASP:O	1:C:161:TYR:CD1	2.50	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:C	1:C:211:ASP:N	2.55	0.64
2:D:92:PHE:HD1	2:D:118:VAL:HG22	1.61	0.64
2:D:184:PRO:HB2	2:D:399:PHE:CZ	2.32	0.64
2:D:311:ARG:HB2	2:D:344:VAL:N	2.12	0.64
2:D:377:PHE:O	2:D:378:ILE:HG12	1.98	0.64
1:A:345:ASP:C	1:A:347:CYS:H	2.06	0.64
2:B:413:MET:HE1	2:B:418:PHE:CE2	2.33	0.64
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.32	0.64
1:C:331:ALA:HA	1:C:334:THR:OG1	1.98	0.64
2:D:59:ASN:ND2	2:D:60:LYS:N	2.45	0.64
2:D:129:CYS:O	2:D:130:ASP:O	2.15	0.64
2:D:391:ILE:H	2:D:391:ILE:CD1	2.10	0.64
2:B:123:ARG:CZ	2:B:160:GLU:OE2	2.45	0.64
2:B:385:GLN:NE2	2:B:433:GLN:HE21	1.96	0.64
1:C:104:ALA:HA	1:C:108:TYR:CD2	2.31	0.64
2:D:385:GLN:HG2	2:D:433:GLN:HE21	1.62	0.64
2:D:416:MET:C	2:D:418:PHE:N	2.56	0.64
1:A:186:ASN:HD22	1:A:391:LEU:HD11	1.63	0.63
2:B:59:ASN:HB2	2:B:64:ARG:CZ	2.28	0.63
2:B:371:LEU:HB3	2:B:373:MET:O	1.97	0.63
2:B:427:ASP:O	2:B:429:VAL:N	2.31	0.63
1:C:27:GLU:CG	1:C:28:HIS:H	2.10	0.63
2:D:140:SER:OG	2:D:171:VAL:HB	1.99	0.63
1:A:5:ILE:HD12	1:A:125:LEU:HD22	1.80	0.63
2:B:16:ILE:HG12	2:B:17:GLY:N	2.13	0.63
2:B:320:ARG:N	2:B:374:SER:O	2.29	0.63
2:B:416:MET:C	2:B:418:PHE:N	2.56	0.63
1:C:363:VAL:H	1:C:367:ASP:HB2	1.61	0.63
2:D:102:ASN:HD22	2:D:105:LYS:CG	2.11	0.63
2:D:345:GLU:HG2	2:D:345:GLU:O	1.96	0.63
1:A:158:SER:HB3	1:A:166:LYS:NZ	2.13	0.63
1:A:217:LEU:O	1:A:219:ILE:HG13	1.99	0.63
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.79	0.63
1:A:307:PRO:HB3	1:A:381:THR:HG21	1.80	0.63
2:B:104:ALA:O	2:B:108:TYR:HB2	1.98	0.63
2:B:140:SER:OG	2:B:171:VAL:HB	1.98	0.63
1:C:75:ILE:HG12	1:C:75:ILE:O	1.97	0.63
1:C:215:ARG:HH22	1:C:300:ASN:HD21	1.45	0.63
2:D:287:THR:OG1	2:D:290:GLU:HB2	1.98	0.63
1:A:87:PHE:CD2	1:A:87:PHE:N	2.63	0.63
1:A:180:ALA:C	1:A:182:VAL:N	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HD11	1:A:368:LEU:HD22	1.81	0.63
1:A:241:SER:HA	1:A:320:ARG:NH2	2.13	0.63
1:A:263:PRO:O	1:A:265:ALA:N	2.28	0.63
1:A:269:LEU:HD12	1:A:269:LEU:C	2.23	0.63
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.80	0.63
2:B:174:SER:HB2	2:B:207:GLU:N	2.12	0.63
2:B:357:ASP:HB3	2:B:358:ILE:HD12	1.81	0.63
1:C:404:PHE:HD1	1:C:404:PHE:N	1.95	0.63
1:C:413:MET:C	1:C:414:GLU:OE1	2.41	0.63
2:D:158:ARG:O	2:D:160:GLU:N	2.31	0.63
2:D:251:ASP:CG	2:D:252:LEU:N	2.56	0.63
2:B:288:VAL:N	2:B:289:PRO:HD2	2.14	0.63
1:C:243:ARG:CZ	1:C:243:ARG:HA	2.28	0.63
1:C:355:ILE:HD12	1:C:355:ILE:N	2.13	0.63
1:C:404:PHE:N	1:C:404:PHE:CD1	2.67	0.63
1:A:215:ARG:NH2	1:A:216:ASN:OD1	2.32	0.63
1:A:256:GLN:HA	1:A:260:VAL:HG23	1.81	0.63
2:B:385:GLN:HG2	2:B:433:GLN:HE21	1.62	0.63
1:C:78:VAL:HG11	1:C:92:LEU:HD21	1.80	0.63
2:D:123:ARG:C	2:D:125:GLU:H	2.06	0.63
2:D:179:ASP:C	2:D:181:VAL:N	2.47	0.63
2:D:5:VAL:HB	2:D:135:PHE:HD2	1.62	0.63
1:A:72:PRO:HB3	1:A:94:THR:OG1	1.98	0.63
1:C:243:ARG:HH12	1:C:250:VAL:CG1	2.11	0.63
1:C:295:CYS:HG	1:C:377:MET:HE2	1.62	0.63
2:D:187:ALA:HA	2:D:425:MET:HE2	1.81	0.63
1:A:291:ILE:HD12	1:A:373:ARG:HG3	1.80	0.63
1:A:311:LYS:CG	1:A:344:VAL:HG22	2.28	0.63
2:B:71:GLU:HB2	2:B:72:PRO:HD2	1.79	0.63
2:B:158:ARG:HD3	2:B:197:ASN:CG	2.23	0.63
2:B:399:PHE:CE2	2:B:404:PHE:HB3	2.34	0.63
1:C:206:ASN:HB3	1:C:210:TYR:HE2	1.61	0.63
1:C:373:ARG:HB3	1:C:373:ARG:NH1	2.12	0.63
1:C:385:ALA:HB2	1:C:432:TYR:HD2	1.63	0.63
1:C:409:VAL:C	1:C:411:GLU:H	2.05	0.63
2:D:107:HIS:CD2	2:D:151:THR:HG23	2.33	0.63
1:A:172:TYR:HB3	1:A:205:ASP:N	2.14	0.62
1:C:93:ILE:HD13	1:C:118:VAL:CG2	2.26	0.62
1:C:296:PHE:CD2	1:C:377:MET:HE1	2.34	0.62
2:D:196:GLU:O	2:D:197:ASN:C	2.39	0.62
2:D:215:ARG:NE	2:D:215:ARG:HA	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:LEU:HD13	2:D:371:LEU:O	1.99	0.62
1:A:70:LEU:HD12	1:A:145:THR:CA	2.17	0.62
1:A:102:ASN:ND2	2:B:257:VAL:HG11	2.09	0.62
1:A:362:VAL:HG21	1:A:369:ALA:O	1.98	0.62
1:A:409:VAL:C	1:A:411:GLU:H	2.07	0.62
2:B:183:GLU:C	2:B:185:TYR:N	2.54	0.62
2:B:241:CYS:C	2:B:243:ARG:H	2.04	0.62
2:B:390:ARG:C	2:B:392:SER:N	2.53	0.62
2:B:417:GLU:HG3	2:B:417:GLU:O	1.98	0.62
1:C:156:ARG:O	1:C:159:VAL:HB	2.00	0.62
2:D:107:HIS:HD2	2:D:151:THR:HG23	1.64	0.62
2:D:264:ARG:HG3	2:D:264:ARG:NH1	2.12	0.62
2:D:398:MET:O	2:D:400:ARG:N	2.32	0.62
1:A:160:ASP:O	1:A:161:TYR:CD1	2.52	0.62
1:A:171:ILE:HD12	1:A:171:ILE:H	1.62	0.62
2:B:292:THR:HG23	2:B:319:PHE:HZ	1.63	0.62
2:D:258:ASN:OD1	2:D:352:LYS:NZ	2.29	0.62
2:D:405:LEU:HD22	2:D:405:LEU:C	2.24	0.62
3:E:35:UNK:O	3:E:39:UNK:N	2.32	0.62
1:A:293:ASN:O	1:A:297:GLU:OE1	2.17	0.62
2:B:251:ASP:CG	2:B:252:LEU:N	2.55	0.62
2:B:267:PHE:HB2	2:B:384:ILE:HD13	1.80	0.62
3:E:75:UNK:O	3:E:76:UNK:C	2.47	0.62
1:A:88:HIS:HB3	1:A:91:GLN:CD	2.24	0.62
1:A:258:ASN:O	1:A:259:LEU:CB	2.48	0.62
1:A:280:LYS:O	1:A:282:TYR:HE2	1.82	0.62
2:B:165:ILE:HD13	2:B:199:ASP:OD1	1.99	0.62
2:B:292:THR:HG23	2:B:319:PHE:CZ	2.35	0.62
2:B:396:THR:CG2	2:B:400:ARG:HD3	2.28	0.62
1:C:154:MET:SD	1:C:197:HIS:CD2	2.93	0.62
1:C:307:PRO:HB3	1:C:381:THR:HG21	1.81	0.62
2:D:267:PHE:HB2	2:D:384:ILE:HD13	1.81	0.62
2:D:385:GLN:HG2	2:D:433:GLN:NE2	2.13	0.62
1:A:156:ARG:O	1:A:159:VAL:HB	1.99	0.62
1:A:393:HIS:C	1:A:395:PHE:H	2.06	0.62
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.32	0.62
2:B:132:LEU:HD23	2:B:132:LEU:O	2.00	0.62
2:D:191:VAL:CG1	2:D:421:ALA:HA	2.29	0.62
1:A:373:ARG:HB3	1:A:373:ARG:NH1	2.15	0.62
2:B:102:ASN:C	2:B:185:TYR:OH	2.43	0.62
2:B:130:ASP:OD2	2:B:131:CYS:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:ARG:NE	2:B:215:ARG:HA	2.13	0.62
1:C:407:TRP:CZ2	2:D:256:ALA:O	2.53	0.62
2:D:282:GLN:HA	2:D:285:ALA:HB2	1.80	0.62
1:A:267:PHE:N	1:A:267:PHE:HD1	1.96	0.62
1:A:344:VAL:HG11	1:A:346:TRP:HE1	1.63	0.62
2:B:2:ARG:HE	2:B:243:ARG:HD2	1.64	0.62
2:B:196:GLU:O	2:B:197:ASN:C	2.43	0.62
1:C:27:GLU:HG3	1:C:28:HIS:ND1	2.14	0.62
1:C:291:ILE:HG21	1:C:375:VAL:HG21	1.82	0.62
1:C:311:LYS:HD3	1:C:344:VAL:HG22	1.80	0.62
1:C:344:VAL:HG12	1:C:345:ASP:N	2.15	0.62
2:D:2:ARG:O	2:D:57:ALA:HB1	1.99	0.62
2:D:24:ILE:HG22	2:D:24:ILE:O	1.98	0.62
2:D:333:LEU:HG	2:D:337:ASN:ND2	2.15	0.62
2:D:348:PRO:O	2:D:349:ASN:HB3	2.00	0.62
1:A:132:LEU:HB3	1:A:164:LYS:HD3	1.80	0.62
1:A:407:TRP:CZ2	2:B:256:ALA:O	2.53	0.62
2:B:102:ASN:ND2	2:B:105:LYS:H	1.98	0.62
2:B:105:LYS:HA	2:B:109:THR:OG1	1.99	0.62
2:B:153:LEU:O	2:B:157:ILE:N	2.33	0.62
2:B:344:VAL:HG23	2:B:345:GLU:N	2.15	0.62
2:D:206:ASN:ND2	2:D:227:LEU:HD21	2.07	0.62
1:A:181:VAL:HG13	1:A:408:TYR:OH	2.00	0.62
1:A:244:PHE:O	1:A:245:ASP:C	2.41	0.62
1:A:365:GLY:O	1:A:368:LEU:HD11	2.00	0.62
1:C:345:ASP:O	1:C:347:CYS:N	2.31	0.62
2:D:2:ARG:HH11	2:D:251:ASP:HA	1.64	0.62
2:D:158:ARG:HA	2:D:197:ASN:ND2	2.15	0.62
3:E:58:UNK:O	3:E:60:UNK:N	2.33	0.62
2:B:280:SER:O	2:B:282:GLN:HG2	1.99	0.61
2:B:385:GLN:HG2	2:B:433:GLN:NE2	2.14	0.61
1:C:191:THR:HB	1:C:421:ALA:HB1	1.79	0.61
1:C:242:LEU:O	1:C:243:ARG:NH1	2.33	0.61
1:C:267:PHE:HD1	1:C:267:PHE:H	1.45	0.61
1:C:344:VAL:HG11	1:C:346:TRP:HE1	1.63	0.61
2:D:358:ILE:H	2:D:358:ILE:CD1	2.13	0.61
1:A:210:TYR:CE2	1:A:227:LEU:HD23	2.34	0.61
1:A:317:LEU:HD23	1:A:377:MET:CB	2.30	0.61
2:B:22:GLU:N	2:B:22:GLU:OE2	2.33	0.61
1:C:362:VAL:CG2	1:C:370:LYS:HA	2.28	0.61
2:D:280:SER:O	2:D:282:GLN:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:CD	1:A:196:GLU:N	2.58	0.61
1:A:413:MET:SD	3:E:15:UNK:CA	2.83	0.61
2:B:326:LYS:O	2:B:330:GLU:HG3	2.00	0.61
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.34	0.61
1:C:182:VAL:O	1:C:183:GLU:C	2.43	0.61
1:C:238:ILE:HG22	1:C:239:THR:N	2.15	0.61
2:D:123:ARG:NE	2:D:160:GLU:OE2	2.32	0.61
2:D:162:PRO:O	2:D:163:ASP:C	2.43	0.61
2:D:413:MET:HE1	2:D:418:PHE:CE2	2.35	0.61
1:A:175:PRO:O	1:A:177:VAL:HG23	2.00	0.61
1:A:386:GLU:C	1:A:388:TRP:H	2.06	0.61
1:A:425:MET:O	1:A:425:MET:HE3	2.01	0.61
2:B:5:VAL:HB	2:B:135:PHE:HD2	1.65	0.61
2:B:218:LYS:NZ	2:B:278:ARG:N	2.46	0.61
2:B:241:CYS:SG	2:B:320:ARG:NH1	2.73	0.61
1:C:2:ARG:NH2	1:C:133:GLN:NE2	2.46	0.61
1:C:86:LEU:CD2	1:C:89:PRO:HD3	2.29	0.61
1:C:236:SER:C	1:C:238:ILE:H	2.08	0.61
2:D:237:GLY:O	2:D:376:THR:HG21	2.01	0.61
3:E:4:UNK:O	3:E:6:UNK:N	2.33	0.61
1:A:362:VAL:CG2	1:A:370:LYS:HA	2.31	0.61
2:B:353:THR:CG2	2:B:354:ALA:H	2.14	0.61
2:B:396:THR:HG23	2:B:400:ARG:CD	2.27	0.61
1:C:36:MET:HE3	1:C:37:PRO:HD2	1.82	0.61
1:C:258:ASN:HD22	1:C:258:ASN:H	1.48	0.61
2:D:264:ARG:HH22	2:D:431:GLU:HG3	1.64	0.61
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.82	0.61
1:A:88:HIS:N	1:A:91:GLN:OE1	2.33	0.61
2:B:2:ARG:NH1	2:B:251:ASP:HA	2.15	0.61
2:B:191:VAL:HG13	2:B:421:ALA:HA	1.83	0.61
2:B:312:TYR:HA	2:B:381:SER:HA	1.81	0.61
2:D:287:THR:O	2:D:290:GLU:HB3	2.01	0.61
1:A:398:MET:O	1:A:400:ALA:N	2.34	0.61
2:B:102:ASN:HD22	2:B:105:LYS:CG	2.13	0.61
2:B:404:PHE:O	2:B:404:PHE:HD2	1.83	0.61
1:C:78:VAL:O	1:C:82:THR:HA	2.01	0.61
1:C:166:LYS:HZ1	1:C:197:HIS:HB2	1.66	0.61
1:A:139:HIS:NE2	1:A:150:THR:HG21	2.16	0.61
2:B:92:PHE:HD1	2:B:118:VAL:HG22	1.63	0.61
1:C:65:ALA:O	1:C:91:GLN:HB2	2.01	0.61
1:C:72:PRO:HB3	1:C:94:THR:OG1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASN:OD1	2:D:254:LYS:NZ	2.30	0.61
1:C:171:ILE:CG2	1:C:206:ASN:OD1	2.48	0.61
1:C:258:ASN:ND2	1:C:258:ASN:H	1.99	0.61
1:C:331:ALA:C	1:C:333:ALA:H	2.08	0.61
2:D:94:PHE:HB2	2:D:114:LEU:CD1	2.31	0.61
2:D:241:CYS:C	2:D:243:ARG:H	2.07	0.61
1:A:27:GLU:CG	1:A:28:HIS:H	2.12	0.61
1:A:101:ASN:O	1:A:185:TYR:OH	2.19	0.61
1:A:103:TYR:CG	1:A:188:ILE:HD13	2.36	0.61
1:A:321:GLY:N	1:A:356:ASN:O	2.34	0.61
2:B:223:THR:N	2:B:226:ASP:OD2	2.30	0.61
1:C:188:ILE:HG22	1:C:417:GLU:O	2.01	0.61
1:C:259:LEU:HD21	1:C:378:LEU:HB3	1.81	0.61
2:D:60:LYS:N	2:D:60:LYS:NZ	2.49	0.61
2:D:154:ILE:C	2:D:156:LYS:H	2.08	0.61
2:D:261:PRO:HB2	2:D:262:PHE:CD1	2.36	0.61
2:B:140:SER:CB	2:B:171:VAL:HB	2.31	0.61
2:D:5:VAL:HG22	2:D:64:ARG:HD3	1.83	0.61
2:D:132:LEU:HD23	2:D:132:LEU:C	2.26	0.61
3:E:35:UNK:HA	3:E:38:UNK:CB	2.31	0.61
3:E:50:UNK:C	3:E:52:UNK:N	2.62	0.61
1:A:103:TYR:HB2	1:A:185:TYR:CD1	2.36	0.60
1:A:143:GLY:O	1:A:144:GLY:O	2.18	0.60
1:A:218:ASP:CG	1:A:219:ILE:H	2.09	0.60
1:A:242:LEU:HB3	1:A:250:VAL:HG11	1.83	0.60
2:B:59:ASN:HB2	2:B:64:ARG:HE	1.63	0.60
2:B:161:TYR:O	2:B:162:PRO:C	2.42	0.60
2:B:226:ASP:C	2:B:228:ASN:H	2.08	0.60
2:B:240:THR:C	2:B:243:ARG:HB2	2.26	0.60
2:B:311:ARG:HG3	2:B:311:ARG:HH11	1.65	0.60
1:C:221:ARG:CD	1:C:221:ARG:H	2.13	0.60
2:D:296:PHE:HA	2:D:377:PHE:CE2	2.35	0.60
2:D:350:ASN:ND2	2:D:351:VAL:HG23	2.16	0.60
2:D:385:GLN:HE21	2:D:433:GLN:HG2	1.65	0.60
1:A:195:LEU:C	1:A:197:HIS:H	2.09	0.60
1:A:282:TYR:N	1:A:282:TYR:HD2	1.98	0.60
1:A:283:HIS:O	1:A:284:GLU:HB3	2.00	0.60
2:B:66:ILE:O	2:B:66:ILE:HG12	2.01	0.60
2:B:286:LEU:HD13	2:B:371:LEU:O	2.00	0.60
2:B:321:GLY:CA	2:B:359:PRO:HB3	2.27	0.60
1:C:8:HIS:N	1:C:8:HIS:HD1	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:THR:HG21	2:D:411:GLU:CG	2.30	0.60
2:D:118:VAL:O	2:D:120:ASP:N	2.32	0.60
2:D:153:LEU:O	2:D:157:ILE:N	2.34	0.60
1:A:318:LEU:HB2	1:A:376:CYS:O	2.01	0.60
2:B:62:VAL:HG23	2:B:62:VAL:O	1.99	0.60
2:B:134:GLY:HA3	2:B:165:ILE:O	2.02	0.60
2:B:287:THR:O	2:B:290:GLU:HB3	2.01	0.60
2:B:308:ARG:NH2	2:B:342:TYR:CD1	2.61	0.60
2:B:348:PRO:O	2:B:349:ASN:HB3	2.01	0.60
1:C:16:ILE:HD12	1:C:171:ILE:HD11	1.83	0.60
1:C:90:GLU:O	1:C:121:ARG:NH1	2.34	0.60
1:C:126:ALA:HB1	1:C:132:LEU:HD11	1.83	0.60
1:C:183:GLU:HB2	1:C:184:PRO:CD	2.30	0.60
1:C:185:TYR:O	1:C:188:ILE:HD12	2.01	0.60
2:D:192:HIS:C	2:D:194:LEU:N	2.56	0.60
1:A:7:ILE:HG22	1:A:66:VAL:CB	2.23	0.60
1:A:350:GLY:C	1:A:351:PHE:CD1	2.72	0.60
2:B:118:VAL:O	2:B:120:ASP:N	2.28	0.60
2:B:149:MET:O	2:B:152:LEU:HB3	2.01	0.60
1:C:158:SER:HB3	1:C:166:LYS:NZ	2.17	0.60
2:D:265:LEU:O	2:D:266:HIS:ND1	2.34	0.60
2:D:312:TYR:HA	2:D:381:SER:HA	1.83	0.60
1:A:222:PRO:CB	1:A:227:LEU:HD11	2.19	0.60
1:A:257:THR:OG1	1:A:258:ASN:ND2	2.35	0.60
2:B:2:ARG:CG	2:B:133:GLN:NE2	2.58	0.60
1:C:276:ILE:O	1:C:369:ALA:HB3	2.01	0.60
2:D:191:VAL:HG13	2:D:421:ALA:HA	1.82	0.60
1:A:175:PRO:HD2	1:A:207:GLU:CB	2.05	0.60
1:A:269:LEU:HD21	1:A:301:GLN:NE2	2.17	0.60
2:B:11:GLN:HG3	2:B:15:GLN:NE2	2.17	0.60
2:B:107:HIS:CD2	2:B:151:THR:HG23	2.35	0.60
2:B:184:PRO:HB2	2:B:399:PHE:CZ	2.35	0.60
2:B:191:VAL:CG1	2:B:421:ALA:HA	2.30	0.60
1:C:332:ILE:HD11	1:C:353:VAL:HG21	1.84	0.60
2:D:339:ASN:O	2:D:341:SER:N	2.34	0.60
2:D:399:PHE:CE2	2:D:404:PHE:HB3	2.37	0.60
1:A:344:VAL:HG12	1:A:345:ASP:N	2.17	0.60
2:B:296:PHE:HA	2:B:377:PHE:CE2	2.36	0.60
1:C:9:VAL:HA	1:C:68:VAL:O	2.02	0.60
1:C:21:TRP:HA	1:C:24:TYR:HB2	1.82	0.60
1:C:77:GLU:O	1:C:83:TYR:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:HIS:NE2	1:C:150:THR:HG21	2.16	0.60
1:C:197:HIS:NE2	1:C:198:SER:HB3	2.17	0.60
1:C:305:CYS:SG	1:C:384:ILE:HA	2.42	0.60
1:C:371:VAL:HG12	1:C:372:GLN:N	2.17	0.60
1:A:220:GLU:OE2	2:B:326:LYS:HD3	2.01	0.60
1:A:291:ILE:HG22	1:A:292:THR:N	2.17	0.60
1:C:280:LYS:O	1:C:282:TYR:HE2	1.84	0.60
2:D:159:GLU:OE2	3:E:82:UNK:CB	2.50	0.60
1:A:9:VAL:HG21	1:A:150:THR:HB	1.84	0.60
1:A:31:GLN:CB	1:A:32:PRO:HD2	2.27	0.60
1:A:69:ASP:OD1	1:A:71:GLU:HG3	2.02	0.60
1:A:215:ARG:NH2	1:A:300:ASN:HD21	1.99	0.60
1:A:360:PRO:HB3	1:A:374:ALA:HB2	1.83	0.60
2:B:311:ARG:HH11	2:B:344:VAL:HA	1.67	0.60
1:C:26:LEU:HG	1:C:361:THR:CB	2.32	0.60
1:C:209:ILE:HD12	1:C:209:ILE:H	1.65	0.60
1:C:287:SER:OG	1:C:290:GLU:HG3	2.02	0.60
2:D:102:ASN:ND2	2:D:105:LYS:H	1.99	0.60
2:D:102:ASN:HB3	2:D:105:LYS:HB2	1.83	0.60
2:D:239:THR:O	2:D:241:CYS:O	2.20	0.60
1:A:100:ALA:HA	1:A:105:ARG:HD2	1.83	0.60
1:A:413:MET:HE2	1:A:413:MET:N	2.14	0.60
2:B:194:LEU:HD11	2:B:428:LEU:HD11	1.84	0.60
1:C:46:ASP:OD2	1:C:46:ASP:N	2.34	0.60
1:C:332:ILE:CD1	1:C:353:VAL:HG21	2.31	0.60
3:E:83:UNK:C	3:E:85:UNK:N	2.63	0.60
1:A:39:ASP:CG	1:A:40:LYS:N	2.60	0.59
1:A:69:ASP:HB3	1:A:75:ILE:CG2	2.26	0.59
1:A:236:SER:C	1:A:238:ILE:H	2.09	0.59
2:B:60:LYS:N	2:B:60:LYS:NZ	2.50	0.59
2:B:218:LYS:O	2:B:219:LEU:HB2	2.00	0.59
2:B:266:HIS:HB2	2:B:380:ASN:OD1	2.02	0.59
1:C:329:ASN:HA	1:C:332:ILE:HB	1.83	0.59
1:C:386:GLU:C	1:C:388:TRP:H	2.10	0.59
2:D:102:ASN:O	2:D:105:LYS:HB2	2.01	0.59
2:D:166:MET:HG3	2:D:167:ASN:N	2.16	0.59
2:D:263:PRO:O	2:D:265:LEU:N	2.33	0.59
2:B:243:ARG:HH12	2:B:252:LEU:HD12	1.67	0.59
2:B:303:ALA:HB1	2:B:387:LEU:CD1	2.32	0.59
2:B:322:ARG:NE	2:B:357:ASP:HB3	2.17	0.59
2:B:350:ASN:HD22	2:B:351:VAL:HG23	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:HG23	1:C:9:VAL:O	2.01	0.59
1:C:88:HIS:HB3	1:C:91:GLN:CD	2.26	0.59
1:C:264:ARG:NH2	1:C:424:ASP:OD1	2.35	0.59
1:C:321:GLY:HA2	1:C:357:TYR:O	2.02	0.59
1:C:423:GLU:O	1:C:427:ALA:N	2.28	0.59
2:D:218:LYS:HZ2	2:D:277:SER:HB3	1.67	0.59
1:A:77:GLU:O	1:A:83:TYR:CB	2.50	0.59
1:A:182:VAL:CG1	1:A:183:GLU:N	2.65	0.59
2:D:58:GLY:O	2:D:64:ARG:NE	2.34	0.59
2:D:99:ALA:HA	2:D:105:LYS:HD3	1.83	0.59
2:D:266:HIS:ND1	2:D:432:TYR:CZ	2.70	0.59
1:A:44:GLY:HA3	1:A:47:ASP:HA	1.84	0.59
1:A:238:ILE:N	1:A:241:SER:HB3	2.18	0.59
2:B:12:CYS:HB3	5:B:501:GDP:C8	2.37	0.59
1:C:86:LEU:HD22	1:C:89:PRO:HD3	1.84	0.59
1:C:166:LYS:HZ2	1:C:197:HIS:HB2	1.64	0.59
1:C:237:SER:CA	1:C:241:SER:HB2	2.28	0.59
2:D:87:PHE:O	2:D:90:ASP:OD1	2.19	0.59
2:D:141:LEU:HB3	2:D:186:ASN:CB	2.32	0.59
1:A:68:VAL:HG21	1:A:118:VAL:HG21	1.83	0.59
1:A:87:PHE:CE2	1:A:92:LEU:HD21	2.38	0.59
1:A:433:GLU:C	1:A:435:VAL:H	2.07	0.59
2:B:102:ASN:HD22	2:B:105:LYS:N	2.01	0.59
2:B:247:GLN:HG2	2:B:325:MET:SD	2.42	0.59
2:B:391:ILE:H	2:B:391:ILE:CD1	2.15	0.59
1:C:110:ILE:O	1:C:111:GLY:C	2.45	0.59
1:C:261:PRO:CG	1:C:380:ASN:HD21	2.13	0.59
1:A:331:ALA:C	1:A:333:ALA:N	2.58	0.59
2:B:79:ARG:HA	2:B:84:GLY:HA2	1.83	0.59
2:B:94:PHE:HB2	2:B:114:LEU:CD1	2.33	0.59
2:B:202:TYR:CE1	2:B:378:ILE:HD12	2.38	0.59
2:D:169:PHE:CD2	2:D:235:MET:SD	2.95	0.59
2:D:276:THR:HG21	2:D:281:GLN:HB3	1.84	0.59
2:D:312:TYR:CD2	2:D:381:SER:HB2	2.37	0.59
2:D:396:THR:HA	2:D:400:ARG:HB3	1.83	0.59
1:A:101:ASN:OD1	2:B:254:LYS:HD3	2.02	0.59
1:A:103:TYR:O	1:A:104:ALA:C	2.45	0.59
2:B:18:ALA:O	2:B:22:GLU:OE2	2.20	0.59
2:B:239:THR:O	2:B:241:CYS:O	2.19	0.59
1:C:258:ASN:O	1:C:259:LEU:HB2	2.02	0.59
2:D:259:MET:HE2	2:D:316:ALA:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:ARG:NH2	2:D:342:TYR:HB2	2.17	0.59
2:D:404:PHE:HD2	2:D:404:PHE:O	1.85	0.59
3:E:67:UNK:O	3:E:71:UNK:N	2.35	0.59
2:B:2:ARG:NE	2:B:243:ARG:CD	2.64	0.59
2:B:181:VAL:O	2:B:183:GLU:N	2.35	0.59
2:B:253:ARG:HG3	2:B:253:ARG:NH1	2.17	0.59
2:B:395:PHE:HB3	2:B:422:GLU:OE1	2.03	0.59
1:C:36:MET:HE2	1:C:38:SER:OG	2.03	0.59
1:C:103:TYR:N	1:C:185:TYR:HE1	2.01	0.59
1:C:195:LEU:C	1:C:197:HIS:H	2.11	0.59
1:C:345:ASP:C	1:C:347:CYS:H	2.10	0.59
2:D:102:ASN:C	2:D:185:TYR:OH	2.46	0.59
3:E:37:UNK:O	3:E:38:UNK:C	2.49	0.59
3:E:54:UNK:O	3:E:56:UNK:N	2.35	0.59
1:A:171:ILE:CG2	1:A:206:ASN:OD1	2.50	0.59
2:B:18:ALA:O	2:B:20:PHE:N	2.35	0.59
2:B:80:SER:OG	2:B:81:GLY:N	2.34	0.59
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.38	0.59
1:C:69:ASP:OD2	1:C:74:VAL:CG1	2.50	0.59
2:D:428:LEU:O	2:D:432:TYR:HB2	2.03	0.59
1:A:183:GLU:HB2	1:A:184:PRO:HD3	1.85	0.58
2:B:75:MET:O	2:B:76:ASP:O	2.21	0.58
2:B:385:GLN:OE1	2:B:429:VAL:HA	2.03	0.58
1:C:244:PHE:O	1:C:245:ASP:C	2.46	0.58
1:C:256:GLN:C	1:C:258:ASN:N	2.57	0.58
2:D:51:VAL:N	2:D:245:PRO:HB2	2.18	0.58
2:D:66:ILE:O	2:D:66:ILE:HG12	2.02	0.58
2:D:102:ASN:HB3	2:D:105:LYS:HD2	1.83	0.58
2:D:179:ASP:HB3	2:D:181:VAL:H	1.66	0.58
1:A:389:ALA:O	1:A:392:ASP:HB3	2.03	0.58
1:C:238:ILE:O	1:C:239:THR:C	2.47	0.58
1:C:286:LEU:O	1:C:373:ARG:HD2	2.02	0.58
2:D:19:LYS:HA	2:D:22:GLU:OE2	2.02	0.58
2:D:129:CYS:O	2:D:130:ASP:C	2.46	0.58
2:D:189:LEU:C	2:D:191:VAL:N	2.55	0.58
2:B:179:ASP:HB2	2:B:182:VAL:CG2	2.33	0.58
2:B:197:ASN:O	2:B:198:THR:HB	2.02	0.58
2:B:200:GLU:CG	2:B:268:PHE:CE2	2.86	0.58
2:B:274:PRO:HA	2:B:294:GLN:CD	2.28	0.58
1:C:23:LEU:C	1:C:25:CYS:H	2.11	0.58
1:C:217:LEU:HD23	1:C:219:ILE:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLN:O	1:C:258:ASN:N	2.36	0.58
2:D:2:ARG:HG3	2:D:133:GLN:CD	2.26	0.58
1:A:241:SER:HB3	1:A:242:LEU:HD12	1.85	0.58
1:A:419:SER:O	1:A:422:ARG:HG2	2.02	0.58
1:A:423:GLU:O	1:A:427:ALA:N	2.29	0.58
2:B:308:ARG:NH2	2:B:342:TYR:HB2	2.19	0.58
2:B:339:ASN:C	2:B:341:SER:N	2.60	0.58
2:D:9:ALA:HA	2:D:68:VAL:O	2.02	0.58
2:D:134:GLY:HA3	2:D:165:ILE:O	2.03	0.58
2:D:149:MET:HA	2:D:149:MET:CE	2.29	0.58
1:A:23:LEU:O	1:A:26:LEU:HD12	2.03	0.58
1:A:26:LEU:HG	1:A:361:THR:OG1	2.04	0.58
2:B:5:VAL:HA	2:B:64:ARG:CD	2.33	0.58
2:B:289:PRO:HB2	2:B:331:GLN:HE21	1.68	0.58
2:B:395:PHE:HD2	2:B:422:GLU:OE1	1.86	0.58
1:C:231:ILE:O	1:C:235:VAL:HG23	2.04	0.58
1:C:420:GLU:C	1:C:420:GLU:OE1	2.46	0.58
2:D:307:PRO:O	2:D:309:HIS:N	2.36	0.58
2:D:321:GLY:CA	2:D:359:PRO:HB3	2.32	0.58
2:D:408:TYR:CB	2:D:413:MET:HE3	2.32	0.58
3:E:66:UNK:O	3:E:69:UNK:N	2.37	0.58
1:A:186:ASN:O	1:A:189:LEU:HB3	2.03	0.58
2:B:51:VAL:C	2:B:53:TYR:N	2.61	0.58
2:B:413:MET:SD	2:B:417:GLU:HG2	2.43	0.58
1:C:39:ASP:CG	1:C:40:LYS:N	2.62	0.58
2:D:12:CYS:HB2	5:D:503:GDP:PA	2.43	0.58
1:A:38:SER:O	1:A:39:ASP:HB3	2.04	0.58
2:B:130:ASP:OD2	2:B:130:ASP:C	2.46	0.58
2:B:198:THR:O	2:B:200:GLU:N	2.37	0.58
1:C:160:ASP:O	1:C:161:TYR:CG	2.57	0.58
2:D:409:THR:HA	2:D:412:GLY:O	2.03	0.58
3:E:58:UNK:C	3:E:60:UNK:N	2.66	0.58
1:A:371:VAL:HG12	1:A:373:ARG:N	2.17	0.58
2:B:79:ARG:HA	2:B:84:GLY:CA	2.34	0.58
1:C:143:GLY:H	1:C:147:SER:CB	2.17	0.58
2:D:165:ILE:HG13	2:D:253:ARG:HG3	1.86	0.58
2:D:183:GLU:HB3	2:D:184:PRO:CD	2.34	0.58
1:A:164:LYS:HB2	1:A:164:LYS:NZ	2.19	0.58
1:A:402:ARG:HD2	2:B:346:TRP:CE3	2.38	0.58
2:B:282:GLN:HA	2:B:285:ALA:HB2	1.86	0.58
2:B:284:ARG:O	2:B:285:ALA:C	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD11	1:C:378:LEU:HD13	1.85	0.58
1:A:7:ILE:HD12	1:A:153:LEU:HD21	1.85	0.58
2:B:107:HIS:HA	2:B:152:LEU:HD22	1.86	0.58
1:C:103:TYR:HB2	1:C:185:TYR:CD1	2.38	0.58
1:C:333:ALA:O	1:C:334:THR:C	2.47	0.58
2:D:59:ASN:OD1	2:D:60:LYS:HD2	2.04	0.58
2:D:226:ASP:C	2:D:228:ASN:H	2.12	0.58
2:D:295:MET:HE3	2:D:377:PHE:CD2	2.39	0.58
1:A:132:LEU:O	1:A:133:GLN:HB2	2.04	0.57
2:B:102:ASN:ND2	2:B:105:LYS:N	2.52	0.57
2:B:258:ASN:OD1	2:B:352:LYS:NZ	2.34	0.57
2:B:276:THR:HB	2:B:281:GLN:OE1	2.03	0.57
2:B:386:GLU:O	2:B:388:PHE:N	2.34	0.57
1:C:215:ARG:NH2	1:C:216:ASN:OD1	2.37	0.57
1:C:336:LYS:HE2	1:C:336:LYS:HA	1.85	0.57
2:D:187:ALA:HB2	2:D:391:ILE:HG22	1.85	0.57
2:D:247:GLN:HG2	2:D:325:MET:SD	2.43	0.57
2:D:274:PRO:HA	2:D:294:GLN:CD	2.29	0.57
3:E:17:UNK:O	3:E:19:UNK:N	2.35	0.57
1:A:287:SER:C	1:A:289:ALA:N	2.60	0.57
2:B:114:LEU:O	2:B:117:SER:N	2.36	0.57
2:B:158:ARG:HA	2:B:197:ASN:ND2	2.19	0.57
2:B:335:VAL:HA	2:B:338:LYS:HB2	1.86	0.57
2:B:381:SER:C	2:B:383:ALA:H	2.11	0.57
1:C:317:LEU:HD23	1:C:377:MET:CB	2.34	0.57
2:D:140:SER:CB	2:D:171:VAL:HB	2.34	0.57
2:D:223:THR:C	2:D:225:GLY:N	2.60	0.57
2:D:289:PRO:HB2	2:D:331:GLN:HE21	1.69	0.57
1:A:9:VAL:HG23	1:A:9:VAL:O	2.03	0.57
1:A:258:ASN:N	1:A:258:ASN:ND2	2.43	0.57
1:A:363:VAL:H	1:A:367:ASP:HB2	1.69	0.57
2:B:167:ASN:HA	2:B:200:GLU:O	2.04	0.57
2:B:313:LEU:HA	2:B:344:VAL:CG1	2.32	0.57
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.86	0.57
1:C:183:GLU:HB2	1:C:184:PRO:HD3	1.85	0.57
1:C:285:GLN:C	1:C:286:LEU:HD23	2.29	0.57
1:C:363:VAL:HG13	1:C:367:ASP:OD2	2.05	0.57
2:D:123:ARG:CZ	2:D:160:GLU:OE2	2.53	0.57
2:D:282:GLN:C	2:D:285:ALA:H	2.12	0.57
1:A:46:ASP:OD2	1:A:46:ASP:N	2.37	0.57
1:A:93:ILE:HD13	1:A:118:VAL:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:HD2	1:A:340:THR:N	2.19	0.57
1:A:404:PHE:N	1:A:404:PHE:CD1	2.73	0.57
1:C:43:GLY:O	1:C:47:ASP:CG	2.47	0.57
1:C:77:GLU:O	1:C:83:TYR:CB	2.53	0.57
1:C:413:MET:H	1:C:413:MET:CE	2.15	0.57
2:D:7:ILE:HB	2:D:137:LEU:HA	1.86	0.57
2:D:276:THR:HB	2:D:281:GLN:OE1	2.04	0.57
3:E:35:UNK:O	3:E:38:UNK:N	2.36	0.57
1:A:236:SER:O	1:A:238:ILE:N	2.31	0.57
1:A:387:ALA:HA	1:A:390:ARG:CD	2.29	0.57
2:B:59:ASN:N	2:B:64:ARG:HE	2.01	0.57
2:B:59:ASN:OD1	2:B:60:LYS:HD2	2.05	0.57
2:B:132:LEU:HB3	2:B:164:ARG:CZ	2.34	0.57
2:B:296:PHE:HE1	2:B:332:MET:HE1	1.67	0.57
1:C:286:LEU:HB2	1:C:291:ILE:HG13	1.86	0.57
1:C:293:ASN:C	1:C:296:PHE:H	2.13	0.57
2:D:311:ARG:HG3	2:D:311:ARG:HH11	1.70	0.57
1:A:101:ASN:C	1:A:185:TYR:OH	2.46	0.57
1:A:212:ILE:C	1:A:214:ARG:H	2.13	0.57
1:A:229:ARG:HH11	1:A:229:ARG:HG3	1.69	0.57
1:A:311:LYS:HB2	1:A:344:VAL:HG22	1.87	0.57
1:A:333:ALA:O	1:A:334:THR:C	2.48	0.57
1:A:398:MET:HE3	1:A:399:TYR:HE1	1.69	0.57
1:A:404:PHE:N	1:A:404:PHE:HD1	2.01	0.57
2:B:223:THR:C	2:B:225:GLY:N	2.61	0.57
1:C:123:ARG:HA	1:C:161:TYR:OH	2.05	0.57
1:C:409:VAL:O	1:C:412:GLY:O	2.22	0.57
1:A:110:ILE:O	1:A:111:GLY:C	2.46	0.57
1:A:206:ASN:ND2	1:A:210:TYR:HE2	1.98	0.57
1:A:209:ILE:HD12	1:A:209:ILE:N	2.19	0.57
1:A:336:LYS:HE2	1:A:336:LYS:HA	1.86	0.57
2:B:409:THR:HG23	2:B:414:ASP:HA	1.86	0.57
1:C:82:THR:HG22	1:C:83:TYR:H	1.70	0.57
1:C:87:PHE:N	1:C:87:PHE:CD2	2.64	0.57
1:C:134:GLY:H	1:C:164:LYS:HG2	1.69	0.57
1:C:292:THR:HA	1:C:295:CYS:HB3	1.86	0.57
2:D:292:THR:HG23	2:D:319:PHE:HZ	1.70	0.57
2:D:305:CYS:O	2:D:306:ASP:C	2.47	0.57
1:A:371:VAL:HG12	1:A:372:GLN:H	1.69	0.57
2:B:223:THR:HG23	2:B:225:GLY:N	2.20	0.57
2:B:395:PHE:HE2	2:B:418:PHE:O	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASN:HD22	1:C:101:ASN:C	2.13	0.57
1:C:101:ASN:O	1:C:185:TYR:OH	2.22	0.57
1:C:102:ASN:ND2	2:D:257:VAL:HG11	2.12	0.57
1:C:142:GLY:O	1:C:182:VAL:HG23	2.04	0.57
2:D:80:SER:OG	2:D:81:GLY:N	2.36	0.57
2:D:206:ASN:HD22	2:D:227:LEU:CD2	2.09	0.57
2:D:215:ARG:HA	2:D:215:ARG:CZ	2.35	0.57
1:A:155:GLU:O	1:A:159:VAL:HG23	2.04	0.57
1:A:291:ILE:CD1	1:A:373:ARG:HG3	2.34	0.57
1:A:386:GLU:CG	1:A:387:ALA:H	2.13	0.57
1:A:401:LYS:O	1:A:402:ARG:CB	2.53	0.57
2:B:114:LEU:O	2:B:115:VAL:C	2.46	0.57
2:B:311:ARG:HH21	2:B:437:ASP:CB	1.97	0.57
1:C:35:GLN:OE1	1:C:88:HIS:NE2	2.38	0.57
1:C:78:VAL:HG11	1:C:87:PHE:HE2	1.69	0.57
1:C:111:GLY:O	1:C:113:GLU:N	2.37	0.57
1:C:220:GLU:HB3	1:C:221:ARG:NE	2.20	0.57
2:D:282:GLN:O	2:D:284:ARG:N	2.38	0.57
2:D:391:ILE:O	2:D:391:ILE:HG22	2.05	0.57
2:D:416:MET:O	2:D:417:GLU:HB3	2.04	0.57
1:A:139:HIS:HB3	1:A:170:SER:HA	1.87	0.57
1:A:267:PHE:HD1	1:A:267:PHE:H	1.53	0.57
1:A:284:GLU:O	1:A:285:GLN:HG3	2.05	0.57
1:A:417:GLU:HB3	1:A:418:PHE:HD2	1.68	0.57
2:B:9:ALA:HA	2:B:68:VAL:O	2.04	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.39	0.57
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.86	0.57
2:B:149:MET:HA	2:B:149:MET:CE	2.34	0.57
2:B:163:ASP:OD1	2:B:164:ARG:HG2	2.05	0.57
2:B:287:THR:C	2:B:289:PRO:HD2	2.29	0.57
1:C:143:GLY:H	1:C:147:SER:HB2	1.70	0.57
2:D:198:THR:O	2:D:200:GLU:N	2.37	0.57
2:D:371:LEU:C	2:D:373:MET:H	2.10	0.57
2:D:417:GLU:HG3	2:D:417:GLU:O	2.04	0.57
1:A:264:ARG:NH2	1:A:424:ASP:OD1	2.38	0.56
2:B:103:TRP:O	2:B:104:ALA:C	2.48	0.56
2:B:350:ASN:ND2	2:B:351:VAL:HG23	2.19	0.56
1:C:108:TYR:CG	1:C:413:MET:HE3	2.39	0.56
1:C:193:THR:HG23	1:C:193:THR:O	2.05	0.56
1:C:293:ASN:O	1:C:297:GLU:OE1	2.23	0.56
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:OD2	1:A:74:VAL:CG1	2.52	0.56
1:A:209:ILE:O	1:A:211:ASP:N	2.38	0.56
2:B:139:HIS:HD2	2:B:139:HIS:O	1.88	0.56
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.41	0.56
1:C:101:ASN:C	1:C:185:TYR:OH	2.47	0.56
1:C:137:VAL:HG21	1:C:154:MET:SD	2.45	0.56
2:D:333:LEU:O	2:D:337:ASN:N	2.38	0.56
1:A:7:ILE:CG1	1:A:137:VAL:HG22	2.35	0.56
1:A:256:GLN:C	1:A:258:ASN:N	2.58	0.56
1:A:401:LYS:O	1:A:402:ARG:HB3	2.05	0.56
1:A:414:GLU:CD	1:A:414:GLU:N	2.64	0.56
2:B:120:ASP:O	2:B:124:LYS:HE3	2.06	0.56
2:B:200:GLU:CG	2:B:268:PHE:HE2	2.19	0.56
2:B:400:ARG:C	2:B:402:LYS:H	2.13	0.56
2:B:416:MET:O	2:B:417:GLU:HB3	2.06	0.56
1:C:23:LEU:O	1:C:26:LEU:HD12	2.06	0.56
1:C:247:ALA:O	1:C:249:ASN:CG	2.48	0.56
1:C:257:THR:OG1	1:C:258:ASN:ND2	2.39	0.56
1:C:398:MET:C	1:C:400:ALA:H	2.13	0.56
1:C:399:TYR:HH	1:C:408:TYR:HE2	1.52	0.56
2:D:69:ASP:CB	2:D:74:THR:HG23	2.35	0.56
2:D:130:ASP:OD2	2:D:131:CYS:N	2.38	0.56
2:D:133:GLN:OE1	2:D:133:GLN:HA	2.05	0.56
2:D:198:THR:C	2:D:200:GLU:N	2.59	0.56
2:D:218:LYS:O	2:D:219:LEU:HB2	2.04	0.56
2:D:263:PRO:HG2	2:D:264:ARG:H	1.71	0.56
1:A:188:ILE:HG22	1:A:417:GLU:O	2.04	0.56
1:A:285:GLN:C	1:A:286:LEU:HD23	2.31	0.56
2:B:2:ARG:NH2	2:B:243:ARG:HA	2.20	0.56
2:B:103:TRP:O	2:B:105:LYS:O	2.23	0.56
2:B:249:ASN:CG	2:B:250:ALA:N	2.62	0.56
2:B:405:LEU:HD22	2:B:405:LEU:C	2.30	0.56
2:D:194:LEU:CD1	2:D:428:LEU:HD21	2.35	0.56
2:D:223:THR:N	2:D:226:ASP:OD2	2.33	0.56
2:D:385:GLN:NE2	2:D:433:GLN:HE21	2.01	0.56
2:D:419:THR:O	2:D:423:SER:N	2.39	0.56
3:E:10:UNK:HA	3:E:13:UNK:CB	2.36	0.56
1:A:286:LEU:HB2	1:A:291:ILE:HG13	1.88	0.56
1:A:402:ARG:CG	1:A:403:ALA:N	2.68	0.56
2:B:198:THR:C	2:B:200:GLU:N	2.62	0.56
2:B:307:PRO:O	2:B:309:HIS:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:TYR:CD2	2:B:381:SER:HB2	2.40	0.56
1:C:282:TYR:N	1:C:282:TYR:HD2	2.00	0.56
1:C:423:GLU:O	1:C:426:ALA:HB3	2.04	0.56
2:D:98:GLY:N	2:D:110:GLU:OE1	2.38	0.56
2:D:133:GLN:HE21	2:D:252:LEU:CB	2.18	0.56
3:E:46:UNK:C	3:E:48:UNK:N	2.62	0.56
1:A:209:ILE:HG12	1:A:231:ILE:HD11	1.88	0.56
1:A:329:ASN:HA	1:A:332:ILE:HB	1.87	0.56
2:B:141:LEU:HB3	2:B:186:ASN:CB	2.30	0.56
2:B:183:GLU:O	2:B:185:TYR:N	2.38	0.56
2:B:241:CYS:O	2:B:242:LEU:C	2.49	0.56
1:C:389:ALA:O	1:C:392:ASP:HB3	2.06	0.56
1:C:398:MET:O	1:C:400:ALA:N	2.38	0.56
2:D:151:THR:HG21	2:D:189:LEU:CD2	2.36	0.56
3:E:57:UNK:O	3:E:58:UNK:C	2.53	0.56
1:A:86:LEU:CD1	1:A:89:PRO:HD3	2.35	0.56
1:A:184:PRO:HG3	1:A:399:TYR:CE1	2.41	0.56
1:A:293:ASN:C	1:A:296:PHE:H	2.14	0.56
1:A:311:LYS:CD	1:A:344:VAL:HG22	2.36	0.56
2:B:371:LEU:C	2:B:373:MET:H	2.14	0.56
1:C:115:ILE:O	1:C:119:LEU:HB2	2.05	0.56
1:C:174:ALA:O	1:C:176:GLN:N	2.39	0.56
1:C:185:TYR:CE1	1:C:408:TYR:HE1	2.22	0.56
1:C:288:VAL:HA	1:C:373:ARG:HD3	1.86	0.56
1:C:399:TYR:OH	1:C:408:TYR:HE2	1.89	0.56
1:C:401:LYS:O	1:C:402:ARG:CB	2.53	0.56
2:D:158:ARG:CZ	2:D:197:ASN:HA	2.36	0.56
1:A:213:CYS:SG	1:A:217:LEU:HD23	2.46	0.56
1:A:316:CYS:O	1:A:316:CYS:SG	2.64	0.56
2:B:97:SER:HG	2:B:110:GLU:CD	2.13	0.56
1:C:69:ASP:HB3	1:C:75:ILE:CG2	2.35	0.56
1:C:387:ALA:HA	1:C:390:ARG:CD	2.30	0.56
2:D:133:GLN:HG3	2:D:252:LEU:HD22	1.87	0.56
2:D:372:LYS:O	2:D:373:MET:HG3	2.06	0.56
1:A:102:ASN:HD21	2:B:257:VAL:CG1	2.12	0.56
1:A:151:SER:HB3	1:A:192:HIS:NE2	2.20	0.56
1:A:189:LEU:CD1	1:A:193:THR:HG21	2.35	0.56
1:A:243:ARG:NH1	1:A:250:VAL:HG13	2.16	0.56
1:A:296:PHE:CD2	1:A:377:MET:HE1	2.41	0.56
1:A:385:ALA:HB2	1:A:432:TYR:CD2	2.39	0.56
2:B:151:THR:HG21	2:B:189:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:HD21	2:D:257:VAL:CG1	2.14	0.56
1:C:108:TYR:CD1	1:C:413:MET:HE3	2.41	0.56
1:C:182:VAL:CG1	1:C:183:GLU:N	2.68	0.56
1:C:258:ASN:O	1:C:259:LEU:CB	2.54	0.56
1:C:289:ALA:HA	1:C:292:THR:HG22	1.87	0.56
2:D:51:VAL:N	2:D:245:PRO:HG2	2.21	0.56
2:D:88:ARG:HH11	2:D:88:ARG:HA	1.70	0.56
2:D:273:ALA:O	2:D:275:LEU:N	2.37	0.56
2:D:292:THR:HG23	2:D:319:PHE:CZ	2.41	0.56
2:D:389:LYS:C	2:D:392:SER:HG	2.13	0.56
1:A:69:ASP:OD2	1:A:74:VAL:HG12	2.05	0.56
1:A:143:GLY:H	1:A:147:SER:CB	2.19	0.56
1:A:362:VAL:CG1	1:A:367:ASP:HB2	2.29	0.56
1:C:36:MET:HA	1:C:36:MET:CE	2.34	0.56
2:D:59:ASN:CB	2:D:64:ARG:HB2	2.35	0.56
2:D:132:LEU:HD23	2:D:132:LEU:O	2.05	0.56
2:D:165:ILE:HG13	2:D:253:ARG:CG	2.36	0.56
