



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FFX  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

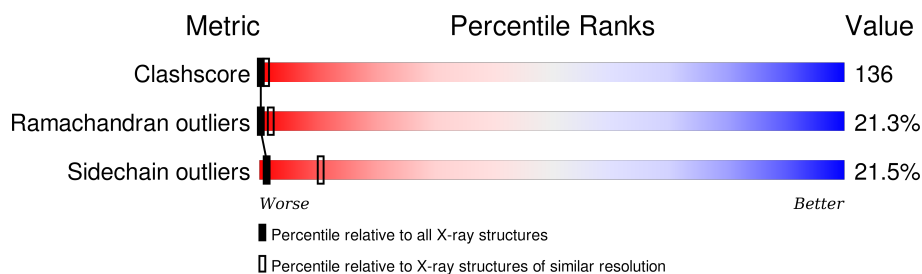
# 1 Overall quality at a glance

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	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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).

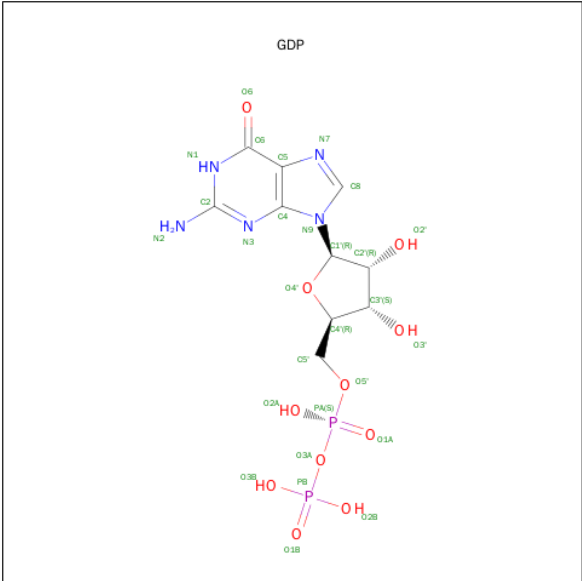
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	91	Total	C	N	O	0	0	0
			456	273	91	92			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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 (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

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

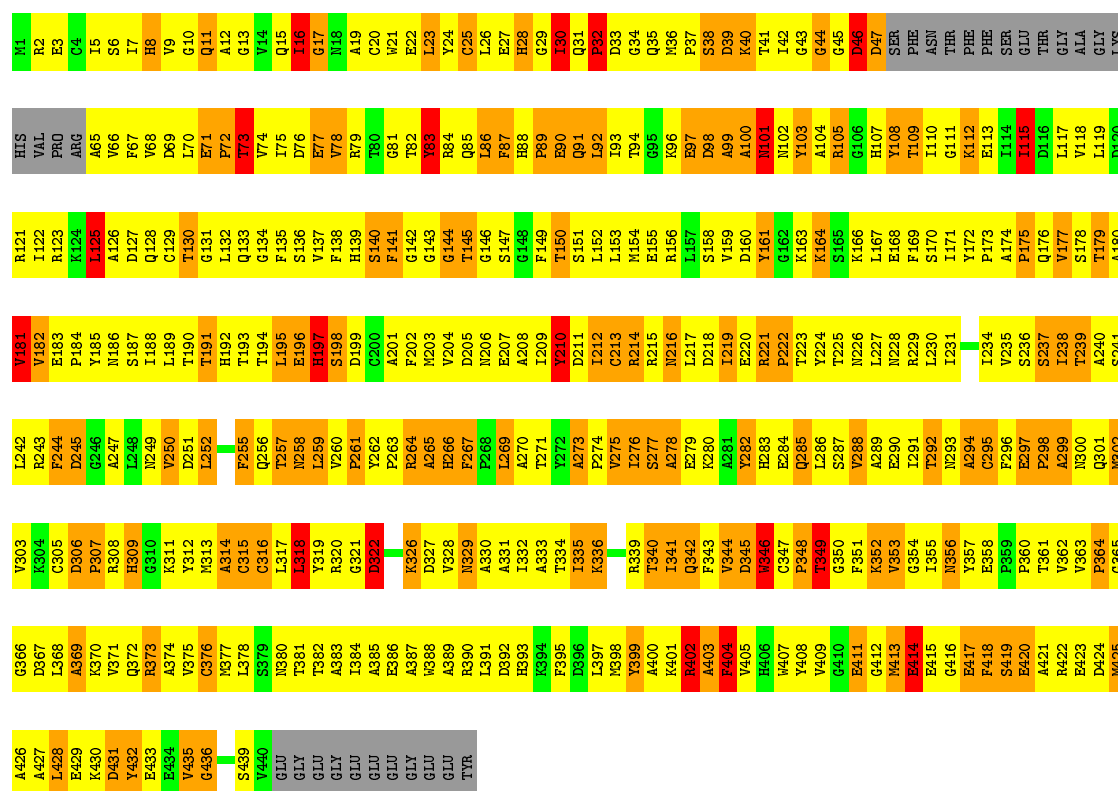
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

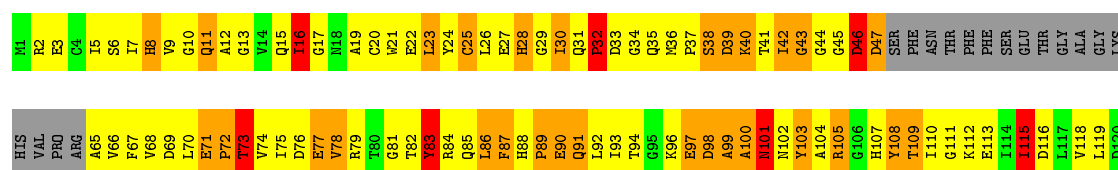
#### • Molecule 1: PROTEIN (TUBULIN)

Chain A: 



#### • Molecule 1: PROTEIN (TUBULIN)

Chain C: 



R121	R181	S241	M302	P364	D424
I122	V182	L242	V303	G365	M425
R123	E183	R243	R304	G366	A426
K124	P184	R244	C305	G367	A427
L125	Y185	D245	D306	L368	L428
A126	M186	G246	P307	A369	E429
D127	S187	K247	R308	K370	K430
Q128	L188	L248	G309	K372	D431
G129	L189	L249	G310	G373	D432
T130	T190	V250	K311	K374	E433
G131	T191	D251	Y312	A374	E434
L132	H192	L252	K313	G375	V435
Q133	T193	T253	A314	G376	G436
G134	T194	E254	C315	K377	S439
F135	L195	F255	C316	L378	V440
S136	E196	Q256	L317	S379	GLU
V137	H197	T257	L318	K380	GLY
F138	S198	N258	Y319	T381	GLY
H139	D199	L259	R320	T382	GLU
S140	G200	V260	G321	K383	GLY
F141	A201	P261	R322	L384	GLU
G142	F202	Y262	K326	I385	GLU
G143	M203	P263	D327	E386	GLU
G144	V204	R264	D327	A387	GLY
T145	D205	G265	V328	K388	GLY
G146	N206	H266	N329	A389	GLU
S147	E207	P267	A330	K390	TYR
G148	A208	F268	A331	L391	
F149	T209	L269	I332	D392	
I150	Y210	K270	A333	H393	
S151	D211	A271	T334	K394	
L152	L212	A273	I335	P395	
L153	C213	P274	K336	D396	
M154	R214	V275	T337	L397	
E155	R215	L276	K338	K398	
R156	N216	S277	K339	Y399	
L157	L217	A278	T340	GLY	
S158	D218	E279	I341	A400	
V159	I219	K280	Q342	R402	
D160	E220	A281	F343	A403	
Y161	R221	Y282	V344	F404	
G162	P222	H283	D345	V405	
K163	T223	E284	K346	H406	
Y164	Y224	Q285	C347	H407	
S165	T225	L286	P348	Y408	
K166	N226	S287	T349	V409	
L167	L227	V288	G350	G410	
E168	N228	A289	F351	E411	
F169	R229	E290	K352	G412	
S170	L230	L291	V353	H413	
I171	I231	T292	G354	E414	
Y172	G232	N293	I355	E415	
P173	Q233	A294	N356	A416	
A174	I234	C295	Y357	A417	
P175	V235	F296	E358	G418	
O176	S236	E297	P359	S419	
V177	S237	P298	P360	E420	
T178	L238	A299	T361	A421	
G179	T239	N300	V362	L242	
A180	A240	Q301	V363	E423	

• Molecule 2: PROTEIN (TUBULIN)

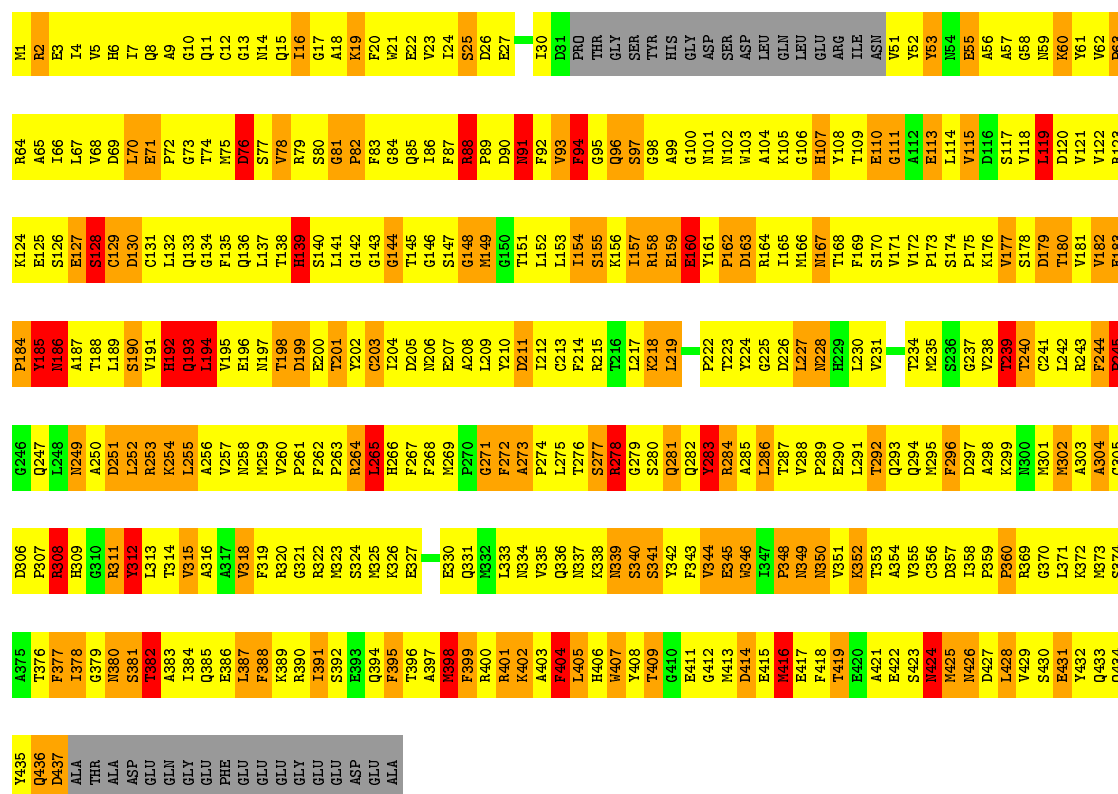
Chain B: 6% 57% 25% 5% 8%

M1	R2	R64	K124	P184	F244	A304	M373	Q433
R2	A65	A65	E125	Y185	P245	C305	S374	Q434
I4	L67	L66	E126	N186	G246	D306	A375	Y435
H6	V68	V68	S128	T188	Q247	P307	T376	Q436
I7	D69	D69	L248	L189	N249	R309	F377	D437
Q8	L70	L70	D130	S190	A250	G310	K378	ALA
G9	E71	E71	C131	Y191	D251	R311	G379	THR
G10	P72	P72	L132	H192	L252	Y312	M380	ALA
Q11	G73	G73	Q133	Q193	R253	L313	S381	ASP
C12	T74	T74	K134	L194	K254	T314	T382	GLU
G13	M75	M75	F135	V195	L255	V315	K383	GLN
N14	S77	S77	L136	E196	A256	A316	K384	GLY
Q15	R78	R78	L137	N197	V257	K317	K385	GLU
I16	R79	R79	T138	T198	N258	V318	E386	PHE
G17	S80	S80	H139	D199	M259	F319	L387	GLU
A18	G81	G81	L141	E200	V260	K320	F388	GLU
K19	P82	P82	G142	T201	P261	G321	K389	GLU
F20	F83	F83	G143	Y202	F262	R322	K390	GLY
M21	G84	G84	G144	C203	P263	K323	I391	GLU
G95	R85	R85	T145	L204	R264	S324	S392	GLU
V23	G86	G86	G146	D205	H266	K325	E393	ASP
I24	F87	F87	S147	N206	H266	K326	Q394	GLU
S25	K88	K88	G148	E207	F267	E327	T395	ALA
D26	P89	P89	M149	A208	F268	A397	T396	
E27	D90	D90	G150	L209	M269	E330	K397	
I30	N91	N91	T151	Y210	P270	K331	K398	
D31	F92	F92	L152	T212	F272	L333	P399	
THR	V93	V93	L153	C213	A273	K334	R400	
P90	F94	F94	I154	F214	P274	V335	K402	
K96	G95	G95	S155	R215	L275	Q336	A403	
GLY	Q96	Q96	T216	L217	T276	R337	R404	
THR	S97	S97	L157	K218	S277	K338	L405	
GLY	HIS	HIS	R158	E159	G279	N339	H407	
ASP	GLY	GLY	E159	L219	S280	S340	Y408	
ASP	ASP	ASP	N101	G100	Q281	Y342	T409	
ASP	ASP	ASP	M102	N102	Q282	F343	G410	
ASP	ASP	ASP	M103	P162	Q283	Y344	E411	
LEU	LEU	LEU	R164	R164	R284	E345	G412	
LEU	LEU	LEU	K105	G225	A285	K346	M413	
LEU	LEU	LEU	M166	D226	L266	L347	D414	
ARG	ARG	ARG	M167	L227	T287	P348	E415	
ILE	ILE	ILE	T168	N228	V288	R349	M416	
V51	V51	V51	F169	H229	P289	N350	E417	
Y52	Y52	Y52	S170	E110	E290	V351	F418	
Y53	Y53	Y53	V171	G111	L230	T352	T419	
E54	E54	E54	V172	A112	S232	K353	A421	
E55	E55	E55	E143	E143	Q233	A354	E422	
A56	A56	A56	S174	L114	Q294	C356	S423	
A57	S117	S117	P175	V115	M295	D357	R424	
G58	V118	V118	K176	D116	S236	F296	M425	
N59	L119	L119	S178	E143	D297	L297	M426	
K60	D120	D120	S178	D179	A298	D427	L428	
V62	V121	V121	T180	T238	K360	P360	V429	
P63	L123	L123	V181	T240	R301	R369	S430	
			V182	C241	M302	G370	E431	
			E183	L242	L242	L371	Y432	