2:D:320:ARG:N	2:D:374:SER:O	2.33	0.56
1:A:16:ILE:O	1:A:19:ALA:N	2.30	0.55
1:A:16:ILE:O	1:A:17:GLY:C	2.49	0.55
1:A:26:LEU:HD12	1:A:26:LEU:H	1.71	0.55
1:A:78:VAL:O	1:A:82:THR:HA	2.05	0.55
1:A:101:ASN:C	1:A:101:ASN:HD22	2.14	0.55
1:A:112:LYS:NZ	3:E:12:UNK:CB	2.69	0.55
1:A:393:HIS:O	1:A:397:LEU:HB2	2.06	0.55
1:A:404:PHE:HD1	1:A:404:PHE:H	1.54	0.55
2:B:3:GLU:OE2	2:B:128:SER:O	2.24	0.55
2:B:241:CYS:O	2:B:243:ARG:N	2.39	0.55
1:C:140:SER:HB3	1:C:171:ILE:HD13	1.86	0.55
1:C:229:ARG:HH11	1:C:229:ARG:HG3	1.72	0.55
1:C:413:MET:SD	3:E:66:UNK:C	2.94	0.55
2:D:149:MET:O	2:D:152:LEU:HB3	2.06	0.55
2:D:192:HIS:CA	2:D:195:VAL:HG22	2.23	0.55
1:A:234:ILE:CD1	1:A:302:MET:SD	2.94	0.55
1:A:238:ILE:O	1:A:239:THR:C	2.48	0.55
2:B:59:ASN:ND2	2:B:60:LYS:N	2.54	0.55
2:B:132:LEU:HD22	2:B:164:ARG:NE	2.22	0.55
1:C:166:LYS:HE3	1:C:198:SER:N	2.12	0.55
1:C:238:ILE:N	1:C:241:SER:HB3	2.21	0.55
1:C:247:ALA:O	1:C:249:ASN:ND2	2.39	0.55
2:D:12:CYS:HB3	5:D:503:GDP:N7	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:VAL:C	2:D:53:TYR:N	2.64	0.55
2:D:59:ASN:HB3	2:D:64:ARG:HB2	1.87	0.55
2:D:69:ASP:HB2	2:D:74:THR:HG23	1.87	0.55
2:D:93:VAL:HG23	2:D:94:PHE:N	2.21	0.55
2:D:158:ARG:O	2:D:159:GLU:C	2.49	0.55
2:D:241:CYS:O	2:D:242:LEU:C	2.50	0.55
1:A:12:ALA:HB3	1:A:140:SER:CB	2.36	0.55
1:A:247:ALA:O	1:A:249:ASN:CG	2.49	0.55
2:B:97:SER:OG	2:B:98:GLY:N	2.39	0.55
1:C:88:HIS:N	1:C:91:GLN:OE1	2.39	0.55
1:C:142:GLY:O	1:C:182:VAL:CG2	2.55	0.55
2:D:159:GLU:CD	3:E:82:UNK:CB	2.80	0.55
2:D:212:ILE:C	2:D:214:PHE:H	2.13	0.55
1:A:143:GLY:H	1:A:147:SER:HB2	1.71	0.55
1:A:154:MET:CE	1:A:197:HIS:NE2	2.70	0.55
1:A:273:ALA:HB2	1:A:295:CYS:HA	1.89	0.55
2:B:99:ALA:HA	2:B:105:LYS:HD3	1.89	0.55
2:B:169:PHE:CG	2:B:235:MET:SD	2.99	0.55
2:B:272:PHE:HD1	2:B:275:LEU:HD23	1.71	0.55
1:C:186:ASN:O	1:C:189:LEU:HB3	2.06	0.55
1:C:284:GLU:O	1:C:285:GLN:HG3	2.06	0.55
2:D:102:ASN:HD21	2:D:104:ALA:HB3	1.71	0.55
2:D:395:PHE:HE2	2:D:418:PHE:O	1.90	0.55
3:E:31:UNK:O	3:E:32:UNK:C	2.51	0.55
1:A:36:MET:HE2	1:A:38:SER:OG	2.07	0.55
1:A:75:ILE:O	1:A:75:ILE:CG1	2.54	0.55
2:B:162:PRO:O	2:B:163:ASP:C	2.47	0.55
2:B:192:HIS:C	2:B:194:LEU:N	2.49	0.55
1:C:2:ARG:HH22	1:C:133:GLN:HE22	1.54	0.55
1:C:100:ALA:CA	1:C:105:ARG:HD2	2.36	0.55
1:C:381:THR:C	1:C:383:ALA:H	2.14	0.55
1:C:401:LYS:O	1:C:402:ARG:HB3	2.05	0.55
2:D:274:PRO:HG3	2:D:374:SER:CB	2.37	0.55
1:A:103:TYR:H	1:A:185:TYR:HE1	1.54	0.55
1:A:187:SER:C	1:A:189:LEU:H	2.15	0.55
1:A:258:ASN:ND2	1:A:258:ASN:H	2.03	0.55
1:A:409:VAL:O	1:A:412:GLY:O	2.25	0.55
2:B:51:VAL:HG22	2:B:245:PRO:CG	2.36	0.55
1:C:96:LYS:O	1:C:98:ASP:N	2.39	0.55
1:C:171:ILE:H	1:C:171:ILE:CD1	2.20	0.55
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:338:LYS:O	2:D:340:SER:N	2.34	0.55
2:D:357:ASP:HB3	2:D:358:ILE:HD12	1.88	0.55
2:D:398:MET:C	2:D:400:ARG:N	2.65	0.55
1:A:139:HIS:CG	1:A:140:SER:H	2.23	0.55
2:B:158:ARG:CB	2:B:197:ASN:HD22	2.19	0.55
2:B:191:VAL:HG22	2:B:421:ALA:O	2.07	0.55
1:C:222:PRO:CB	1:C:227:LEU:HD11	2.20	0.55
1:C:417:GLU:HB3	1:C:418:PHE:HD2	1.67	0.55
2:D:11:GLN:C	2:D:13:GLY:H	2.15	0.55
2:D:59:ASN:N	2:D:64:ARG:HE	2.04	0.55
2:B:127:GLU:O	2:B:128:SER:C	2.50	0.55
2:B:212:ILE:C	2:B:214:PHE:H	2.13	0.55
2:B:320:ARG:HB2	2:B:374:SER:OG	2.07	0.55
2:B:345:GLU:O	2:B:345:GLU:CG	2.55	0.55
1:C:72:PRO:HG3	1:C:96:LYS:HA	1.89	0.55
1:C:427:ALA:HA	1:C:430:LYS:HB2	1.88	0.55
2:D:120:ASP:O	2:D:124:LYS:HE3	2.06	0.55
1:A:107:HIS:CE1	1:A:151:SER:HB2	2.41	0.55
1:A:197:HIS:NE2	1:A:198:SER:HB3	2.22	0.55
2:B:10:GLY:CA	2:B:146:GLY:HA3	2.37	0.55
2:B:133:GLN:HG3	2:B:252:LEU:HD22	1.88	0.55
2:B:180:THR:HB	2:B:404:PHE:CE1	2.42	0.55
2:B:194:LEU:CD1	2:B:428:LEU:HD21	2.37	0.55
2:B:227:LEU:HD23	2:B:227:LEU:O	2.06	0.55
2:B:264:ARG:NH2	2:B:431:GLU:HG3	2.20	0.55
1:C:217:LEU:O	1:C:217:LEU:HG	2.06	0.55
1:C:286:LEU:HD12	1:C:291:ILE:HG12	1.89	0.55
1:C:407:TRP:C	1:C:409:VAL:N	2.65	0.55
2:D:230:LEU:H	2:D:230:LEU:CD1	2.19	0.55
2:D:277:SER:O	2:D:278:ARG:O	2.25	0.55
1:A:259:LEU:HD21	1:A:378:LEU:CB	2.37	0.55
1:A:331:ALA:HA	1:A:334:THR:OG1	2.07	0.55
1:A:398:MET:C	1:A:400:ALA:H	2.14	0.55
1:A:413:MET:C	1:A:414:GLU:OE1	2.49	0.55
2:B:12:CYS:HB2	5:B:501:GDP:O1A	2.07	0.55
2:B:132:LEU:HD11	2:B:135:PHE:CZ	2.42	0.55
2:B:226:ASP:O	2:B:228:ASN:N	2.37	0.55
2:B:284:ARG:O	2:B:287:THR:N	2.40	0.55
1:C:425:MET:HE3	1:C:425:MET:O	2.06	0.55
2:D:242:LEU:O	2:D:243:ARG:HD3	2.07	0.55
2:D:395:PHE:HB3	2:D:422:GLU:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:O	1:A:195:LEU:C	2.49	0.54
2:B:223:THR:HG23	2:B:225:GLY:CA	2.36	0.54
2:B:263:PRO:HG2	2:B:264:ARG:H	1.72	0.54
1:C:11:GLN:NE2	4:C:502:GTP:O2A	2.40	0.54
1:C:103:TYR:O	1:C:104:ALA:C	2.47	0.54
1:C:119:LEU:HD22	1:C:156:ARG:NE	2.21	0.54
1:C:236:SER:O	1:C:238:ILE:N	2.34	0.54
1:C:318:LEU:HB2	1:C:376:CYS:O	2.07	0.54
2:D:107:HIS:HA	2:D:152:LEU:HD22	1.88	0.54
2:D:133:GLN:HE22	2:D:252:LEU:H	1.54	0.54
2:D:200:GLU:CG	2:D:268:PHE:CE2	2.90	0.54
2:D:243:ARG:HH12	2:D:252:LEU:HD12	1.72	0.54
2:D:306:ASP:HB3	2:D:309:HIS:CD2	2.42	0.54
2:D:395:PHE:HD2	2:D:422:GLU:OE1	1.89	0.54
1:A:317:LEU:HD23	1:A:377:MET:HB3	1.88	0.54
1:A:386:GLU:C	1:A:388:TRP:N	2.66	0.54
1:A:399:TYR:OH	1:A:408:TYR:HE2	1.90	0.54
2:B:218:LYS:O	2:B:219:LEU:CB	2.55	0.54
1:C:71:GLU:O	1:C:73:THR:N	2.40	0.54
1:C:77:GLU:C	1:C:83:TYR:HB2	2.32	0.54
1:C:100:ALA:HA	1:C:105:ARG:HD2	1.89	0.54
1:C:175:PRO:HD2	1:C:207:GLU:CB	2.11	0.54
1:C:194:THR:O	1:C:195:LEU:C	2.50	0.54
2:D:288:VAL:N	2:D:289:PRO:CD	2.70	0.54
2:D:297:ASP:OD1	2:D:298:ALA:N	2.40	0.54
2:D:339:ASN:C	2:D:341:SER:N	2.58	0.54
1:A:427:ALA:HA	1:A:430:LYS:HB2	1.89	0.54
2:B:154:ILE:C	2:B:156:LYS:H	2.15	0.54
2:B:218:LYS:HZ2	2:B:277:SER:HB3	1.72	0.54
2:B:377:PHE:O	2:B:378:ILE:HG12	2.07	0.54
2:B:400:ARG:C	2:B:402:LYS:N	2.62	0.54
1:C:189:LEU:CD1	1:C:193:THR:HG21	2.37	0.54
1:C:316:CYS:O	1:C:316:CYS:SG	2.65	0.54
1:C:344:VAL:CG1	1:C:346:TRP:NE1	2.69	0.54
2:D:22:GLU:OE2	2:D:22:GLU:N	2.41	0.54
2:D:100:GLY:C	2:D:101:ASN:HD22	2.15	0.54
2:D:168:THR:OG1	2:D:201:THR:CB	2.54	0.54
2:D:428:LEU:HD12	2:D:428:LEU:H	1.73	0.54
1:A:137:VAL:O	1:A:168:GLU:HA	2.07	0.54
1:A:331:ALA:C	1:A:333:ALA:H	2.16	0.54
2:B:59:ASN:CB	2:B:64:ARG:HB2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:LYS:N	2:B:60:LYS:HZ2	2.04	0.54
2:B:158:ARG:C	2:B:160:GLU:N	2.64	0.54
2:B:394:GLN:O	2:B:398:MET:CB	2.56	0.54
1:C:209:ILE:H	1:C:209:ILE:CD1	2.20	0.54
1:C:350:GLY:C	1:C:351:PHE:CD1	2.80	0.54
2:D:59:ASN:HA	2:D:60:LYS:HZ3	1.71	0.54
2:D:102:ASN:HD22	2:D:105:LYS:N	2.05	0.54
2:D:114:LEU:O	2:D:117:SER:N	2.40	0.54
2:D:132:LEU:HD11	2:D:135:PHE:CE2	2.41	0.54
2:D:189:LEU:O	2:D:191:VAL:N	2.38	0.54
2:D:303:ALA:O	2:D:387:LEU:HD12	2.08	0.54
1:A:190:THR:HG21	1:A:425:MET:SD	2.47	0.54
1:A:381:THR:C	1:A:383:ALA:H	2.15	0.54
2:B:215:ARG:HA	2:B:215:ARG:CZ	2.37	0.54
2:B:378:ILE:O	2:B:378:ILE:HG22	2.06	0.54
2:B:428:LEU:CD1	2:B:428:LEU:H	2.20	0.54
2:B:437:ASP:OD2	2:B:437:ASP:N	2.39	0.54
1:C:314:ALA:O	1:C:315:CYS:CB	2.56	0.54
1:C:419:SER:O	1:C:422:ARG:N	2.41	0.54
2:D:2:ARG:NH1	2:D:251:ASP:HA	2.23	0.54
2:D:114:LEU:O	2:D:115:VAL:C	2.49	0.54
2:D:192:HIS:O	2:D:194:LEU:N	2.36	0.54
2:D:344:VAL:HG23	2:D:345:GLU:N	2.21	0.54
1:A:389:ALA:CB	1:A:429:GLU:OE2	2.55	0.54
1:C:12:ALA:HB3	1:C:140:SER:OG	2.07	0.54
1:C:26:LEU:HD12	1:C:26:LEU:H	1.73	0.54
1:C:134:GLY:H	1:C:164:LYS:HG3	1.72	0.54
1:C:169:PHE:HE1	1:C:238:ILE:HD12	1.73	0.54
1:C:184:PRO:HG3	1:C:399:TYR:CE1	2.43	0.54
1:C:287:SER:C	1:C:289:ALA:N	2.59	0.54
2:D:5:VAL:O	2:D:5:VAL:HG12	2.06	0.54
2:D:409:THR:HG23	2:D:414:ASP:HA	1.89	0.54
3:E:71:UNK:C	3:E:73:UNK:N	2.70	0.54
1:A:273:ALA:HB2	1:A:295:CYS:CA	2.38	0.54
2:B:98:GLY:N	2:B:110:GLU:OE1	2.40	0.54
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.89	0.54
1:C:9:VAL:HG21	1:C:150:THR:CG2	2.38	0.54
1:C:393:HIS:C	1:C:395:PHE:N	2.65	0.54
1:C:413:MET:C	1:C:414:GLU:CD	2.76	0.54
2:D:132:LEU:HD11	2:D:135:PHE:CZ	2.42	0.54
2:D:148:GLY:HA2	2:D:151:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD13	1:A:118:VAL:CG2	2.29	0.54
1:A:123:ARG:HG2	1:A:161:TYR:OH	2.08	0.54
1:A:242:LEU:HG	1:A:318:LEU:HD11	1.89	0.54
2:B:18:ALA:C	2:B:20:PHE:N	2.66	0.54
2:B:187:ALA:HB2	2:B:391:ILE:HG22	1.88	0.54
1:C:5:ILE:O	1:C:135:PHE:HA	2.07	0.54
1:C:78:VAL:HG11	1:C:87:PHE:CE2	2.42	0.54
1:C:177:VAL:HG11	2:D:349:ASN:HB3	1.90	0.54
1:C:322:ASP:N	1:C:357:TYR:O	2.38	0.54
1:C:416:GLY:C	1:C:418:PHE:N	2.55	0.54
2:D:385:GLN:OE1	2:D:429:VAL:HA	2.08	0.54
1:A:103:TYR:HB2	1:A:185:TYR:HD1	1.72	0.54
1:A:322:ASP:N	1:A:357:TYR:O	2.38	0.54
2:B:60:LYS:H	2:B:60:LYS:NZ	2.06	0.54
2:B:69:ASP:HB2	2:B:74:THR:HG23	1.90	0.54
1:C:139:HIS:CG	1:C:140:SER:H	2.26	0.54
1:C:256:GLN:HA	1:C:260:VAL:HG23	1.88	0.54
2:D:102:ASN:ND2	2:D:105:LYS:N	2.55	0.54
1:A:169:PHE:HE1	1:A:238:ILE:HD12	1.73	0.54
2:B:179:ASP:HB3	2:B:181:VAL:CG1	2.37	0.54
2:B:288:VAL:N	2:B:289:PRO:CD	2.71	0.54
2:B:331:GLN:HA	2:B:331:GLN:OE1	2.08	0.54
1:C:241:SER:HB3	1:C:242:LEU:HD12	1.90	0.54
1:C:283:HIS:C	1:C:285:GLN:H	2.16	0.54
1:C:417:GLU:C	1:C:418:PHE:HD2	2.15	0.54
1:A:35:GLN:OE1	1:A:88:HIS:NE2	2.41	0.53
1:A:182:VAL:HG12	1:A:183:GLU:N	2.23	0.53
1:A:190:THR:CG2	1:A:425:MET:HG2	2.38	0.53
2:B:344:VAL:CG2	2:B:345:GLU:N	2.71	0.53
1:C:186:ASN:ND2	1:C:391:LEU:HD21	2.23	0.53
2:D:191:VAL:O	2:D:191:VAL:CG1	2.55	0.53
2:D:223:THR:O	2:D:226:ASP:N	2.39	0.53
2:B:158:ARG:O	2:B:159:GLU:C	2.51	0.53
1:C:86:LEU:CD1	1:C:89:PRO:HD3	2.38	0.53
1:C:92:LEU:N	1:C:92:LEU:CD1	2.71	0.53
1:C:242:LEU:HB3	1:C:250:VAL:CG1	2.38	0.53
1:C:395:PHE:C	1:C:397:LEU:N	2.61	0.53
2:D:398:MET:SD	2:D:399:PHE:CD2	3.01	0.53
1:A:16:ILE:CG2	1:A:17:GLY:N	2.59	0.53
1:A:20:CYS:C	1:A:22:GLU:H	2.16	0.53
1:A:87:PHE:H	1:A:87:PHE:HD2	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:C	1:A:176:GLN:N	2.65	0.53
1:A:193:THR:HG23	1:A:193:THR:O	2.07	0.53
1:A:405:VAL:O	1:A:409:VAL:HG23	2.08	0.53
2:B:189:LEU:O	2:B:191:VAL:N	2.39	0.53
1:C:185:TYR:O	1:C:186:ASN:C	2.51	0.53
1:C:214:ARG:CA	1:C:218:ASP:O	2.53	0.53
1:C:242:LEU:HG	1:C:318:LEU:HD11	1.89	0.53
2:D:174:SER:C	2:D:176:LYS:H	2.16	0.53
2:D:308:ARG:NH2	2:D:342:TYR:CG	2.76	0.53
2:D:400:ARG:C	2:D:402:LYS:N	2.63	0.53
1:A:183:GLU:OE2	2:B:348:PRO:HB2	2.09	0.53
1:A:408:TYR:O	1:A:414:GLU:HG3	2.08	0.53
2:B:174:SER:OG	2:B:207:GLU:HA	2.09	0.53
2:B:204:ILE:HG21	2:B:209:LEU:HD11	1.89	0.53
2:B:371:LEU:O	2:B:372:LYS:HB2	2.08	0.53
2:B:388:PHE:C	2:B:390:ARG:H	2.14	0.53
1:C:24:TYR:HA	1:C:26:LEU:HD12	1.91	0.53
2:D:17:GLY:O	2:D:20:PHE:HB3	2.07	0.53
2:D:51:VAL:HG22	2:D:245:PRO:CG	2.38	0.53
2:D:102:ASN:HD22	2:D:105:LYS:CB	2.20	0.53
2:D:154:ILE:C	2:D:156:LYS:N	2.65	0.53
2:D:283:TYR:O	2:D:290:GLU:OE1	2.25	0.53
2:D:283:TYR:C	2:D:285:ALA:H	2.15	0.53
2:D:315:VAL:HG23	2:D:351:VAL:HG22	1.90	0.53
2:D:386:GLU:C	2:D:388:PHE:N	2.66	0.53
1:A:82:THR:O	1:A:83:TYR:HB2	2.09	0.53
1:A:220:GLU:HB3	1:A:221:ARG:NE	2.23	0.53
1:A:273:ALA:HB2	1:A:295:CYS:HB2	1.91	0.53
1:A:275:VAL:HG12	1:A:275:VAL:O	2.09	0.53
1:A:395:PHE:C	1:A:397:LEU:N	2.63	0.53
2:B:297:ASP:OD1	2:B:298:ALA:N	2.42	0.53
1:C:20:CYS:C	1:C:22:GLU:N	2.66	0.53
1:C:82:THR:O	1:C:83:TYR:HB2	2.07	0.53
2:D:206:ASN:HD21	5:D:503:GDP:N2	2.06	0.53
1:A:20:CYS:C	1:A:22:GLU:N	2.63	0.53
1:A:65:ALA:O	1:A:91:GLN:HB2	2.08	0.53
1:A:92:LEU:N	1:A:92:LEU:CD1	2.70	0.53
1:A:305:CYS:SG	1:A:384:ILE:HA	2.49	0.53
1:A:331:ALA:O	1:A:335:ILE:HG23	2.08	0.53
2:B:185:TYR:O	2:B:188:THR:HG22	2.08	0.53
2:B:387:LEU:O	2:B:387:LEU:CD2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LEU:HD23	1:C:219:ILE:HD12	1.89	0.53
1:C:238:ILE:O	1:C:242:LEU:HD12	2.09	0.53
2:D:179:ASP:HB2	2:D:182:VAL:CG2	2.38	0.53
1:A:271:THR:HG23	1:A:300:ASN:O	2.08	0.53
1:A:283:HIS:C	1:A:285:GLN:H	2.16	0.53
2:B:88:ARG:CB	2:B:89:PRO:HD3	2.32	0.53
2:B:209:LEU:HD21	2:B:302:MET:HG3	1.89	0.53
2:B:223:THR:O	2:B:226:ASP:N	2.41	0.53
2:B:274:PRO:HG3	2:B:374:SER:CB	2.38	0.53
2:B:358:ILE:H	2:B:358:ILE:CD1	2.18	0.53
1:C:181:VAL:HG22	1:C:408:TYR:OH	2.09	0.53
1:C:184:PRO:HA	1:C:395:PHE:HD2	1.74	0.53
2:D:223:THR:HG23	2:D:225:GLY:CA	2.39	0.53
2:D:241:CYS:O	2:D:243:ARG:N	2.42	0.53
2:B:59:ASN:HA	2:B:60:LYS:HZ3	1.73	0.53
2:B:181:VAL:C	2:B:184:PRO:HD2	2.34	0.53
1:C:339:ARG:HD2	1:C:340:THR:N	2.24	0.53
2:D:79:ARG:HA	2:D:84:GLY:HA2	1.90	0.53
2:D:103:TRP:O	2:D:104:ALA:C	2.52	0.53
2:D:322:ARG:HG2	2:D:357:ASP:CA	2.30	0.53
2:D:345:GLU:O	2:D:345:GLU:CG	2.57	0.53
1:A:216:ASN:HB3	1:A:275:VAL:CG1	2.39	0.53
2:B:6:HIS:O	2:B:66:ILE:HG22	2.09	0.53
2:B:62:VAL:O	2:B:63:PRO:C	2.51	0.53
1:C:206:ASN:O	1:C:210:TYR:HD2	1.92	0.53
2:D:166:MET:HE3	2:D:197:ASN:HB3	1.91	0.53
2:D:190:SER:CB	2:D:425:MET:HG3	2.28	0.53
2:D:200:GLU:CG	2:D:268:PHE:HE2	2.22	0.53
2:D:392:SER:HB2	2:D:426:ASN:ND2	2.24	0.53
1:A:23:LEU:C	1:A:25:CYS:N	2.67	0.53
1:A:286:LEU:O	1:A:287:SER:C	2.50	0.53
1:A:341:ILE:HG22	1:A:342:GLN:N	2.23	0.53
1:A:426:ALA:C	1:A:428:LEU:H	2.17	0.53
2:B:111:GLY:O	2:B:114:LEU:N	2.42	0.53
2:B:191:VAL:CG2	2:B:421:ALA:HB1	2.25	0.53
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.44	0.53
2:B:311:ARG:HG3	2:B:311:ARG:NH1	2.23	0.53
2:B:385:GLN:HE21	2:B:433:GLN:HG2	1.72	0.53
2:B:386:GLU:C	2:B:388:PHE:N	2.66	0.53
2:B:402:LYS:NZ	1:C:440:VAL:O	2.42	0.53
2:B:403:ALA:HB1	2:B:405:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLY:C	1:C:46:ASP:N	2.61	0.53
2:D:194:LEU:HD12	2:D:428:LEU:HD21	1.91	0.53
2:D:206:ASN:ND2	5:D:503:GDP:N3	2.54	0.53
1:A:101:ASN:CG	2:B:254:LYS:HD3	2.34	0.52
2:B:51:VAL:CG2	2:B:53:TYR:HB2	2.39	0.52
2:B:88:ARG:HH11	2:B:88:ARG:HA	1.73	0.52
2:B:139:HIS:C	2:B:139:HIS:HD2	2.17	0.52
1:C:15:GLN:HE22	1:C:224:TYR:HD1	1.56	0.52
1:C:40:LYS:HD2	1:C:41:THR:H	1.73	0.52
1:C:218:ASP:CG	1:C:219:ILE:H	2.16	0.52
2:D:2:ARG:CG	2:D:133:GLN:NE2	2.61	0.52
2:D:253:ARG:C	2:D:255:LEU:N	2.62	0.52
2:D:287:THR:C	2:D:289:PRO:HD2	2.34	0.52
2:D:400:ARG:C	2:D:402:LYS:H	2.17	0.52
3:E:30:UNK:O	3:E:33:UNK:N	2.42	0.52
1:A:77:GLU:C	1:A:83:TYR:HB2	2.35	0.52
1:A:237:SER:HG	1:A:272:TYR:HE2	1.56	0.52
1:A:256:GLN:O	1:A:258:ASN:N	2.43	0.52
1:C:401:LYS:O	1:C:402:ARG:CD	2.57	0.52
2:D:25:SER:HB3	2:D:369:ARG:HH22	1.74	0.52
2:D:154:ILE:O	2:D:156:LYS:N	2.42	0.52
2:D:381:SER:C	2:D:383:ALA:H	2.16	0.52
2:D:383:ALA:C	2:D:385:GLN:N	2.67	0.52
2:D:413:MET:SD	2:D:417:GLU:HG2	2.49	0.52
2:D:437:ASP:OD2	2:D:437:ASP:N	2.43	0.52
1:A:289:ALA:HA	1:A:292:THR:HG22	1.89	0.52
2:B:402:LYS:CE	1:C:440:VAL:C	2.82	0.52
1:C:107:HIS:CE1	1:C:151:SER:HB2	2.43	0.52
1:C:276:ILE:CG1	1:C:282:TYR:CD2	2.92	0.52
1:C:276:ILE:HD12	1:C:277:SER:N	2.25	0.52
1:C:322:ASP:OD1	1:C:357:TYR:O	2.27	0.52
2:D:264:ARG:NH2	2:D:431:GLU:HG3	2.24	0.52
2:D:283:TYR:C	2:D:285:ALA:N	2.67	0.52
2:D:428:LEU:CD1	2:D:428:LEU:H	2.23	0.52
3:E:73:UNK:C	3:E:75:UNK:N	2.66	0.52
1:A:46:ASP:O	1:A:47:ASP:C	2.52	0.52
1:A:108:TYR:CD1	1:A:413:MET:HE3	2.44	0.52
1:A:213:CYS:SG	1:A:230:LEU:HD23	2.50	0.52
1:A:314:ALA:O	1:A:315:CYS:CB	2.57	0.52
2:B:306:ASP:HB3	2:B:309:HIS:NE2	2.24	0.52
1:C:16:ILE:O	1:C:17:GLY:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:VAL:HG13	1:C:408:TYR:OH	2.09	0.52
1:C:321:GLY:HA2	1:C:358:GLU:O	2.09	0.52
2:D:130:ASP:C	2:D:130:ASP:OD2	2.52	0.52
2:D:143:GLY:O	5:D:503:GDP:O3B	2.28	0.52
2:D:350:ASN:HD22	2:D:350:ASN:C	2.17	0.52
2:D:371:LEU:O	2:D:372:LYS:HB2	2.07	0.52
1:A:163:LYS:C	1:A:164:LYS:HZ2	2.17	0.52
1:A:174:ALA:C	1:A:176:GLN:H	2.18	0.52
1:A:243:ARG:HA	1:A:243:ARG:NE	2.24	0.52
1:A:298:PRO:O	1:A:300:ASN:N	2.42	0.52
1:A:417:GLU:C	1:A:418:PHE:HD2	2.17	0.52
2:B:16:ILE:HD12	2:B:231:VAL:CG1	2.38	0.52
2:B:70:LEU:HD11	2:B:110:GLU:O	2.09	0.52
2:B:200:GLU:CD	2:B:268:PHE:HE2	2.17	0.52
2:B:265:LEU:O	2:B:266:HIS:CG	2.63	0.52
2:B:276:THR:HG21	2:B:281:GLN:HB3	1.92	0.52
2:B:308:ARG:HH21	2:B:342:TYR:HD1	1.50	0.52
2:B:409:THR:HA	2:B:412:GLY:O	2.10	0.52
1:C:103:TYR:HB2	1:C:185:TYR:HD1	1.74	0.52
1:C:137:VAL:O	1:C:168:GLU:HA	2.10	0.52
2:D:161:TYR:O	2:D:162:PRO:C	2.52	0.52
2:D:179:ASP:HB3	2:D:181:VAL:CG1	2.37	0.52
2:D:182:VAL:O	2:D:182:VAL:CG1	2.57	0.52
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.91	0.52
1:A:252:LEU:HD22	1:A:255:PHE:HD2	1.74	0.52
2:B:183:GLU:HB3	2:B:184:PRO:HD3	1.91	0.52
2:B:283:TYR:C	2:B:285:ALA:H	2.16	0.52
2:B:322:ARG:HG2	2:B:357:ASP:CA	2.30	0.52
2:B:427:ASP:O	2:B:428:LEU:C	2.53	0.52
1:C:35:GLN:HE22	1:C:88:HIS:CD2	2.28	0.52
1:C:102:ASN:O	1:C:105:ARG:N	2.38	0.52
1:C:172:TYR:HB3	1:C:205:ASP:H	1.74	0.52
1:C:294:ALA:HA	1:C:297:GLU:OE1	2.09	0.52
1:C:311:LYS:CG	1:C:344:VAL:HG22	2.40	0.52
2:D:260:VAL:O	2:D:260:VAL:HG12	2.09	0.52
2:D:405:LEU:C	2:D:407:TRP:H	2.17	0.52
2:D:415:GLU:O	2:D:416:MET:O	2.27	0.52
1:A:142:GLY:O	1:A:182:VAL:CG2	2.57	0.52
2:B:129:CYS:O	2:B:130:ASP:O	2.27	0.52
1:C:68:VAL:HG21	1:C:118:VAL:HG21	1.91	0.52
1:C:152:LEU:O	1:C:156:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:CD1	1:C:302:MET:SD	2.97	0.52
1:C:402:ARG:CG	1:C:403:ALA:N	2.69	0.52
2:D:59:ASN:ND2	2:D:60:LYS:H	2.07	0.52
2:D:127:GLU:O	2:D:128:SER:O	2.28	0.52
2:D:132:LEU:HB3	2:D:164:ARG:CZ	2.38	0.52
2:D:140:SER:HA	2:D:171:VAL:H	1.74	0.52
1:A:134:GLY:H	1:A:164:LYS:HG3	1.73	0.52
1:A:172:TYR:HB3	1:A:205:ASP:H	1.75	0.52
1:A:286:LEU:HD12	1:A:291:ILE:HG12	1.90	0.52
2:B:69:ASP:CB	2:B:74:THR:HG23	2.39	0.52
2:B:154:ILE:C	2:B:156:LYS:N	2.64	0.52
2:B:179:ASP:HB3	2:B:181:VAL:H	1.75	0.52
2:B:312:TYR:O	2:B:344:VAL:HG13	2.09	0.52
2:B:325:MET:HG2	2:B:355:VAL:HG11	1.91	0.52
1:C:71:GLU:OE2	4:C:502:GTP:O1B	2.28	0.52
1:C:307:PRO:HA	1:C:383:ALA:HB3	1.92	0.52
1:C:341:ILE:HG22	1:C:342:GLN:N	2.25	0.52
1:C:388:TRP:HZ3	1:C:428:LEU:HD22	1.71	0.52
1:C:426:ALA:C	1:C:428:LEU:H	2.17	0.52
2:D:239:THR:O	2:D:241:CYS:N	2.43	0.52
1:A:401:LYS:O	1:A:402:ARG:CD	2.58	0.52
2:B:51:VAL:HG22	2:B:245:PRO:HG2	1.90	0.52
2:B:100:GLY:C	2:B:101:ASN:HD22	2.18	0.52
2:B:132:LEU:HD11	2:B:135:PHE:CE2	2.45	0.52
2:B:293:GLN:C	2:B:295:MET:N	2.67	0.52
2:B:399:PHE:HE2	2:B:404:PHE:HB3	1.74	0.52
1:C:108:TYR:O	1:C:109:THR:C	2.52	0.52
1:C:139:HIS:O	1:C:140:SER:CB	2.58	0.52
1:C:190:THR:CG2	1:C:425:MET:HG2	2.40	0.52
1:C:213:CYS:O	1:C:219:ILE:HB	2.10	0.52
1:C:286:LEU:O	1:C:287:SER:C	2.51	0.52
2:D:1:MET:C	2:D:3:GLU:N	2.68	0.52
2:D:93:VAL:HG23	2:D:95:GLY:N	2.25	0.52
2:D:142:GLY:HA2	2:D:185:TYR:CB	2.35	0.52
2:D:265:LEU:O	2:D:266:HIS:CG	2.63	0.52
1:A:2:ARG:NH2	1:A:133:GLN:NE2	2.53	0.52
1:A:212:ILE:HD11	1:A:230:LEU:HD21	1.91	0.52
1:A:414:GLU:CA	1:A:417:GLU:HB2	2.39	0.52
2:B:158:ARG:HG3	2:B:159:GLU:HG3	1.92	0.52
2:B:282:GLN:C	2:B:285:ALA:H	2.17	0.52
2:B:391:ILE:O	2:B:391:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:THR:O	1:C:292:THR:OG1	2.22	0.52
1:C:389:ALA:CB	1:C:429:GLU:OE2	2.58	0.52
2:D:2:ARG:HE	2:D:243:ARG:HD2	1.75	0.52
2:D:174:SER:C	2:D:176:LYS:N	2.66	0.52
2:D:197:ASN:O	2:D:198:THR:HB	2.08	0.52
1:A:115:ILE:O	1:A:119:LEU:HB2	2.09	0.51
1:A:152:LEU:O	1:A:153:LEU:C	2.52	0.51
1:A:221:ARG:CD	1:A:221:ARG:H	2.23	0.51
1:A:387:ALA:HB1	1:A:390:ARG:CZ	2.40	0.51
2:B:58:GLY:O	2:B:64:ARG:CZ	2.59	0.51
2:B:129:CYS:O	2:B:130:ASP:C	2.52	0.51
2:B:264:ARG:HG3	2:B:264:ARG:NH1	2.25	0.51
2:B:396:THR:HA	2:B:400:ARG:HB3	1.92	0.51
1:C:44:GLY:HA3	1:C:47:ASP:HA	1.91	0.51
1:C:88:HIS:CB	1:C:91:GLN:HE22	2.18	0.51
1:C:298:PRO:O	1:C:300:ASN:N	2.43	0.51
1:C:344:VAL:HG11	1:C:346:TRP:CE2	2.45	0.51
2:D:320:ARG:HB2	2:D:374:SER:OG	2.10	0.51
1:A:264:ARG:HH22	1:A:427:ALA:HB3	1.75	0.51
1:A:426:ALA:C	1:A:428:LEU:N	2.67	0.51
2:B:179:ASP:CB	2:B:182:VAL:HG23	2.37	0.51
2:B:253:ARG:C	2:B:255:LEU:N	2.68	0.51
1:C:296:PHE:CE2	1:C:377:MET:HE1	2.44	0.51
2:D:75:MET:O	2:D:76:ASP:O	2.27	0.51
2:D:97:SER:OG	2:D:98:GLY:N	2.38	0.51
1:A:206:ASN:O	1:A:207:GLU:C	2.53	0.51
2:B:104:ALA:HB1	2:B:411:GLU:HB2	1.93	0.51
2:B:247:GLN:OE1	2:B:355:VAL:O	2.28	0.51
2:B:273:ALA:O	2:B:275:LEU:N	2.40	0.51
2:B:293:GLN:C	2:B:295:MET:H	2.17	0.51
2:B:333:LEU:O	2:B:337:ASN:N	2.43	0.51
2:B:357:ASP:CB	2:B:358:ILE:HD12	2.41	0.51
2:B:415:GLU:O	2:B:416:MET:O	2.28	0.51
1:C:322:ASP:HA	1:C:357:TYR:CD1	2.37	0.51
1:C:386:GLU:C	1:C:388:TRP:N	2.68	0.51
1:C:388:TRP:CZ3	1:C:428:LEU:HD13	2.45	0.51
2:D:223:THR:HG23	2:D:225:GLY:N	2.25	0.51
2:D:415:GLU:HG2	2:D:416:MET:H	1.75	0.51
1:A:202:PHE:CE1	1:A:378:LEU:HD22	2.42	0.51
1:A:416:GLY:C	1:A:418:PHE:N	2.62	0.51
2:B:5:VAL:HG22	2:B:64:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:NH2	2:B:160:GLU:OE2	2.44	0.51
2:B:234:THR:O	2:B:238:VAL:HG23	2.11	0.51
1:C:168:GLU:HG3	1:C:201:ALA:CB	2.39	0.51
1:C:216:ASN:HB3	1:C:275:VAL:CG1	2.40	0.51
2:D:87:PHE:O	2:D:89:PRO:N	2.43	0.51
1:A:5:ILE:O	1:A:135:PHE:HA	2.10	0.51
1:A:37:PRO:HA	1:A:45:GLY:O	2.10	0.51
1:A:102:ASN:O	1:A:103:TYR:C	2.54	0.51
2:B:7:ILE:HB	2:B:137:LEU:HA	1.91	0.51
2:B:24:ILE:O	2:B:24:ILE:HG22	2.10	0.51
2:B:401:ARG:O	2:B:402:LYS:HG3	2.10	0.51
1:C:277:SER:O	1:C:278:ALA:HB2	2.10	0.51
1:C:365:GLY:O	1:C:368:LEU:CD1	2.59	0.51
1:C:426:ALA:C	1:C:428:LEU:N	2.67	0.51
2:D:51:VAL:CG2	2:D:53:TYR:HB2	2.40	0.51
2:D:59:ASN:CA	2:D:60:LYS:HZ3	2.24	0.51
2:D:60:LYS:H	2:D:60:LYS:HD2	1.74	0.51
2:D:154:ILE:HD11	2:D:168:THR:HG21	1.92	0.51
2:D:318:VAL:HG12	2:D:318:VAL:O	2.11	0.51
1:A:41:THR:O	1:A:42:ILE:HB	2.09	0.51
1:A:44:GLY:C	1:A:46:ASP:N	2.69	0.51
1:A:160:ASP:O	1:A:161:TYR:CG	2.64	0.51
1:A:184:PRO:HA	1:A:395:PHE:HD2	1.76	0.51
1:A:288:VAL:HA	1:A:373:ARG:HD3	1.92	0.51
1:A:320:ARG:CB	1:A:374:ALA:HB3	2.37	0.51
2:B:118:VAL:C	2:B:120:ASP:N	2.65	0.51
2:B:166:MET:HG3	2:B:167:ASN:N	2.24	0.51
2:B:179:ASP:OD1	1:C:352:LYS:NZ	2.43	0.51
2:B:305:CYS:O	2:B:306:ASP:C	2.53	0.51
2:B:402:LYS:HE3	1:C:440:VAL:C	2.35	0.51
1:C:78:VAL:HG11	1:C:92:LEU:CD2	2.39	0.51
1:C:212:ILE:C	1:C:214:ARG:H	2.17	0.51
2:D:59:ASN:CA	2:D:64:ARG:HH21	2.19	0.51
2:D:63:PRO:C	2:D:65:ALA:N	2.67	0.51
2:D:179:ASP:HB2	2:D:182:VAL:N	2.25	0.51
1:A:15:GLN:HE22	1:A:224:TYR:HD1	1.58	0.51
1:A:72:PRO:HG3	1:A:96:LYS:HA	1.91	0.51
1:A:294:ALA:C	1:A:296:PHE:N	2.67	0.51
1:A:393:HIS:C	1:A:395:PHE:N	2.68	0.51
2:B:2:ARG:O	2:B:57:ALA:HB1	2.11	0.51
2:B:253:ARG:HG3	2:B:253:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:LEU:C	2:B:407:TRP:H	2.18	0.51
2:B:408:TYR:CB	2:B:413:MET:HE3	2.40	0.51
1:C:69:ASP:OD2	1:C:74:VAL:HG12	2.11	0.51
1:C:171:ILE:HA	1:C:204:VAL:HB	1.92	0.51
2:D:6:HIS:ND1	2:D:21:TRP:HZ2	2.09	0.51
2:D:11:GLN:HG3	2:D:15:GLN:NE2	2.26	0.51
2:D:103:TRP:O	2:D:105:LYS:O	2.28	0.51
2:D:297:ASP:OD1	2:D:299:LYS:N	2.32	0.51
2:D:397:ALA:O	2:D:398:MET:HB2	2.10	0.51
3:E:90:UNK:O	3:E:91:UNK:O	2.29	0.51
1:A:84:ARG:C	1:A:85:GLN:HG2	2.36	0.51
2:B:372:LYS:O	2:B:373:MET:HG3	2.11	0.51
2:D:59:ASN:HB2	2:D:64:ARG:HE	1.74	0.51
2:D:242:LEU:O	2:D:243:ARG:NE	2.44	0.51
2:D:297:ASP:O	2:D:301:MET:HG2	2.11	0.51
2:D:424:ASN:O	2:D:427:ASP:N	2.44	0.51
1:A:423:GLU:O	1:A:426:ALA:HB3	2.11	0.51
2:B:90:ASP:OD1	2:B:91:ASN:ND2	2.44	0.51
2:B:391:ILE:N	2:B:391:ILE:CD1	2.74	0.51
1:C:38:SER:O	1:C:39:ASP:HB3	2.11	0.51
1:C:215:ARG:NH2	1:C:300:ASN:HD21	2.07	0.51
1:C:220:GLU:HB3	1:C:221:ARG:CZ	2.40	0.51
1:C:344:VAL:HG12	1:C:345:ASP:CG	2.36	0.51
1:C:405:VAL:O	1:C:409:VAL:HG23	2.11	0.51
2:D:86:ILE:H	2:D:88:ARG:CZ	2.24	0.51
2:D:179:ASP:HB3	2:D:182:VAL:H	1.73	0.51
2:D:264:ARG:O	2:D:265:LEU:O	2.29	0.51
2:D:283:TYR:O	2:D:283:TYR:CG	2.64	0.51
2:D:307:PRO:C	2:D:309:HIS:N	2.68	0.51
1:A:21:TRP:HA	1:A:24:TYR:HB2	1.93	0.51
1:A:218:ASP:CG	1:A:219:ILE:N	2.69	0.51
2:B:79:ARG:HG3	2:B:88:ARG:HE	1.75	0.51
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.93	0.51
2:B:283:TYR:C	2:B:285:ALA:N	2.68	0.51
1:C:186:ASN:HD21	1:C:391:LEU:HD11	1.75	0.51
2:D:259:MET:HE1	2:D:316:ALA:N	2.26	0.51
2:D:313:LEU:HD21	2:D:435:TYR:HD2	1.76	0.51
1:A:143:GLY:O	4:A:500:GTP:O3G	2.29	0.50
1:A:177:VAL:HG11	2:B:349:ASN:HB3	1.93	0.50
1:A:180:ALA:O	1:A:182:VAL:N	2.44	0.50
2:B:203:CYS:SG	2:B:384:ILE:HD11	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:LYS:HE3	1:C:440:VAL:CG1	2.41	0.50
2:B:430:SER:O	2:B:431:GLU:C	2.54	0.50
1:C:5:ILE:CD1	1:C:125:LEU:HD22	2.41	0.50
1:C:239:THR:OG1	1:C:240:ALA:N	2.41	0.50
1:C:273:ALA:HB2	1:C:295:CYS:CA	2.41	0.50
2:D:186:ASN:HA	2:D:189:LEU:HD12	1.93	0.50
2:D:249:ASN:CG	2:D:250:ALA:N	2.68	0.50
3:E:4:UNK:C	3:E:6:UNK:N	2.74	0.50
1:A:101:ASN:ND2	1:A:185:TYR:OH	2.44	0.50
1:A:265:ALA:O	1:A:266:HIS:C	2.54	0.50
1:A:294:ALA:HA	1:A:297:GLU:OE1	2.11	0.50
1:A:368:LEU:N	1:A:368:LEU:HD12	2.26	0.50
2:B:11:GLN:C	2:B:13:GLY:H	2.18	0.50
2:B:277:SER:O	2:B:278:ARG:O	2.29	0.50
2:B:395:PHE:CE2	2:B:418:PHE:O	2.64	0.50
1:C:75:ILE:O	1:C:75:ILE:CG1	2.58	0.50
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.93	0.50
2:D:218:LYS:NZ	2:D:277:SER:HB3	2.26	0.50
3:E:4:UNK:O	3:E:5:UNK:C	2.59	0.50
1:A:333:ALA:O	1:A:336:LYS:N	2.43	0.50
2:B:6:HIS:CE1	2:B:21:TRP:HE1	2.30	0.50
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.93	0.50
1:C:181:VAL:HG13	1:C:181:VAL:O	2.11	0.50
1:C:208:ALA:HB2	1:C:302:MET:O	2.11	0.50
1:C:260:VAL:O	1:C:260:VAL:HG12	2.10	0.50
1:C:311:LYS:HB2	1:C:344:VAL:HG22	1.92	0.50
1:C:341:ILE:HD12	1:C:341:ILE:N	2.26	0.50
1:C:414:GLU:CG	1:C:415:GLU:N	2.69	0.50
2:D:123:ARG:NH2	2:D:160:GLU:OE2	2.44	0.50
2:D:296:PHE:HE1	2:D:332:MET:HE1	1.74	0.50
2:D:308:ARG:HH21	2:D:342:TYR:HD1	1.48	0.50
1:A:38:SER:O	1:A:39:ASP:CB	2.59	0.50
1:A:82:THR:HG22	1:A:83:TYR:H	1.76	0.50
1:A:363:VAL:HG22	1:A:367:ASP:OD2	2.10	0.50
1:A:413:MET:C	1:A:414:GLU:CD	2.80	0.50
2:B:403:ALA:HB3	1:C:262:TYR:HE2	1.76	0.50
1:C:20:CYS:C	1:C:22:GLU:H	2.19	0.50
1:C:25:CYS:O	1:C:25:CYS:SG	2.69	0.50
1:C:317:LEU:HD23	1:C:377:MET:HB3	1.92	0.50
1:C:350:GLY:O	1:C:351:PHE:HD1	1.93	0.50
1:C:419:SER:O	1:C:420:GLU:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:ILE:CD1	2:D:252:LEU:HD13	2.42	0.50
2:D:10:GLY:CA	2:D:146:GLY:HA3	2.41	0.50
2:D:191:VAL:HG22	2:D:421:ALA:O	2.11	0.50
2:D:289:PRO:O	2:D:292:THR:OG1	2.25	0.50
1:A:10:GLY:O	1:A:11:GLN:C	2.54	0.50
1:A:152:LEU:O	1:A:156:ARG:HG2	2.10	0.50
2:B:51:VAL:N	2:B:245:PRO:HG2	2.27	0.50
2:B:71:GLU:CB	2:B:72:PRO:CD	2.90	0.50
2:B:133:GLN:OE1	2:B:133:GLN:HA	2.11	0.50
2:B:179:ASP:HB3	2:B:182:VAL:H	1.73	0.50
2:B:228:ASN:O	2:B:231:VAL:HB	2.11	0.50
2:B:343:PHE:HB3	2:B:350:ASN:OD1	2.11	0.50
1:C:102:ASN:O	1:C:103:TYR:C	2.53	0.50
2:D:111:GLY:O	2:D:114:LEU:N	2.44	0.50
2:D:212:ILE:O	2:D:217:LEU:HB3	2.10	0.50
2:D:326:LYS:O	2:D:330:GLU:HG3	2.11	0.50
1:A:101:ASN:O	1:A:101:ASN:ND2	2.39	0.50
1:A:206:ASN:O	1:A:210:TYR:HD2	1.95	0.50
1:A:399:TYR:HH	1:A:408:TYR:HE2	1.58	0.50
2:B:93:VAL:HG23	2:B:94:PHE:N	2.25	0.50
2:B:140:SER:HA	2:B:171:VAL:H	1.76	0.50
2:B:158:ARG:CZ	2:B:197:ASN:HA	2.41	0.50
2:B:174:SER:C	2:B:176:LYS:H	2.19	0.50
1:C:66:VAL:HG21	1:C:122:ILE:HG12	1.93	0.50
1:C:155:GLU:O	1:C:159:VAL:HG23	2.12	0.50
1:C:174:ALA:HB2	1:C:206:ASN:HB2	1.94	0.50
2:D:295:MET:O	2:D:297:ASP:N	2.43	0.50
1:A:9:VAL:HA	1:A:68:VAL:O	2.12	0.50
1:A:40:LYS:HD2	1:A:41:THR:H	1.76	0.50
1:A:74:VAL:HG13	1:A:75:ILE:N	2.27	0.50
1:A:181:VAL:HG23	1:A:404:PHE:HB2	1.93	0.50
1:A:258:ASN:HD22	1:A:258:ASN:H	1.52	0.50
1:A:332:ILE:HG23	1:A:351:PHE:CE2	2.46	0.50
1:A:344:VAL:CG1	1:A:346:TRP:NE1	2.73	0.50
2:B:211:ASP:O	2:B:215:ARG:N	2.44	0.50
2:B:266:HIS:ND1	2:B:432:TYR:CE1	2.79	0.50
2:B:311:ARG:NH1	2:B:344:VAL:HA	2.26	0.50
1:C:190:THR:CA	1:C:193:THR:HG22	2.36	0.50
1:C:266:HIS:H	1:C:266:HIS:HD1	1.60	0.50
1:C:417:GLU:HB3	1:C:418:PHE:HE2	1.74	0.50
2:D:2:ARG:NE	2:D:243:ARG:CD	2.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:ARG:HH11	2:D:284:ARG:HG3	1.77	0.50
1:A:143:GLY:O	1:A:144:GLY:C	2.55	0.50
1:A:184:PRO:CG	1:A:399:TYR:CZ	2.93	0.50
1:A:208:ALA:O	1:A:212:ILE:HG23	2.12	0.50
1:A:244:PHE:HE1	1:A:358:GLU:OE2	1.95	0.50
1:A:363:VAL:HG22	1:A:367:ASP:CG	2.36	0.50
1:A:401:LYS:O	1:A:402:ARG:NE	2.45	0.50
2:B:107:HIS:ND1	2:B:107:HIS:O	2.44	0.50
2:B:115:VAL:CG1	2:B:156:LYS:NZ	2.73	0.50
2:B:313:LEU:HD21	2:B:435:TYR:HD2	1.76	0.50
2:B:383:ALA:C	2:B:385:GLN:N	2.68	0.50
1:C:181:VAL:O	1:C:184:PRO:HG2	2.11	0.50
1:C:183:GLU:OE2	2:D:348:PRO:HB2	2.12	0.50
1:C:184:PRO:O	1:C:188:ILE:HG13	2.11	0.50
1:C:206:ASN:O	1:C:207:GLU:C	2.55	0.50
1:C:380:ASN:CG	1:C:380:ASN:O	2.53	0.50
2:D:272:PHE:HD1	2:D:275:LEU:HD23	1.77	0.50
2:D:306:ASP:HB3	2:D:309:HIS:NE2	2.26	0.50
2:D:311:ARG:HH11	2:D:344:VAL:HA	1.77	0.50
3:E:50:UNK:O	3:E:53:UNK:N	2.44	0.50
1:A:9:VAL:HG21	1:A:150:THR:CG2	2.42	0.50
1:A:108:TYR:O	1:A:109:THR:C	2.55	0.50
1:A:144:GLY:CA	1:A:147:SER:HB3	2.42	0.50
1:A:171:ILE:H	1:A:171:ILE:CD1	2.25	0.50
1:A:194:THR:O	1:A:196:GLU:N	2.45	0.50
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.26	0.50
1:A:311:LYS:HD3	1:A:344:VAL:CG2	2.42	0.50
1:A:346:TRP:HZ2	1:A:435:VAL:HB	1.76	0.50
1:A:364:PRO:C	1:A:366:GLY:H	2.20	0.50
2:B:84:GLY:HA2	2:B:88:ARG:HH21	1.77	0.50
2:B:96:GLN:OE1	1:C:130:THR:HB	2.12	0.50
1:C:177:VAL:HG11	2:D:349:ASN:CB	2.42	0.50
1:C:210:TYR:CE2	1:C:227:LEU:CD2	2.95	0.50
1:C:269:LEU:HD21	1:C:301:GLN:NE2	2.27	0.50
2:D:241:CYS:SG	2:D:320:ARG:NH1	2.85	0.50
2:D:284:ARG:O	2:D:285:ALA:C	2.54	0.50
3:E:71:UNK:O	3:E:72:UNK:C	2.60	0.50
1:A:71:GLU:O	1:A:73:THR:N	2.44	0.49
2:B:280:SER:O	2:B:282:GLN:N	2.45	0.49
2:B:315:VAL:HG23	2:B:351:VAL:HG22	1.94	0.49
1:C:242:LEU:O	1:C:243:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:CYS:SG	1:C:306:ASP:N	2.77	0.49