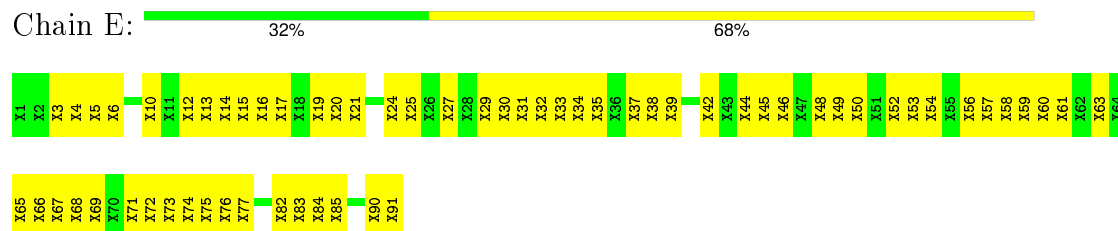
• Molecule 2: PROTEIN (TUBULIN)

Chain D: 6% 56% 24% 6% 8%





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



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	67.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.59	0/3367	0.86	5/4570 (0.1%)
1	C	0.56	0/3367	0.84	5/4570 (0.1%)
2	B	0.56	0/3270	0.82	1/4428 (0.0%)
2	D	0.58	0/3270	0.84	0/4428
All	All	0.57	0/13274	0.84	11/17996 (0.1%)

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

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	417	GLU	N-CA-C	-5.93	94.99	111.00
1	C	318	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	417	GLU	N-CA-C	-5.77	95.43	111.00
1	A	318	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	294	ALA	N-CA-C	-5.38	96.46	111.00
1	C	294	ALA	N-CA-C	-5.33	96.61	111.00
2	B	356	CYS	N-CA-C	5.20	125.05	111.00
1	A	44	GLY	N-CA-C	-5.15	100.23	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	GLY	N-CA-C	-5.13	100.27	113.10
1	C	43	GLY	N-CA-C	-5.05	100.47	113.10
1	A	81	GLY	N-CA-C	-5.04	100.49	113.10

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 ⓘ

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	883	0
1	C	3295	0	3202	910	0
2	B	3201	0	3091	916	0
2	D	3201	0	3091	883	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
All	All	13568	0	12737	3585	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 136.

All (3585) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:311:ARG:HH21	2:D:437:ASP:HB2	1.03	1.13
1:C:222:PRO:HB2	1:C:227:LEU:HD11	1.31	1.12
2:B:179:ASP:HA	1:C:352:LYS:HE2	1.20	1.12
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
2:D:240:THR:O	2:D:243:ARG:HB2	1.56	1.06
1:A:133:GLN:H	1:A:164:LYS:HD3	1.12	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
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
1:C:7:ILE:HG22	1:C:66:VAL:HB	1.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:HG3	2:D:133:GLN:NE2	1.73	1.03
2:B:278:ARG:HA	2:B:278:ARG:HH11	0.91	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
2:B:264:ARG:HH21	2:B:428:LEU:HD12	1.22	1.02
1:A:141:PHE:HE2	1:A:172:TYR:HA	1.23	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
2:D:278:ARG:HA	2:D:278:ARG:NH1	1.76	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: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
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.45	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:C:166:LYS:HE3	1:C:198:SER:H	1.31	0.96
1:A:322:ASP:H	1:A:357:TYR:HA	1.30	0.96
1:C:409:VAL:HA	1:C:414:GLU:OE1	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CA	2:B:278:ARG:HH11	1.79	0.95
1:C:214:ARG:NH2	1:C:220:GLU:HA	1.80	0.95
2:B:91:ASN:HD22	2:B:91:ASN:H	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:196:GLU:O	2:D:198:THR:HG22	1.66	0.94
2:D:77:SER:HA	2:D:80:SER:HB3	1.48	0.94
1:A:93:ILE:HD13	1:A:118:VAL:HG22	1.48	0.94
2:B:407:TRP:HZ2	1:C:256:GLN:HB2	1.30	0.94
2:D:218:LYS:HZ3	2:D:278:ARG:N	1.65	0.93
1:A:79:ARG:HD3	1:A:89:PRO:HB3	1.50	0.93
1:A:175:PRO:CD	1:A:207:GLU:HB2	1.97	0.93
2:D:263:PRO:C	2:D:265:LEU:H	1.68	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
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:B:218:LYS:HZ3	2:B:278:ARG:H	0.96	0.92
1:C:383:ALA:O	1:C:386:GLU:HG2	1.68	0.92
1:C:87:PHE:HE2	1:C:92:LEU:HD21	1.34	0.92
1:A:322:ASP:N	1:A:357:TYR:HA	1.84	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:C:137:VAL:HG11	1:C:154:MET:HE2	1.51	0.92
1:C:175:PRO:C	1:C:177:VAL:H	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:137:VAL:HG11	1:A:154:MET:HE2	1.50	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
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:263:PRO:C	2:B:265:LEU:H	1.64	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
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:223:THR:HB	1:A:226:ASN:OD1	1.71	0.90
2:B:286:LEU:HD12	2:B:373:MET:HB2	1.54	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
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:311:ARG:NH2	2:B:437:ASP:HB2	1.88	0.89
2:B:96:GLN:HE22	1:C:130:THR:HG22	1.35	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
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
1:A:166:LYS:NZ	1:A:197:HIS:HB2	1.88	0.88
1:A:9:VAL:HG12	1:A:68:VAL:CG1	2.03	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:N	1:A:418:PHE:HD2	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:69:ASP:OD1	1:C:70:LEU:N	2.05	0.88
1:C:31:GLN:HB3	1:C:32:PRO:HD2	1.56	0.88
2:B:133:GLN:NE2	2:B:252:LEU:HB3	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:284:ARG:O	2:B:287:THR:HG23	1.73	0.87
1:A:287:SER:H	1:A:290:GLU:CD	1.77	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: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:409:VAL:HG13	1:A:414:GLU:OE2	1.75	0.87
1:A:216:ASN:HD22	1:A:275:VAL:HG12	1.38	0.87
1:A:144:GLY:N	1:A:147:SER:HB3	1.89	0.87
2:B:176:LYS:HD2	2:B:210:TYR:CZ	2.10	0.87
1:A:320:ARG:HB3	1:A:374:ALA:HB3	1.56	0.87
1:A:261:PRO:HG2	1:A:380:ASN:HD21	1.38	0.87
1:C:243:ARG:HH12	1:C:250:VAL:HG13	1.39	0.86
1:C:27:GLU:HG3	1:C:28:HIS:H	1.40	0.86
2:B:396:THR:HG23	2:B:400:ARG:HD3	1.54	0.86
2:D:396:THR:HG23	2:D:400:ARG:HD3	1.57	0.86
2:D:223:THR:HG22	2:D:226:ASP:OD2	1.76	0.86
2:D:88:ARG:HB2	2:D:89:PRO:HD3	1.56	0.86
2:B:311:ARG:HB2	2:B:344:VAL:H	1.40	0.86
2:B:88:ARG:HB2	2:B:89:PRO:HD3	1.55	0.86
1:A:322:ASP:H	1:A:357:TYR:CA	1.88	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
2:B:223:THR:HG22	2:B:226:ASP:CG	1.97	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:C:409:VAL:HG13	1:C:414:GLU:OE2	1.75	0.85
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.58	0.85
1:C:322:ASP:H	1:C:357:TYR:CA	1.88	0.85
1:C:223:THR:HB	1:C:226:ASN:OD1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:O	1:C:104:ALA:N	2.09	0.85
2:D:344:VAL:HB	2:D:346:TRP:NE1	1.91	0.85
2:D:103:TRP:HE1	2:D:189:LEU:HD21	1.40	0.85
1:A:332:ILE:HD11	1:A:353:VAL:HG21	1.58	0.85
1:C:344:VAL:HG11	1:C:346:TRP:NE1	1.91	0.85
3:E:35:UNK:C	3:E:37:UNK:N	2.35	0.85
2:D:59:ASN:HB2	2:D:64:ARG:NE	1.90	0.85
1:C:386:GLU:HG3	1:C:387:ALA:N	1.90	0.85
2:B:19:LYS:HZ1	2:B:82:PRO:HG3	1.42	0.85
2:D:158:ARG:HG3	2:D:159:GLU:N	1.91	0.85
2:B:91:ASN:N	2:B:91:ASN:HD22	1.75	0.84
2:B:141:LEU:HB3	2:B:186:ASN:HB3	1.57	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:418:PHE:CD2	1:C:418:PHE:N	2.45	0.84
2:D:176:LYS:HD2	2:D:210:TYR:CZ	2.13	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
2:B:51:VAL:HG23	2:B:53:TYR:H	1.42	0.84
1:C:216:ASN:HD22	1:C:275:VAL:HG12	1.42	0.84
1:A:2:ARG:NH2	1:A:133:GLN:HE22	1.76	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: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
2:B:121:VAL:HA	2:B:124:LYS:HG2	1.57	0.83
2:D:58:GLY:C	2:D:64:ARG:HE	1.81	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
2:D:19:LYS:NZ	2:D:82:PRO:HG3	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:192:HIS:C	2:B:194:LEU:H	1.82	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:100:ALA:HB1	1:A:105:ARG:O	1.78	0.82
2:D:132:LEU:HB3	2:D:164:ARG:HH21	1.42	0.82
1:A:350:GLY:C	1:A:351:PHE:HD1	1.82	0.82
1:A:92:LEU:N	1:A:92:LEU:HD12	1.94	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:C:9:VAL:HG12	1:C:68:VAL:CG1	2.08	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
3:E:42:UNK:C	3:E:44:UNK:N	2.41	0.82
2:B:175:PRO:HD2	2:B:207:GLU:CB	2.09	0.82
1:A:88:HIS:HB3	1:A:91:GLN:HE22	1.45	0.82
1:A:339:ARG:HD2	1:A:339:ARG:C	1.98	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
2:B:189:LEU:C	2:B:191:VAL:H	1.83	0.82
1:C:208:ALA:O	1:C:211:ASP:HB2	1.80	0.82
2:D:313:LEU:HA	2:D:344:VAL:HG11	1.60	0.82
2:D:109:THR:O	2:D:111:GLY:N	2.13	0.82
2:D:189:LEU:C	2:D:191:VAL:H	1.83	0.82
1:A:373:ARG:HB3	1:A:373:ARG:HH11	1.45	0.82
1:A:206:ASN:HD22	1:A:210:TYR:HE2	1.26	0.82
2:B:58:GLY:C	2:B:64:ARG:HE	1.83	0.82
2:D:59:ASN:HA	2:D:64:ARG:HH21	1.45	0.82
2:B:358:ILE:H	2:B:358:ILE:HD12	1.44	0.82
2:D:287:THR:HB	2:D:289:PRO:HD2	1.61	0.81
1:C:287:SER:H	1:C:290:GLU:CD	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:A:115:ILE:O	1.80	0.81
1:A:386:GLU:HG3	1:A:387:ALA:N	1.93	0.81
1:C:115:ILE:HD13	1:C:115:ILE:O	1.81	0.81
1:C:388:TRP:CH2	1:C:428:LEU:HD13	2.15	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
1:C:409:VAL:HG13	1:C:414:GLU:CD	2.01	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: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
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:311:ARG:HH21	2:D:437:ASP:CB	1.91	0.80
2:D:184:PRO:HB2	2:D:399:PHE:CE1	2.17	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
2:D:264:ARG:HH11	2:D:264:ARG:HG3	1.47	0.80
1:C:373:ARG:HH11	1:C:373:ARG:HB3	1.46	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:D:286:LEU:HG	2:D:373:MET:HE3	1.62	0.80
2:B:401:ARG:NH1	1:C:440:VAL:HA	1.95	0.80
2:B:115:VAL:HG11	2:B:156:LYS:HZ2	1.46	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:O	2:B:286:LEU:HG	1.79	0.80
2:D:133:GLN:NE2	2:D:252:LEU:HB3	1.97	0.80
1:C:291:ILE:HD12	1:C:373:ARG:HG3	1.63	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
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
2:B:103:TRP:NE1	2:B:189:LEU:HD21	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:LYS:HZ1	2:D:278:ARG:HB2	1.46	0.79
1:A:133:GLN:N	1:A:164:LYS:HD3	1.94	0.79
2:D:391:ILE:HD12	2:D:391:ILE:H	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:180:ALA:C	1:A:182:VAL:H	1.86	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
2:D:102:ASN:HD22	2:D:105:LYS:HG3	1.47	0.79
1:C:311:LYS:HD3	1:C:344:VAL:HG13	1.62	0.79
2:D:353:THR:HG22	2:D:354:ALA:N	1.96	0.79
1:C:339:ARG:C	1:C:339:ARG:HD2	2.03	0.79
2:B:102:ASN:ND2	2:B:105:LYS:HG3	1.98	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:417:GLU:HB3	1:C:418:PHE:CE2	2.17	0.79
1:C:92:LEU:HD12	1:C:92:LEU:N	1.97	0.79
1:A:388:TRP:HH2	1:A:428:LEU:HD13	1.47	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:175:PRO:C	1:C:177:VAL:N	2.36	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
1:C:107:HIS:HD1	1:C:151:SER:HB2	1.49	0.78
2:B:217:LEU:HG	2:B:218:LYS:N	1.98	0.78
1:C:362:VAL:HG13	1:C:367:ASP:CB	2.13	0.78
3:E:31:UNK:O	3:E:34:UNK:N	2.17	0.78
2:D:2:ARG:HG3	2:D:133:GLN:HE21	1.48	0.78
1:C:371:VAL:HG12	1:C:373:ARG:H	1.48	0.78
1:C:144:GLY:N	1:C:147:SER:HB3	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:THR:HG22	2:D:226:ASP:CG	2.03	0.78
2:B:285:ALA:O	2:B:286:LEU:HD23	1.84	0.78
1:A:33:ASP:HA	1:A:36:MET:HB3	1.66	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
1:A:30:ILE:HG13	1:A:31:GLN:N	1.97	0.78
2:B:179:ASP:HB2	2:B:182:VAL:HG23	1.63	0.78
1:C:402:ARG:HG2	1:C:403:ALA:H	1.46	0.78
1:C:388:TRP:HH2	1:C:428:LEU:HD13	1.49	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:158:ARG:HG3	2:B:159:GLU:N	1.98	0.77
2:B:87:PHE:O	2:B:87:PHE:HD1	1.67	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
3:E:35:UNK:O	3:E:37:UNK:N	2.18	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
2:B:402:LYS:HE3	1:C:440:VAL:HB	1.65	0.77
1:C:413:MET:HG3	3:E:66:UNK:CB	2.14	0.77
2:D:274:PRO:HB2	2:D:371:LEU:CD1	2.15	0.77
2:B:213:CYS:HA	2:B:217:LEU:HD23	1.67	0.77
1:C:298:PRO:O	1:C:301:GLN:HG3	1.85	0.77
2:D:179:ASP:CB	2:D:182:VAL:H	1.98	0.77
1:A:413:MET:CE	1:A:413:MET:H	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:183:GLU:C	2:D:185:TYR:H	1.88	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: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
2:B:172:VAL:HG13	2:B:173:PRO:HD2	1.67	0.77
1:A:258:ASN:HD22	1:A:258:ASN:N	1.82	0.77
1:C:322:ASP:HA	1:C:357:TYR:HD1	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:HZ1	2:D:82:PRO:HG3	1.48	0.77
1:C:180:ALA:C	1:C:182:VAL:H	1.84	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:311:ARG:HG3	2:B:344:VAL:HA	1.65	0.76
2:B:266:HIS:ND1	2:B:432:TYR:CZ	2.53	0.76
1:C:151:SER:HB3	1:C:192:HIS:CE1	2.20	0.76
1:C:33:ASP:HA	1:C:36:MET:HB3	1.66	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:149:MET:HA	2:B:149:MET:HE3	1.68	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
2:D:115:VAL:HG11	2:D:156:LYS:NZ	2.00	0.76
1:A:164:LYS:HZ2	1:A:164:LYS:N	1.83	0.76
3:E:42:UNK:O	3:E:44:UNK:N	2.18	0.76
1:C:388:TRP:CZ3	1:C:428:LEU:HD22	2.21	0.76
2:D:19:LYS:HA	2:D:22:GLU:CD	2.06	0.76
2:D:180:THR:HB	2:D:404:PHE:CE1	2.19	0.76
1:A:371:VAL:HG12	1:A:373:ARG:H	1.50	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
2:B:91:ASN:ND2	2:B:91:ASN:H	1.82	0.76
1:C:88:HIS:HB3	1:C:91:GLN:HE22	1.48	0.76
2:D:194:LEU:CD2	2:D:195:VAL:HG13	2.16	0.76
2:D:175:PRO:CD	2:D:207:GLU:HB2	2.12	0.76
2:D:202:TYR:CE1	2:D:378:ILE:HD12	2.20	0.76
1:A:243:ARG:HH12	1:A:250:VAL:CG1	1.99	0.76
1:C:311:LYS:HD2	1:C:436:GLY:HA2	1.66	0.76
1:A:98:ASP:OD1	2:B:1:MET:HB3	1.85	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
2:B:401:ARG:HH11	1:C:440:VAL:HA	1.48	0.76
1:A:398:MET:HG3	1:A:399:TYR:CD1	2.21	0.76
1:A:409:VAL:HG13	1:A:414:GLU:CD	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:ARG:O	2:B:392:SER:N	2.17	0.76
2:B:385:GLN:HE21	2:B:433:GLN:HE21	1.31	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
1:C:89:PRO:O	1:C:90:GLU:HB2	1.85	0.76
2:D:182:VAL:HG12	2:D:182:VAL:O	1.85	0.76
2:D:390:ARG:C	2:D:392:SER:H	1.88	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:D:91:ASN:ND2	2:D:91:ASN:H	1.84	0.75
2:B:179:ASP:CB	2:B:182:VAL:H	1.99	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
2:B:244:PHE:HB2	2:B:245:PRO:HD2	1.65	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
1:C:398:MET:HB3	2:D:346:TRP:O	1.87	0.75
3:E:54:UNK:C	3:E:56:UNK:N	2.48	0.75
1:C:340:THR:OG1	1:C:341:ILE:HD12	1.86	0.75
2:B:100:GLY:HA3	1:C:254:GLU:OE1	1.86	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:D:174:SER:OG	2:D:176:LYS:HG3	1.87	0.75