2:D:6:HIS:O	2:D:66:ILE:HG22	2.12	0.49
2:D:218:LYS:O	2:D:219:LEU:CB	2.60	0.49
2:D:223:THR:C	2:D:225:GLY:H	2.20	0.49
1:A:100:ALA:CA	1:A:105:ARG:HD2	2.41	0.49
1:A:102:ASN:O	1:A:105:ARG:N	2.34	0.49
1:A:174:ALA:CB	1:A:176:GLN:HG2	2.42	0.49
1:A:409:VAL:HA	1:A:414:GLU:CD	2.32	0.49
2:B:51:VAL:N	2:B:245:PRO:HB2	2.26	0.49
2:B:282:GLN:O	2:B:284:ARG:N	2.45	0.49
2:B:427:ASP:O	2:B:430:SER:N	2.45	0.49
1:C:41:THR:O	1:C:42:ILE:HB	2.11	0.49
1:C:402:ARG:HD2	2:D:346:TRP:CE3	2.47	0.49
2:D:87:PHE:O	2:D:89:PRO:HD2	2.12	0.49
2:D:204:ILE:HG21	2:D:209:LEU:HD11	1.93	0.49
2:D:390:ARG:HB2	2:D:391:ILE:HD12	1.94	0.49
2:B:4:ILE:CD1	2:B:252:LEU:HD13	2.42	0.49
2:B:59:ASN:HB3	2:B:64:ARG:HB2	1.93	0.49
2:B:344:VAL:O	2:B:345:GLU:HB3	2.13	0.49
2:B:428:LEU:HD12	2:B:428:LEU:H	1.76	0.49
1:C:213:CYS:SG	1:C:217:LEU:CD2	2.99	0.49
1:C:283:HIS:O	1:C:284:GLU:HB3	2.12	0.49
2:D:2:ARG:CG	2:D:133:GLN:HE21	2.23	0.49
2:D:107:HIS:ND1	2:D:107:HIS:O	2.46	0.49
1:A:190:THR:CA	1:A:193:THR:HG22	2.37	0.49
1:A:306:ASP:OD1	1:A:306:ASP:O	2.30	0.49
1:A:307:PRO:HA	1:A:383:ALA:CB	2.41	0.49
1:A:343:PHE:CD2	1:A:349:THR:HB	2.47	0.49
2:B:5:VAL:HA	2:B:64:ARG:HD2	1.93	0.49
2:B:126:SER:O	2:B:127:GLU:C	2.54	0.49
2:B:271:GLY:O	2:B:272:PHE:O	2.30	0.49
2:B:290:GLU:O	2:B:291:LEU:C	2.55	0.49
2:B:398:MET:O	2:B:401:ARG:N	2.45	0.49
2:B:428:LEU:O	2:B:429:VAL:C	2.54	0.49
1:C:414:GLU:CG	1:C:415:GLU:H	2.17	0.49
2:D:79:ARG:O	2:D:79:ARG:HG2	2.13	0.49
2:D:184:PRO:CB	2:D:399:PHE:CZ	2.95	0.49
2:D:382:THR:HB	2:D:436:GLN:HG2	1.95	0.49
2:D:424:ASN:O	2:D:427:ASP:HB2	2.12	0.49
1:A:139:HIS:CG	1:A:140:SER:N	2.77	0.49
1:A:181:VAL:HG22	1:A:408:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:MET:O	2:B:297:ASP:N	2.44	0.49
1:C:93:ILE:HD13	1:C:118:VAL:HA	1.95	0.49
1:C:194:THR:O	1:C:196:GLU:N	2.45	0.49
1:C:202:PHE:CE1	1:C:378:LEU:HD22	2.43	0.49
1:C:264:ARG:HH22	1:C:427:ALA:HB3	1.78	0.49
1:C:433:GLU:C	1:C:435:VAL:N	2.69	0.49
2:D:71:GLU:CB	2:D:72:PRO:CD	2.90	0.49
2:D:158:ARG:HB2	2:D:197:ASN:CB	2.31	0.49
1:A:108:TYR:CG	1:A:413:MET:HE3	2.47	0.49
1:A:123:ARG:O	1:A:127:ASP:HB2	2.12	0.49
1:A:142:GLY:O	1:A:182:VAL:HG23	2.13	0.49
1:A:213:CYS:SG	1:A:230:LEU:CD2	3.01	0.49
1:A:238:ILE:O	1:A:242:LEU:HD12	2.12	0.49
1:A:428:LEU:C	1:A:430:LYS:N	2.66	0.49
2:B:189:LEU:O	2:B:192:HIS:ND1	2.38	0.49
1:C:37:PRO:HA	1:C:45:GLY:O	2.13	0.49
1:C:171:ILE:N	1:C:171:ILE:CD1	2.76	0.49
2:D:242:LEU:O	2:D:243:ARG:CD	2.60	0.49
3:E:25:UNK:O	3:E:27:UNK:N	2.44	0.49
1:A:93:ILE:CD1	1:A:118:VAL:HA	2.42	0.49
2:B:59:ASN:CB	2:B:64:ARG:HE	2.25	0.49
2:B:132:LEU:CB	2:B:164:ARG:HH21	2.15	0.49
2:B:286:LEU:HA	2:B:290:GLU:CD	2.37	0.49
2:B:395:PHE:CD2	2:B:422:GLU:OE1	2.66	0.49
1:C:7:ILE:HG21	1:C:122:ILE:CD1	2.42	0.49
1:C:255:PHE:CD1	1:C:259:LEU:HD12	2.48	0.49
1:C:393:HIS:O	1:C:397:LEU:HB2	2.13	0.49
1:C:409:VAL:C	1:C:411:GLU:N	2.71	0.49
2:D:2:ARG:NH2	2:D:243:ARG:HA	2.28	0.49
2:D:60:LYS:N	2:D:60:LYS:HZ3	2.11	0.49
2:D:289:PRO:CB	2:D:331:GLN:HE21	2.25	0.49
2:D:325:MET:HG2	2:D:355:VAL:HG11	1.95	0.49
1:A:2:ARG:HH22	1:A:133:GLN:HE22	1.57	0.49
1:A:68:VAL:HG13	1:A:68:VAL:O	2.13	0.49
1:A:168:GLU:HG3	1:A:201:ALA:CB	2.42	0.49
1:A:241:SER:CB	1:A:242:LEU:HD12	2.43	0.49
1:A:420:GLU:C	1:A:420:GLU:OE1	2.54	0.49
2:B:102:ASN:HD22	2:B:105:LYS:CB	2.26	0.49
2:B:188:THR:HA	2:B:191:VAL:HG21	1.95	0.49
2:B:381:SER:O	2:B:383:ALA:N	2.46	0.49
1:C:183:GLU:N	1:C:184:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:GLU:OE1	1:C:420:GLU:O	2.30	0.49
2:D:144:GLY:HA3	2:D:185:TYR:OH	2.13	0.49
2:D:403:ALA:O	2:D:404:PHE:HB2	2.12	0.49
1:A:186:ASN:HD21	1:A:391:LEU:HD11	1.70	0.49
1:A:311:LYS:HB2	1:A:344:VAL:CG2	2.43	0.49
1:A:427:ALA:HA	1:A:430:LYS:CB	2.43	0.49
1:C:9:VAL:HG21	1:C:150:THR:HB	1.93	0.49
1:C:68:VAL:HG21	1:C:149:PHE:HE1	1.77	0.49
1:C:102:ASN:HB2	1:C:105:ARG:HB3	1.91	0.49
1:C:176:GLN:OE1	1:C:210:TYR:CE1	2.66	0.49
1:C:291:ILE:HG22	1:C:292:THR:N	2.28	0.49
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.31	0.49
3:E:58:UNK:O	3:E:59:UNK:C	2.58	0.49
1:A:26:LEU:HG	1:A:361:THR:HB	1.95	0.49
1:A:111:GLY:C	1:A:113:GLU:N	2.71	0.49
1:A:317:LEU:HD13	1:A:319:TYR:CE1	2.48	0.49
2:B:73:GLY:C	2:B:75:MET:H	2.20	0.49
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.93	0.49
2:B:133:GLN:NE2	2:B:252:LEU:CB	2.65	0.49
2:B:149:MET:CE	2:B:152:LEU:HD23	2.43	0.49
2:B:242:LEU:O	2:B:243:ARG:HD3	2.12	0.49
1:C:46:ASP:O	1:C:47:ASP:C	2.56	0.49
1:C:163:LYS:C	1:C:164:LYS:HZ1	2.20	0.49
1:C:294:ALA:C	1:C:296:PHE:N	2.67	0.49
1:C:350:GLY:O	1:C:351:PHE:CD1	2.66	0.49
1:C:428:LEU:C	1:C:430:LYS:H	2.21	0.49
2:D:60:LYS:H	2:D:60:LYS:NZ	2.11	0.49
2:D:181:VAL:O	2:D:183:GLU:N	2.42	0.49
2:D:188:THR:HA	2:D:191:VAL:HG21	1.95	0.49
2:D:395:PHE:CE2	2:D:418:PHE:O	2.66	0.49
1:A:126:ALA:HB1	1:A:132:LEU:HD11	1.93	0.48
1:A:256:GLN:HA	1:A:260:VAL:CG2	2.43	0.48
2:B:119:LEU:HD13	2:B:123:ARG:NH2	2.28	0.48
2:B:238:VAL:HG22	2:B:376:THR:HG21	1.95	0.48
1:C:256:GLN:C	1:C:258:ASN:H	2.19	0.48
2:D:8:GLN:O	2:D:67:LEU:HA	2.13	0.48
2:D:87:PHE:O	2:D:89:PRO:CD	2.61	0.48
2:D:106:GLY:O	2:D:149:MET:HA	2.13	0.48
2:D:204:ILE:HD13	2:D:231:VAL:HG13	1.94	0.48
2:D:344:VAL:CG2	2:D:345:GLU:N	2.76	0.48
1:A:102:ASN:HB2	1:A:105:ARG:HB3	1.88	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLN:C	1:A:258:ASN:H	2.20	0.48
1:A:294:ALA:HA	1:A:297:GLU:HB2	1.95	0.48
1:A:307:PRO:HA	1:A:383:ALA:HB3	1.95	0.48
1:A:344:VAL:HG12	1:A:345:ASP:CG	2.38	0.48
2:B:20:PHE:HZ	2:B:239:THR:HG21	1.78	0.48
2:B:102:ASN:HB3	2:B:105:LYS:CD	2.43	0.48
2:B:262:PHE:O	2:B:265:LEU:CA	2.57	0.48
2:B:265:LEU:O	2:B:266:HIS:ND1	2.46	0.48
1:C:31:GLN:HB3	1:C:32:PRO:CD	2.37	0.48
1:C:265:ALA:O	1:C:266:HIS:C	2.55	0.48
1:C:303:VAL:HG21	1:C:384:ILE:HD11	1.94	0.48
2:D:118:VAL:C	2:D:120:ASP:N	2.66	0.48
2:D:291:LEU:H	2:D:291:LEU:CD2	2.26	0.48
2:D:313:LEU:O	2:D:314:THR:CG2	2.61	0.48
2:D:394:GLN:O	2:D:398:MET:CB	2.59	0.48
2:D:430:SER:O	2:D:431:GLU:C	2.56	0.48
2:D:436:GLN:HE21	2:D:436:GLN:C	2.20	0.48
3:E:34:UNK:O	3:E:38:UNK:N	2.47	0.48
1:A:284:GLU:OE2	1:A:285:GLN:NE2	2.46	0.48
2:B:25:SER:HB3	2:B:369:ARG:HH22	1.79	0.48
2:B:154:ILE:O	2:B:156:LYS:N	2.46	0.48
2:B:239:THR:O	2:B:241:CYS:N	2.46	0.48
2:B:269:MET:SD	2:B:381:SER:HB3	2.54	0.48
2:B:289:PRO:CB	2:B:331:GLN:HE21	2.26	0.48
1:C:152:LEU:O	1:C:153:LEU:C	2.55	0.48
1:C:174:ALA:CB	1:C:176:GLN:HG2	2.43	0.48
1:C:344:VAL:HG12	1:C:345:ASP:OD2	2.13	0.48
2:D:311:ARG:HG3	2:D:311:ARG:NH1	2.29	0.48
3:E:35:UNK:O	3:E:37:UNK:C	2.61	0.48
1:A:96:LYS:O	1:A:98:ASP:N	2.46	0.48
1:A:179:THR:HB	1:A:182:VAL:HB	1.94	0.48
1:A:305:CYS:C	1:A:386:GLU:OE1	2.56	0.48
2:B:4:ILE:HG12	2:B:133:GLN:HG2	1.95	0.48
2:B:223:THR:HG23	2:B:225:GLY:C	2.38	0.48
2:B:407:TRP:HE1	1:C:257:THR:HA	1.79	0.48
1:C:10:GLY:O	1:C:11:GLN:C	2.56	0.48
1:C:77:GLU:OE2	1:C:83:TYR:CG	2.66	0.48
1:C:139:HIS:CG	1:C:140:SER:N	2.80	0.48
1:C:256:GLN:O	1:C:257:THR:C	2.57	0.48
1:C:393:HIS:O	1:C:395:PHE:N	2.38	0.48
1:C:395:PHE:C	1:C:395:PHE:HD1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ALA:HA	1:C:430:LYS:CB	2.43	0.48
2:D:79:ARG:HA	2:D:84:GLY:CA	2.44	0.48
2:D:163:ASP:OD1	2:D:164:ARG:HG2	2.13	0.48
2:D:198:THR:C	2:D:200:GLU:H	2.21	0.48
2:D:286:LEU:CD1	2:D:371:LEU:O	2.61	0.48
2:D:320:ARG:HB3	2:D:320:ARG:CZ	2.42	0.48
2:B:398:MET:C	2:B:400:ARG:N	2.57	0.48
1:C:101:ASN:CB	2:D:254:LYS:HD3	2.42	0.48
1:C:181:VAL:HG23	1:C:404:PHE:HB2	1.96	0.48
1:C:244:PHE:HE1	1:C:358:GLU:OE2	1.97	0.48
1:C:274:PRO:HG3	1:C:373:ARG:O	2.13	0.48
1:C:414:GLU:CA	1:C:417:GLU:HB2	2.44	0.48
2:D:51:VAL:HG22	2:D:245:PRO:HG2	1.96	0.48
2:D:90:ASP:OD1	2:D:91:ASN:ND2	2.47	0.48
2:D:179:ASP:CB	2:D:182:VAL:HG23	2.41	0.48
2:D:279:GLY:O	2:D:281:GLN:N	2.47	0.48
2:D:427:ASP:C	2:D:429:VAL:N	2.72	0.48
1:A:217:LEU:O	1:A:217:LEU:HG	2.12	0.48
1:A:408:TYR:HB2	1:A:418:PHE:HZ	1.79	0.48
2:B:137:LEU:CD2	2:B:154:ILE:HG13	2.43	0.48
1:C:33:ASP:O	1:C:34:GLY:C	2.57	0.48
1:C:174:ALA:C	1:C:176:GLN:N	2.71	0.48
1:C:229:ARG:HB3	1:C:366:GLY:O	2.14	0.48
2:D:132:LEU:HD22	2:D:164:ARG:NE	2.29	0.48
2:D:132:LEU:CB	2:D:164:ARG:HH21	2.21	0.48
2:D:383:ALA:C	2:D:385:GLN:H	2.20	0.48
3:E:48:UNK:C	3:E:50:UNK:N	2.75	0.48
1:A:26:LEU:CG	1:A:361:THR:OG1	2.62	0.48
1:A:139:HIS:CD2	1:A:146:GLY:O	2.66	0.48
1:A:176:GLN:OE1	1:A:210:TYR:CE1	2.67	0.48
1:A:213:CYS:O	1:A:219:ILE:HB	2.14	0.48
2:B:93:VAL:HG23	2:B:95:GLY:N	2.28	0.48
2:B:189:LEU:HA	2:B:192:HIS:CE1	2.48	0.48
2:B:223:THR:C	2:B:225:GLY:H	2.20	0.48
2:B:284:ARG:HB3	2:B:287:THR:OG1	2.14	0.48
2:B:397:ALA:O	2:B:398:MET:HB2	2.13	0.48
1:C:143:GLY:O	1:C:144:GLY:C	2.56	0.48
1:C:343:PHE:CD1	1:C:349:THR:HA	2.49	0.48
1:C:398:MET:HB2	1:C:403:ALA:HB2	1.96	0.48
2:D:158:ARG:HD3	2:D:197:ASN:HD22	1.67	0.48
2:D:284:ARG:HB2	2:D:290:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:H	1:A:21:TRP:CD1	2.32	0.48
1:A:104:ALA:CA	1:A:108:TYR:HD2	2.23	0.48
1:A:205:ASP:OD2	1:A:205:ASP:C	2.56	0.48
1:A:209:ILE:CG2	1:A:227:LEU:HG	2.44	0.48
1:A:220:GLU:HB3	1:A:221:ARG:CZ	2.43	0.48
1:A:239:THR:OG1	1:A:240:ALA:N	2.45	0.48
1:A:321:GLY:HA2	1:A:358:GLU:O	2.14	0.48
1:A:322:ASP:HA	1:A:357:TYR:CD1	2.42	0.48
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.27	0.48
2:B:182:VAL:O	2:B:182:VAL:CG1	2.53	0.48
2:B:212:ILE:HG21	2:B:230:LEU:HD21	1.96	0.48
1:C:103:TYR:CG	1:C:188:ILE:HD13	2.48	0.48
2:D:84:GLY:HA2	2:D:88:ARG:HH21	1.78	0.48
2:D:158:ARG:C	2:D:160:GLU:N	2.71	0.48
1:A:174:ALA:HB2	1:A:206:ASN:HB2	1.94	0.48
1:A:417:GLU:HB3	1:A:418:PHE:HE2	1.74	0.48
2:B:59:ASN:CA	2:B:64:ARG:HH21	2.23	0.48
2:B:148:GLY:HA2	2:B:151:THR:HG22	1.95	0.48
2:B:424:ASN:O	2:B:427:ASP:N	2.46	0.48
1:C:69:ASP:OD1	1:C:71:GLU:HG3	2.14	0.48
1:C:221:ARG:H	1:C:221:ARG:NE	2.11	0.48
1:C:256:GLN:HA	1:C:260:VAL:CG2	2.44	0.48
1:C:289:ALA:HA	1:C:292:THR:HG23	1.95	0.48
1:C:403:ALA:C	1:C:405:VAL:H	2.22	0.48
2:D:62:VAL:O	2:D:62:VAL:CG2	2.62	0.48
2:D:253:ARG:HG3	2:D:253:ARG:NH1	2.27	0.48
1:A:182:VAL:HG12	1:A:183:GLU:H	1.79	0.48
1:A:242:LEU:HB3	1:A:250:VAL:CG1	2.44	0.48
1:A:326:LYS:HG2	1:A:326:LYS:O	2.13	0.48
2:B:2:ARG:NH2	2:B:243:ARG:CA	2.76	0.48
2:B:22:GLU:HG3	2:B:83:PHE:CE1	2.49	0.48
2:B:59:ASN:CG	2:B:60:LYS:HD2	2.39	0.48
2:B:106:GLY:O	2:B:149:MET:HA	2.14	0.48
2:B:297:ASP:OD1	2:B:299:LYS:N	2.36	0.48
1:C:71:GLU:CD	4:C:502:GTP:O3G	2.57	0.48
1:C:180:ALA:O	1:C:182:VAL:N	2.47	0.48
1:C:296:PHE:HZ	1:C:317:LEU:HD21	1.79	0.48
2:D:16:ILE:HG12	2:D:17:GLY:N	2.24	0.48
2:D:262:PHE:HB3	2:D:263:PRO:CD	2.36	0.48
1:A:164:LYS:NZ	1:A:164:LYS:CB	2.77	0.47
1:A:311:LYS:CB	1:A:344:VAL:HG22	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:MET:CE	1:A:399:TYR:HE1	2.27	0.47
2:B:121:VAL:CG1	2:B:121:VAL:O	2.61	0.47
2:B:224:TYR:O	2:B:228:ASN:HB2	2.14	0.47
2:B:297:ASP:O	2:B:301:MET:HG2	2.13	0.47
2:B:320:ARG:HG2	2:B:320:ARG:NH1	2.29	0.47
1:C:346:TRP:HZ2	1:C:435:VAL:HB	1.79	0.47
2:D:18:ALA:O	2:D:22:GLU:OE2	2.32	0.47
1:A:7:ILE:HG21	1:A:122:ILE:CD1	2.40	0.47
1:A:36:MET:HA	1:A:36:MET:CE	2.36	0.47
1:A:115:ILE:HG12	1:A:149:PHE:HE2	1.80	0.47
1:A:355:ILE:N	1:A:355:ILE:CD1	2.76	0.47
2:B:429:VAL:O	2:B:433:GLN:HG2	2.13	0.47
1:C:103:TYR:N	1:C:185:TYR:CE1	2.82	0.47
1:C:255:PHE:HD1	1:C:259:LEU:HD12	1.79	0.47
1:C:284:GLU:OE2	1:C:285:GLN:NE2	2.46	0.47
1:C:296:PHE:CZ	1:C:317:LEU:HD21	2.48	0.47
2:D:3:GLU:O	2:D:133:GLN:N	2.38	0.47
2:D:63:PRO:C	2:D:65:ALA:H	2.20	0.47
1:A:185:TYR:O	1:A:186:ASN:C	2.56	0.47
1:A:209:ILE:CD1	1:A:209:ILE:H	2.28	0.47
1:A:428:LEU:C	1:A:430:LYS:H	2.22	0.47
2:B:14:ASN:O	2:B:18:ALA:N	2.47	0.47
2:B:79:ARG:O	2:B:79:ARG:HG2	2.13	0.47
1:C:128:GLN:OE1	1:C:128:GLN:HA	2.14	0.47
1:C:137:VAL:HB	1:C:154:MET:HE1	1.95	0.47
1:C:243:ARG:HA	1:C:243:ARG:NE	2.29	0.47
1:C:294:ALA:C	1:C:296:PHE:H	2.22	0.47
1:C:409:VAL:HA	1:C:414:GLU:CD	2.38	0.47
2:D:389:LYS:HA	2:D:392:SER:OG	2.14	0.47
1:A:189:LEU:HD13	1:A:189:LEU:C	2.40	0.47
1:A:217:LEU:HD23	1:A:219:ILE:CD1	2.44	0.47
1:A:296:PHE:CE2	1:A:377:MET:HE1	2.49	0.47
1:A:395:PHE:C	1:A:397:LEU:H	2.20	0.47
2:B:335:VAL:C	2:B:338:LYS:H	2.22	0.47
2:B:350:ASN:HD22	2:B:350:ASN:C	2.21	0.47
1:C:307:PRO:HA	1:C:383:ALA:CB	2.45	0.47
2:D:142:GLY:HA3	2:D:186:ASN:OD1	2.15	0.47
2:D:212:ILE:HG21	2:D:230:LEU:HD21	1.95	0.47
2:D:283:TYR:HD1	2:D:284:ARG:HH21	1.62	0.47
2:D:303:ALA:HB1	2:D:387:LEU:HD12	1.95	0.47
2:D:387:LEU:O	2:D:387:LEU:CD2	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PHE:CG	1:A:349:THR:HB	2.49	0.47
2:B:51:VAL:HG23	2:B:53:TYR:HB2	1.95	0.47
2:B:144:GLY:HA3	2:B:185:TYR:OH	2.14	0.47
2:B:154:ILE:HD11	2:B:168:THR:HG21	1.96	0.47
2:B:206:ASN:ND2	2:B:227:LEU:CD2	2.71	0.47
2:B:223:THR:HG23	2:B:225:GLY:H	1.79	0.47
2:B:235:MET:O	2:B:239:THR:OG1	2.31	0.47
2:B:242:LEU:O	2:B:243:ARG:NE	2.46	0.47
1:C:241:SER:HA	1:C:320:ARG:CZ	2.43	0.47
1:C:305:CYS:C	1:C:386:GLU:OE1	2.57	0.47
1:C:311:LYS:HD3	1:C:344:VAL:CG1	2.39	0.47
1:C:327:ASP:O	1:C:330:ALA:HB3	2.14	0.47
1:C:408:TYR:HB2	1:C:418:PHE:HZ	1.79	0.47
2:D:137:LEU:O	2:D:137:LEU:HG	2.15	0.47
2:D:200:GLU:CD	2:D:268:PHE:HE2	2.21	0.47
2:D:255:LEU:HD21	2:D:259:MET:HG3	1.95	0.47
2:D:315:VAL:HA	2:D:379:GLY:HA2	1.97	0.47
3:E:57:UNK:O	3:E:60:UNK:N	2.48	0.47
1:A:189:LEU:HD13	1:A:193:THR:CG2	2.44	0.47
1:A:217:LEU:HD23	1:A:219:ILE:HD12	1.95	0.47
1:A:433:GLU:C	1:A:435:VAL:N	2.72	0.47
2:B:119:LEU:CD1	2:B:123:ARG:NH2	2.78	0.47
2:B:133:GLN:NE2	2:B:252:LEU:N	2.59	0.47
2:B:174:SER:C	2:B:176:LYS:N	2.68	0.47
2:B:174:SER:O	2:B:176:LYS:N	2.47	0.47
2:B:178:SER:O	2:B:179:ASP:O	2.32	0.47
2:B:179:ASP:HB2	2:B:182:VAL:N	2.29	0.47
1:C:73:THR:HG23	1:C:74:VAL:H	1.79	0.47
1:C:137:VAL:HG21	1:C:154:MET:CE	2.45	0.47
1:C:187:SER:C	1:C:189:LEU:H	2.21	0.47
1:C:286:LEU:HB3	1:C:290:GLU:HB3	1.97	0.47
1:C:295:CYS:SG	1:C:295:CYS:O	2.73	0.47
2:D:115:VAL:HG21	2:D:152:LEU:HD21	1.95	0.47
2:D:139:HIS:HD2	2:D:139:HIS:O	1.98	0.47
2:D:158:ARG:HG3	2:D:159:GLU:HG3	1.97	0.47
2:D:181:VAL:C	2:D:184:PRO:HD2	2.40	0.47
2:D:202:TYR:HE1	2:D:378:ILE:HD12	1.76	0.47
1:A:137:VAL:HB	1:A:154:MET:HE1	1.97	0.47
1:A:154:MET:C	1:A:156:ARG:N	2.70	0.47
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.49	0.47
1:A:242:LEU:HD11	1:A:318:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:C	1:A:341:ILE:HD12	2.40	0.47
2:B:154:ILE:HG23	2:B:197:ASN:HB3	1.97	0.47
2:B:174:SER:HB2	2:B:206:ASN:C	2.39	0.47
2:B:286:LEU:CD1	2:B:371:LEU:O	2.63	0.47
2:B:383:ALA:C	2:B:385:GLN:H	2.23	0.47
1:C:35:GLN:HE22	1:C:88:HIS:CG	2.32	0.47
1:C:179:THR:HG22	1:C:180:ALA:O	2.15	0.47
1:C:190:THR:HG21	1:C:425:MET:SD	2.55	0.47
1:C:294:ALA:HA	1:C:297:GLU:HB2	1.96	0.47
1:C:312:TYR:O	1:C:344:VAL:HG23	2.14	0.47
1:C:368:LEU:HD12	1:C:368:LEU:N	2.29	0.47
1:C:385:ALA:HB1	1:C:429:GLU:HG3	1.97	0.47
2:D:19:LYS:HA	2:D:22:GLU:CG	2.45	0.47
2:D:81:GLY:N	2:D:82:PRO:HD2	2.29	0.47
2:D:93:VAL:CG2	2:D:94:PHE:N	2.78	0.47
2:D:124:LYS:HG3	2:D:124:LYS:O	2.15	0.47
2:D:271:GLY:O	2:D:272:PHE:O	2.33	0.47
2:D:295:MET:HG2	2:D:377:PHE:HD2	1.79	0.47
1:A:77:GLU:OE2	1:A:83:TYR:CG	2.68	0.47
1:A:86:LEU:HD13	1:A:89:PRO:HD3	1.97	0.47
1:A:184:PRO:O	1:A:188:ILE:HG13	2.14	0.47
1:A:311:LYS:CD	1:A:344:VAL:HG13	2.31	0.47
1:A:314:ALA:O	1:A:315:CYS:HB3	2.15	0.47
1:C:23:LEU:O	1:C:26:LEU:CD1	2.63	0.47
1:C:111:GLY:C	1:C:113:GLU:N	2.73	0.47
1:C:401:LYS:O	1:C:402:ARG:NE	2.47	0.47
2:D:126:SER:O	2:D:127:GLU:C	2.57	0.47
2:D:209:LEU:CB	2:D:227:LEU:HG	2.45	0.47
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.32	0.47
1:A:164:LYS:HZ2	1:A:164:LYS:CA	2.28	0.47
1:A:274:PRO:HG3	1:A:373:ARG:O	2.14	0.47
1:A:306:ASP:HB3	1:A:386:GLU:OE1	2.15	0.47
2:B:218:LYS:NZ	2:B:277:SER:HB3	2.29	0.47
2:B:243:ARG:HA	2:B:243:ARG:HD3	1.47	0.47
1:C:9:VAL:HG21	1:C:150:THR:HG22	1.96	0.47
1:C:16:ILE:CG2	1:C:17:GLY:N	2.67	0.47
1:C:20:CYS:O	1:C:24:TYR:N	2.34	0.47
1:C:243:ARG:NH1	1:C:250:VAL:HG13	2.19	0.47
1:C:256:GLN:HB3	1:C:260:VAL:CB	2.41	0.47
1:C:311:LYS:CD	1:C:344:VAL:HG22	2.44	0.47
1:C:419:SER:O	1:C:422:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:ILE:HD12	2:D:231:VAL:CG1	2.42	0.47
2:D:22:GLU:HG3	2:D:83:PHE:CE1	2.50	0.47
1:A:144:GLY:H	1:A:147:SER:HB3	1.76	0.47
1:A:177:VAL:HG11	2:B:349:ASN:CB	2.45	0.47
1:A:209:ILE:HG22	1:A:227:LEU:HG	1.97	0.47
1:A:294:ALA:C	1:A:296:PHE:H	2.23	0.47
2:B:178:SER:C	2:B:182:VAL:HB	2.35	0.47
2:B:220:THR:HB	1:C:326:LYS:CE	2.45	0.47
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.79	0.47
2:B:298:ALA:HB2	2:B:307:PRO:CD	2.45	0.47
1:C:73:THR:HA	1:C:76:ASP:HB2	1.96	0.47
1:C:416:GLY:O	1:C:420:GLU:HB3	2.14	0.47
1:C:431:ASP:C	1:C:433:GLU:H	2.23	0.47
2:D:4:ILE:HG12	2:D:133:GLN:HG2	1.97	0.47
2:D:58:GLY:O	2:D:64:ARG:CZ	2.63	0.47
2:D:141:LEU:HG	2:D:170:SER:HB3	1.97	0.47
2:D:186:ASN:O	2:D:189:LEU:HB2	2.15	0.47
2:D:203:CYS:SG	2:D:384:ILE:CD1	3.02	0.47
2:D:320:ARG:HH11	2:D:320:ARG:CG	2.25	0.47
2:D:357:ASP:CB	2:D:358:ILE:HD12	2.45	0.47
3:E:42:UNK:O	3:E:45:UNK:N	2.48	0.47
1:A:123:ARG:HA	1:A:161:TYR:OH	2.15	0.46
1:A:185:TYR:O	1:A:188:ILE:HD12	2.15	0.46
1:A:185:TYR:CE1	1:A:408:TYR:HE1	2.33	0.46
1:A:264:ARG:O	1:A:266:HIS:ND1	2.48	0.46
1:A:265:ALA:O	1:A:266:HIS:O	2.33	0.46
1:A:313:MET:HE3	1:A:346:TRP:HH2	1.81	0.46
1:A:362:VAL:O	1:A:370:LYS:NZ	2.48	0.46
2:B:123:ARG:C	2:B:125:GLU:N	2.72	0.46
2:B:191:VAL:O	2:B:191:VAL:CG1	2.58	0.46
1:C:164:LYS:HB2	1:C:164:LYS:NZ	2.29	0.46
1:C:192:HIS:C	1:C:194:THR:H	2.23	0.46
1:C:273:ALA:HB2	1:C:295:CYS:HA	1.97	0.46
1:C:343:PHE:CG	1:C:349:THR:HB	2.50	0.46
1:C:385:ALA:HB2	1:C:432:TYR:CD2	2.47	0.46
2:D:84:GLY:C	2:D:85:GLN:HG2	2.39	0.46
2:D:238:VAL:HG22	2:D:376:THR:HG21	1.96	0.46
3:E:61:UNK:C	3:E:63:UNK:N	2.78	0.46
2:B:1:MET:C	2:B:3:GLU:N	2.73	0.46
2:B:320:ARG:HH11	2:B:320:ARG:CG	2.25	0.46
1:C:26:LEU:HG	1:C:361:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TYR:CG	1:C:173:PRO:HD2	2.50	0.46
2:D:3:GLU:HG2	2:D:58:GLY:O	2.15	0.46
2:D:335:VAL:C	2:D:338:LYS:H	2.23	0.46
2:D:401:ARG:O	2:D:402:LYS:HG3	2.15	0.46
1:A:132:LEU:O	1:A:133:GLN:CB	2.61	0.46
1:A:317:LEU:HD23	1:A:377:MET:HB2	1.96	0.46
1:A:402:ARG:NH1	2:B:346:TRP:CD2	2.83	0.46
2:B:1:MET:C	2:B:3:GLU:H	2.20	0.46
2:B:75:MET:SD	2:B:79:ARG:CZ	3.02	0.46
2:B:114:LEU:HD12	2:B:114:LEU:HA	1.78	0.46
2:B:142:GLY:HA2	2:B:185:TYR:CB	2.39	0.46
1:C:9:VAL:O	1:C:9:VAL:CG2	2.63	0.46
1:C:68:VAL:HG13	1:C:68:VAL:O	2.14	0.46
1:C:161:TYR:O	1:C:162:GLY:C	2.59	0.46
2:D:60:LYS:H	2:D:60:LYS:CD	2.28	0.46
2:D:243:ARG:HD3	2:D:243:ARG:HA	1.52	0.46
2:D:313:LEU:O	2:D:314:THR:HG23	2.15	0.46
1:A:33:ASP:O	1:A:34:GLY:C	2.59	0.46
1:A:181:VAL:O	1:A:185:TYR:CD2	2.69	0.46
1:A:243:ARG:NH1	1:A:250:VAL:CG1	2.72	0.46
1:A:275:VAL:O	1:A:275:VAL:CG1	2.63	0.46
1:A:403:ALA:C	1:A:405:VAL:H	2.23	0.46
2:B:103:TRP:N	2:B:185:TYR:OH	2.48	0.46
2:B:224:TYR:C	2:B:226:ASP:H	2.22	0.46
2:B:296:PHE:CE1	2:B:332:MET:HE1	2.48	0.46
2:B:313:LEU:O	2:B:314:THR:CG2	2.64	0.46
2:B:389:LYS:HA	2:B:392:SER:OG	2.14	0.46
1:C:24:TYR:HA	1:C:26:LEU:CD1	2.46	0.46
1:C:101:ASN:OD1	2:D:254:LYS:CD	2.59	0.46
1:C:269:LEU:C	1:C:269:LEU:CD1	2.84	0.46
1:C:273:ALA:HB2	1:C:295:CYS:CB	2.42	0.46
2:D:3:GLU:OE2	2:D:128:SER:O	2.33	0.46
2:D:132:LEU:H	2:D:164:ARG:HH21	1.62	0.46
2:D:137:LEU:CD2	2:D:154:ILE:HG13	2.46	0.46
1:A:122:ILE:HG22	1:A:123:ARG:N	2.30	0.46
1:A:209:ILE:HD12	1:A:209:ILE:H	1.79	0.46
1:A:237:SER:C	1:A:241:SER:CB	2.88	0.46
1:A:388:TRP:CZ3	1:A:428:LEU:HD13	2.50	0.46
1:C:344:VAL:CG1	1:C:345:ASP:N	2.75	0.46
1:C:398:MET:CE	1:C:399:TYR:HE1	2.29	0.46
2:D:286:LEU:HA	2:D:290:GLU:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:ARG:NE	2:D:357:ASP:CB	2.74	0.46
2:D:350:ASN:ND2	2:D:350:ASN:H	2.13	0.46
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.51	0.46
1:A:287:SER:O	1:A:289:ALA:N	2.49	0.46
2:B:60:LYS:H	2:B:60:LYS:HD2	1.79	0.46
2:B:73:GLY:O	2:B:78:VAL:HG21	2.16	0.46
2:B:320:ARG:HB3	2:B:320:ARG:CZ	2.45	0.46
1:C:69:ASP:CG	1:C:71:GLU:H	2.23	0.46
1:C:122:ILE:O	1:C:125:LEU:N	2.48	0.46
1:C:265:ALA:O	1:C:266:HIS:O	2.33	0.46
1:C:363:VAL:HG22	1:C:367:ASP:CG	2.41	0.46
2:D:148:GLY:CA	2:D:151:THR:HG22	2.46	0.46
2:D:239:THR:HB	2:D:240:THR:H	1.42	0.46
1:A:23:LEU:O	1:A:26:LEU:CD1	2.63	0.46
1:A:112:LYS:HZ1	3:E:12:UNK:CB	2.29	0.46
1:A:341:ILE:HD12	1:A:341:ILE:N	2.30	0.46
1:A:416:GLY:O	1:A:420:GLU:HB3	2.16	0.46
2:B:137:LEU:HD23	2:B:154:ILE:CD1	2.45	0.46
2:B:232:SER:C	2:B:234:THR:H	2.22	0.46
2:B:313:LEU:C	2:B:314:THR:HG23	2.41	0.46
1:C:121:ARG:O	1:C:122:ILE:C	2.57	0.46
1:C:149:PHE:CD2	1:C:149:PHE:O	2.69	0.46
1:C:159:VAL:HG21	3:E:56:UNK:HA	1.98	0.46
1:C:245:ASP:O	1:C:249:ASN:OD1	2.33	0.46
2:D:18:ALA:O	2:D:21:TRP:N	2.46	0.46
2:D:223:THR:HG23	2:D:225:GLY:C	2.41	0.46
2:D:378:ILE:O	2:D:378:ILE:HG22	2.16	0.46
1:A:398:MET:HB2	1:A:403:ALA:HB2	1.96	0.46
1:A:409:VAL:C	1:A:411:GLU:N	2.73	0.46
1:A:419:SER:O	1:A:420:GLU:C	2.59	0.46
2:B:194:LEU:HD12	2:B:428:LEU:HD21	1.97	0.46
2:B:289:PRO:O	2:B:292:THR:OG1	2.32	0.46
2:B:308:ARG:HG3	2:B:342:TYR:CZ	2.51	0.46
2:B:315:VAL:HA	2:B:379:GLY:HA2	1.98	0.46
2:B:427:ASP:C	2:B:429:VAL:N	2.73	0.46
1:C:144:GLY:O	1:C:145:THR:C	2.59	0.46
1:C:159:VAL:CG2	3:E:56:UNK:HA	2.46	0.46
1:C:166:LYS:HD2	1:C:197:HIS:HD2	1.81	0.46
1:C:171:ILE:CG2	4:C:502:GTP:HN22	2.29	0.46
1:C:182:VAL:HG12	1:C:183:GLU:N	2.31	0.46
1:C:251:ASP:O	1:C:254:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:PRO:HB3	1:C:291:ILE:CD1	2.45	0.46
2:D:20:PHE:O	2:D:23:VAL:N	2.48	0.46
2:D:174:SER:O	2:D:176:LYS:N	2.49	0.46
2:D:291:LEU:HD22	2:D:291:LEU:N	2.30	0.46
2:D:331:GLN:OE1	2:D:331:GLN:HA	2.15	0.46
2:D:350:ASN:ND2	2:D:350:ASN:N	2.62	0.46
1:A:103:TYR:CD1	1:A:188:ILE:HD13	2.51	0.46
1:A:149:PHE:CD2	1:A:149:PHE:O	2.69	0.46
1:A:206:ASN:O	1:A:210:TYR:CD2	2.69	0.46
1:A:225:THR:HA	1:A:228:ASN:HB2	1.98	0.46
1:A:409:VAL:HG22	1:A:414:GLU:CD	2.40	0.46
2:B:236:SER:C	2:B:238:VAL:H	2.24	0.46
2:B:279:GLY:O	2:B:281:GLN:N	2.49	0.46
2:B:398:MET:HG3	1:C:346:TRP:O	2.16	0.46
2:B:428:LEU:HD12	2:B:428:LEU:N	2.31	0.46
1:C:175:PRO:HB2	1:C:207:GLU:OE2	2.16	0.46
2:D:169:PHE:CG	2:D:235:MET:SD	3.09	0.46
2:D:215:ARG:NE	2:D:215:ARG:CA	2.78	0.46
2:D:238:VAL:HG21	2:D:378:ILE:HD11	1.98	0.46
1:A:30:ILE:C	1:A:30:ILE:HD12	2.40	0.46
1:A:306:ASP:OD1	1:A:309:HIS:NE2	2.49	0.46
1:A:335:ILE:O	1:A:336:LYS:C	2.59	0.46
1:A:371:VAL:CG1	1:A:372:GLN:N	2.78	0.46
1:A:371:VAL:HG11	1:A:373:ARG:O	2.15	0.46
2:B:6:HIS:ND1	2:B:21:TRP:HZ2	2.14	0.46
2:B:11:GLN:OE1	2:B:73:GLY:HA3	2.15	0.46
2:B:119:LEU:HD13	2:B:123:ARG:CZ	2.46	0.46
2:B:238:VAL:HG21	2:B:378:ILE:HD11	1.98	0.46
2:B:269:MET:HE2	2:B:301:MET:CE	2.45	0.46
2:B:271:GLY:C	2:B:272:PHE:O	2.58	0.46
2:B:283:TYR:HD1	2:B:284:ARG:HH21	1.64	0.46
1:C:42:ILE:HD12	1:C:43:GLY:H	1.81	0.46
1:C:184:PRO:CG	1:C:399:TYR:CZ	2.98	0.46
1:C:331:ALA:O	1:C:335:ILE:HG23	2.15	0.46
1:C:395:PHE:C	1:C:397:LEU:H	2.23	0.46
1:C:428:LEU:C	1:C:430:LYS:N	2.68	0.46
2:D:59:ASN:CG	2:D:60:LYS:HD2	2.41	0.46
2:D:122:VAL:CG1	2:D:123:ARG:N	2.78	0.46
2:D:253:ARG:C	2:D:255:LEU:H	2.22	0.46
2:D:416:MET:HA	2:D:419:THR:OG1	2.16	0.46
1:A:21:TRP:CD1	1:A:21:TRP:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:CD	1:A:97:GLU:H	2.23	0.45
1:A:210:TYR:CE2	1:A:227:LEU:CD2	2.98	0.45
1:A:242:LEU:O	1:A:250:VAL:HG12	2.16	0.45
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.35	0.45
1:A:276:ILE:CG1	1:A:282:TYR:CD2	2.98	0.45
1:A:339:ARG:C	1:A:339:ARG:CD	2.75	0.45
2:B:287:THR:CB	2:B:289:PRO:HD2	2.41	0.45
1:C:23:LEU:C	1:C:25:CYS:N	2.73	0.45
1:C:84:ARG:C	1:C:85:GLN:HG2	2.41	0.45
1:C:104:ALA:CA	1:C:108:TYR:HD2	2.23	0.45
1:C:316:CYS:HB2	1:C:352:LYS:CB	2.24	0.45
2:D:20:PHE:HZ	2:D:239:THR:HG21	1.81	0.45
2:D:226:ASP:C	2:D:228:ASN:N	2.74	0.45
2:D:290:GLU:HG2	2:D:294:GLN:HB2	1.97	0.45
2:D:351:VAL:O	2:D:352:LYS:HG3	2.17	0.45
2:D:351:VAL:HG12	2:D:352:LYS:N	2.32	0.45
1:A:244:PHE:H	1:A:244:PHE:HD2	1.63	0.45
1:A:280:LYS:O	1:A:282:TYR:CD2	2.69	0.45
2:B:81:GLY:N	2:B:82:PRO:HD2	2.32	0.45
2:B:103:TRP:C	2:B:105:LYS:N	2.74	0.45
2:B:154:ILE:HG23	2:B:166:MET:HE3	1.98	0.45
2:B:158:ARG:HB2	2:B:197:ASN:HD22	1.81	0.45
2:B:208:ALA:HB2	2:B:304:ALA:CB	2.47	0.45
2:B:211:ASP:O	2:B:215:ARG:HB2	2.16	0.45
2:B:247:GLN:OE1	2:B:356:CYS:HA	2.16	0.45
1:C:206:ASN:O	1:C:210:TYR:CD2	2.69	0.45
2:D:58:GLY:O	2:D:64:ARG:NH2	2.49	0.45
2:D:119:LEU:HD13	2:D:123:ARG:NH2	2.30	0.45
2:D:298:ALA:HB2	2:D:307:PRO:CD	2.46	0.45
1:A:74:VAL:CG1	1:A:75:ILE:N	2.78	0.45
1:A:242:LEU:O	1:A:250:VAL:CG1	2.64	0.45
1:A:255:PHE:HD1	1:A:259:LEU:HD12	1.81	0.45
2:B:5:VAL:O	2:B:5:VAL:HG12	2.17	0.45
2:B:313:LEU:O	2:B:314:THR:HG23	2.16	0.45
1:C:139:HIS:CD2	1:C:146:GLY:O	2.69	0.45
1:C:197:HIS:CG	1:C:198:SER:N	2.83	0.45
2:D:14:ASN:O	2:D:18:ALA:N	2.46	0.45
2:D:178:SER:C	2:D:182:VAL:HB	2.35	0.45
2:D:247:GLN:OE1	2:D:356:CYS:HA	2.16	0.45
2:D:276:THR:HG21	2:D:281:GLN:CG	2.47	0.45
1:A:221:ARG:HA	1:A:222:PRO:HD2	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:O	1:A:239:THR:O	2.35	0.45
1:A:414:GLU:HA	1:A:417:GLU:HB2	1.98	0.45
1:C:5:ILE:O	1:C:136:SER:N	2.48	0.45
1:C:99:ALA:O	1:C:100:ALA:HB2	2.17	0.45
1:C:189:LEU:HD13	1:C:193:THR:CG2	2.45	0.45
1:C:416:GLY:C	1:C:418:PHE:H	2.19	0.45
2:D:276:THR:HG21	2:D:281:GLN:CB	2.47	0.45
2:D:350:ASN:C	2:D:351:VAL:CG2	2.89	0.45
2:D:399:PHE:HE2	2:D:404:PHE:HB3	1.80	0.45
3:E:10:UNK:C	3:E:12:UNK:N	2.71	0.45
1:A:179:THR:HB	1:A:182:VAL:CG2	2.47	0.45
1:A:277:SER:O	1:A:278:ALA:CB	2.62	0.45
1:A:380:ASN:O	1:A:380:ASN:CG	2.60	0.45
2:B:51:VAL:HG13	2:B:245:PRO:HB2	1.99	0.45
2:B:60:LYS:H	2:B:60:LYS:CD	2.29	0.45
2:B:87:PHE:O	2:B:89:PRO:N	2.49	0.45
2:B:403:ALA:O	2:B:404:PHE:HB2	2.16	0.45
2:B:424:ASN:O	2:B:427:ASP:HB2	2.17	0.45
1:C:67:PHE:O	1:C:92:LEU:HA	2.16	0.45
1:C:119:LEU:HD22	1:C:156:ARG:HE	1.81	0.45
1:C:197:HIS:CE1	1:C:198:SER:HB3	2.52	0.45
1:C:365:GLY:O	1:C:368:LEU:HD11	2.17	0.45
1:C:413:MET:HE2	1:C:413:MET:N	2.24	0.45
2:D:2:ARG:O	2:D:2:ARG:HG2	2.17	0.45
2:D:427:ASP:O	2:D:428:LEU:C	2.59	0.45
1:A:431:ASP:C	1:A:433:GLU:H	2.22	0.45
2:B:124:LYS:HG3	2:B:124:LYS:O	2.15	0.45
2:B:176:LYS:HD2	2:B:210:TYR:CE1	2.52	0.45
2:B:272:PHE:CE1	2:B:274:PRO:HG2	2.51	0.45
1:C:115:ILE:HG12	1:C:149:PHE:HE2	1.80	0.45
1:C:287:SER:O	1:C:289:ALA:N	2.50	0.45
1:C:332:ILE:HG23	1:C:351:PHE:CE2	2.52	0.45
2:D:59:ASN:HA	2:D:60:LYS:NZ	2.32	0.45
2:D:62:VAL:O	2:D:63:PRO:C	2.59	0.45
2:D:140:SER:O	2:D:147:SER:OG	2.33	0.45
2:D:211:ASP:O	2:D:215:ARG:N	2.50	0.45
2:D:234:THR:O	2:D:238:VAL:HG23	2.17	0.45
2:D:311:ARG:NE	2:D:436:GLN:O	2.50	0.45
2:D:405:LEU:HD22	2:D:405:LEU:O	2.16	0.45
1:A:327:ASP:O	1:A:330:ALA:HB3	2.16	0.45
2:B:133:GLN:CG	2:B:252:LEU:HD22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:GLN:HE21	2:B:436:GLN:C	2.23	0.45
1:C:16:ILE:HG22	1:C:17:GLY:H	1.79	0.45
1:C:174:ALA:C	1:C:176:GLN:H	2.25	0.45
1:C:236:SER:C	1:C:238:ILE:N	2.75	0.45
1:C:371:VAL:HG12	1:C:372:GLN:H	1.81	0.45
1:C:398:MET:HE2	1:C:399:TYR:CE1	2.52	0.45
1:C:408:TYR:O	1:C:414:GLU:HG3	2.17	0.45
2:D:206:ASN:ND2	5:D:503:GDP:N2	2.64	0.45
2:D:334:ASN:O	2:D:338:LYS:N	2.50	0.45
1:A:171:ILE:HG21	4:A:500:GTP:HN22	1.81	0.45
1:A:206:ASN:CB	1:A:210:TYR:HE2	2.28	0.45
1:A:344:VAL:CG1	1:A:345:ASP:N	2.76	0.45
2:B:102:ASN:HB3	2:B:105:LYS:CG	2.47	0.45
1:C:164:LYS:HB2	1:C:164:LYS:HZ2	1.80	0.45
1:C:172:TYR:H	1:C:205:ASP:H	1.65	0.45
1:C:344:VAL:HG12	1:C:345:ASP:H	1.81	0.45
1:C:355:ILE:N	1:C:355:ILE:CD1	2.79	0.45
2:D:80:SER:C	2:D:82:PRO:CD	2.86	0.45
2:D:209:LEU:HD21	2:D:302:MET:HG3	1.98	0.45
2:D:290:GLU:O	2:D:291:LEU:C	2.59	0.45
1:A:155:GLU:OE2	1:A:196:GLU:HB3	2.17	0.45
2:B:198:THR:O	2:B:199:ASP:C	2.60	0.45
2:B:198:THR:C	2:B:200:GLU:H	2.25	0.45
2:B:298:ALA:HA	2:B:301:MET:CG	2.47	0.45
1:C:31:GLN:CB	1:C:32:PRO:CD	2.94	0.45
1:C:171:ILE:HG21	4:C:502:GTP:N3	2.32	0.45
1:C:223:THR:O	1:C:226:ASN:N	2.50	0.45
1:C:343:PHE:CD2	1:C:349:THR:HB	2.52	0.45
1:C:396:ASP:O	1:C:400:ALA:HB3	2.17	0.45
2:D:85:GLN:HA	2:D:88:ARG:HG2	1.98	0.45
2:D:158:ARG:HB2	2:D:197:ASN:ND2	2.30	0.45
2:D:403:ALA:HB1	2:D:405:LEU:HD12	1.99	0.45
1:A:5:ILE:HG22	1:A:6:SER:N	2.31	0.45
1:A:83:TYR:O	1:A:84:ARG:HB2	2.17	0.45
1:A:171:ILE:N	1:A:171:ILE:CD1	2.78	0.45
1:A:255:PHE:CD1	1:A:259:LEU:HD12	2.52	0.45
1:A:346:TRP:CD1	1:A:346:TRP:N	2.74	0.45
1:A:351:PHE:HB3	1:A:352:LYS:H	1.63	0.45
2:B:115:VAL:HG21	2:B:152:LEU:CD2	2.47	0.45
2:B:217:LEU:CG	2:B:218:LYS:N	2.75	0.45
2:B:351:VAL:HG12	2:B:352:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:PHE:C	2:B:390:ARG:N	2.75	0.45
1:C:101:ASN:O	1:C:101:ASN:ND2	2.44	0.45
1:C:101:ASN:ND2	1:C:185:TYR:OH	2.50	0.45
1:C:197:HIS:CD2	1:C:198:SER:HB3	2.52	0.45
1:C:402:ARG:O	1:C:405:VAL:HG12	2.17	0.45
2:D:388:PHE:C	2:D:390:ARG:H	2.24	0.45
3:E:3:UNK:C	3:E:5:UNK:N	2.80	0.45
1:A:125:LEU:C	1:A:127:ASP:H	2.25	0.44
1:A:284:GLU:O	1:A:285:GLN:CG	2.65	0.44
1:A:407:TRP:C	1:A:409:VAL:N	2.67	0.44
2:B:59:ASN:CA	2:B:60:LYS:HZ3	2.29	0.44
2:B:395:PHE:C	2:B:397:ALA:N	2.73	0.44
1:C:185:TYR:HA	1:C:188:ILE:CD1	2.33	0.44
1:C:209:ILE:O	1:C:211:ASP:N	2.49	0.44
2:D:19:LYS:NZ	2:D:77:SER:O	2.49	0.44
2:D:73:GLY:C	2:D:75:MET:H	2.24	0.44
2:D:98:GLY:H	2:D:110:GLU:CD	2.25	0.44
2:D:178:SER:O	2:D:179:ASP:O	2.35	0.44
1:A:88:HIS:HA	1:A:89:PRO:HD2	1.87	0.44
1:A:187:SER:C	1:A:189:LEU:N	2.74	0.44
2:B:51:VAL:O	2:B:53:TYR:N	2.50	0.44
2:B:242:LEU:O	2:B:243:ARG:CD	2.64	0.44
2:B:255:LEU:C	2:B:257:VAL:N	2.75	0.44
1:C:86:LEU:HD13	1:C:89:PRO:HD3	1.99	0.44