2:D:196:GLU:OE2	2:D:196:GLU:HA	1.86	0.75
2:B:218:LYS:HZ1	2:B:278:ARG:HB2	1.50	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
2:B:292:THR:HG21	2:B:331:GLN:HB3	1.69	0.75
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
1:C:276:ILE:HG12	1:C:282:TYR:CD2	2.22	0.74
2:B:179:ASP:CA	1:C:352:LYS:HE2	2.11	0.74
1:A:322:ASP:CA	1:A:357:TYR:HA	2.17	0.74
1:A:184:PRO:HG3	1:A:399:TYR:CZ	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:GLY:O	2:B:145:THR:N	2.18	0.74
1:C:107:HIS:ND1	1:C:151:SER:HB2	2.01	0.74
2:B:220:THR:HB	1:C:326:LYS:CD	2.17	0.74
1:A:335:ILE:HG13	1:A:336:LYS:N	2.01	0.74
1:A:39:ASP:CG	1:A:40:LYS:H	1.88	0.74
2:B:274:PRO:HB2	2:B:371:LEU:CD1	2.16	0.74
2:B:387:LEU:HD23	2:B:387:LEU:O	1.86	0.74
2:D:241:CYS:O	2:D:243:ARG:HG2	1.87	0.74
2:D:385:GLN:HE21	2:D:433:GLN:HE21	1.35	0.74
2:B:286:LEU:HG	2:B:373:MET:HE3	1.69	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
2:D:192:HIS:C	2:D:194:LEU:H	1.89	0.74
1:C:350:GLY:C	1:C:351:PHE:HD1	1.90	0.74
1:C:289:ALA:HA	1:C:292:THR:CG2	2.17	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:269:LEU:HD12	1:A:270:ALA:N	2.03	0.74
1:A:214:ARG:HA	1:A:218:ASP:O	1.86	0.74
2:B:179:ASP:C	2:B:181:VAL:H	1.88	0.74
1:C:166:LYS:HZ2	1:C:197:HIS:HB2	1.51	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
1:A:77:GLU:HB3	1:A:83:TYR:CD2	2.23	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: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
2:B:322:ARG:HE	2:B:357:ASP:HB3	1.53	0.74
1:C:101:ASN:OD1	2:D:254:LYS:HD3	1.86	0.74
2:D:179:ASP:C	2:D:181:VAL:H	1.90	0.74
1:A:291:ILE:HG21	1:A:375:VAL:CG2	2.18	0.74
1:C:183:GLU:N	1:C:184:PRO:HD2	2.03	0.74
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.70	0.74
2:D:80:SER:C	2:D:82:PRO:HD2	2.07	0.74
2:B:94:PHE:HB2	2:B:114:LEU:HD13	1.69	0.73
1:A:209:ILE:C	1:A:211:ASP:H	1.90	0.73
2:D:371:LEU:HB3	2:D:373:MET:O	1.86	0.73
2:B:385:GLN:NE2	2:B:433:GLN:HG2	2.03	0.73
2:B:145:THR:HB	5:B:501:GDP:O2B	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:ASP:HB2	2:D:182:VAL:H	1.53	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
2:B:166:MET:HE3	2:B:197:ASN:HB3	1.69	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
1:A:190:THR:O	1:A:192:HIS:N	2.22	0.73
1:A:175:PRO:C	1:A:177:VAL:N	2.39	0.73
2:B:77:SER:HA	2:B:80:SER:CB	2.18	0.73
1:C:262:TYR:HB3	1:C:263:PRO:HD2	1.70	0.73
2:D:343:PHE:O	2:D:345:GLU:N	2.21	0.73
2:D:142:GLY:CA	2:D:185:TYR:HB3	2.18	0.73
2:D:394:GLN:O	2:D:398:MET:HB3	1.87	0.73
1:A:238:ILE:HG22	1:A:239:THR:N	2.03	0.73
2:B:339:ASN:HB3	2:B:342:TYR:CD1	2.23	0.73
1:A:385:ALA:HB2	1:A:432:TYR:HD2	1.53	0.73
2:B:168:THR:OG1	2:B:201:THR:HB	1.88	0.73
2:D:407:TRP:HA	2:D:407:TRP:CE3	2.22	0.73
1:C:132:LEU:HB3	1:C:164:LYS:HD3	1.71	0.73
2:B:390:ARG:C	2:B:392:SER:H	1.92	0.73
2:D:191:VAL:O	2:D:191:VAL:HG12	1.87	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:D:179:ASP:HB2	2:D:182:VAL:HG23	1.71	0.73
2:D:77:SER:HA	2:D:80:SER:CB	2.19	0.73
1:A:298:PRO:O	1:A:301:GLN:HG3	1.89	0.73
1:A:27:GLU:HG3	1:A:28:HIS:ND1	2.04	0.73
2:D:385:GLN:NE2	2:D:433:GLN:HG2	2.04	0.73
2:D:77:SER:CA	2:D:80:SER:HB3	2.19	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
1:A:267:PHE:CD1	1:A:267:PHE:N	2.57	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:HE3	2:B:407:TRP:HA	1.54	0.72
1:C:194:THR:O	1:C:197:HIS:O	2.07	0.72
2:D:115:VAL:HG11	2:D:156:LYS:HZ2	1.52	0.72
2:D:18:ALA:C	2:D:20:PHE:H	1.92	0.72
1:C:322:ASP:HA	1:C:357:TYR:HA	1.71	0.72
2:D:263:PRO:C	2:D:265:LEU:N	2.42	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:LEU:O	2:D:286:LEU:HG	1.89	0.72
2:B:190:SER:CB	2:B:425:MET:HG3	2.16	0.72
1:C:322:ASP:H	1:C:357:TYR:C	1.92	0.72
3:E:25:UNK:C	3:E:27:UNK:N	2.49	0.72
2:B:266:HIS:HA	2:B:432:TYR:OH	1.89	0.72
1:C:100:ALA:HB1	1:C:105:ARG:HD2	1.70	0.72
1:C:70:LEU:HD12	1:C:145:THR:CA	2.12	0.72
2:B:16:ILE:HB	2:B:228:ASN:HD21	1.53	0.72
1:A:215:ARG:HH22	1:A:300:ASN:ND2	1.87	0.72
1:C:267:PHE:CD1	1:C:267:PHE:N	2.55	0.72
2:B:158:ARG:CG	2:B:159:GLU:H	1.99	0.72
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:D:18:ALA:O	2:D:20:PHE:N	2.21	0.72
1:A:202:PHE:HE1	1:A:378:LEU:HD22	1.55	0.72
1:A:345:ASP:O	1:A:347:CYS:N	2.23	0.72
2:B:133:GLN:NE2	2:B:252:LEU:H	1.87	0.72
2:B:274:PRO:HB2	2:B:371:LEU:HD12	1.70	0.72
2:B:77:SER:CA	2:B:80:SER:HB3	2.20	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
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
2:B:353:THR:HG22	2:B:354:ALA:N	2.04	0.72
2:B:158:ARG:O	2:B:160:GLU:N	2.22	0.72
2:D:158:ARG:CA	2:D:197:ASN:HD22	2.02	0.72
1:C:285:GLN:OE1	1:C:372:GLN:HG2	1.90	0.72
1:C:44:GLY:C	1:C:46:ASP:H	1.92	0.72
2:D:273:ALA:HB2	2:D:295:MET:HB2	1.70	0.72
2:D:194:LEU:HD11	2:D:428:LEU:HD11	1.72	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
2:D:353:THR:CG2	2:D:354:ALA:N	2.52	0.72
1:A:97:GLU:O	1:A:99:ALA:N	2.22	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
1:C:39:ASP:CG	1:C:40:LYS:H	1.91	0.72
2:B:138:THR:O	2:B:139:HIS:HB3	1.90	0.72
2:B:92:PHE:CE1	2:B:118:VAL:CA	2.70	0.71
2:D:16:ILE:HB	2:D:228:ASN:HD21	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:THR:O	1:C:197:HIS:N	2.22	0.71
2:D:396:THR:HG23	2:D:400:ARG:CD	2.19	0.71
1:C:348:PRO:O	1:C:350:GLY:N	2.23	0.71
2:B:422:GLU:O	2:B:426:ASN:HB2	1.90	0.71
1:A:256:GLN:HB3	1:A:260:VAL:HB	1.71	0.71
2:B:263:PRO:C	2:B:265:LEU:N	2.39	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
1:A:291:ILE:HG21	1:A:375:VAL:HG21	1.73	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:OE2	2:B:196:GLU:HA	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
2:B:398:MET:C	2:B:400:ARG:H	1.94	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
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:243:ARG:CZ	1:A:243:ARG:HA	2.21	0.71
1:A:31:GLN:O	1:A:33:ASP:N	2.23	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
2:D:427:ASP:O	2:D:429:VAL:N	2.24	0.71
2:D:4:ILE:O	2:D:58:GLY:HA2	1.91	0.71
1:A:78:VAL:HG11	1:A:87:PHE:HE2	1.54	0.71
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:215:ARG:HH22	1:A:300:ASN:HD21	1.39	0.70
1:A:26:LEU:HG	1:A:361:THR:CB	2.21	0.70
2:B:87:PHE:O	2:B:90:ASP:OD1	2.08	0.70
1:C:264:ARG:O	1:C:266:HIS:N	2.24	0.70
1:A:322:ASP:HA	1:A:357:TYR:HA	1.73	0.70
1:C:284:GLU:HG2	1:C:285:GLN:NE2	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.27	0.70
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
2:B:191:VAL:HG12	2:B:191:VAL:O	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:255:LEU:CD2	2:D:259:MET:HG3	2.21	0.70
1:A:332:ILE:CD1	1:A:353:VAL:HG21	2.21	0.70
1:A:399:TYR:HH	1:A:408:TYR:HE2	1.37	0.70
1:C:98:ASP:OD1	2:D:1:MET:HB3	1.91	0.70
1:A:340:THR:OG1	1:A:341:ILE:HD12	1.90	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
1:C:7:ILE:HD12	1:C:153:LEU:HD21	1.74	0.70
2:B:230:LEU:H	2:B:230:LEU:HD12	1.55	0.70
1:A:209:ILE:HG23	1:A:213:CYS:HB2	1.73	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
1:C:5:ILE:HD12	1:C:125:LEU:HD22	1.74	0.70
1:A:350:GLY:O	1:A:351:PHE:HD1	1.74	0.70
2:D:51:VAL:HG23	2:D:53:TYR:N	2.07	0.70
1:A:418:PHE:O	1:A:420:GLU:N	2.25	0.70
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.54	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
1:A:7:ILE:HG21	1:A:122:ILE:HD11	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
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
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
1:C:78:VAL:C	1:C:82:THR:HA	2.13	0.70
2:D:385:GLN:HE21	2:D:433:GLN:NE2	1.90	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:H	1:A:357:TYR:C	1.94	0.69
1:C:190:THR:O	1:C:192:HIS:N	2.25	0.69
1:C:184:PRO:HG3	1:C:399:TYR:CZ	2.28	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:N	2:D:391:ILE:HD12	2.07	0.69
1:A:280:LYS:O	1:A:282:TYR:CE2	2.45	0.69
1:A:89:PRO:O	1:A:90:GLU:HB2	1.90	0.69
1:A:284:GLU:HG2	1:A:285:GLN:NE2	2.07	0.69
1:C:291:ILE:HG21	1:C:375:VAL:CG2	2.22	0.69
1:A:205:ASP:OD2	1:A:207:GLU:HB3	1.92	0.69
1:A:11:GLN:HB3	4:A:500:GTP:O2A	1.91	0.69
2:B:133:GLN:HE21	2:B:252:LEU:CB	2.05	0.69
2:D:183:GLU:O	2:D:185:TYR:N	2.24	0.69
2:D:59:ASN:HB2	2:D:64:ARG:CZ	2.22	0.69
2:D:218:LYS:NZ	2:D:278:ARG:HB2	2.07	0.69
1:C:414:GLU:HG2	1:C:415:GLU:H	1.58	0.69
2:D:262:PHE:O	2:D:265:LEU:HA	1.93	0.69
2:D:218:LYS:NZ	2:D:278:ARG:N	2.39	0.69
1:A:78:VAL:O	1:A:82:THR:HG23	1.92	0.69
2:D:138:THR:O	2:D:139:HIS:HB3	1.91	0.69
2:B:345:GLU:O	2:B:345:GLU:HG2	1.92	0.69
2:D:396:THR:CG2	2:D:400:ARG:HD3	2.23	0.69
2:D:416:MET:C	2:D:418:PHE:H	1.95	0.69
1:C:31:GLN:CB	1:C:32:PRO:HD2	2.23	0.69
2:B:255:LEU:CD2	2:B:259:MET:HG3	2.22	0.69
1:C:100:ALA:HB1	1:C:105:ARG:O	1.92	0.69
1:C:205:ASP:OD2	1:C:207:GLU:HB3	1.93	0.69
1:C:78:VAL:O	1:C:82:THR:HG23	1.91	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
1:C:202:PHE:HE1	1:C:378:LEU:HD22	1.57	0.69
2:D:259:MET:HE1	2:D:316:ALA:N	2.08	0.69
2:D:59:ASN:CG	2:D:60:LYS:H	1.95	0.69
2:B:218:LYS:NZ	2:B:278:ARG:H	1.83	0.69
1:A:86:LEU:CD2	1:A:89:PRO:HD3	2.23	0.69
1:C:30:ILE:HG13	1:C:31:GLN:N	2.07	0.69
1:C:287:SER:N	1:C:290:GLU:HB2	2.07	0.69
1:A:78:VAL:HG11	1:A:92:LEU:HD21	1.73	0.69
2:B:183:GLU:C	2:B:185:TYR:H	1.95	0.69
2:B:274:PRO:HA	2:B:294:GLN:NE2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:C	1:C:269:LEU:HD12	2.13	0.69
2:D:422:GLU:O	2:D:426:ASN:HB2	1.93	0.69
2:B:179:ASP:C	2:B:181:VAL:N	2.45	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:191:THR:CB	1:A:421:ALA:HB1	2.23	0.69
1:A:413:MET:O	1:A:414:GLU:HB3	1.92	0.68
2:D:105:LYS:HA	2:D:109:THR:OG1	1.93	0.68
1:C:286:LEU:HA	1:C:290:GLU:OE1	1.93	0.68
3:E:71:UNK:O	3:E:73:UNK:N	2.27	0.68
2:B:333:LEU:HG	2:B:337:ASN:ND2	2.08	0.68
2:B:132:LEU:HD22	2:B:164:ARG:HG3	1.75	0.68
1:C:258:ASN:ND2	1:C:258:ASN:N	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
2:B:344:VAL:HB	2:B:346:TRP:CE2	2.28	0.68
2:B:296:PHE:HA	2:B:377:PHE:HE2	1.59	0.68
2:B:416:MET:C	2:B:418:PHE:H	1.96	0.68
1:A:259:LEU:HD21	1:A:378:LEU:HB3	1.74	0.68
1:A:10:GLY:O	1:A:13:GLY:N	2.26	0.68
2:B:111:GLY:C	2:B:113:GLU:H	1.94	0.68
1:C:209:ILE:C	1:C:211:ASP:H	1.95	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:HE3	2:D:407:TRP:HA	1.56	0.68
1:A:75:ILE:HG12	1:A:75:ILE:O	1.92	0.68
2:B:175:PRO:O	2:B:177:VAL:HG23	1.93	0.68
2:D:430:SER:O	2:D:434:GLN:HG3	1.93	0.68
1:A:330:ALA:O	1:A:334:THR:HG23	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
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.29	0.68
2:D:175:PRO:O	2:D:177:VAL:HG23	1.93	0.68
2:B:391:ILE:HD12	2:B:391:ILE:H	1.57	0.68
1:A:305:CYS:SG	1:A:306:ASP:N	2.65	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
2:D:126:SER:OG	2:D:127:GLU:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:GLU:OE1	1:C:433:GLU:HA	1.92	0.68
2:D:71:GLU:HB2	2:D:72:PRO:CD	2.24	0.68
1:A:153:LEU:O	1:A:156:ARG:HB2	1.93	0.68
1:A:171:ILE:N	1:A:171:ILE:HD12	2.08	0.68
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.75	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
1:A:134:GLY:H	1:A:164:LYS:HG2	1.58	0.68
2:D:55:GLU:HB2	2:D:244:PHE:HA	1.75	0.68
2:B:51:VAL:HG23	2:B:53:TYR:N	2.08	0.68
1:A:258:ASN:O	1:A:259:LEU:HB2	1.93	0.68
2:B:163:ASP:CG	2:B:164:ARG:N	2.47	0.68
1:C:147:SER:O	1:C:189:LEU:HD23	1.93	0.68
2:D:179:ASP:C	2:D:181:VAL:N	2.47	0.68
1:A:321:GLY:HA2	1:A:357:TYR:O	1.94	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: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
1:C:31:GLN:O	1:C:33:ASP:N	2.28	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:D:104:ALA:O	2:D:108:TYR:HB2	1.94	0.67
2:B:398:MET:N	2:B:401:ARG:HB2	2.09	0.67
2:B:102:ASN:HD21	2:B:104:ALA:HB3	1.58	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:311:LYS:HD2	1:A:436:GLY:HA2	1.76	0.67
1:A:413:MET:HE2	1:A:413:MET:H	1.58	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:263:PRO:O	2:B:265:LEU:N	2.27	0.67
2:B:331:GLN:O	2:B:334:ASN:HB3	1.95	0.67
2:B:237:GLY:O	2:B:376:THR:HG21	1.95	0.67
1:C:287:SER:OG	1:C:290:GLU:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD1	1:C:404:PHE:H	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:C:177:VAL:HB	2:D:349:ASN:CG	2.15	0.67
2:D:205:ASP:OD2	2:D:207:GLU:HB3	1.95	0.67
2:D:266:HIS:HB2	2:D:380:ASN:OD1	1.95	0.67
1:A:287:SER:OG	1:A:290:GLU:HG3	1.94	0.67
2:D:386:GLU:C	2:D:388:PHE:H	1.98	0.67
1:A:44:GLY:C	1:A:46:ASP:H	1.97	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: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
1:C:291:ILE:CD1	1:C:373:ARG:HG3	2.24	0.67