1:C:154:MET:C	1:C:156:ARG:N	2.72	0.44
2:D:102:ASN:HA	2:D:408:TYR:HE1	1.82	0.44
2:D:155:SER:HB2	2:D:196:GLU:HG2	1.98	0.44
2:D:185:TYR:O	2:D:188:THR:HG22	2.16	0.44
2:D:287:THR:CB	2:D:289:PRO:HD2	2.39	0.44
1:A:9:VAL:O	1:A:9:VAL:CG2	2.66	0.44
1:A:24:TYR:HA	1:A:26:LEU:HD12	1.99	0.44
1:A:100:ALA:CB	1:A:105:ARG:HD2	2.47	0.44
1:A:137:VAL:HG21	1:A:154:MET:SD	2.57	0.44
1:A:169:PHE:HE1	1:A:238:ILE:CD1	2.30	0.44
1:A:276:ILE:HD12	1:A:277:SER:H	1.79	0.44
2:B:2:ARG:CZ	2:B:243:ARG:HD3	2.47	0.44
2:B:184:PRO:CB	2:B:399:PHE:CZ	3.00	0.44
2:B:226:ASP:C	2:B:228:ASN:N	2.70	0.44
1:C:218:ASP:CG	1:C:219:ILE:N	2.75	0.44
1:C:331:ALA:O	1:C:333:ALA:N	2.51	0.44
2:D:25:SER:HB3	2:D:369:ARG:NH2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ARG:CB	2:D:89:PRO:HD3	2.34	0.44
2:D:154:ILE:HG23	2:D:166:MET:HE3	1.99	0.44
2:D:280:SER:O	2:D:282:GLN:N	2.50	0.44
2:D:284:ARG:O	2:D:287:THR:N	2.51	0.44
1:A:345:ASP:C	1:A:347:CYS:N	2.73	0.44
2:B:20:PHE:C	2:B:22:GLU:H	2.25	0.44
2:B:138:THR:HG22	2:B:139:HIS:N	2.32	0.44
2:B:298:ALA:HB2	2:B:307:PRO:HD2	2.00	0.44
2:B:308:ARG:NH2	2:B:342:TYR:CG	2.83	0.44
2:B:409:THR:O	2:B:410:GLY:C	2.60	0.44
1:C:11:GLN:OE1	4:C:502:GTP:O1B	2.35	0.44
1:C:16:ILE:O	1:C:19:ALA:N	2.41	0.44
1:C:45:GLY:C	1:C:46:ASP:OD2	2.60	0.44
1:C:273:ALA:CB	1:C:295:CYS:HB2	2.45	0.44
1:C:363:VAL:HG22	1:C:367:ASP:OD2	2.18	0.44
1:C:380:ASN:O	1:C:380:ASN:OD1	2.35	0.44
2:D:139:HIS:O	2:D:170:SER:HA	2.17	0.44
2:D:151:THR:HG21	2:D:189:LEU:HD21	1.99	0.44
2:D:236:SER:C	2:D:238:VAL:H	2.25	0.44
2:D:428:LEU:O	2:D:429:VAL:C	2.60	0.44
1:A:139:HIS:NE2	1:A:150:THR:CG2	2.79	0.44
1:A:214:ARG:CA	1:A:218:ASP:O	2.61	0.44
1:A:344:VAL:HG12	1:A:345:ASP:OD2	2.17	0.44
2:B:4:ILE:N	2:B:58:GLY:HA2	2.33	0.44
2:B:63:PRO:C	2:B:65:ALA:N	2.74	0.44
2:B:338:LYS:O	2:B:340:SER:N	2.43	0.44
2:B:381:SER:C	2:B:383:ALA:N	2.74	0.44
2:B:407:TRP:HE1	1:C:257:THR:CA	2.31	0.44
1:C:7:ILE:HG13	1:C:7:ILE:O	2.18	0.44
1:C:67:PHE:O	1:C:75:ILE:HD11	2.17	0.44
1:C:96:LYS:HE3	1:C:96:LYS:HB2	1.77	0.44
1:C:188:ILE:HG13	1:C:188:ILE:H	1.62	0.44
1:C:189:LEU:HD13	1:C:189:LEU:C	2.42	0.44
1:C:344:VAL:CG1	1:C:345:ASP:H	2.30	0.44
1:C:347:CYS:O	1:C:349:THR:N	2.50	0.44
1:C:424:ASP:C	1:C:426:ALA:H	2.26	0.44
2:D:95:GLY:O	2:D:96:GLN:HB3	2.18	0.44
2:D:187:ALA:HB2	2:D:391:ILE:CG2	2.48	0.44
2:D:344:VAL:O	2:D:346:TRP:CD1	2.70	0.44
2:D:419:THR:C	2:D:422:GLU:H	2.24	0.44
1:A:69:ASP:CG	1:A:71:GLU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:SER:C	1:A:241:SER:HB2	2.43	0.44
1:A:414:GLU:CG	1:A:415:GLU:H	2.13	0.44
2:B:2:ARG:CZ	2:B:243:ARG:CD	2.96	0.44
2:B:12:CYS:HB2	5:B:501:GDP:PA	2.58	0.44
2:B:58:GLY:O	2:B:64:ARG:NH2	2.50	0.44
2:B:59:ASN:ND2	2:B:60:LYS:H	2.16	0.44
2:B:271:GLY:O	2:B:377:PHE:HB2	2.18	0.44
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.48	0.44
2:B:286:LEU:CG	2:B:373:MET:HE3	2.43	0.44
2:B:295:MET:HE2	2:B:296:PHE:CD1	2.53	0.44
2:B:334:ASN:O	2:B:338:LYS:N	2.51	0.44
2:B:407:TRP:HE1	1:C:257:THR:N	2.15	0.44
1:C:326:LYS:O	1:C:326:LYS:HG2	2.16	0.44
1:C:340:THR:O	1:C:342:GLN:HG2	2.17	0.44
1:C:398:MET:C	1:C:403:ALA:HB2	2.43	0.44
2:D:174:SER:HB2	2:D:206:ASN:C	2.43	0.44
2:D:179:ASP:HB2	2:D:182:VAL:CB	2.47	0.44
3:E:13:UNK:C	3:E:15:UNK:N	2.77	0.44
1:A:142:GLY:HA2	1:A:185:TYR:HB2	1.98	0.44
2:B:6:HIS:HD2	2:B:136:GLN:CD	2.25	0.44
2:B:103:TRP:O	2:B:105:LYS:N	2.50	0.44
2:B:182:VAL:HG11	5:B:501:GDP:O3'	2.17	0.44
2:B:283:TYR:O	2:B:290:GLU:OE1	2.36	0.44
2:B:303:ALA:HB1	2:B:387:LEU:HD13	1.99	0.44
1:C:177:VAL:HG21	2:D:349:ASN:HB2	1.99	0.44
1:C:227:LEU:N	1:C:227:LEU:CD1	2.81	0.44
1:C:259:LEU:HD21	1:C:378:LEU:CB	2.45	0.44
1:C:312:TYR:H	1:C:312:TYR:HD1	1.65	0.44
2:D:358:ILE:HD12	2:D:358:ILE:N	2.21	0.44
3:E:71:UNK:O	3:E:74:UNK:N	2.51	0.44
1:A:289:ALA:HA	1:A:292:THR:HG23	1.96	0.44
1:A:395:PHE:C	1:A:395:PHE:HD1	2.24	0.44
2:B:121:VAL:O	2:B:121:VAL:HG12	2.16	0.44
2:B:165:ILE:HG13	2:B:253:ARG:CG	2.48	0.44
2:B:274:PRO:HB2	2:B:371:LEU:HD11	1.99	0.44
2:B:320:ARG:NH1	2:B:320:ARG:CG	2.79	0.44
1:C:277:SER:O	1:C:368:LEU:HB3	2.17	0.44
1:C:288:VAL:HA	1:C:373:ARG:CD	2.47	0.44
2:D:51:VAL:HG23	2:D:53:TYR:HB2	1.99	0.44
2:D:273:ALA:H	2:D:274:PRO:HD2	1.83	0.44
1:A:126:ALA:O	1:A:132:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG13	1:A:181:VAL:O	2.18	0.44
1:A:184:PRO:HB2	1:A:399:TYR:CE2	2.53	0.44
2:B:179:ASP:HB2	2:B:182:VAL:CB	2.48	0.44
2:B:324:SER:HB3	2:B:327:GLU:OE1	2.18	0.44
2:B:428:LEU:O	2:B:432:TYR:HB2	2.18	0.44
1:C:206:ASN:CB	1:C:210:TYR:HE2	2.28	0.44
1:C:244:PHE:CZ	1:C:358:GLU:OE1	2.71	0.44
1:C:284:GLU:O	1:C:285:GLN:CG	2.65	0.44
1:C:349:THR:O	1:C:349:THR:OG1	2.29	0.44
1:C:402:ARG:HG2	1:C:403:ALA:N	2.24	0.44
2:D:75:MET:SD	2:D:79:ARG:CZ	3.06	0.44
2:D:106:GLY:HA2	2:D:111:GLY:HA3	1.99	0.44
2:D:224:TYR:C	2:D:226:ASP:H	2.25	0.44
2:D:264:ARG:O	2:D:265:LEU:C	2.60	0.44
2:D:380:ASN:C	2:D:380:ASN:ND2	2.75	0.44
2:D:381:SER:O	2:D:383:ALA:N	2.51	0.44
2:D:427:ASP:O	2:D:430:SER:N	2.51	0.44
1:A:67:PHE:O	1:A:92:LEU:HA	2.18	0.43
1:A:411:GLU:OE2	1:A:411:GLU:O	2.36	0.43
2:B:150:GLY:C	2:B:152:LEU:N	2.76	0.43
2:B:322:ARG:NE	2:B:357:ASP:CB	2.81	0.43
1:C:320:ARG:CB	1:C:374:ALA:HB3	2.40	0.43
1:C:398:MET:O	1:C:401:LYS:N	2.42	0.43
2:D:185:TYR:HB3	2:D:186:ASN:H	1.56	0.43
2:D:293:GLN:C	2:D:295:MET:N	2.76	0.43
2:D:431:GLU:HA	2:D:434:GLN:HE21	1.83	0.43
1:A:306:ASP:O	1:A:308:ARG:N	2.51	0.43
1:A:307:PRO:CB	1:A:381:THR:HG21	2.48	0.43
2:B:3:GLU:HG2	2:B:58:GLY:O	2.18	0.43
2:B:137:LEU:O	2:B:168:THR:HA	2.18	0.43
2:B:272:PHE:HD1	2:B:275:LEU:CD2	2.31	0.43
2:B:333:LEU:O	2:B:336:GLN:HB3	2.18	0.43
1:C:3:GLU:O	1:C:3:GLU:HG3	2.18	0.43
1:C:91:GLN:HG2	1:C:92:LEU:CD1	2.47	0.43
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.53	0.43
1:C:132:LEU:HB3	1:C:133:GLN:H	1.63	0.43
1:C:171:ILE:HG21	4:C:502:GTP:HN22	1.82	0.43
2:D:18:ALA:C	2:D:20:PHE:N	2.60	0.43
2:D:51:VAL:N	2:D:245:PRO:CB	2.81	0.43
2:D:88:ARG:HA	2:D:91:ASN:ND2	2.33	0.43
2:D:133:GLN:NE2	2:D:252:LEU:CB	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ASP:CG	2:D:253:ARG:H	2.25	0.43
2:D:305:CYS:O	2:D:383:ALA:HB1	2.18	0.43
2:D:308:ARG:NH2	2:D:342:TYR:CB	2.81	0.43
1:A:303:VAL:O	1:A:305:CYS:N	2.51	0.43
1:A:402:ARG:HG2	1:A:403:ALA:N	2.22	0.43
2:B:19:LYS:HA	2:B:22:GLU:OE2	2.18	0.43
2:B:139:HIS:O	2:B:170:SER:HA	2.17	0.43
2:B:216:THR:C	2:B:217:LEU:O	2.62	0.43
2:B:284:ARG:HB2	2:B:290:GLU:OE1	2.17	0.43
1:C:229:ARG:HD2	1:C:366:GLY:HA3	1.99	0.43
1:C:264:ARG:C	1:C:266:HIS:H	2.22	0.43
1:C:306:ASP:C	1:C:308:ARG:N	2.69	0.43
1:C:328:VAL:O	1:C:330:ALA:N	2.52	0.43
2:D:115:VAL:O	2:D:116:ASP:C	2.61	0.43
2:D:320:ARG:NH1	2:D:320:ARG:CG	2.80	0.43
1:A:88:HIS:O	1:A:90:GLU:N	2.51	0.43
1:A:174:ALA:HB1	1:A:176:GLN:HG2	2.01	0.43
1:A:209:ILE:N	1:A:209:ILE:CD1	2.81	0.43
1:A:371:VAL:CG1	1:A:372:GLN:H	2.32	0.43
2:B:3:GLU:O	2:B:133:GLN:N	2.40	0.43
2:B:107:HIS:HB2	2:B:148:GLY:O	2.17	0.43
2:B:154:ILE:O	2:B:157:ILE:N	2.50	0.43
2:B:159:GLU:OE2	3:E:30:UNK:HA	2.17	0.43
2:B:194:LEU:HD23	2:B:194:LEU:C	2.44	0.43
2:B:264:ARG:O	2:B:265:LEU:C	2.61	0.43
1:C:93:ILE:CD1	1:C:118:VAL:HA	2.48	0.43
1:C:217:LEU:HD23	1:C:219:ILE:HD11	1.99	0.43
1:C:371:VAL:HG11	1:C:373:ARG:O	2.18	0.43
2:D:137:LEU:HD23	2:D:154:ILE:CD1	2.47	0.43
2:D:174:SER:OG	2:D:207:GLU:HA	2.18	0.43
2:D:291:LEU:CD2	2:D:291:LEU:N	2.81	0.43
2:D:411:GLU:O	2:D:412:GLY:C	2.60	0.43
2:D:413:MET:HE1	2:D:418:PHE:CZ	2.54	0.43
1:A:9:VAL:HG21	1:A:150:THR:CB	2.46	0.43
1:A:178:SER:O	1:A:179:THR:CB	2.66	0.43
1:A:195:LEU:C	1:A:197:HIS:N	2.77	0.43
1:A:266:HIS:HD1	1:A:266:HIS:H	1.67	0.43
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.52	0.43
2:B:209:LEU:CB	2:B:227:LEU:HG	2.48	0.43
2:B:327:GLU:O	2:B:331:GLN:HB2	2.19	0.43
2:B:380:ASN:C	2:B:380:ASN:ND2	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLU:CG	1:C:28:HIS:N	2.81	0.43
1:C:242:LEU:HD11	1:C:318:LEU:HG	2.00	0.43
1:C:262:TYR:C	1:C:264:ARG:N	2.76	0.43
1:C:276:ILE:HG12	1:C:282:TYR:HD2	1.79	0.43
1:C:328:VAL:C	1:C:330:ALA:N	2.75	0.43
2:D:91:ASN:N	2:D:91:ASN:ND2	2.50	0.43
2:D:238:VAL:CG2	2:D:376:THR:HG21	2.49	0.43
2:D:287:THR:O	2:D:291:LEU:HD23	2.18	0.43
2:D:313:LEU:C	2:D:314:THR:HG23	2.42	0.43
2:D:343:PHE:O	2:D:344:VAL:C	2.61	0.43
2:D:351:VAL:C	2:D:352:LYS:HG3	2.43	0.43
1:A:15:GLN:O	1:A:16:ILE:O	2.36	0.43
1:A:111:GLY:C	1:A:113:GLU:H	2.26	0.43
1:A:278:ALA:HA	1:A:282:TYR:OH	2.19	0.43
2:B:18:ALA:O	2:B:21:TRP:N	2.51	0.43
2:B:151:THR:HG21	2:B:189:LEU:HD21	1.99	0.43
1:C:154:MET:CE	1:C:197:HIS:NE2	2.79	0.43
1:C:263:PRO:C	1:C:265:ALA:N	2.76	0.43
1:C:286:LEU:C	1:C:290:GLU:HB2	2.44	0.43
2:D:193:GLN:HE21	2:D:193:GLN:HB3	1.66	0.43
1:A:23:LEU:O	1:A:25:CYS:N	2.42	0.43
1:A:45:GLY:C	1:A:46:ASP:OD2	2.61	0.43
1:A:179:THR:HG22	1:A:180:ALA:O	2.18	0.43
2:B:132:LEU:H	2:B:164:ARG:HH21	1.66	0.43
2:B:346:TRP:HZ2	2:B:435:TYR:HB3	1.82	0.43
1:C:179:THR:HB	1:C:182:VAL:HB	2.01	0.43
1:C:333:ALA:O	1:C:336:LYS:N	2.52	0.43
2:D:51:VAL:N	2:D:245:PRO:CG	2.81	0.43
2:D:180:THR:CB	2:D:404:PHE:CE1	2.97	0.43
2:D:343:PHE:HB3	2:D:350:ASN:OD1	2.17	0.43
2:D:353:THR:HG23	2:D:354:ALA:H	1.83	0.43
1:A:43:GLY:O	1:A:47:ASP:OD2	2.37	0.43
1:A:197:HIS:CG	1:A:198:SER:N	2.85	0.43
1:A:256:GLN:HB3	1:A:260:VAL:CB	2.46	0.43
2:B:200:GLU:HG2	2:B:268:PHE:CE2	2.53	0.43
2:B:272:PHE:HB3	2:B:275:LEU:HD21	2.00	0.43
2:B:419:THR:O	2:B:423:SER:N	2.51	0.43
1:C:78:VAL:O	1:C:82:THR:CG2	2.63	0.43
1:C:122:ILE:HG22	1:C:123:ARG:N	2.34	0.43
2:D:60:LYS:H	2:D:60:LYS:HZ3	1.66	0.43
2:D:152:LEU:O	2:D:153:LEU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ALA:O	2:D:212:ILE:HG13	2.19	0.43
1:A:26:LEU:HD23	1:A:361:THR:OG1	2.18	0.43
1:A:77:GLU:HB3	1:A:83:TYR:HD2	1.76	0.43
1:A:100:ALA:HA	1:A:105:ARG:CD	2.49	0.43
1:A:163:LYS:HB2	1:A:163:LYS:NZ	2.34	0.43
1:A:171:ILE:HA	1:A:204:VAL:HB	2.01	0.43
1:A:182:VAL:O	1:A:183:GLU:C	2.62	0.43
1:A:229:ARG:HG3	1:A:229:ARG:NH1	2.34	0.43
1:A:292:THR:O	1:A:292:THR:OG1	2.33	0.43
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.00	0.43
2:B:59:ASN:CA	2:B:64:ARG:HE	2.32	0.43
2:B:276:THR:HG21	2:B:281:GLN:CG	2.49	0.43
1:C:270:ALA:O	1:C:302:MET:HE2	2.19	0.43
1:C:345:ASP:C	1:C:347:CYS:N	2.77	0.43
1:C:346:TRP:CE3	1:C:347:CYS:SG	3.12	0.43
2:D:10:GLY:HA3	2:D:146:GLY:HA3	1.99	0.43
2:D:92:PHE:CZ	2:D:117:SER:O	2.71	0.43
2:D:348:PRO:O	2:D:349:ASN:CB	2.66	0.43
2:D:428:LEU:HD12	2:D:428:LEU:N	2.33	0.43
3:E:68:UNK:O	3:E:72:UNK:CB	2.66	0.43
3:E:83:UNK:O	3:E:85:UNK:N	2.51	0.43
1:A:100:ALA:HB1	1:A:105:ARG:HD2	2.00	0.43
1:A:186:ASN:CG	1:A:391:LEU:HD21	2.43	0.43
1:A:242:LEU:CG	1:A:318:LEU:HD11	2.47	0.43
1:A:262:TYR:C	1:A:264:ARG:N	2.77	0.43
2:B:59:ASN:HA	2:B:60:LYS:NZ	2.33	0.43
2:B:132:LEU:O	2:B:164:ARG:NE	2.41	0.43
2:B:181:VAL:C	2:B:183:GLU:N	2.77	0.43
2:B:402:LYS:HE3	1:C:440:VAL:HG12	1.99	0.43
1:C:270:ALA:HB3	1:C:302:MET:HG2	2.00	0.43
2:D:121:VAL:O	2:D:121:VAL:CG1	2.66	0.43
2:D:183:GLU:HB3	2:D:184:PRO:HD3	2.01	0.43
2:D:194:LEU:HD23	2:D:194:LEU:C	2.44	0.43
1:A:39:ASP:OD2	1:A:40:LYS:HB2	2.19	0.42
1:A:181:VAL:HG13	1:A:185:TYR:CE2	2.53	0.42
2:B:88:ARG:O	2:B:91:ASN:ND2	2.52	0.42
2:B:111:GLY:O	2:B:113:GLU:N	2.52	0.42
2:B:189:LEU:HA	2:B:192:HIS:HE1	1.82	0.42
2:B:211:ASP:OD1	2:B:211:ASP:N	2.52	0.42
2:B:273:ALA:HB3	2:B:274:PRO:HD3	2.01	0.42
1:C:217:LEU:CD2	1:C:219:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:ILE:H	2:D:88:ARG:NH2	2.17	0.42
2:D:211:ASP:O	2:D:215:ARG:HB2	2.19	0.42
2:D:273:ALA:HB3	2:D:274:PRO:HD3	2.00	0.42
2:D:283:TYR:HE2	2:D:294:GLN:NE2	2.17	0.42
2:D:311:ARG:HD3	2:D:311:ARG:H	1.84	0.42
2:D:312:TYR:CE2	2:D:377:PHE:CZ	3.06	0.42
3:E:14:UNK:C	3:E:16:UNK:N	2.81	0.42
1:A:46:ASP:O	1:A:47:ASP:O	2.37	0.42
1:A:306:ASP:N	1:A:307:PRO:HD3	2.33	0.42
2:B:283:TYR:O	2:B:283:TYR:CG	2.72	0.42
2:B:287:THR:OG1	2:B:290:GLU:CB	2.67	0.42
2:B:343:PHE:O	2:B:344:VAL:C	2.61	0.42
2:B:344:VAL:O	2:B:346:TRP:CD1	2.72	0.42
2:B:425:MET:HE3	2:B:425:MET:HB3	1.69	0.42
1:C:209:ILE:HG12	1:C:231:ILE:HD11	2.00	0.42
1:C:237:SER:C	1:C:241:SER:CB	2.92	0.42
1:C:273:ALA:HB3	1:C:291:ILE:HG23	2.01	0.42
1:C:284:GLU:CG	1:C:285:GLN:HE21	2.22	0.42
1:C:306:ASP:HB3	1:C:386:GLU:OE1	2.18	0.42
1:C:312:TYR:CD1	1:C:312:TYR:N	2.87	0.42
2:D:52:TYR:CG	2:D:52:TYR:O	2.72	0.42
2:D:206:ASN:O	2:D:207:GLU:C	2.61	0.42
2:D:226:ASP:O	2:D:228:ASN:N	2.44	0.42
2:D:311:ARG:NH1	2:D:344:VAL:HA	2.35	0.42
2:D:327:GLU:O	2:D:331:GLN:HB2	2.19	0.42
3:E:75:UNK:C	3:E:77:UNK:N	2.78	0.42
1:A:228:ASN:C	1:A:230:LEU:H	2.26	0.42
1:A:242:LEU:CD2	1:A:318:LEU:HD21	2.33	0.42
1:A:284:GLU:CG	1:A:285:GLN:HE21	2.24	0.42
2:B:2:ARG:HH21	2:B:243:ARG:HB3	1.84	0.42
2:B:10:GLY:HA3	2:B:146:GLY:HA3	2.01	0.42
2:B:212:ILE:O	2:B:217:LEU:HB3	2.19	0.42
2:B:322:ARG:CG	2:B:357:ASP:HA	2.33	0.42
1:C:31:GLN:OE1	1:C:32:PRO:HD3	2.19	0.42
1:C:88:HIS:O	1:C:89:PRO:C	2.60	0.42
1:C:119:LEU:HD22	1:C:156:ARG:CZ	2.49	0.42
1:C:264:ARG:HD3	1:C:264:ARG:HA	1.97	0.42
1:C:305:CYS:SG	1:C:383:ALA:C	3.02	0.42
2:D:176:LYS:NZ	2:D:210:TYR:CG	2.84	0.42
2:D:232:SER:C	2:D:234:THR:H	2.25	0.42
2:D:312:TYR:HE2	2:D:377:PHE:CZ	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:PHE:CD2	2:D:422:GLU:OE1	2.71	0.42
1:A:411:GLU:OE2	1:A:411:GLU:CA	2.68	0.42
2:B:22:GLU:HG3	2:B:83:PHE:CD1	2.55	0.42
2:B:93:VAL:CG2	2:B:94:PHE:N	2.82	0.42
2:B:95:GLY:O	2:B:96:GLN:O	2.37	0.42
2:B:256:ALA:O	2:B:260:VAL:HB	2.19	0.42
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.38	0.42
2:B:327:GLU:O	2:B:331:GLN:N	2.53	0.42
1:C:20:CYS:SG	1:C:232:GLY:HA2	2.59	0.42
1:C:125:LEU:C	1:C:127:ASP:H	2.26	0.42
1:C:143:GLY:C	1:C:144:GLY:O	2.63	0.42
1:C:187:SER:C	1:C:189:LEU:N	2.77	0.42
1:C:241:SER:CB	1:C:242:LEU:HD12	2.48	0.42
1:C:321:GLY:N	1:C:356:ASN:O	2.52	0.42
2:D:4:ILE:HD11	2:D:252:LEU:HD13	2.00	0.42
2:D:322:ARG:CG	2:D:357:ASP:HA	2.34	0.42
1:A:164:LYS:HB2	1:A:164:LYS:HZ3	1.84	0.42
1:A:283:HIS:C	1:A:285:GLN:N	2.75	0.42
1:A:291:ILE:CG2	1:A:375:VAL:HG21	2.44	0.42
1:A:311:LYS:CE	1:A:344:VAL:HA	2.50	0.42
2:B:3:GLU:HB3	2:B:132:LEU:HA	2.01	0.42
2:B:101:ASN:H	1:C:254:GLU:CD	2.27	0.42
2:B:259:MET:HE2	2:B:316:ALA:CB	2.44	0.42
1:C:5:ILE:HG22	1:C:6:SER:N	2.34	0.42
1:C:44:GLY:O	1:C:46:ASP:N	2.52	0.42
1:C:83:TYR:O	1:C:84:ARG:HB2	2.20	0.42
1:C:123:ARG:O	1:C:127:ASP:HB2	2.19	0.42
1:C:190:THR:O	1:C:193:THR:N	2.52	0.42
1:C:207:GLU:O	1:C:208:ALA:C	2.62	0.42
1:C:286:LEU:HD12	1:C:291:ILE:CG1	2.48	0.42
1:C:332:ILE:HG23	1:C:351:PHE:CZ	2.55	0.42
2:D:165:ILE:HD13	2:D:199:ASP:OD1	2.18	0.42
3:E:30:UNK:O	3:E:31:UNK:C	2.67	0.42
1:A:73:THR:O	1:A:76:ASP:N	2.48	0.42
1:A:126:ALA:O	1:A:132:LEU:CD1	2.67	0.42
1:A:216:ASN:HB3	1:A:275:VAL:HG11	2.01	0.42
1:A:305:CYS:O	1:A:306:ASP:HB2	2.19	0.42
2:B:88:ARG:HA	2:B:91:ASN:ND2	2.35	0.42
2:B:230:LEU:H	2:B:230:LEU:CD1	2.25	0.42
2:B:255:LEU:C	2:B:257:VAL:H	2.27	0.42
1:C:21:TRP:CD1	1:C:21:TRP:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:O	1:C:90:GLU:N	2.52	0.42
1:C:190:THR:HA	1:C:193:THR:CG2	2.39	0.42
1:C:335:ILE:O	1:C:338:LYS:HG2	2.19	0.42
1:C:398:MET:CG	1:C:399:TYR:H	2.33	0.42
2:D:22:GLU:HG3	2:D:83:PHE:CD1	2.55	0.42
2:D:95:GLY:O	2:D:96:GLN:O	2.38	0.42
2:D:346:TRP:HZ2	2:D:435:TYR:HB3	1.85	0.42
2:D:408:TYR:C	2:D:410:GLY:N	2.77	0.42
2:D:415:GLU:HG2	2:D:416:MET:SD	2.59	0.42
1:A:119:LEU:HD22	1:A:156:ARG:NE	2.34	0.42
1:A:190:THR:O	1:A:193:THR:N	2.50	0.42
1:A:286:LEU:HD12	1:A:291:ILE:CG1	2.49	0.42
2:B:20:PHE:C	2:B:22:GLU:N	2.78	0.42
2:B:63:PRO:C	2:B:65:ALA:H	2.27	0.42
2:B:396:THR:HG1	2:B:422:GLU:CD	2.26	0.42
2:B:411:GLU:O	2:B:412:GLY:C	2.62	0.42
2:B:415:GLU:HG2	2:B:416:MET:H	1.85	0.42
1:C:91:GLN:HE21	1:C:91:GLN:HB3	1.58	0.42
1:C:185:TYR:CE1	1:C:408:TYR:CE1	3.06	0.42
1:C:209:ILE:CG2	1:C:213:CYS:HB2	2.43	0.42
1:C:239:THR:O	1:C:243:ARG:HB2	2.19	0.42
2:D:115:VAL:CG1	2:D:156:LYS:NZ	2.77	0.42
2:D:311:ARG:HB3	2:D:343:PHE:N	2.35	0.42
1:A:209:ILE:CG2	1:A:213:CYS:HB2	2.47	0.42
1:A:368:LEU:O	1:A:369:ALA:HB3	2.19	0.42
2:B:98:GLY:H	2:B:110:GLU:CD	2.27	0.42
2:B:323:MET:HE2	2:B:323:MET:HB3	1.99	0.42
2:B:350:ASN:ND2	2:B:350:ASN:N	2.67	0.42
1:C:97:GLU:H	1:C:97:GLU:CD	2.27	0.42
1:C:320:ARG:HH21	1:C:356:ASN:ND2	2.18	0.42
1:C:405:VAL:O	1:C:405:VAL:CG2	2.68	0.42
1:C:413:MET:O	1:C:414:GLU:CB	2.66	0.42
2:D:88:ARG:HA	2:D:91:ASN:HD21	1.85	0.42
2:D:224:TYR:O	2:D:228:ASN:HB2	2.20	0.42
2:D:255:LEU:C	2:D:257:VAL:N	2.77	0.42
2:D:269:MET:HG2	2:D:384:ILE:HB	2.01	0.42
2:D:320:ARG:HG2	2:D:320:ARG:NH1	2.32	0.42
1:A:69:ASP:CG	1:A:70:LEU:N	2.77	0.42
1:A:144:GLY:O	1:A:145:THR:C	2.63	0.42
1:A:241:SER:C	1:A:242:LEU:HD12	2.45	0.42
1:A:312:TYR:HD1	1:A:312:TYR:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:MET:C	1:A:403:ALA:HB2	2.43	0.42
2:B:6:HIS:HD2	2:B:136:GLN:OE1	2.03	0.42
2:B:216:THR:O	2:B:217:LEU:C	2.63	0.42
2:B:251:ASP:OD2	2:B:251:ASP:C	2.63	0.42
2:B:333:LEU:HG	2:B:337:ASN:HD21	1.82	0.42
2:B:346:TRP:CZ2	2:B:435:TYR:HB3	2.54	0.42
2:B:405:LEU:HD13	2:B:406:HIS:H	1.79	0.42
2:B:408:TYR:C	2:B:410:GLY:N	2.76	0.42
1:C:88:HIS:HA	1:C:89:PRO:HD2	1.84	0.42
1:C:125:LEU:C	1:C:127:ASP:N	2.78	0.42
1:C:157:LEU:C	1:C:159:VAL:N	2.77	0.42
1:C:229:ARG:HG3	1:C:229:ARG:NH1	2.33	0.42
2:D:102:ASN:HD22	2:D:105:LYS:H	1.62	0.42
2:D:123:ARG:C	2:D:125:GLU:N	2.74	0.42
1:A:7:ILE:C	1:A:8:HIS:HD1	2.27	0.42
1:A:72:PRO:HB3	1:A:94:THR:HG1	1.85	0.42
1:A:208:ALA:HB2	1:A:302:MET:O	2.20	0.42
2:B:273:ALA:H	2:B:274:PRO:HD2	1.84	0.42
1:C:174:ALA:HB1	1:C:176:GLN:HG2	2.02	0.42
1:C:208:ALA:O	1:C:212:ILE:HG23	2.20	0.42
1:C:275:VAL:HG12	1:C:275:VAL:O	2.18	0.42
1:C:277:SER:HA	1:C:368:LEU:HB3	2.02	0.42
1:C:321:GLY:CA	1:C:358:GLU:O	2.68	0.42
1:C:364:PRO:C	1:C:366:GLY:H	2.27	0.42
2:D:69:ASP:HB3	2:D:74:THR:HG23	2.02	0.42
2:D:104:ALA:HB1	2:D:411:GLU:HB2	2.02	0.42
1:A:115:ILE:HG12	1:A:149:PHE:CE2	2.54	0.41
1:A:197:HIS:CD2	1:A:198:SER:HB3	2.55	0.41
1:A:256:GLN:O	1:A:257:THR:C	2.63	0.41
2:B:122:VAL:CG1	2:B:123:ARG:N	2.82	0.41
1:C:181:VAL:HG22	1:C:399:TYR:OH	2.18	0.41
1:C:209:ILE:HA	1:C:212:ILE:HG12	2.01	0.41
2:D:179:ASP:OD2	2:D:181:VAL:HG12	2.20	0.41
1:A:181:VAL:O	1:A:184:PRO:HG2	2.20	0.41
1:A:182:VAL:HA	1:A:185:TYR:HD2	1.86	0.41
1:A:245:ASP:O	1:A:249:ASN:OD1	2.37	0.41
1:A:328:VAL:C	1:A:330:ALA:N	2.78	0.41
1:A:420:GLU:OE1	1:A:420:GLU:O	2.38	0.41
2:B:86:ILE:H	2:B:88:ARG:CZ	2.33	0.41
1:C:21:TRP:CD1	1:C:21:TRP:H	2.37	0.41
1:C:168:GLU:HG3	1:C:168:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:HG2	1:C:216:ASN:N	2.36	0.41
1:C:242:LEU:CG	1:C:318:LEU:HD11	2.50	0.41
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.49	0.41
3:E:16:UNK:O	3:E:20:UNK:N	2.53	0.41
1:A:5:ILE:O	1:A:136:SER:N	2.47	0.41
1:A:111:GLY:O	1:A:112:LYS:C	2.63	0.41
1:A:117:LEU:O	1:A:121:ARG:HB2	2.21	0.41
1:A:189:LEU:O	1:A:190:THR:C	2.62	0.41
1:A:214:ARG:O	1:A:214:ARG:HG3	2.20	0.41
1:A:312:TYR:HD2	1:A:315:CYS:HB2	1.84	0.41
2:B:165:ILE:HG13	2:B:253:ARG:HG2	2.02	0.41
2:B:291:LEU:CD2	2:B:291:LEU:H	2.32	0.41
1:C:38:SER:O	1:C:39:ASP:CB	2.68	0.41
1:C:42:ILE:HD12	1:C:42:ILE:HA	1.87	0.41
1:C:163:LYS:HB2	1:C:163:LYS:NZ	2.34	0.41
1:C:312:TYR:HD1	1:C:312:TYR:N	2.17	0.41
2:D:73:GLY:O	2:D:78:VAL:HG21	2.20	0.41
2:D:121:VAL:O	2:D:121:VAL:HG12	2.20	0.41
2:D:214:PHE:CE2	2:D:215:ARG:NE	2.88	0.41
2:D:377:PHE:C	2:D:378:ILE:HG12	2.44	0.41
1:A:3:GLU:O	1:A:3:GLU:HG3	2.19	0.41
1:A:30:ILE:HG13	1:A:31:GLN:H	1.81	0.41
1:A:35:GLN:HE22	1:A:88:HIS:CD2	2.38	0.41
1:A:229:ARG:HB3	1:A:366:GLY:O	2.20	0.41
1:A:261:PRO:CB	1:A:313:MET:HE2	2.50	0.41
1:A:387:ALA:CB	1:A:390:ARG:NH1	2.83	0.41
1:A:414:GLU:HB2	1:A:417:GLU:CB	2.46	0.41
2:B:103:TRP:HE1	2:B:151:THR:HG21	1.85	0.41
2:B:215:ARG:NE	2:B:215:ARG:CA	2.80	0.41
2:B:395:PHE:CE1	2:B:399:PHE:CD1	3.08	0.41
2:B:404:PHE:O	2:B:404:PHE:CD2	2.69	0.41
1:C:10:GLY:O	1:C:12:ALA:N	2.54	0.41
1:C:253:THR:OG1	1:C:254:GLU:N	2.53	0.41
1:C:317:LEU:HD23	1:C:377:MET:HB2	2.00	0.41
1:C:381:THR:C	1:C:383:ALA:N	2.77	0.41
2:D:3:GLU:OE2	2:D:130:ASP:CB	2.60	0.41
2:D:60:LYS:N	2:D:60:LYS:HZ2	2.17	0.41
2:D:132:LEU:HD22	2:D:164:ARG:CG	2.48	0.41
2:D:139:HIS:C	2:D:139:HIS:HD2	2.28	0.41
2:D:208:ALA:HB2	2:D:304:ALA:CB	2.51	0.41
2:D:218:LYS:NZ	2:D:278:ARG:CB	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:283:TYR:O	2:D:284:ARG:HB2	2.20	0.41
2:D:323:MET:HE2	2:D:323:MET:HB3	1.93	0.41
1:A:27:GLU:OE1	1:A:28:HIS:CE1	2.73	0.41
1:A:90:GLU:C	1:A:90:GLU:OE2	2.64	0.41
1:A:177:VAL:HG21	2:B:349:ASN:HB2	2.03	0.41
1:A:203:MET:SD	1:A:388:TRP:CD1	3.13	0.41
2:B:190:SER:O	2:B:425:MET:HB2	2.21	0.41
2:B:191:VAL:HG21	2:B:421:ALA:CB	2.28	0.41
2:B:295:MET:HE3	2:B:377:PHE:CD2	2.56	0.41
2:B:314:THR:C	2:B:315:VAL:HG22	2.45	0.41
2:B:407:TRP:NE1	1:C:257:THR:HA	2.34	0.41
2:B:413:MET:O	2:B:414:ASP:C	2.63	0.41
1:C:107:HIS:HB2	1:C:148:GLY:O	2.21	0.41
1:C:115:ILE:HG23	1:C:116:ASP:OD1	2.20	0.41
1:C:122:ILE:O	1:C:123:ARG:C	2.63	0.41
1:C:139:HIS:HB3	1:C:170:SER:CA	2.44	0.41
1:C:158:SER:HB3	1:C:166:LYS:HZ1	1.83	0.41
1:C:262:TYR:O	1:C:263:PRO:C	2.64	0.41
2:D:176:LYS:HD2	2:D:210:TYR:CE1	2.55	0.41
2:D:212:ILE:C	2:D:214:PHE:N	2.78	0.41
2:D:265:LEU:HB2	2:D:266:HIS:H	1.58	0.41
1:A:105:ARG:HG3	1:A:411:GLU:HG3	2.03	0.41
1:A:167:LEU:HD13	1:A:252:LEU:HD11	2.03	0.41
1:A:180:ALA:HB3	2:B:258:ASN:ND2	2.36	0.41
1:A:238:ILE:N	1:A:241:SER:CB	2.84	0.41
2:B:115:VAL:HG23	2:B:149:MET:HE1	2.03	0.41
2:B:158:ARG:HD3	2:B:197:ASN:HD22	1.73	0.41
2:B:212:ILE:HD12	2:B:302:MET:HE2	2.03	0.41
2:B:351:VAL:O	2:B:352:LYS:HG3	2.21	0.41
1:C:174:ALA:HB2	1:C:206:ASN:CB	2.50	0.41
1:C:228:ASN:ND2	4:C:502:GTP:O6	2.53	0.41
1:C:340:THR:C	1:C:341:ILE:HD12	2.45	0.41
2:D:277:SER:C	2:D:278:ARG:O	2.64	0.41
2:D:320:ARG:HE	2:D:360:PRO:HG3	1.85	0.41
2:D:333:LEU:O	2:D:336:GLN:HB3	2.20	0.41
2:D:372:LYS:HE2	2:D:372:LYS:HA	2.02	0.41
2:D:389:LYS:C	2:D:392:SER:OG	2.62	0.41
1:A:24:TYR:HA	1:A:26:LEU:CD1	2.50	0.41
1:A:139:HIS:O	1:A:140:SER:CB	2.68	0.41
1:A:239:THR:O	1:A:243:ARG:HB2	2.19	0.41
1:A:242:LEU:HD21	1:A:318:LEU:CD2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:OD2	1:A:252:LEU:N	2.54	0.41
1:A:317:LEU:HA	1:A:377:MET:HB2	2.02	0.41
2:B:4:ILE:HD13	2:B:252:LEU:HD13	2.03	0.41
2:B:103:TRP:H	2:B:408:TYR:HE1	1.69	0.41
2:B:103:TRP:HB2	2:B:185:TYR:CE2	2.56	0.41
2:B:262:PHE:CE1	2:B:435:TYR:CE2	3.08	0.41
2:B:304:ALA:O	2:B:305:CYS:SG	2.77	0.41
2:B:310:GLY:HA3	2:B:436:GLN:HG2	2.03	0.41
2:B:313:LEU:HD21	2:B:435:TYR:CD2	2.54	0.41
1:C:69:ASP:CG	1:C:70:LEU:N	2.75	0.41
1:C:283:HIS:C	1:C:285:GLN:N	2.78	0.41
2:D:102:ASN:N	2:D:185:TYR:OH	2.53	0.41
2:D:103:TRP:HE1	2:D:151:THR:HG21	1.85	0.41
2:D:289:PRO:HA	2:D:292:THR:OG1	2.21	0.41
1:A:197:HIS:O	1:A:198:SER:OG	2.35	0.41
1:A:335:ILE:CG1	1:A:336:LYS:N	2.77	0.41
1:A:343:PHE:CD1	1:A:349:THR:HA	2.55	0.41
1:A:344:VAL:HG12	1:A:345:ASP:H	1.83	0.41
2:B:95:GLY:O	2:B:96:GLN:HB3	2.21	0.41
2:B:102:ASN:HD22	2:B:105:LYS:H	1.58	0.41
1:C:142:GLY:HA2	1:C:185:TYR:HB2	2.03	0.41
1:C:205:ASP:OD2	1:C:205:ASP:C	2.63	0.41
1:C:255:PHE:O	1:C:259:LEU:HB2	2.21	0.41
1:C:419:SER:C	1:C:421:ALA:N	2.79	0.41
2:D:176:LYS:O	2:D:177:VAL:HB	2.21	0.41
2:D:267:PHE:CD2	2:D:267:PHE:N	2.89	0.41
1:A:115:ILE:HG13	1:A:152:LEU:CG	2.50	0.41
1:A:178:SER:O	1:A:182:VAL:HG21	2.21	0.41
1:A:184:PRO:CB	1:A:399:TYR:CE2	3.04	0.41
1:A:273:ALA:HB2	1:A:295:CYS:CB	2.51	0.41
1:A:311:LYS:HD3	1:A:344:VAL:CB	2.51	0.41
1:A:339:ARG:HD2	1:A:339:ARG:O	2.21	0.41
1:A:365:GLY:O	1:A:368:LEU:HD12	2.20	0.41
1:A:388:TRP:HZ3	1:A:428:LEU:HD22	1.82	0.41
1:A:398:MET:CG	1:A:399:TYR:H	2.34	0.41
2:B:51:VAL:HG22	2:B:245:PRO:CB	2.51	0.41
2:B:52:TYR:O	2:B:52:TYR:CG	2.74	0.41
2:B:76:ASP:HB2	2:B:77:SER:H	1.46	0.41
2:B:136:GLN:HG3	2:B:136:GLN:O	2.21	0.41
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.51	0.41
2:B:247:GLN:HG2	2:B:355:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:VAL:C	2:B:352:LYS:HG3	2.46	0.41
2:B:384:ILE:O	2:B:384:ILE:HG12	2.20	0.41
2:B:404:PHE:HZ	1:C:257:THR:O	2.04	0.41
1:C:9:VAL:HG21	1:C:150:THR:CB	2.51	0.41
1:C:137:VAL:CB	1:C:154:MET:HE1	2.50	0.41
1:C:228:ASN:C	1:C:230:LEU:H	2.29	0.41
1:C:306:ASP:N	1:C:307:PRO:HD3	2.35	0.41
1:C:311:LYS:HB2	1:C:344:VAL:CG2	2.50	0.41
1:C:371:VAL:CG1	1:C:372:GLN:N	2.82	0.41
2:D:8:GLN:O	2:D:68:VAL:N	2.54	0.41
2:D:16:ILE:CD1	2:D:231:VAL:CG1	2.99	0.41
2:D:51:VAL:HG22	2:D:245:PRO:CB	2.51	0.41
2:D:88:ARG:O	2:D:91:ASN:ND2	2.54	0.41
2:D:103:TRP:H	2:D:408:TYR:HE1	1.68	0.41
2:D:158:ARG:NH1	2:D:197:ASN:OD1	2.54	0.41
2:D:198:THR:O	2:D:199:ASP:C	2.63	0.41
2:D:245:PRO:O	2:D:246:GLY:C	2.64	0.41
1:A:36:MET:CE	1:A:37:PRO:HD2	2.48	0.41
1:A:128:GLN:HA	1:A:128:GLN:OE1	2.21	0.41
1:A:158:SER:HB3	1:A:166:LYS:HZ1	1.86	0.41
1:A:174:ALA:HB2	1:A:206:ASN:CB	2.51	0.41
1:A:204:VAL:O	1:A:205:ASP:HB3	2.21	0.41
2:B:19:LYS:HA	2:B:22:GLU:CG	2.51	0.41
2:B:25:SER:HB3	2:B:369:ARG:NH2	2.34	0.41
2:B:148:GLY:CA	2:B:151:THR:HG22	2.51	0.41
2:B:179:ASP:CB	2:B:181:VAL:HG12	2.46	0.41
2:B:325:MET:CG	2:B:355:VAL:HG11	2.51	0.41
2:B:407:TRP:CZ2	1:C:256:GLN:CB	2.91	0.41
1:C:137:VAL:HG11	1:C:154:MET:CE	2.46	0.41
1:C:238:ILE:O	1:C:239:THR:O	2.38	0.41
1:C:244:PHE:H	1:C:244:PHE:HD2	1.67	0.41
1:C:244:PHE:N	1:C:244:PHE:CD2	2.89	0.41
1:C:389:ALA:C	1:C:392:ASP:H	2.29	0.41
1:C:414:GLU:HA	1:C:417:GLU:HB2	2.02	0.41
2:D:182:VAL:O	2:D:183:GLU:HB2	2.21	0.41
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.40
1:A:244:PHE:CE1	1:A:358:GLU:OE2	2.74	0.40
1:A:269:LEU:HD11	1:A:301:GLN:HB3	2.03	0.40
1:A:295:CYS:SG	1:A:295:CYS:O	2.78	0.40
1:A:384:ILE:O	1:A:385:ALA:C	2.64	0.40
2:B:158:ARG:C	2:B:160:GLU:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:PRO:HG2	2:B:163:ASP:H	1.86	0.40
2:B:269:MET:HG2	2:B:384:ILE:HB	2.03	0.40
1:C:107:HIS:HA	1:C:148:GLY:O	2.21	0.40
1:C:150:THR:C	1:C:152:LEU:N	2.77	0.40
1:C:320:ARG:N	1:C:374:ALA:O	2.49	0.40
2:D:87:PHE:O	2:D:88:ARG:C	2.64	0.40
2:D:114:LEU:HD12	2:D:114:LEU:HA	1.78	0.40
2:D:115:VAL:HG21	2:D:152:LEU:CD2	2.51	0.40
2:D:269:MET:HE2	2:D:301:MET:CE	2.51	0.40
2:D:293:GLN:C	2:D:295:MET:H	2.29	0.40
2:D:371:LEU:C	2:D:373:MET:N	2.76	0.40
2:D:381:SER:C	2:D:383:ALA:N	2.79	0.40
3:E:83:UNK:O	3:E:84:UNK:C	2.67	0.40
1:A:101:ASN:OD1	2:B:254:LYS:NZ	2.39	0.40
1:A:346:TRP:CZ2	1:A:435:VAL:HB	2.56	0.40
2:B:7:ILE:HG21	2:B:137:LEU:HD13	2.03	0.40
2:B:174:SER:CB	2:B:207:GLU:N	2.82	0.40
2:B:264:ARG:O	2:B:265:LEU:O	2.38	0.40
2:B:408:TYR:CD2	2:B:418:PHE:CZ	3.09	0.40
1:C:109:THR:OG1	1:C:110:ILE:N	2.53	0.40
1:C:214:ARG:HG3	1:C:214:ARG:NH1	2.35	0.40
1:C:223:THR:O	1:C:224:TYR:C	2.64	0.40
1:C:362:VAL:HG12	1:C:363:VAL:N	2.36	0.40
1:C:405:VAL:O	1:C:405:VAL:HG22	2.20	0.40
2:D:154:ILE:O	2:D:157:ILE:N	2.46	0.40
2:D:180:THR:HB	2:D:404:PHE:CZ	2.55	0.40
2:D:346:TRP:CZ2	2:D:435:TYR:HB3	2.57	0.40
1:A:132:LEU:HB3	1:A:133:GLN:H	1.66	0.40
1:A:175:PRO:HB2	1:A:207:GLU:OE2	2.22	0.40
1:A:322:ASP:OD1	1:A:357:TYR:O	2.39	0.40
1:A:409:VAL:HA	1:A:412:GLY:O	2.22	0.40
2:B:132:LEU:CD2	2:B:164:ARG:NE	2.83	0.40
2:B:172:VAL:CG1	2:B:173:PRO:HD2	2.42	0.40
2:B:212:ILE:C	2:B:214:PHE:N	2.79	0.40
2:B:333:LEU:O	2:B:334:ASN:C	2.64	0.40
2:B:405:LEU:C	2:B:407:TRP:N	2.79	0.40
1:C:139:HIS:NE2	1:C:150:THR:CG2	2.84	0.40
1:C:225:THR:HA	1:C:228:ASN:HB2	2.04	0.40
1:C:305:CYS:O	1:C:306:ASP:HB2	2.22	0.40
1:C:411:GLU:OE2	1:C:411:GLU:O	2.39	0.40
2:D:144:GLY:N	2:D:185:TYR:CZ	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:ASP:CB	2:D:181:VAL:HG12	2.42	0.40
2:D:286:LEU:CG	2:D:373:MET:HE3	2.45	0.40
2:D:333:LEU:O	2:D:334:ASN:C	2.64	0.40
2:D:429:VAL:O	2:D:433:GLN:HG2	2.22	0.40
1:A:79:ARG:HD3	1:A:86:LEU:HD11	2.04	0.40
1:A:142:GLY:O	1:A:182:VAL:HG22	2.20	0.40
1:A:145:THR:CB	4:A:500:GTP:PG	3.10	0.40
2:B:102:ASN:O	2:B:103:TRP:C	2.63	0.40
2:B:109:THR:O	2:B:112:ALA:N	2.49	0.40
2:B:147:SER:O	2:B:189:LEU:HD11	2.22	0.40
2:B:192:HIS:CA	2:B:195:VAL:HG22	2.26	0.40
2:B:267:PHE:CD2	2:B:267:PHE:N	2.89	0.40
2:B:295:MET:C	2:B:297:ASP:H	2.28	0.40
2:B:403:ALA:HB1	2:B:405:LEU:CD1	2.51	0.40
1:C:107:HIS:CB	1:C:148:GLY:O	2.69	0.40
1:C:111:GLY:C	1:C:113:GLU:H	2.30	0.40
1:C:184:PRO:HB2	1:C:399:TYR:CE2	2.56	0.40
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.04	0.40
2:D:12:CYS:HB3	5:D:503:GDP:H8	1.79	0.40
2:D:223:THR:HG23	2:D:225:GLY:H	1.85	0.40
2:D:308:ARG:NH2	2:D:339:ASN:CB	2.85	0.40
2:D:350:ASN:O	2:D:351:VAL:HG22	2.21	0.40
3:E:21:UNK:O	3:E:24:UNK:CA	2.69	0.40
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.39	0.40
1:A:125:LEU:C	1:A:127:ASP:N	2.78	0.40
1:A:221:ARG:NE	1:A:221:ARG:H	2.20	0.40
1:A:317:LEU:CD2	1:A:377:MET:HB3	2.50	0.40
1:A:402:ARG:O	1:A:405:VAL:HG12	2.21	0.40
2:B:87:PHE:O	2:B:88:ARG:C	2.65	0.40
2:B:88:ARG:HA	2:B:91:ASN:HD21	1.87	0.40
2:B:117:SER:O	2:B:120:ASP:HB2	2.21	0.40
2:B:144:GLY:N	2:B:185:TYR:CZ	2.90	0.40
2:B:151:THR:HG21	2:B:189:LEU:HD22	2.03	0.40
2:B:153:LEU:O	2:B:156:LYS:HB3	2.21	0.40
2:B:168:THR:OG1	2:B:201:THR:CB	2.64	0.40
2:B:258:ASN:OD1	2:B:352:LYS:HD2	2.21	0.40
1:C:115:ILE:CD1	1:C:156:ARG:HG3	2.34	0.40
2:D:333:LEU:HA	2:D:336:GLN:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	419/451 (93%)	221 (53%)	111 (26%)	87 (21%)	0	1
1	C	419/451 (93%)	219 (52%)	114 (27%)	86 (20%)	0	1
2	B	406/445 (91%)	184 (45%)	133 (33%)	89 (22%)	0	1
2	D	406/445 (91%)	186 (46%)	130 (32%)	90 (22%)	0	1
All	All	1650/1792 (92%)	810 (49%)	488 (30%)	352 (21%)	0	1

All (352) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	32	PRO
1	A	46	ASP
1	A	83	TYR
1	A	90	GLU
1	A	97	GLU
1	A	98	ASP
1	A	100	ALA
1	A	103	TYR
1	A	109	THR
1	A	140	SER
1	A	177	VAL
1	A	181	VAL
1	A	191	THR
1	A	197	HIS
1	A	222	PRO
1	A	238	ILE
1	A	239	THR
1	A	265	ALA
1	A	266	HIS
1	A	278	ALA
1	A	322	ASP

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Mol	Chain	Res	Type
1	A	346	TRP
1	A	349	THR
1	A	352	LYS
1	A	399	TYR
1	A	402	ARG
1	A	403	ALA
1	A	414	GLU
2	B	19	LYS
2	B	76	ASP
2	B	82	PRO
2	B	88	ARG
2	B	110	GLU
2	B	127	GLU
2	B	129	CYS
2	B	130	ASP
2	B	144	GLY
2	B	159	GLU
2	B	179	ASP
2	B	183	GLU
2	B	198	THR
2	B	240	THR
2	B	245	PRO
2	B	265	LEU
2	B	272	PHE
2	B	278	ARG
2	B	281	GLN
2	B	296	PHE
2	B	308	ARG
2	B	324	SER
2	B	344	VAL
2	B	360	PRO
2	B	378	ILE
2	B	391	ILE
2	B	398	MET
2	B	399	PHE
2	B	402	LYS
2	B	404	PHE
2	B	416	MET
2	B	428	LEU
1	C	11	GLN
1	C	32	PRO
1	C	83	TYR