1:C:180:ALA:C	1:C:182:VAL:N	2.48	0.67
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:255:LEU:HD23	2:D:259:MET:CG	2.25	0.66
2:D:87:PHE:O	2:D:87:PHE:CD1	2.48	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:305:CYS:SG	2:B:387:LEU:HB2	2.35	0.66
2:D:62:VAL:HG23	2:D:62:VAL:O	1.94	0.66
2:D:4:ILE:O	2:D:64:ARG:HD2	1.95	0.66
1:A:164:LYS:HZ3	1:A:164:LYS:HB2	1.59	0.66
2:B:70:LEU:HG	2:B:99:ALA:CB	2.24	0.66
1:A:355:ILE:HD12	1:A:355:ILE:N	2.10	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
1:A:306:ASP:C	1:A:308:ARG:H	1.98	0.66
2:B:19:LYS:HA	2:B:22:GLU:CD	2.16	0.66
1:C:306:ASP:C	1:C:308:ARG:H	1.99	0.66
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ALA:HB2	1:C:295:CYS:HB2	1.76	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:386:GLU:C	2:B:388:PHE:H	1.99	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: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:102:ASN:O	2:B:105:LYS:HB2	1.96	0.66
2:D:320:ARG:HG2	2:D:320:ARG:HH11	1.59	0.66
1:C:242:LEU:HB3	1:C:250:VAL:HG11	1.78	0.66
3:E:48:UNK:O	3:E:49:UNK:C	2.44	0.66
2:B:353:THR:CG2	2:B:354:ALA:N	2.58	0.66
2:B:111:GLY:C	2:B:113:GLU:N	2.47	0.66
2:B:118:VAL:C	2:B:120:ASP:H	1.97	0.66
2:D:149:MET:HA	2:D:149:MET:HE3	1.78	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
1:A:78:VAL:C	1:A:82:THR:HA	2.15	0.66
3:E:25:UNK:O	3:E:29:UNK:N	2.29	0.66
2:B:126:SER:OG	2:B:127:GLU:N	2.28	0.66
1:C:172:TYR:HB3	1:C:205:ASP:N	2.11	0.66
1:C:7:ILE:HG22	1:C:66:VAL:CB	2.18	0.66
1:A:286:LEU:HA	1:A:290:GLU:OE1	1.96	0.66
1:A:261:PRO:CG	1:A:380:ASN:HD21	2.09	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
1:A:276:ILE:HG12	1:A:282:TYR:CD2	2.32	0.65
2:D:118:VAL:C	2:D:120:ASP:H	1.99	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
2:B:1:MET:O	2:B:3:GLU:N	2.26	0.65
1:C:217:LEU:O	1:C:219:ILE:HG13	1.97	0.65
1:C:217:LEU:HD11	1:C:368:LEU:HD22	1.79	0.65
1:C:407:TRP:C	1:C:409:VAL:H	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:231:ILE:O	1:A:235:VAL:HG23	1.96	0.65
1:A:363:VAL:HG13	1:A:367:ASP:OD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ALA:C	2:B:20:PHE:H	2.00	0.65
2:B:58:GLY:O	2:B:64:ARG:NE	2.30	0.65
1:C:151:SER:HB3	1:C:192:HIS:NE2	2.12	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:C:134:GLY:H	1:C:164:LYS:CG	2.09	0.65
1:A:206:ASN:HB3	1:A:210:TYR:HE2	1.58	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:92:PHE:CD1	2:D:118:VAL:HG22	2.31	0.65
2:D:303:ALA:HB1	2:D:387:LEU:HD13	1.78	0.65
2:D:5:VAL:HA	2:D:64:ARG:CD	2.26	0.65
2:D:278:ARG:H	2:D:278:ARG:HD2	1.59	0.65
1:A:388:TRP:CZ3	1:A:428:LEU:HD22	2.31	0.65
2:B:255:LEU:HD23	2:B:259:MET:CG	2.27	0.65
2:B:218:LYS:NZ	2:B:278:ARG:HB2	2.11	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
2:B:264:ARG:HH11	2:B:264:ARG:HG3	1.60	0.65
2:D:227:LEU:HD23	2:D:227:LEU:O	1.96	0.65
2:D:59:ASN:CG	2:D:60:LYS:N	2.50	0.65
1:C:330:ALA:O	1:C:334:THR:HG23	1.96	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:392:SER:HB2	2:B:426:ASN:ND2	2.11	0.65
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:247:ALA:O	1:A:249:ASN:ND2	2.30	0.65
1:A:287:SER:C	1:A:289:ALA:H	1.98	0.65
1:A:177:VAL:HB	2:B:349:ASN:CG	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:ASP:CG	2:D:164:ARG:N	2.50	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:258:ASN:ND2	1:A:258:ASN:N	2.43	0.65
2:B:139:HIS:CD2	2:B:139:HIS:C	2.69	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:183:GLU:C	2:D:185:TYR:N	2.47	0.65
1:A:133:GLN:HA	1:A:164:LYS:HG3	1.79	0.65
2:B:339:ASN:C	2:B:341:SER:H	2.00	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
1:A:407:TRP:C	1:A:409:VAL:H	2.00	0.64
2:B:205:ASP:OD2	2:B:207:GLU:HB3	1.96	0.64
1:C:8:HIS:N	1:C:8:HIS:ND1	2.44	0.64
1:C:133:GLN:HA	1:C:164:LYS:HG3	1.79	0.64
1:A:180:ALA:C	1:A:182:VAL:N	2.51	0.64
1:C:362:VAL:CG1	1:C:367:ASP:HB2	2.26	0.64
2:D:137:LEU:HD23	2:D:154:ILE:HD11	1.80	0.64
2:D:5:VAL:HA	2:D:64:ARG:HD2	1.79	0.64
1:A:277:SER:O	1:A:278:ALA:HB2	1.97	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
2:B:59:ASN:CG	2:B:60:LYS:H	1.99	0.64
1:C:100:ALA:CB	1:C:105:ARG:HD2	2.27	0.64
2:B:96:GLN:NE2	1:C:130:THR:HG22	2.11	0.64
1:C:360:PRO:HB3	1:C:374:ALA:HB2	1.79	0.64
1:A:183:GLU:HB2	1:A:184:PRO:CD	2.27	0.64
1:C:138:PHE:CZ	1:C:235:VAL:HG11	2.30	0.64
2:B:278:ARG:HD2	2:B:278:ARG:H	1.59	0.64
1:A:78:VAL:HG11	1:A:87:PHE:CE2	2.32	0.64
1:A:138:PHE:CZ	1:A:235:VAL:HG11	2.26	0.64
1:A:433:GLU:HA	1:A:433:GLU:OE1	1.97	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
2:D:288:VAL:N	2:D:289:PRO:HD2	2.12	0.64
1:A:292:THR:HA	1:A:295:CYS:HB3	1.80	0.64
1:A:285:GLN:OE1	1:A:372:GLN:HG2	1.96	0.64
2:B:51:VAL:C	2:B:53:TYR:H	2.00	0.64
1:C:267:PHE:N	1:C:267:PHE:HD1	1.94	0.64
2:B:71:GLU:HB2	2:B:72:PRO:CD	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:192:HIS:O	2:B:194:LEU:N	2.30	0.64
2:B:2:ARG:HG3	2:B:133:GLN:HE21	1.58	0.64
2:D:255:LEU:HD23	2:D:259:MET:HG3	1.80	0.64
1:A:191:THR:HB	1:A:421:ALA:HB1	1.79	0.64
1:C:191:THR:CB	1:C:421:ALA:HB1	2.27	0.64
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.26	0.64
1:A:86:LEU:HD22	1:A:89:PRO:HD3	1.79	0.64
1:A:350:GLY:O	1:A:351:PHE:CD1	2.50	0.64
1:A:287:SER:N	1:A:290:GLU:HB2	2.13	0.64
2:B:339:ASN:O	2:B:341:SER:N	2.30	0.64
1:A:77:GLU:O	1:A:83:TYR:HB2	1.97	0.64
2:D:386:GLU:O	2:D:388:PHE:N	2.31	0.64
1:A:276:ILE:O	1:A:369:ALA:HB3	1.98	0.64
1:C:160:ASP:O	1:C:161:TYR:CD1	2.50	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
2:D:184:PRO:HB2	2:D:399:PHE:CZ	2.32	0.64
2:D:92:PHE:HD1	2:D:118:VAL:HG22	1.61	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:C:172:TYR:CE2	1:C:391:LEU:HD22	2.32	0.64
2:D:111:GLY:C	2:D:113:GLU:H	1.99	0.64
2:D:129:CYS:O	2:D:130:ASP:O	2.15	0.64
2:D:59:ASN:ND2	2:D:60:LYS:N	2.45	0.64
2:D:391:ILE:CD1	2:D:391:ILE:H	2.10	0.64
1:C:331:ALA:HA	1:C:334:THR:OG1	1.98	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
2:B:80:SER:C	2:B:82:PRO:HD2	2.18	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
1:A:186:ASN:HD22	1:A:391:LEU:HD11	1.63	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
2:B:59:ASN:HB2	2:B:64:ARG:CZ	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:VAL:H	1:C:367:ASP:HB2	1.61	0.63
2:D:345:GLU:O	2:D:345:GLU:HG2	1.96	0.63
2:D:102:ASN:HD22	2:D:105:LYS:CG	2.11	0.63
1:C:287:SER:C	1:C:289:ALA:H	2.00	0.63
1:A:5:ILE:HD12	1:A:125:LEU:HD22	1.80	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: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
1:C:101:ASN:CG	2:D:254:LYS:HD3	2.17	0.63
1:C:215:ARG:HH22	1:C:300:ASN:HD21	1.45	0.63
1:C:75:ILE:HG12	1:C:75:ILE:O	1.97	0.63
2:D:287:THR:OG1	2:D:290:GLU:HB2	1.98	0.63
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.79	0.63
2:B:140:SER:OG	2:B:171:VAL:HB	1.98	0.63
1:A:217:LEU:HD11	1:A:368:LEU:HD22	1.81	0.63
1:A:263:PRO:O	1:A:265:ALA:N	2.28	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
1:C:404:PHE:HD1	1:C:404:PHE:N	1.95	0.63
2:D:158:ARG:O	2:D:160:GLU:N	2.31	0.63
1:A:241:SER:HA	1:A:320:ARG:NH2	2.13	0.63
2:B:357:ASP:HB3	2:B:358:ILE:HD12	1.81	0.63
1:A:87:PHE:CD2	1:A:87:PHE:N	2.63	0.63
1:A:43:GLY:O	1:A:47:ASP:CG	2.37	0.63
2:B:288:VAL:N	2:B:289:PRO:HD2	2.14	0.63
1:C:404:PHE:N	1:C:404:PHE:CD1	2.67	0.63
1:C:243:ARG:CZ	1:C:243:ARG:HA	2.28	0.63
1:C:355:ILE:N	1:C:355:ILE:HD12	2.13	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:339:ASN:C	2:D:341:SER:H	2.01	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: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
2:B:390:ARG:C	2:B:392:SER:N	2.53	0.63
2:D:158:ARG:HD3	2:D:197:ASN:CG	2.18	0.63
1:C:243:ARG:HH12	1:C:250:VAL:CG1	2.11	0.63
1:A:311:LYS:CG	1:A:344:VAL:HG22	2.28	0.63
2:B:399:PHE:CE2	2:B:404:PHE:HB3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:HB3	1:C:210:TYR:HE2	1.61	0.63
2:D:107:HIS:CD2	2:D:151:THR:HG23	2.33	0.63
1:A:291:ILE:HD12	1:A:373:ARG:HG3	1.80	0.63
1:C:373:ARG:NH1	1:C:373:ARG:HB3	2.12	0.63
2:B:71:GLU:HB2	2:B:72:PRO:HD2	1.79	0.63
1:C:385:ALA:HB2	1:C:432:TYR:HD2	1.63	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
2:D:286:LEU:HD13	2:D:371:LEU:O	1.99	0.62
2:D:215:ARG:HA	2:D:215:ARG:NE	2.13	0.62
2:D:391:ILE:O	2:D:425:MET:HE1	1.98	0.62
1:A:362:VAL:HG21	1:A:369:ALA:O	1.98	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
2:B:417:GLU:O	2:B:417:GLU:HG3	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:NH1	2:D:264:ARG:HG3	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
3:E:35:UNK:O	3:E:39:UNK:N	2.32	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:293:ASN:O	1:A:297:GLU:OE1	2.17	0.62
1:A:280:LYS:O	1:A:282:TYR:HE2	1.82	0.62
2:B:192:HIS:C	2:B:194:LEU:N	2.49	0.62
2:B:165:ILE:HD13	2:B:199:ASP:OD1	1.99	0.62
2:B:241:CYS:C	2:B:243:ARG:N	2.48	0.62
2:B:292:THR:HG23	2:B:319:PHE:CZ	2.35	0.62
2:B:62:VAL:O	2:B:62:VAL:HG23	1.99	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:166:MET:HE3	2:D:197:ASN:HB3	1.82	0.62
2:D:385:GLN:HG2	2:D:433:GLN:NE2	2.13	0.62
2:B:396:THR:CG2	2:B:400:ARG:HD3	2.28	0.62
1:A:258:ASN:O	1:A:259:LEU:CB	2.48	0.62
2:D:267:PHE:HB2	2:D:384:ILE:HD13	1.81	0.62
1:A:156:ARG:O	1:A:159:VAL:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.32	0.62
2:B:132:LEU:O	2:B:132:LEU:HD23	2.00	0.62
2:D:191:VAL:CG1	2:D:421:ALA:HA	2.29	0.62
2:B:130:ASP:OD2	2:B:131:CYS:N	2.32	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:373:ARG:HB3	1:A:373:ARG:NH1	2.15	0.62
2:B:215:ARG:HA	2:B:215:ARG:NE	2.13	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:D:348:PRO:O	2:D:349:ASN:HB3	2.00	0.62
2:D:2:ARG:O	2:D:57:ALA:HB1	1.99	0.62
2:B:218:LYS:O	2:B:219:LEU:HB2	2.00	0.62
1:C:331:ALA:C	1:C:333:ALA:N	2.51	0.62
1:C:27:GLU:HG3	1:C:28:HIS:ND1	2.14	0.62
1:C:344:VAL:HG12	1:C:345:ASP:N	2.15	0.62
1:C:311:LYS:HD3	1:C:344:VAL:HG22	1.80	0.62
1:C:291:ILE:HG21	1:C:375:VAL:HG21	1.82	0.62
1:A:267:PHE:HD1	1:A:267:PHE:N	1.96	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: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
1:A:407:TRP:CZ2	2:B:256:ALA:O	2.53	0.62
2:B:344:VAL:HG23	2:B:345:GLU:N	2.15	0.62
2:B:58:GLY:C	2:B:64:ARG:NE	2.52	0.62
2:D:149:MET:HA	2:D:149:MET:CE	2.29	0.62
2:D:206:ASN:ND2	2:D:227:LEU:HD21	2.07	0.62
1:A:132:LEU:HB3	1:A:164:LYS:HD3	1.80	0.62
1:A:365:GLY:O	1:A:368:LEU:HD11	2.00	0.62
1:A:181:VAL:HG13	1:A:408:TYR:OH	2.00	0.62
2:B:163:ASP:CG	2:B:164:ARG:H	2.03	0.62
2:D:158:ARG:HA	2:D:197:ASN:ND2	2.15	0.62
2:D:2:ARG:HH11	2:D:251:ASP:HA	1.64	0.62
1:C:345:ASP:O	1:C:347:CYS:N	2.31	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
2:D:358:ILE:CD1	2:D:358:ILE:H	2.13	0.61
1:C:242:LEU:O	1:C:243:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:HG11	1:C:346:TRP:HE1	1.63	0.61
1:C:267:PHE:H	1:C:267:PHE:HD1	1.45	0.61
1:C:191:THR:HB	1:C:421:ALA:HB1	1.79	0.61
1:A:210:TYR:CE2	1:A:227:LEU:HD23	2.34	0.61
2:B:22:GLU:OE2	2:B:22:GLU:N	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
1:A:317:LEU:HD23	1:A:377:MET:CB	2.30	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
2:D:123:ARG:NE	2:D:160:GLU:OE2	2.32	0.61
1:C:238:ILE:HG22	1:C:239:THR:N	2.15	0.61
1:A:175:PRO:O	1:A:177:VAL:HG23	2.00	0.61
2:B:5:VAL:HB	2:B:135:PHE:HD2	1.65	0.61
2:B:241:CYS:SG	2:B:320:ARG:NH1	2.73	0.61
1:C:414:GLU:CD	1:C:414:GLU:N	2.54	0.61
1:C:86:LEU:CD2	1:C:89:PRO:HD3	2.29	0.61
2:D:237:GLY:O	2:D:376:THR:HG21	2.01	0.61
2:B:218:LYS:NZ	2:B:278:ARG:N	2.46	0.61
1:C:2:ARG:NH2	1:C:133:GLN:NE2	2.46	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
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
2:B:396:THR:HG23	2:B:400:ARG:CD	2.27	0.61
2:B:353:THR:CG2	2:B:354:ALA:H	2.14	0.61
2:B:191:VAL:HG13	2:B:421:ALA:HA	1.83	0.61
2:B:2:ARG:NH1	2:B:251:ASP:HA	2.15	0.61
2:B:312:TYR:HA	2:B:381:SER:HA	1.81	0.61
2:B:59:ASN:CG	2:B:60:LYS:N	2.54	0.61
2:D:287:THR:O	2:D:290:GLU:HB3	2.01	0.61
1:A:88:HIS:N	1:A:91:GLN:OE1	2.33	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:HD2	2:B:404:PHE:O	1.83	0.61
1:C:78:VAL:O	1:C:82:THR:HA	2.01	0.61
1:C:164:LYS:HZ1	1:C:164:LYS:N	1.98	0.61
2:D:51:VAL:C	2:D:53:TYR:H	2.03	0.61
1:A:139:HIS:NE2	1:A:150:THR:HG21	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:PHE:HD1	2:B:118:VAL:HG22	1.63	0.61
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: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
2:D:94:PHE:HB2	2:D:114:LEU:CD1	2.31	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