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Mol	Chain	Res	Type
1	C	90	GLU
1	C	97	GLU
1	C	98	ASP
1	C	99	ALA
1	C	100	ALA
1	C	103	TYR
1	C	109	THR
1	C	140	SER
1	C	144	GLY
1	C	177	VAL
1	C	181	VAL
1	C	191	THR
1	C	197	HIS
1	C	222	PRO
1	C	238	ILE
1	C	259	LEU
1	C	265	ALA
1	C	266	HIS
1	C	277	SER
1	C	278	ALA
1	C	299	ALA
1	C	322	ASP
1	C	340	THR
1	C	346	TRP
1	C	349	THR
1	C	352	LYS
1	C	399	TYR
1	C	402	ARG
1	C	403	ALA
1	C	414	GLU
2	D	19	LYS
2	D	27	GLU
2	D	61	TYR
2	D	71	GLU
2	D	76	ASP
2	D	82	PRO
2	D	88	ARG
2	D	110	GLU
2	D	127	GLU
2	D	129	CYS
2	D	130	ASP
2	D	144	GLY

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Mol	Chain	Res	Type
2	D	159	GLU
2	D	179	ASP
2	D	183	GLU
2	D	198	THR
2	D	240	THR
2	D	245	PRO
2	D	265	LEU
2	D	272	PHE
2	D	278	ARG
2	D	281	GLN
2	D	296	PHE
2	D	308	ARG
2	D	324	SER
2	D	344	VAL
2	D	360	PRO
2	D	378	ILE
2	D	391	ILE
2	D	398	MET
2	D	402	LYS
2	D	404	PHE
2	D	416	MET
2	D	428	LEU
1	A	11	GLN
1	A	39	ASP
1	A	73	THR
1	A	99	ALA
1	A	112	LYS
1	A	144	GLY
1	A	195	LEU
1	A	237	SER
1	A	245	ASP
1	A	259	LEU
1	A	277	SER
1	A	299	ALA
1	A	340	THR
1	A	341	ILE
1	A	344	VAL
1	A	353	VAL
1	A	419	SER
2	B	26	ASP
2	B	27	GLU
2	B	56	ALA

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Mol	Chain	Res	Type
2	B	60	LYS
2	B	61	TYR
2	B	71	GLU
2	B	96	GLN
2	B	115	VAL
2	B	119	LEU
2	B	128	SER
2	B	139	HIS
2	B	185	TYR
2	B	199	ASP
2	B	219	LEU
2	B	239	THR
2	B	264	ARG
2	B	293	GLN
2	B	304	ALA
2	B	340	SER
2	B	349	ASN
2	B	382	THR
2	B	387	LEU
1	C	16	ILE
1	C	38	SER
1	C	39	ASP
1	C	46	ASP
1	C	73	THR
1	C	112	LYS
1	C	195	LEU
1	C	237	SER
1	C	239	THR
1	C	245	ASP
1	C	257	THR
1	C	264	ARG
1	C	315	CYS
1	C	341	ILE
1	C	344	VAL
1	C	353	VAL
1	C	404	PHE
1	C	419	SER
2	D	2	ARG
2	D	26	ASP
2	D	56	ALA
2	D	96	GLN
2	D	115	VAL

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Mol	Chain	Res	Type
2	D	119	LEU
2	D	128	SER
2	D	139	HIS
2	D	185	TYR
2	D	186	ASN
2	D	199	ASP
2	D	219	LEU
2	D	239	THR
2	D	293	GLN
2	D	340	SER
2	D	382	THR
2	D	387	LEU
2	D	399	PHE
1	A	28	HIS
1	A	29	GLY
1	A	38	SER
1	A	89	PRO
1	A	101	ASN
1	A	115	ILE
1	A	129	CYS
1	A	175	PRO
1	A	198	SER
1	A	210	TYR
1	A	219	ILE
1	A	257	THR
1	A	261	PRO
1	A	264	ARG
1	A	306	ASP
1	A	315	CYS
1	A	404	PHE
2	B	2	ARG
2	B	91	ASN
2	B	94	PHE
2	B	97	SER
2	B	186	ASN
2	B	190	SER
2	B	192	HIS
2	B	194	LEU
2	B	211	ASP
2	B	227	LEU
2	B	273	ALA
2	B	277	SER