2:B:223:THR:N	2:B:226:ASP:OD2	2.30	0.61
1:C:259:LEU:HD21	1:C:378:LEU:HB3	1.81	0.61
1:C:393:HIS:C	1:C:395:PHE:H	2.03	0.61
1:C:188:ILE:HG22	1:C:417:GLU:O	2.01	0.61
2:D:261:PRO:HB2	2:D:262:PHE:CD1	2.36	0.61
2:D:60:LYS:N	2:D:60:LYS:NZ	2.49	0.61
1:A:321:GLY:N	1:A:356:ASN:O	2.34	0.61
1:A:27:GLU:CG	1:A:28:HIS:H	2.12	0.61
1:A:137:VAL:CG1	1:A:154:MET:HE2	2.29	0.61
2:B:189:LEU:C	2:B:191:VAL:N	2.55	0.61
3:E:35:UNK:HA	3:E:38:UNK:CB	2.31	0.61
2:D:5:VAL:HG22	2:D:64:ARG:HD3	1.83	0.61
1:C:164:LYS:HZ2	1:C:164:LYS:HB2	1.66	0.61
3:E:50:UNK:C	3:E:52:UNK:N	2.62	0.61
2:B:140:SER:CB	2:B:171:VAL:HB	2.31	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
2:B:311:ARG:HG3	2:B:311:ARG:HH11	1.65	0.60
2:B:59:ASN:HB2	2:B:64:ARG:HE	1.63	0.60
1:C:221:ARG:H	1:C:221:ARG:CD	2.13	0.60
2:D:350:ASN:ND2	2:D:351:VAL:HG23	2.16	0.60
2:D:296:PHE:HA	2:D:377:PHE:CE2	2.35	0.60
2:D:385:GLN:HE21	2:D:433:GLN:HG2	1.65	0.60
1:A:242:LEU:HB3	1:A:250:VAL:HG11	1.83	0.60
1:A:354:GLY:C	1:A:355:ILE:HD12	2.21	0.60
1:A:282:TYR:HD2	1:A:282:TYR:N	1.98	0.60
2:B:286:LEU:HD13	2:B:371:LEU:O	2.00	0.60
2:B:380:ASN:C	2:B:380:ASN:HD22	2.05	0.60
2:B:66:ILE:O	2:B:66:ILE:HG12	2.01	0.60
2:B:75:MET:O	2:B:76:ASP:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:ASP:CG	2:D:164:ARG:H	2.04	0.60
2:D:307:PRO:C	2:D:309:HIS:H	2.04	0.60
2:D:109:THR:HG21	2:D:411:GLU:CG	2.30	0.60
2:B:321:GLY:CA	2:B:359:PRO:HB3	2.27	0.60
1:A:283:HIS:O	1:A:284:GLU:HB3	2.00	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:348:PRO:O	2:B:349:ASN:HB3	2.01	0.60
1:C:90:GLU:O	1:C:121:ARG:NH1	2.34	0.60
1:C:16:ILE:HD12	1:C:171:ILE: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
1:C:126:ALA:HB1	1:C:132:LEU:HD11	1.83	0.60
1:A:318:LEU:HB2	1:A:376:CYS:O	2.01	0.60
2:B:308:ARG:NH2	2:B:342:TYR:CD1	2.61	0.60
1:A:7:ILE:HG22	1:A:66:VAL:CB	2.23	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
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:257:THR:OG1	1:A:258:ASN:ND2	2.35	0.60
1:A:175:PRO:HD2	1:A:207:GLU:CB	2.05	0.60
2:B:107:HIS:CD2	2:B:151:THR:HG23	2.35	0.60
2:B:11:GLN:HG3	2:B:15:GLN:NE2	2.17	0.60
2:B:191:VAL:CG1	2:B:421:ALA:HA	2.30	0.60
2:B:184:PRO:HB2	2:B:399:PHE:CZ	2.35	0.60
2:D:399:PHE:CE2	2:D:404:PHE:HB3	2.37	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
1:A:269:LEU:HD21	1:A:301:GLN:NE2	2.17	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: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:21:TRP:HA	1:C:24:TYR:HB2	1.82	0.60
1:C:305:CYS:SG	1:C:384:ILE:HA	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLU:O	1:C:83:TYR:HB2	2.02	0.60
1:C:9:VAL:HA	1:C:68:VAL:O	2.02	0.60
2:D:111:GLY:C	2:D:113:GLU:N	2.53	0.60
2:D:139:HIS:C	2:D:139:HIS:CD2	2.75	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:23:LEU:C	1:A:25:CYS:H	2.05	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:291:ILE:HG22	1:A:292:THR:N	2.17	0.60
1:A:9:VAL:HG21	1:A:150:THR:HB	1.84	0.60
1:A:69:ASP:OD1	1:A:71:GLU:HG3	2.02	0.60
2:B:132:LEU:C	2:B:132:LEU:HD23	2.22	0.60
2:B:311:ARG:HH11	2:B:344:VAL:HA	1.67	0.60
1:C:209:ILE:H	1:C:209:ILE:HD12	1.65	0.60
1:C:26:LEU:HG	1:C:361:THR:CB	2.32	0.60
2:D:102:ASN:HB3	2:D:105:LYS:HB2	1.83	0.60
2:D:102:ASN:ND2	2:D:105:LYS:H	1.99	0.60
2:D:239:THR:O	2:D:241:CYS:O	2.20	0.60
2:D:398:MET:C	2:D:400:ARG:H	2.05	0.60
1:A:360:PRO:HB3	1:A:374:ALA:HB2	1.83	0.60
1:A:215:ARG:NH2	1:A:300:ASN:HD21	1.99	0.60
1:A:31:GLN:CB	1:A:32:PRO:HD2	2.27	0.60
1:C:287:SER:OG	1:C:290:GLU:HG3	2.02	0.60
1:C:354:GLY:C	1:C:355:ILE:HD12	2.22	0.60
1:A:100:ALA:HA	1:A:105:ARG:HD2	1.83	0.60
2:B:194:LEU:HD11	2:B:428:LEU:HD11	1.84	0.60
1:C:332:ILE:CD1	1:C:353:VAL:HG21	2.31	0.60
1:C:46:ASP:N	1:C:46:ASP:OD2	2.34	0.60
3:E:83:UNK:C	3:E:85:UNK:N	2.63	0.60
1:A:69:ASP:HB3	1:A:75:ILE:CG2	2.26	0.59
2:B:266:HIS:HB2	2:B:380:ASN:OD1	2.02	0.59
2:B:60:LYS:N	2:B:60:LYS:NZ	2.50	0.59
2:D:102:ASN:O	2:D:105:LYS:HB2	2.01	0.59
2:D:127:GLU:O	2:D:128:SER:C	2.40	0.59
2:D:166:MET:HG3	2:D:167:ASN:N	2.16	0.59
2:D:240:THR:C	2:D:243:ARG:HB2	2.22	0.59
2:D:263:PRO:O	2:D:265:LEU:N	2.33	0.59
2:D:380:ASN:HD22	2:D:380:ASN:C	2.05	0.59
2:D:58:GLY:C	2:D:64:ARG:NE	2.55	0.59
1:C:329:ASN:HA	1:C:332:ILE:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:350:ASN:HD22	2:B:351:VAL:HG23	1.68	0.59
1:C:264:ARG:NH2	1:C:424:ASP:OD1	2.35	0.59
1:C:423:GLU:O	1:C:427:ALA:N	2.28	0.59
1:C:9:VAL:HG23	1:C:9:VAL:O	2.01	0.59
2:D:218:LYS:HZ2	2:D:277:SER:HB3	1.67	0.59
2:B:322:ARG:NE	2:B:357:ASP:HB3	2.17	0.59
1:C:321:GLY:HA2	1:C:357:TYR:O	2.02	0.59
1:C:433:GLU:C	1:C:435:VAL:H	2.04	0.59
1:A:182:VAL:CG1	1:A:183:GLU:N	2.65	0.59
1:A:209:ILE:C	1:A:211:ASP:N	2.51	0.59
2:B:259:MET:HE1	2:B:316:ALA:N	2.16	0.59
1:C:209:ILE:C	1:C:211:ASP:N	2.55	0.59
2:D:266:HIS:ND1	2:D:432:TYR:CZ	2.70	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:390:ARG:C	2:D:392:SER:N	2.51	0.59
1:A:77:GLU:O	1:A:83:TYR:CB	2.50	0.59
1:A:395:PHE:CD1	1:A:395:PHE:C	2.75	0.59
2:B:416:MET:C	2:B:418:PHE:N	2.56	0.59
2:B:12:CYS:HB3	5:B:501:GDP:C8	2.37	0.59
1:C:395:PHE:CD1	1:C:395:PHE:C	2.75	0.59
1:C:413:MET:H	1:C:413:MET:CE	2.15	0.59
1:C:86:LEU:HD22	1:C:89:PRO:HD3	1.84	0.59
2:D:141:LEU:HB3	2:D:186:ASN:CB	2.32	0.59
1:A:238:ILE:N	1:A:241:SER:HB3	2.18	0.59
2:D:75:MET:O	2:D:76:ASP:C	2.40	0.59
2:D:87:PHE:O	2:D:90:ASP:OD1	2.19	0.59
1:C:237:SER:CA	1:C:241:SER:HB2	2.28	0.59
1:A:44:GLY:HA3	1:A:47:ASP:HA	1.84	0.59
1:A:68:VAL:HG21	1:A:118:VAL:HG21	1.83	0.59
2:B:102:ASN:HD22	2:B:105:LYS:N	2.01	0.59
1:C:196:GLU:N	1:C:196:GLU:CD	2.55	0.59
2:D:66:ILE:HG12	2:D:66:ILE:O	2.02	0.59
2:B:391:ILE:CD1	2:B:391:ILE:H	2.15	0.59
1:C:261:PRO:CG	1:C:380:ASN:HD21	2.13	0.59
1:A:87:PHE:CE2	1:A:92:LEU:HD21	2.38	0.59
2:B:247:GLN:HG2	2:B:325:MET:SD	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ARG:HA	2:B:84:GLY:HA2	1.83	0.59
1:C:413:MET:C	1:C:414:GLU:OE1	2.41	0.59
2:D:169:PHE:CD2	2:D:235:MET:SD	2.95	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
2:D:276:THR:HG21	2:D:281:GLN:HB3	1.84	0.59
1:A:345:ASP:C	1:A:347:CYS:H	2.06	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:A:101:ASN:OD1	2:B:254:LYS:HD3	2.02	0.59
2:B:2:ARG:HG3	2:B:133:GLN:CD	2.21	0.59
1:C:258:ASN:O	1:C:259:LEU:HB2	2.02	0.59
2:D:404:PHE:O	2:D:404:PHE:HD2	1.85	0.59
2:D:308:ARG:NH2	2:D:342:TYR:HB2	2.17	0.59
3:E:67:UNK:O	3:E:71:UNK:N	2.35	0.59
2:B:181:VAL:O	2:B:183:GLU:N	2.35	0.59
2:B:2:ARG:NE	2:B:243:ARG:CD	2.64	0.59
2:B:253:ARG:HG3	2:B:253:ARG:NH1	2.17	0.59
2:B:307:PRO:C	2:B:309:HIS:H	2.06	0.59
2:B:395:PHE:HB3	2:B:422:GLU:OE1	2.03	0.59
1:C:103:TYR:N	1:C:185:TYR:HE1	2.01	0.59
1:C:416:GLY:C	1:C:418:PHE:N	2.55	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:241:CYS:C	2:B:243:ARG:H	2.04	0.59
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.38	0.59
2:B:80:SER:OG	2:B:81:GLY:N	2.34	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:385:GLN:OE1	2:B:429:VAL:HA	2.03	0.58
2:B:75:MET:O	2:B:76:ASP:O	2.21	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
2:D:416:MET:C	2:D:418:PHE:N	2.56	0.58
2:D:51:VAL:N	2:D:245:PRO:HB2	2.18	0.58
2:D:19:LYS:HA	2:D:22:GLU:OE2	2.02	0.58
2:D:241:CYS:C	2:D:243:ARG:N	2.49	0.58
2:D:251:ASP:CG	2:D:252:LEU:N	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:C	1:A:269:LEU:HD12	2.23	0.58
1:C:286:LEU:O	1:C:373:ARG:HD2	2.02	0.58
1:A:389:ALA:O	1:A:392:ASP:HB3	2.03	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
1:C:217:LEU:HD23	1:C:219:ILE:CD1	2.33	0.58
1:C:256:GLN:O	1:C:258:ASN:N	2.36	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:123:ARG:C	2:B:125:GLU:H	2.06	0.58
2:D:123:ARG:C	2:D:125:GLU:H	2.06	0.58
2:D:134:GLY:HA3	2:D:165:ILE:O	2.03	0.58
2:D:9:ALA:HA	2:D:68:VAL:O	2.02	0.58
1:A:241:SER:HB3	1:A:242:LEU:HD12	1.85	0.58
2:B:308:ARG:NH2	2:B:342:TYR:HB2	2.19	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: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
2:B:5:VAL:HA	2:B:64:ARG:CD	2.33	0.58
1:C:231:ILE:O	1:C:235:VAL:HG23	2.04	0.58
3:E:66:UNK:O	3:E:69:UNK:N	2.37	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
1:A:186:ASN:O	1:A:189:LEU:HB3	2.03	0.58
2:B:183:GLU:C	2:B:185:TYR:N	2.54	0.58
2:B:413:MET:SD	2:B:417:GLU:HG2	2.43	0.58
2:D:12:CYS:HB2	5:D:503:GDP:PA	2.43	0.58
2:B:158:ARG:HD3	2:B:197:ASN:CG	2.23	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
3:E:58:UNK:C	3:E:60:UNK:N	2.66	0.58
1:A:38:SER:O	1:A:39:ASP:HB3	2.04	0.58
2:D:409:THR:HA	2:D:412:GLY:O	2.03	0.58
1:A:409:VAL:C	1:A:411:GLU:H	2.07	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
1:C:256:GLN:C	1:C:258:ASN:N	2.57	0.58
2:D:183:GLU:HB3	2:D:184:PRO:CD	2.34	0.58
2:D:165:ILE:HG13	2:D:253:ARG:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:VAL:HG12	1:A:373:ARG:N	2.17	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
1:C:259:LEU:HD11	1:C:378:LEU:HD13	1.85	0.58
2:D:196:GLU:O	2:D:197:ASN:C	2.39	0.58
2:D:80:SER:OG	2:D:81:GLY:N	2.36	0.58
1:C:36:MET:HA	1:C:36:MET:CE	2.34	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
2:D:192:HIS:C	2:D:194:LEU:N	2.56	0.58
2:D:405:LEU:HD22	2:D:405:LEU:C	2.24	0.58
2:D:59:ASN:OD1	2:D:60:LYS:HD2	2.04	0.58
2:B:391:ILE:O	2:B:425:MET:HE1	2.03	0.58
2:B:102:ASN:ND2	2:B:105:LYS:N	2.52	0.57
2:B:251:ASP:CG	2:B:252:LEU:N	2.55	0.57
2:B:258:ASN:OD1	2:B:352:LYS:NZ	2.34	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:A:132:LEU:O	1:A:133:GLN:HB2	2.04	0.57
2:D:187:ALA:HB2	2:D:391:ILE:HG22	1.85	0.57
1:C:336:LYS:HA	1:C:336:LYS:HE2	1.85	0.57
3:E:17:UNK:O	3:E:19:UNK:N	2.35	0.57
2:D:247:GLN:HG2	2:D:325:MET:SD	2.43	0.57
2:B:276:THR:HB	2:B:281:GLN:OE1	2.03	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:D:289:PRO:HB2	2:D:331:GLN:HE21	1.69	0.57
1:A:88:HIS:HB3	1:A:91:GLN:CD	2.24	0.57
2:D:140:SER:CB	2:D:171:VAL:HB	2.34	0.57
1:C:317:LEU:HD23	1:C:377:MET:CB	2.34	0.57
1:A:363:VAL:H	1:A:367:ASP:HB2	1.69	0.57
1:A:393:HIS:C	1:A:395:PHE:H	2.06	0.57
1:A:9:VAL:O	1:A:9:VAL:HG23	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD13	1:A:118:VAL:HA	1.86	0.57
1:A:404:PHE:CD1	1:A:404:PHE:N	2.73	0.57
2:B:102:ASN:C	2:B:185:TYR:OH	2.43	0.57
1:C:77:GLU:O	1:C:83:TYR:CB	2.53	0.57
3:E:35:UNK:O	3:E:38:UNK:N	2.36	0.57
2:D:7:ILE:HB	2:D:137:LEU:HA	1.86	0.57
1:A:339:ARG:HD2	1:A:340:THR:N	2.19	0.57
1:A:46:ASP:N	1:A:46:ASP:OD2	2.37	0.57
2:D:276:THR:HB	2:D:281:GLN:OE1	2.04	0.57
1:A:387:ALA:HA	1:A:390:ARG:CD	2.29	0.57
2:B:132:LEU:HB3	2:B:164:ARG:CZ	2.34	0.57
2:B:196:GLU:O	2:B:197:ASN:C	2.43	0.57
2:B:59:ASN:OD1	2:B:60:LYS:HD2	2.05	0.57
2:B:59:ASN:N	2:B:64:ARG:HE	2.01	0.57
1:C:409:VAL:C	1:C:411:GLU:H	2.05	0.57
2:D:311:ARG:HG3	2:D:311:ARG:HH11	1.70	0.57
1:A:236:SER:O	1:A:238:ILE:N	2.31	0.57
1:C:286:LEU:HB2	1:C:291:ILE:HG13	1.86	0.57
1:A:311:LYS:HB2	1:A:344:VAL:HG22	1.87	0.57
1:A:404:PHE:N	1:A:404:PHE:HD1	2.01	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
2:D:417:GLU:O	2:D:417:GLU:HG3	2.04	0.57
1:A:229:ARG:HG3	1:A:229:ARG:HH11	1.69	0.57
1:A:209:ILE:N	1:A:209:ILE:HD12	2.19	0.57
1:A:206:ASN:ND2	1:A:210:TYR:HE2	1.98	0.57
1:C:401:LYS:O	1:C:402:ARG:HB3	2.05	0.57
1:C:82:THR:HG22	1:C:83:TYR:H	1.70	0.57
1:C:87:PHE:CD2	1:C:87:PHE:N	2.64	0.57
2:D:154:ILE:C	2:D:156:LYS:H	2.08	0.57
2:D:292:THR:HG23	2:D:319:PHE:HZ	1.70	0.57
1:C:134:GLY:H	1:C:164:LYS:HG2	1.69	0.57
1:A:244:PHE:O	1:A:245:ASP:C	2.41	0.57
1:A:336:LYS:HA	1:A:336:LYS:HE2	1.86	0.57
1:C:292:THR:HA	1:C:295:CYS:HB3	1.86	0.57
2:B:409:THR:HG23	2:B:414:ASP:HA	1.86	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
1:C:142:GLY:O	1:C:182:VAL:HG23	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:371:VAL:HG12	1:A:372:GLN:H	1.69	0.57
1:A:155:GLU:O	1:A:159:VAL:HG23	2.04	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:311:ARG:HH21	2:B:437:ASP:CB	1.97	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
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
2:D:282:GLN:O	2:D:284:ARG:N	2.38	0.57
1:A:164:LYS:NZ	1:A:164:LYS:HB2	2.19	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:291:ILE:CD1	1:A:373:ARG:HG3	2.34	0.57
1:A:139:HIS:HB3	1:A:170:SER:HA	1.87	0.57
1:A:196:GLU:N	1:A:196:GLU:CD	2.58	0.57
1:A:417:GLU:HB3	1:A:418:PHE:HD2	1.68	0.57
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.86	0.57
2:B:149:MET:CE	2:B:149:MET:HA	2.34	0.57
2:B:163:ASP:OD1	2:B:164:ARG:HG2	2.05	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.39	0.57
1:C:143:GLY:H	1:C:147:SER:HB2	1.70	0.57
1:C:182:VAL:O	1:C:183:GLU:C	2.43	0.57