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Mol	Chain	Res	Type
2	B	348	PRO
2	B	370	GLY
1	C	29	GLY
1	C	72	PRO
1	C	89	PRO
1	C	101	ASN
1	C	129	CYS
1	C	130	THR
1	C	161	TYR
1	C	198	SER
1	C	208	ALA
1	C	219	ILE
1	C	261	PRO
1	C	329	ASN
1	C	364	PRO
1	C	432	TYR
2	D	78	VAL
2	D	81	GLY
2	D	91	ASN
2	D	94	PHE
2	D	97	SER
2	D	155	SER
2	D	190	SER
2	D	192	HIS
2	D	194	LEU
2	D	264	ARG
2	D	273	ALA
2	D	277	SER
2	D	283	TYR
2	D	304	ALA
2	D	339	ASN
2	D	348	PRO
2	D	370	GLY
1	A	72	PRO
1	A	125	LEU
1	A	130	THR
1	A	131	GLY
1	A	145	THR
1	A	314	ALA
1	A	326	LYS
1	A	436	GLY
2	B	30	ILE

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Mol	Chain	Res	Type
2	B	52	TYR
2	B	63	PRO
2	B	78	VAL
2	B	177	VAL
2	B	424	ASN
1	C	28	HIS
1	C	132	LEU
1	C	145	THR
1	C	292	THR
1	C	306	ASP
1	C	314	ALA
1	C	326	LYS
1	C	348	PRO
1	C	382	THR
1	C	408	TYR
1	C	436	GLY
2	D	63	PRO
2	D	154	ILE
2	D	177	VAL
2	D	211	ASP
2	D	227	LEU
2	D	318	VAL
2	D	349	ASN
2	D	424	ASN
2	D	431	GLU
1	A	161	TYR
1	A	329	ASN
1	A	342	GLN
1	A	348	PRO
1	A	364	PRO
1	A	369	ALA
1	A	382	THR
1	A	432	TYR
2	B	3	GLU
2	B	162	PRO
2	B	193	GLN
2	B	339	ASN
1	C	125	LEU
1	C	175	PRO
1	C	369	ALA
2	D	148	GLY
2	D	160	GLU

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Mol	Chain	Res	Type
2	D	193	GLN
1	A	17	GLY
1	A	307	PRO
2	B	81	GLY
2	B	154	ILE
2	B	163	ASP
2	B	182	VAL
2	B	431	GLU
1	C	115	ILE
1	C	298	PRO
1	C	342	GLN
2	D	30	ILE
2	D	107	HIS
2	D	111	GLY
2	D	162	PRO
2	D	182	VAL
1	A	298	PRO
2	B	93	VAL
2	B	222	PRO
2	B	318	VAL
1	C	78	VAL
1	C	131	GLY
2	D	93	VAL
2	D	222	PRO
1	A	288	VAL
2	B	86	ILE
1	A	30	ILE
2	B	111	GLY
1	C	307	PRO
2	D	184	PRO
1	A	78	VAL
2	B	279	GLY
1	C	273	ALA
1	A	273	ALA
1	A	435	VAL
2	D	271	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	354/377 (94%)	268 (76%)	86 (24%)	1	5
1	C	354/377 (94%)	272 (77%)	82 (23%)	1	5
2	B	347/381 (91%)	273 (79%)	74 (21%)	1	7
2	D	347/381 (91%)	274 (79%)	73 (21%)	1	7
All	All	1402/1516 (92%)	1087 (78%)	315 (22%)	1	6

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	8	HIS
1	A	16	ILE
1	A	23	LEU
1	A	25	CYS
1	A	30	ILE
1	A	32	PRO
1	A	40	LYS
1	A	42	ILE
1	A	46	ASP
1	A	47	ASP
1	A	71	GLU
1	A	73	THR
1	A	77	GLU
1	A	82	THR
1	A	86	LEU
1	A	87	PHE
1	A	91	GLN
1	A	92	LEU
1	A	97	GLU
1	A	101	ASN
1	A	105	ARG
1	A	115	ILE
1	A	125	LEU
1	A	130	THR
1	A	141	PHE
1	A	150	THR
1	A	163	LYS
1	A	164	LYS
1	A	171	ILE

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Mol	Chain	Res	Type
1	A	177	VAL
1	A	179	THR
1	A	181	VAL
1	A	182	VAL
1	A	188	ILE
1	A	196	GLU
1	A	197	HIS
1	A	199	ASP
1	A	209	ILE
1	A	210	TYR
1	A	212	ILE
1	A	213	CYS
1	A	214	ARG
1	A	216	ASN
1	A	221	ARG
1	A	244	PHE
1	A	248	LEU
1	A	250	VAL
1	A	252	LEU
1	A	258	ASN
1	A	267	PHE
1	A	269	LEU
1	A	275	VAL
1	A	276	ILE
1	A	279	GLU
1	A	282	TYR
1	A	284	GLU
1	A	285	GLN
1	A	286	LEU
1	A	292	THR
1	A	297	GLU
1	A	302	MET
1	A	309	HIS
1	A	312	TYR
1	A	316	CYS
1	A	318	LEU
1	A	322	ASP
1	A	324	VAL
1	A	335	ILE
1	A	336	LYS
1	A	345	ASP
1	A	349	THR

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Mol	Chain	Res	Type
1	A	364	PRO
1	A	373	ARG
1	A	376	CYS
1	A	398	MET
1	A	402	ARG
1	A	404	PHE
1	A	411	GLU
1	A	413	MET
1	A	414	GLU
1	A	418	PHE
1	A	420	GLU
1	A	428	LEU
1	A	433	GLU
1	A	439	SER
2	B	16	ILE
2	B	25	SER
2	B	53	TYR
2	B	55	GLU
2	B	60	LYS
2	B	70	LEU
2	B	76	ASP
2	B	78	VAL
2	B	86	ILE
2	B	88	ARG
2	B	91	ASN
2	B	113	GLU
2	B	119	LEU
2	B	128	SER
2	B	136	GLN
2	B	137	LEU
2	B	139	HIS
2	B	149	MET
2	B	157	ILE
2	B	160	GLU
2	B	163	ASP
2	B	166	MET
2	B	168	THR
2	B	180	THR
2	B	185	TYR
2	B	186	ASN
2	B	193	GLN
2	B	194	LEU

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Mol	Chain	Res	Type
2	B	201	THR
2	B	203	CYS
2	B	218	LYS
2	B	228	ASN
2	B	239	THR
2	B	244	PHE
2	B	245	PRO
2	B	249	ASN
2	B	251	ASP
2	B	253	ARG
2	B	254	LYS
2	B	255	LEU
2	B	257	VAL
2	B	278	ARG
2	B	283	TYR
2	B	284	ARG
2	B	286	LEU
2	B	292	THR
2	B	302	MET
2	B	308	ARG
2	B	311	ARG
2	B	315	VAL
2	B	323	MET
2	B	341	SER
2	B	345	GLU
2	B	346	TRP
2	B	348	PRO
2	B	350	ASN
2	B	352	LYS
2	B	380	ASN
2	B	382	THR
2	B	388	PHE
2	B	391	ILE
2	B	398	MET
2	B	401	ARG
2	B	405	LEU
2	B	407	TRP
2	B	409	THR
2	B	413	MET
2	B	414	ASP
2	B	416	MET
2	B	419	THR

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Mol	Chain	Res	Type
2	B	425	MET
2	B	426	ASN
2	B	436	GLN
2	B	437	ASP
1	C	8	HIS
1	C	16	ILE
1	C	23	LEU
1	C	25	CYS
1	C	30	ILE
1	C	32	PRO
1	C	40	LYS
1	C	42	ILE
1	C	46	ASP
1	C	47	ASP
1	C	71	GLU
1	C	73	THR
1	C	77	GLU
1	C	82	THR
1	C	86	LEU
1	C	87	PHE
1	C	91	GLN
1	C	92	LEU
1	C	97	GLU
1	C	101	ASN
1	C	115	ILE
1	C	125	LEU
1	C	130	THR
1	C	141	PHE
1	C	150	THR
1	C	163	LYS
1	C	164	LYS
1	C	171	ILE
1	C	175	PRO
1	C	177	VAL
1	C	179	THR
1	C	181	VAL
1	C	182	VAL
1	C	188	ILE
1	C	189	LEU
1	C	196	GLU
1	C	197	HIS
1	C	199	ASP

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Mol	Chain	Res	Type
1	C	209	ILE
1	C	212	ILE
1	C	213	CYS
1	C	214	ARG
1	C	216	ASN
1	C	221	ARG
1	C	244	PHE
1	C	252	LEU
1	C	258	ASN
1	C	267	PHE
1	C	269	LEU
1	C	275	VAL
1	C	276	ILE
1	C	279	GLU
1	C	282	TYR
1	C	284	GLU
1	C	285	GLN
1	C	286	LEU
1	C	292	THR
1	C	297	GLU
1	C	302	MET
1	C	309	HIS
1	C	316	CYS
1	C	318	LEU
1	C	322	ASP
1	C	335	ILE
1	C	336	LYS
1	C	345	ASP
1	C	349	THR
1	C	355	ILE
1	C	373	ARG
1	C	376	CYS
1	C	395	PHE
1	C	398	MET
1	C	402	ARG
1	C	404	PHE
1	C	411	GLU
1	C	413	MET
1	C	414	GLU
1	C	418	PHE
1	C	420	GLU
1	C	428	LEU

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Mol	Chain	Res	Type
1	C	433	GLU
1	C	439	SER
2	D	16	ILE
2	D	25	SER
2	D	53	TYR
2	D	55	GLU
2	D	60	LYS
2	D	70	LEU
2	D	76	ASP
2	D	78	VAL
2	D	88	ARG
2	D	91	ASN
2	D	113	GLU
2	D	119	LEU
2	D	128	SER
2	D	136	GLN
2	D	137	LEU
2	D	139	HIS
2	D	149	MET
2	D	157	ILE
2	D	160	GLU
2	D	163	ASP
2	D	175	PRO
2	D	180	THR
2	D	185	TYR
2	D	186	ASN
2	D	192	HIS
2	D	193	GLN
2	D	194	LEU
2	D	201	THR
2	D	218	LYS
2	D	228	ASN
2	D	230	LEU
2	D	239	THR
2	D	244	PHE
2	D	245	PRO
2	D	249	ASN
2	D	251	ASP
2	D	254	LYS
2	D	255	LEU
2	D	257	VAL
2	D	278	ARG

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Mol	Chain	Res	Type
2	D	283	TYR
2	D	284	ARG
2	D	286	LEU
2	D	292	THR
2	D	302	MET
2	D	308	ARG
2	D	311	ARG
2	D	312	TYR
2	D	315	VAL
2	D	323	MET
2	D	341	SER
2	D	345	GLU
2	D	346	TRP
2	D	350	ASN
2	D	352	LYS
2	D	380	ASN
2	D	381	SER
2	D	382	THR
2	D	388	PHE
2	D	391	ILE
2	D	398	MET
2	D	401	ARG
2	D	405	LEU
2	D	407	TRP
2	D	409	THR
2	D	413	MET
2	D	414	ASP
2	D	416	MET
2	D	419	THR
2	D	425	MET
2	D	426	ASN
2	D	436	GLN
2	D	437	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	35	GLN
1	A	102	ASN
1	A	133	GLN
1	A	176	GLN

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Mol	Chain	Res	Type
1	A	186	ASN
1	A	258	ASN
1	A	285	GLN
1	A	300	ASN
1	A	301	GLN
1	A	356	ASN
1	A	393	HIS
2	B	6	HIS
2	B	14	ASN
2	B	15	GLN
2	B	85	GLN
2	B	91	ASN
2	B	96	GLN
2	B	101	ASN
2	B	102	ASN
2	B	133	GLN
2	B	139	HIS
2	B	193	GLN
2	B	197	ASN
2	B	206	ASN
2	B	228	ASN
2	B	282	GLN
2	B	294	GLN
2	B	337	ASN
2	B	350	ASN
2	B	380	ASN
2	B	424	ASN
2	B	433	GLN
2	B	434	GLN
1	C	15	GLN
1	C	35	GLN
1	C	102	ASN
1	C	133	GLN
1	C	176	GLN
1	C	186	ASN
1	C	258	ASN
1	C	285	GLN
1	C	300	ASN
1	C	301	GLN
1	C	329	ASN
1	C	356	ASN
1	C	393	HIS

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Mol	Chain	Res	Type
2	D	6	HIS
2	D	14	ASN
2	D	15	GLN
2	D	85	GLN
2	D	91	ASN
2	D	101	ASN
2	D	102	ASN
2	D	107	HIS
2	D	133	GLN
2	D	139	HIS
2	D	193	GLN
2	D	197	ASN
2	D	206	ASN
2	D	228	ASN
2	D	282	GLN
2	D	294	GLN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	433	GLN
2	D	434	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
4	GTP	C	502	-	33,34,34	1.47	3 (9%)	50,54,54	0.82	2 (4%)
5	GDP	B	501	-	29,30,30	1.68	4 (13%)	45,47,47	0.82	1 (2%)
4	GTP	A	500	-	33,34,34	2.79	5 (15%)	50,54,54	0.79	0
5	GDP	D	503	-	29,30,30	1.10	3 (10%)	45,47,47	0.85	2 (4%)

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
4	GTP	C	502	-	-	3/22/38/38	0/3/3/3
5	GDP	B	501	-	-	4/16/32/32	0/3/3/3
4	GTP	A	500	-	-	5/22/38/38	0/3/3/3
5	GDP	D	503	-	-	6/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	GTP	PA-O3A	-10.33	1.48	1.59
4	A	500	GTP	PB-O3A	-8.66	1.50	1.59
5	B	501	GDP	PA-O3A	-6.91	1.52	1.59
4	A	500	GTP	PB-O3B	6.48	1.66	1.59
4	C	502	GTP	PB-O3B	5.64	1.65	1.59
5	B	501	GDP	C6-N1	2.49	1.43	1.38
4	C	502	GTP	PB-O3A	2.44	1.62	1.59
5	D	503	GDP	PA-O3A	-2.37	1.56	1.59
4	A	500	GTP	O5'-C5'	-2.22	1.36	1.44
5	D	503	GDP	C6-N1	2.22	1.43	1.38
5	D	503	GDP	PA-O2A	-2.14	1.45	1.55
4	A	500	GTP	PA-O2A	-2.11	1.45	1.55
5	B	501	GDP	PA-O2A	-2.06	1.45	1.55
5	B	501	GDP	O4'-C1'	-2.05	1.37	1.42
4	C	502	GTP	PA-O3A	2.00	1.61	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	GTP	O2G-PG-O3B	2.65	113.51	104.64
4	C	502	GTP	O2A-PA-O3A	2.41	113.79	107.27
5	D	503	GDP	O2B-PB-O3A	2.31	112.38	104.64
5	B	501	GDP	C4'-O4'-C1'	-2.26	104.48	109.47
5	D	503	GDP	O3B-PB-O3A	2.10	111.68	104.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O1A
5	B	501	GDP	C5'-O5'-PA-O2A
5	B	501	GDP	C4'-C5'-O5'-PA
5	D	503	GDP	C5'-O5'-PA-O3A
5	D	503	GDP	C5'-O5'-PA-O1A
5	D	503	GDP	C5'-O5'-PA-O2A
5	D	503	GDP	C4'-C5'-O5'-PA
4	A	500	GTP	C3'-C4'-C5'-O5'
5	D	503	GDP	O4'-C4'-C5'-O5'
5	D	503	GDP	C3'-C4'-C5'-O5'
4	A	500	GTP	O4'-C4'-C5'-O5'
4	A	500	GTP	PG-O3B-PB-O1B
4	C	502	GTP	C3'-C4'-C5'-O5'
4	A	500	GTP	PA-O3A-PB-O1B
4	A	500	GTP	C5'-O5'-PA-O1A
4	C	502	GTP	C5'-O5'-PA-O1A
4	C	502	GTP	O4'-C4'-C5'-O5'

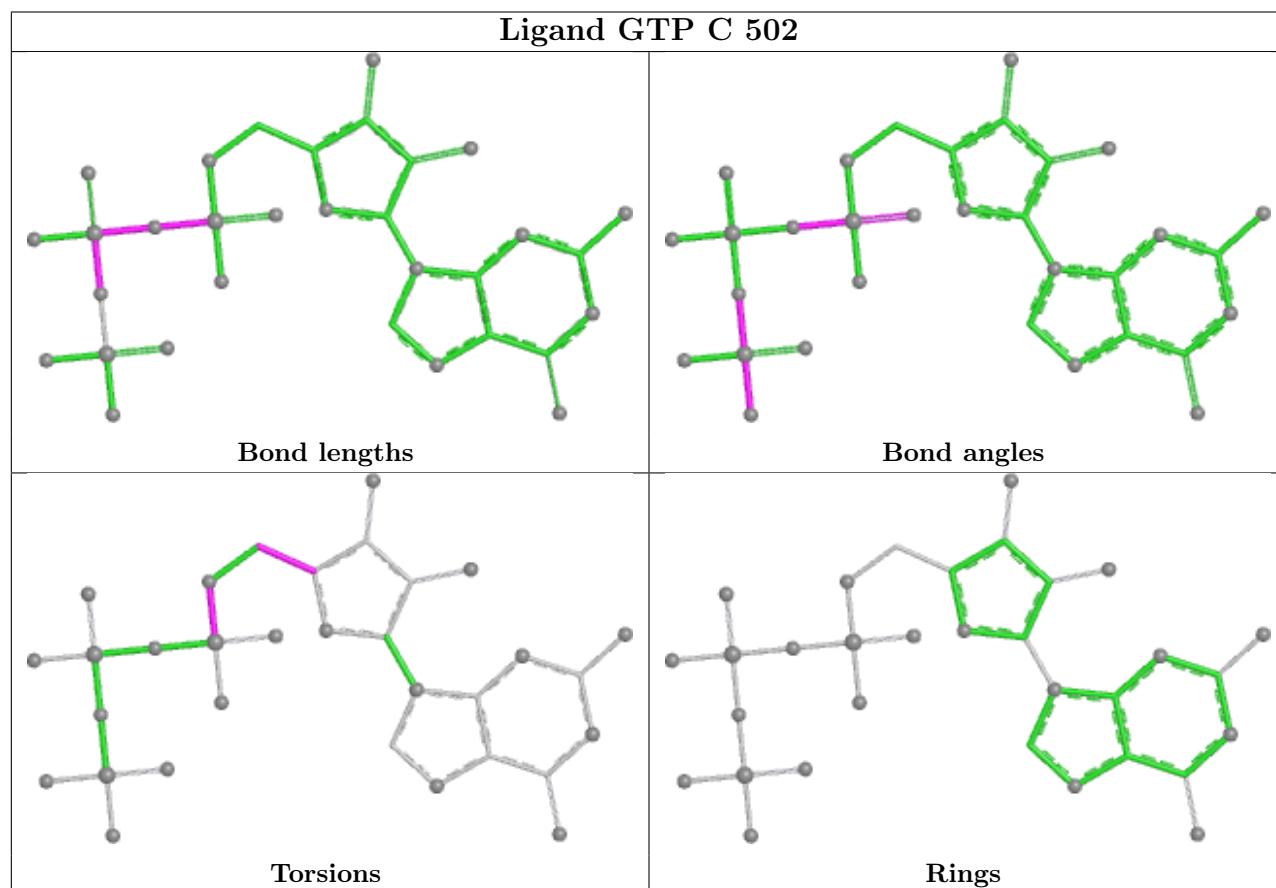
There are no ring outliers.

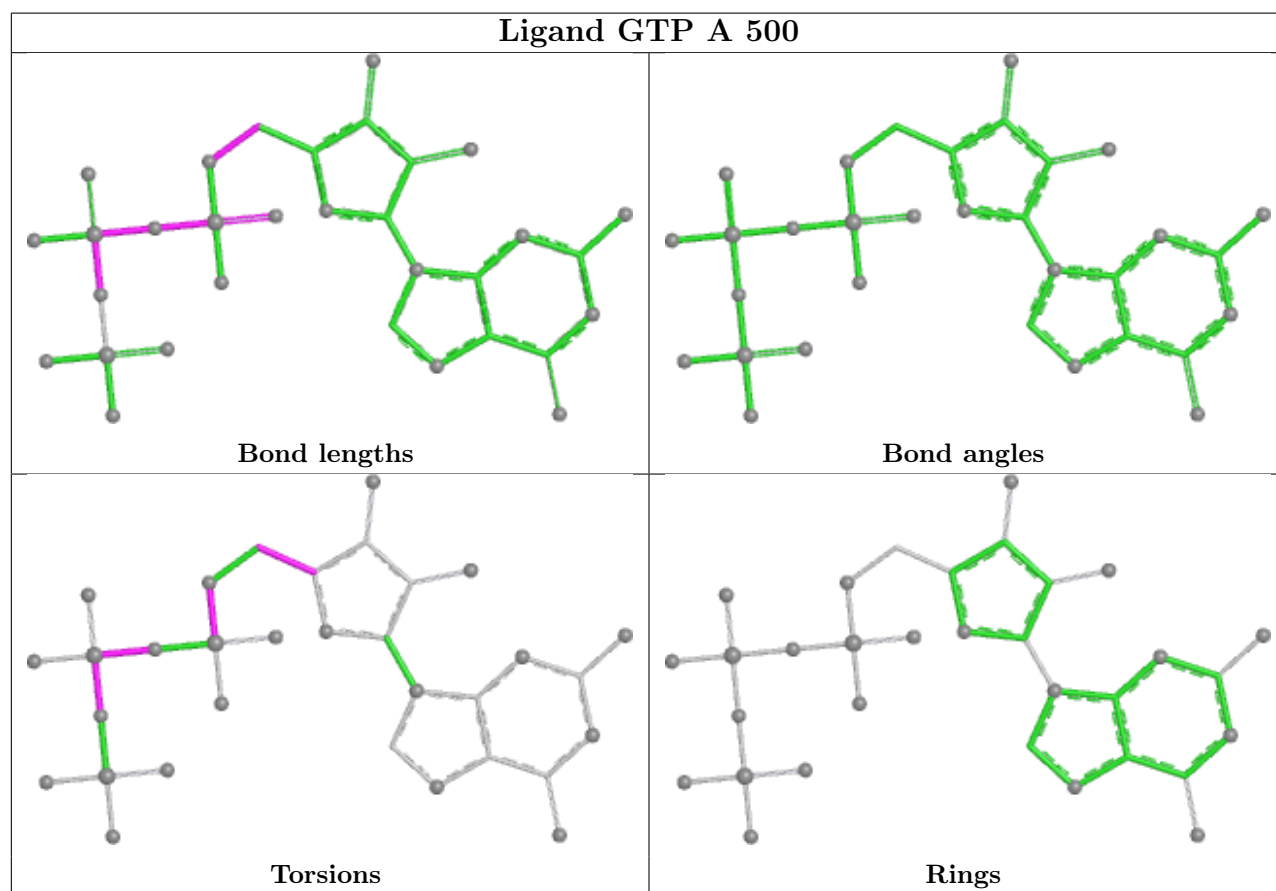
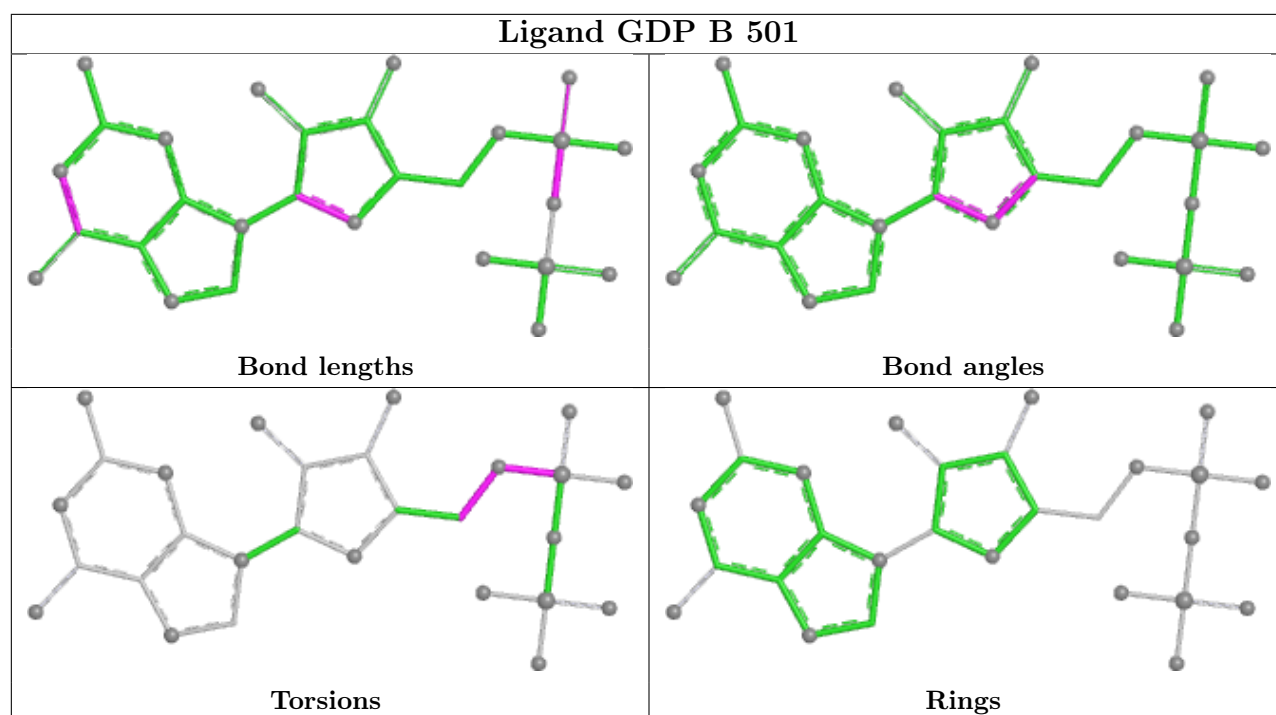
4 monomers are involved in 26 short contacts:

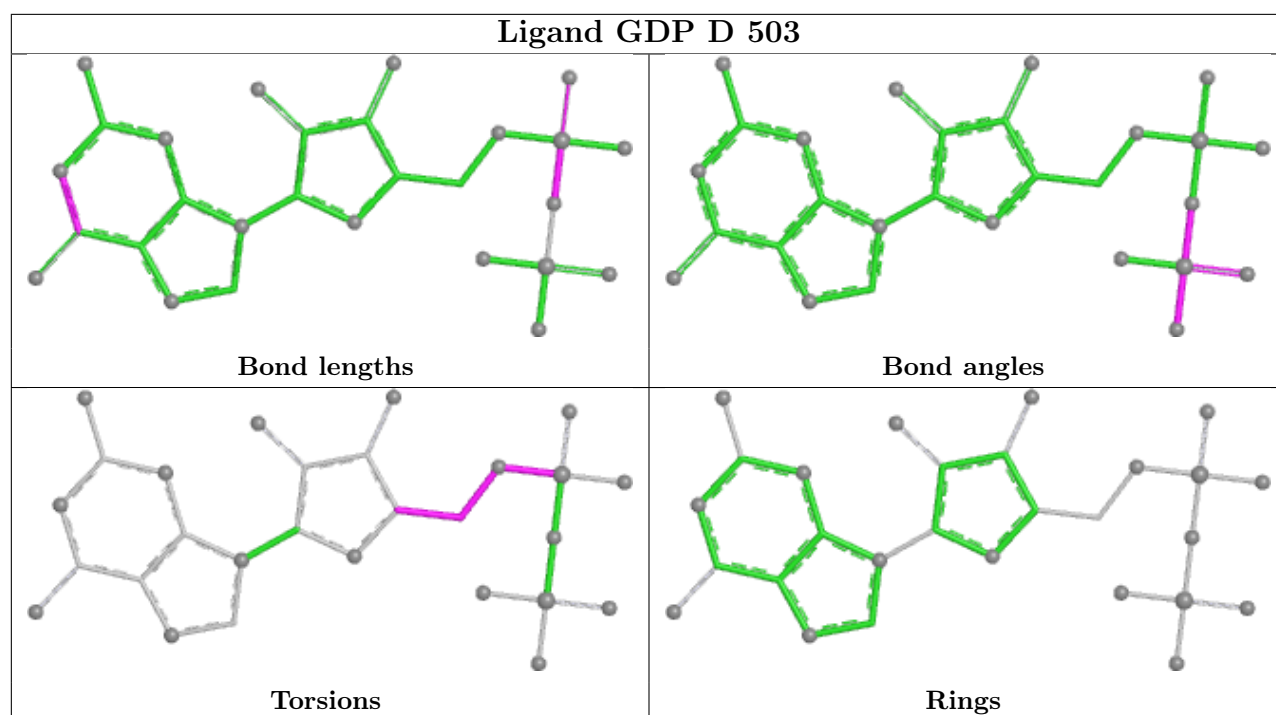
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	GTP	8	0
5	B	501	GDP	5	0
4	A	500	GTP	4	0
5	D	503	GDP	9	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.