2:D:133:GLN:OE1	2:D:133:GLN:HA	2.05	0.57
2:D:198:THR:O	2:D:200:GLU:N	2.37	0.57
1:A:284:GLU:O	1:A:285:GLN:HG3	2.05	0.57
1:A:267:PHE:H	1:A:267:PHE:HD1	1.53	0.57
2:B:9:ALA:HA	2:B:68:VAL:O	2.04	0.57
1:A:386:GLU:C	1:A:388:TRP:H	2.06	0.56
1:A:264:ARG:NH2	1:A:424:ASP:OD1	2.38	0.56
2:B:350:ASN:ND2	2:B:351:VAL:HG23	2.19	0.56
1:C:193:THR:HG23	1:C:193:THR:O	2.05	0.56
2:D:162:PRO:O	2:D:163:ASP:C	2.43	0.56
1:C:293:ASN:O	1:C:297:GLU:OE1	2.23	0.56
1:A:209:ILE:O	1:A:211:ASP:N	2.38	0.56
1:A:69:ASP:OD2	1:A:74:VAL:CG1	2.52	0.56
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.68	0.56
1:C:137:VAL:HG21	1:C:154:MET:SD	2.45	0.56
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:SER:C	1:C:238:ILE:H	2.08	0.56
2:D:339:ASN:C	2:D:341:SER:N	2.58	0.56
2:B:139:HIS:O	2:B:139:HIS:HD2	1.88	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:401:LYS:O	1:A:402:ARG:HB3	2.05	0.56
2:B:120:ASP:O	2:B:124:LYS:HE3	2.06	0.56
2:B:416:MET:O	2:B:417:GLU:HB3	2.06	0.56
1:C:137:VAL:CG1	1:C:154:MET:HE2	2.30	0.56
1:C:23:LEU:O	1:C:26:LEU:HD12	2.06	0.56
1:C:399:TYR:HH	1:C:408:TYR:HE2	1.52	0.56
2:B:200:GLU:CG	2:B:268:PHE:HE2	2.19	0.56
1:C:257:THR:OG1	1:C:258:ASN:ND2	2.39	0.56
2:D:130:ASP:OD2	2:D:131:CYS:N	2.38	0.56
2:D:263:PRO:HG2	2:D:264:ARG:H	1.71	0.56
2:D:218:LYS:O	2:D:219:LEU:HB2	2.04	0.56
2:D:69:ASP:CB	2:D:74:THR:HG23	2.35	0.56
1:A:188:ILE:HG22	1:A:417:GLU:O	2.04	0.56
2:B:103:TRP:O	2:B:105:LYS:O	2.23	0.56
2:B:2:ARG:NH2	2:B:243:ARG:HA	2.20	0.56
3:E:10:UNK:HA	3:E:13:UNK:CB	2.36	0.56
2:D:223:THR:N	2:D:226:ASP:OD2	2.33	0.56
2:D:194:LEU:CD1	2:D:428:LEU:HD21	2.35	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
1:C:331:ALA:C	1:C:333:ALA:H	2.08	0.56
1:A:402:ARG:CG	1:A:403:ALA:N	2.68	0.56
1:A:433:GLU:C	1:A:435:VAL:H	2.07	0.56
2:B:307:PRO:O	2:B:309:HIS:N	2.38	0.56
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
1:A:286:LEU:HB2	1:A:291:ILE:HG13	1.88	0.56
3:E:46:UNK:C	3:E:48:UNK:N	2.62	0.56
1:A:256:GLN:C	1:A:258:ASN:N	2.58	0.56
1:A:209:ILE:HG12	1:A:231:ILE:HD11	1.88	0.56
2:B:183:GLU:O	2:B:185:TYR:N	2.38	0.56
1:C:398:MET:O	1:C:400:ALA:N	2.38	0.56
2:D:132:LEU:HD23	2:D:132:LEU:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:THR:HG21	2:D:189:LEU:CD2	2.36	0.56
2:D:241:CYS:C	2:D:243:ARG:H	2.07	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
3:E:57:UNK:O	3:E:58:UNK:C	2.53	0.56
1:C:389:ALA:O	1:C:392:ASP:HB3	2.06	0.56
1:A:311:LYS:CD	1:A:344:VAL:HG22	2.36	0.56
1:A:184:PRO:HG3	1:A:399:TYR:CE1	2.41	0.56
2:B:161:TYR:O	2:B:162:PRO:C	2.42	0.56
2:B:226:ASP:C	2:B:228:ASN:H	2.08	0.56
2:B:240:THR:C	2:B:243:ARG:HB2	2.26	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:401:LYS:O	1:C:402:ARG:CB	2.53	0.56
1:C:399:TYR:OH	1:C:408:TYR:HE2	1.89	0.56
2:D:158:ARG:CZ	2:D:197:ASN:HA	2.36	0.56
1:A:86:LEU:CD1	1:A:89:PRO:HD3	2.35	0.56
1:A:36:MET:HA	1:A:36:MET:CE	2.36	0.56
1:C:288:VAL:HA	1:C:373:ARG:HD3	1.86	0.56
1:A:195:LEU:C	1:A:197:HIS:H	2.09	0.56
1:A:213:CYS:SG	1:A:217:LEU:HD23	2.46	0.56
1:C:387:ALA:HA	1:C:390:ARG:CD	2.30	0.56
1:C:69:ASP:HB3	1:C:75:ILE:CG2	2.35	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:316:CYS:SG	1:A:316:CYS:O	2.64	0.56
2:B:398:MET:C	2:B:400:ARG:N	2.57	0.56
1:A:102:ASN:HD21	2:B:257:VAL:CG1	2.12	0.56
1:A:189:LEU:CD1	1:A:193:THR:HG21	2.35	0.56
1:A:151:SER:HB3	1:A:192:HIS:NE2	2.20	0.56
2:B:151:THR:HG21	2:B:189:LEU:CD2	2.36	0.56
1:C:102:ASN:HD21	2:D:257:VAL:CG1	2.14	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
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
1:A:243:ARG:NH1	1:A:250:VAL:HG13	2.16	0.56
1:A:350:GLY:C	1:A:351:PHE:CD1	2.72	0.56
2:D:88:ARG:HA	2:D:88:ARG:HH11	1.70	0.56
2:D:51:VAL:N	2:D:245:PRO:HG2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ALA:HA	1:C:292:THR:HG22	1.87	0.56
1:A:78:VAL:O	1:A:82:THR:HA	2.05	0.56
1:A:385:ALA:HB2	1:A:432:TYR:CD2	2.39	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:A:69:ASP:OD2	1:A:74:VAL:HG12	2.05	0.56
2:D:132:LEU:O	2:D:132:LEU:HD23	2.05	0.56
2:D:198:THR:C	2:D:200:GLU:N	2.59	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
2:D:59:ASN:CB	2:D:64:ARG:HB2	2.35	0.56
1:A:112:LYS:NZ	3:E:12:UNK:CB	2.69	0.55
1:A:16:ILE:O	1:A:19:ALA:N	2.30	0.55
1:A:26:LEU:HD12	1:A:26:LEU:H	1.71	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:241:CYS:O	2:B:243:ARG:N	2.39	0.55
2:B:3:GLU:OE2	2:B:128:SER:O	2.24	0.55
1:C:140:SER:HB3	1:C:171:ILE:HD13	1.86	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:C:229:ARG:HG3	1:C:229:ARG:HH11	1.72	0.55
1:A:234:ILE:CD1	1:A:302:MET:SD	2.94	0.55
2:B:132:LEU:HD22	2:B:164:ARG:NE	2.22	0.55
2:B:59:ASN:ND2	2:B:60:LYS:N	2.54	0.55
1:C:166:LYS:HE3	1:C:198:SER:N	2.12	0.55
2:D:12:CYS:HB3	5:D:503:GDP:N7	2.21	0.55
2:D:59:ASN:HB3	2:D:64:ARG:HB2	1.87	0.55
2:D:93:VAL:HG23	2:D:94:PHE:N	2.21	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
1:C:287:SER:C	1:C:289:ALA:N	2.59	0.55
2:D:69:ASP:HB2	2:D:74:THR:HG23	1.87	0.55
1:A:12:ALA:HB3	1:A:140:SER:CB	2.36	0.55
2:B:97:SER:OG	2:B:98:GLY:N	2.39	0.55
1:C:142:GLY:O	1:C:182:VAL:CG2	2.55	0.55
1:C:88:HIS:N	1:C:91:GLN:OE1	2.39	0.55
2:D:97:SER:OG	2:D:98:GLY:N	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:99:ALA:HA	2:B:105:LYS:HD3	1.89	0.55
1:C:186:ASN:O	1:C:189:LEU:HB3	2.06	0.55
3:E:31:UNK:O	3:E:32:UNK:C	2.51	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
1:A:273:ALA:HB2	1:A:295:CYS:HA	1.89	0.55
1:C:284:GLU:O	1:C:285:GLN:HG3	2.06	0.55
1:A:75:ILE:CG1	1:A:75:ILE:O	2.54	0.55
1:C:100:ALA:CA	1:C:105:ARG:HD2	2.36	0.55
2:D:274:PRO:HG3	2:D:374:SER:CB	2.37	0.55
1:C:2:ARG:HH22	1:C:133:GLN:HE22	1.54	0.55
1:A:103:TYR:H	1:A:185:TYR:HE1	1.54	0.55
1:A:409:VAL:O	1:A:412:GLY:O	2.25	0.55
1:C:171:ILE:H	1:C:171:ILE:CD1	2.20	0.55
1:C:386:GLU:C	1:C:388:TRP:H	2.10	0.55
1:C:96:LYS:O	1:C:98:ASP:N	2.39	0.55
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.41	0.55
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:B:51:VAL:HG22	2:B:245:PRO:CG	2.36	0.55
1:A:258:ASN:ND2	1:A:258:ASN:H	2.03	0.55
1:A:139:HIS:CG	1:A:140:SER:H	2.23	0.55
1:A:218:ASP:CG	1:A:219:ILE:H	2.09	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:189:LEU:C	2:D:191:VAL:N	2.55	0.55
2:D:59:ASN:N	2:D:64:ARG:HE	2.04	0.55
1:A:236:SER:C	1:A:238:ILE:H	2.09	0.55
2:B:345:GLU:O	2:B:345:GLU:CG	2.55	0.55
2:B:320:ARG:HB2	2:B:374:SER:OG	2.07	0.55
1:C:427:ALA:HA	1:C:430:LYS:HB2	1.88	0.55
1:C:88:HIS:HB3	1:C:91:GLN:CD	2.26	0.55
1:C:72:PRO:HG3	1:C:96:LYS:HA	1.89	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:133:GLN:HG3	2:B:252:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:LEU:CD1	2:B:428:LEU:HD21	2.37	0.55
2:B:227:LEU:O	2:B:227:LEU:HD23	2.06	0.55
2:B:264:ARG:NH2	2:B:431:GLU:HG3	2.20	0.55
2:B:180:THR:HB	2:B:404:PHE:CE1	2.42	0.55
1:C:217:LEU:HG	1:C:217:LEU:O	2.06	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:C:286:LEU:HD12	1:C:291:ILE:HG12	1.89	0.55
2:B:10:GLY:CA	2:B:146:GLY:HA3	2.37	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
2:D:242:LEU:O	2:D:243:ARG:HD3	2.07	0.55
2:D:59:ASN:HA	2:D:60:LYS:HZ3	1.71	0.55
2:D:395:PHE:HB3	2:D:422:GLU:OE1	2.07	0.55
1:A:331:ALA:HA	1:A:334:THR:OG1	2.07	0.55
1:A:259:LEU:HD21	1:A:378:LEU:CB	2.37	0.55
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:119:LEU:HD22	1:C:156:ARG:NE	2.21	0.54
2:D:107:HIS:HA	2:D:152:LEU:HD22	1.88	0.54
2:D:243:ARG:HH12	2:D:252:LEU:HD12	1.72	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: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: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
1:A:287:SER:C	1:A:289:ALA:N	2.60	0.54
1:A:399:TYR:OH	1:A:408:TYR:HE2	1.90	0.54
1:C:100:ALA:HA	1:C:105:ARG:HD2	1.89	0.54
1:C:110:ILE:O	1:C:111:GLY:C	2.45	0.54
1:C:175:PRO:HD2	1:C:207:GLU:CB	2.11	0.54
1:C:71:GLU:O	1:C:73:THR:N	2.40	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:B:218:LYS:O	2:B:219:LEU:CB	2.55	0.54
1:A:317:LEU:HD23	1:A:377:MET:HB3	1.88	0.54
1:A:103:TYR:O	1:A:104:ALA:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:HA	1:A:430:LYS:HB2	1.89	0.54
2:B:377:PHE:O	2:B:378:ILE:HG12	2.07	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
2:D:168:THR:OG1	2:D:201:THR:CB	2.54	0.54
2:D:22:GLU:OE2	2:D:22:GLU:N	2.41	0.54
2:D:428:LEU:HD12	2:D:428:LEU:H	1.73	0.54
2:B:218:LYS:HZ2	2:B:277:SER:HB3	1.72	0.54
1:C:344:VAL:CG1	1:C:346:TRP:NE1	2.69	0.54
1:A:137:VAL:O	1:A:168:GLU:HA	2.07	0.54
2:B:59:ASN:CB	2:B:64:ARG:HB2	2.37	0.54
2:B:60:LYS:HZ2	2:B:60:LYS:N	2.04	0.54
1:C:209:ILE:CD1	1:C:209:ILE:H	2.20	0.54
2:D:102:ASN:C	2:D:185:TYR:OH	2.46	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
2:B:394:GLN:O	2:B:398:MET:CB	2.56	0.54
1:C:345:ASP:C	1:C:347:CYS:H	2.10	0.54
1:A:190:THR:HG21	1:A:425:MET:SD	2.47	0.54
2:B:378:ILE:HG22	2:B:378:ILE:O	2.06	0.54
2:B:428:LEU:CD1	2:B:428:LEU:H	2.20	0.54
2:B:437:ASP:N	2:B:437:ASP:OD2	2.39	0.54
1:C:419:SER:O	1:C:422:ARG:N	2.41	0.54
2:D:344:VAL:HG23	2:D:345:GLU:N	2.21	0.54
2:D:192:HIS:O	2:D:194:LEU:N	2.36	0.54
2:D:2:ARG:NH1	2:D:251:ASP:HA	2.23	0.54
2:B:215:ARG:HA	2:B:215:ARG:CZ	2.37	0.54
1:C:314:ALA:O	1:C:315:CYS:CB	2.56	0.54
1:C:12:ALA:HB3	1:C:140:SER:OG	2.07	0.54
1:C:26:LEU:H	1:C:26:LEU:HD12	1.73	0.54
1:C:184:PRO:HG3	1:C:399:TYR:CE1	2.43	0.54
2:D:5:VAL:HG12	2:D:5:VAL:O	2.06	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
3:E:71:UNK:C	3:E:73:UNK:N	2.70	0.54
1:A:389:ALA:CB	1:A:429:GLU:OE2	2.55	0.54
2:D:409:THR:HG23	2:D:414:ASP:HA	1.89	0.54
2:B:98:GLY:N	2:B:110:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:244:PHE:O	1:C:245:ASP:C	2.46	0.54
1:A:273:ALA:HB2	1:A:295:CYS:CA	2.38	0.54
1:A:123:ARG:HG2	1:A:161:TYR:OH	2.08	0.54
1:A:93:ILE:HD13	1:A:118:VAL:CG2	2.29	0.54
1:C:177:VAL:HG11	2:D:349:ASN:HB3	1.90	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
2:D:129:CYS:O	2:D:130:ASP:C	2.46	0.54
2:D:385:GLN:OE1	2:D:429:VAL:HA	2.08	0.54
2:B:187:ALA:HB2	2:B:391:ILE:HG22	1.88	0.54
1:A:242:LEU:HG	1:A:318:LEU:HD11	1.89	0.54
1:C:238:ILE:O	1:C:239:THR:C	2.47	0.54
1:C:322:ASP:N	1:C:357:TYR:O	2.38	0.54
1:A:331:ALA:C	1:A:333:ALA:N	2.58	0.54
1:A:103:TYR:HB2	1:A:185:TYR:HD1	1.72	0.54
2:B:60:LYS:NZ	2:B:60:LYS:H	2.06	0.54
1:C:139:HIS:CG	1:C:140:SER:H	2.26	0.54
1:C:195:LEU:C	1:C:197:HIS:H	2.11	0.54
1:C:23:LEU:C	1:C:25:CYS:H	2.11	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
2:D:2:ARG:HG3	2:D:133:GLN:CD	2.26	0.54
2:D:371:LEU:O	2:D:372:LYS:HB2	2.07	0.54
1:A:322:ASP:N	1:A:357:TYR:O	2.38	0.54
2:B:69:ASP:HB2	2:B:74:THR:HG23	1.90	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:A:163:LYS:C	1:A:164:LYS:HZ2	2.10	0.54
1:A:169:PHE:HE1	1:A:238:ILE:HD12	1.73	0.54
1:C:241:SER:HB3	1:C:242:LEU:HD12	1.90	0.54
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
1:C:395:PHE:C	1:C:397:LEU:N	2.61	0.53
2:D:191:VAL:O	2:D:191:VAL:CG1	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:THR:O	2:D:226:ASP:N	2.39	0.53
1:A:35:GLN:OE1	1:A:88:HIS:NE2	2.41	0.53
2:B:51:VAL:C	2:B:53:TYR:N	2.61	0.53
1:C:420:GLU:OE1	1:C:420:GLU:C	2.46	0.53
1:C:86:LEU:CD1	1:C:89:PRO:HD3	2.38	0.53
1:C:92:LEU:CD1	1:C:92:LEU:N	2.71	0.53
2:D:398:MET:SD	2:D:399:PHE:CD2	3.01	0.53
1:C:242:LEU:HB3	1:C:250:VAL:CG1	2.38	0.53
1:A:16:ILE:CG2	1:A:17:GLY:N	2.59	0.53
1:A:193:THR:O	1:A:193:THR:HG23	2.07	0.53
1:A:405:VAL:O	1:A:409:VAL:HG23	2.08	0.53
2:B:130:ASP:OD2	2:B:130:ASP:C	2.46	0.53
2:B:189:LEU:O	2:B:191:VAL:N	2.39	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:308:ARG:NH2	2:D:342:TYR:CG	2.76	0.53
1:A:87:PHE:HD2	1:A:87:PHE:H	1.54	0.53
1:A:408:TYR:O	1:A:414:GLU:HG3	2.08	0.53
2:B:204:ILE:HG21	2:B:209:LEU:HD11	1.89	0.53
2:B:174:SER:OG	2:B:207:GLU:HA	2.09	0.53
1:A:183:GLU:OE2	2:B:348:PRO:HB2	2.09	0.53
2:B:371:LEU:O	2:B:372:LYS:HB2	2.08	0.53
1:C:24:TYR:HA	1:C:26:LEU:HD12	1.91	0.53
2:D:315:VAL:HG23	2:D:351:VAL:HG22	1.90	0.53
2:D:102:ASN:HD22	2:D:105:LYS:CB	2.20	0.53
2:D:17:GLY:O	2:D:20:PHE:HB3	2.07	0.53
2:D:283:TYR:O	2:D:290:GLU:OE1	2.25	0.53
2:D:51:VAL:HG22	2:D:245:PRO:CG	2.38	0.53
1:A:220:GLU:HB3	1:A:221:ARG:NE	2.23	0.53
2:B:284:ARG:O	2:B:285:ALA:C	2.47	0.53
2:B:274:PRO:HA	2:B:294:GLN:CD	2.28	0.53
2:B:297:ASP:OD1	2:B:298:ALA:N	2.42	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: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:82:THR:O	1:A:83:TYR:HB2	2.09	0.53
1:A:305:CYS:SG	1:A:384:ILE:HA	2.49	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
1:C:217:LEU:HD23	1:C:219:ILE:HD12	1.89	0.53

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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	0.53
2:D:179:ASP:HB2	2:D:182:VAL:CG2	2.38	0.53
2:D:274:PRO:HA	2:D:294:GLN:CD	2.29	0.53
1:A:65:ALA:O	1:A:91:GLN:HB2	2.08	0.53
1:C:238:ILE:O	1:C:242:LEU:HD12	2.09	0.53
1:A:331:ALA:O	1:A:335:ILE:HG23	2.08	0.53
1:A:92:LEU:N	1:A:92:LEU:CD1	2.70	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:88:ARG:CB	2:B:89:PRO:HD3	2.32	0.53
1:C:184:PRO:HA	1:C:395:PHE:HD2	1.74	0.53
1:C:181:VAL:HG22	1:C:408:TYR:OH	2.09	0.53
2:D:223:THR:HG23	2:D:225:GLY:CA	2.39	0.53
2:D:226:ASP:C	2:D:228:ASN:H	2.12	0.53
2:D:241:CYS:O	2:D:243:ARG:N	2.42	0.53
2:B:358:ILE:H	2:B:358:ILE:CD1	2.18	0.53
1:C:333:ALA:O	1:C:334:THR:C	2.47	0.53
1:A:271:THR:HG23	1:A:300:ASN:O	2.08	0.53
2:B:59:ASN:HA	2:B:60:LYS:HZ3	1.73	0.53
2:D:345:GLU:CG	2:D:345:GLU:O	2.57	0.53
2:D:79:ARG:HA	2:D:84:GLY:HA2	1.90	0.53
2:D:322:ARG:HG2	2:D:357:ASP:CA	2.30	0.53
1:C:339:ARG:HD2	1:C:340:THR:N	2.24	0.53
2:B:6:HIS:O	2:B:66:ILE:HG22	2.09	0.53
1:C:206:ASN:O	1:C:210:TYR:HD2	1.92	0.53
2:D:200:GLU:CG	2:D:268:PHE:HE2	2.22	0.53
2:D:282:GLN:C	2:D:285:ALA:H	2.12	0.53
2:D:392:SER:HB2	2:D:426:ASN:ND2	2.24	0.53
2:D:190:SER:CB	2:D:425:MET:HG3	2.28	0.53
1:A:216:ASN:HB3	1:A:275:VAL:CG1	2.39	0.53
1:C:285:GLN:C	1:C:286:LEU:HD23	2.29	0.53
2:B:111:GLY:O	2:B:114:LEU:N	2.42	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:403:ALA:HB1	2:B:405:LEU:HD12	1.90	0.53
2:B:191:VAL:CG2	2:B:421:ALA:HB1	2.25	0.53
2:B:91:ASN:N	2:B:91:ASN:ND2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:HG22	1:A:342:GLN:N	2.23	0.53
1:C:43:GLY:O	1:C:47:ASP:CG	2.47	0.53
1:A:212:ILE:C	1:A:214:ARG:H	2.13	0.52
2:B:223:THR:C	2:B:225:GLY:N	2.61	0.52
2:B:381:SER:C	2:B:383:ALA:H	2.11	0.52
2:B:88:ARG:HH11	2:B:88:ARG:HA	1.73	0.52
3:E:30:UNK:O	3:E:33:UNK:N	2.42	0.52
2:D:2:ARG:CG	2:D:133:GLN:NE2	2.61	0.52
2:B:51:VAL:CG2	2:B:53:TYR:HB2	2.39	0.52
1:C:40:LYS:HD2	1:C:41:THR:H	1.73	0.52
1:C:15:GLN:HE22	1:C:224:TYR:HD1	1.56	0.52
1:C:401:LYS:O	1:C:402:ARG:CD	2.57	0.52
2:D:437:ASP:OD2	2:D:437:ASP:N	2.43	0.52
2:D:154:ILE:O	2:D:156:LYS:N	2.42	0.52
2:D:371:LEU:C	2:D:373:MET:H	2.10	0.52
2:D:413:MET:SD	2:D:417:GLU:HG2	2.49	0.52
1:A:256:GLN:O	1:A:258:ASN:N	2.43	0.52
2:D:25:SER:HB3	2:D:369:ARG:HH22	1.74	0.52
1:A:101:ASN:C	1:A:185:TYR:OH	2.46	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
2:D:16:ILE:HG12	2:D:17:GLY:N	2.24	0.52
2:D:223:THR:C	2:D:225:GLY:N	2.60	0.52
2:D:264:ARG:NH2	2:D:431:GLU:HG3	2.24	0.52
2:D:305:CYS:O	2:D:306:ASP:C	2.47	0.52
2:D:428:LEU:H	2:D:428:LEU:CD1	2.23	0.52
1:C:322:ASP:OD1	1:C:357:TYR:O	2.27	0.52
1:A:333:ALA:O	1:A:334:THR:C	2.48	0.52
1:A:289:ALA:HA	1:A:292:THR:HG22	1.89	0.52
3:E:73:UNK:C	3:E:75:UNK:N	2.66	0.52
1:A:110:ILE:O	1:A:111:GLY:C	2.46	0.52
1:A:213:CYS:SG	1:A:230:LEU:HD23	2.50	0.52
1:A:416:GLY:C	1:A:418:PHE:N	2.62	0.52
2:B:306:ASP:HB3	2:B:309:HIS:NE2	2.24	0.52
1:C:101:ASN:HD22	1:C:101:ASN:C	2.13	0.52
1:C:181:VAL:HG13	1:C:408:TYR:OH	2.09	0.52
2:D:143:GLY:O	5:D:503:GDP:O3B	2.28	0.52
1:C:321:GLY:HA2	1:C:358:GLU:O	2.09	0.52
1:A:314:ALA:O	1:A:315:CYS:CB	2.57	0.52
2:B:70:LEU:HD11	2:B:110:GLU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:LEU:O	2:B:115:VAL:C	2.46	0.52
2:B:16:ILE:HD12	2:B:231:VAL:CG1	2.38	0.52
2:B:265:LEU:O	2:B:266:HIS:CG	2.63	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:179:ASP:HB3	2:D:181:VAL:CG1	2.37	0.52
2:D:182:VAL:CG1	2:D:182:VAL:O	2.57	0.52
1:A:243:ARG:NE	1:A:243:ARG:HA	2.24	0.52
1:A:298:PRO:O	1:A:300:ASN:N	2.42	0.52
2:B:308:ARG:HH21	2:B:342:TYR:HD1	1.50	0.52
2:B:276:THR:HG21	2:B:281:GLN:HB3	1.92	0.52
1:C:293:ASN:C	1:C:296:PHE:H	2.13	0.52
2:B:409:THR:HA	2:B:412:GLY:O	2.10	0.52
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.91	0.52
2:B:183:GLU:HB3	2:B:184:PRO:HD3	1.91	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:35:GLN:HE22	1:C:88:HIS:CD2	2.28	0.52
2:B:322:ARG:HG2	2:B:357:ASP:CA	2.30	0.52
2:D:415:GLU:O	2:D:416:MET:O	2.27	0.52
1:C:311:LYS:CG	1:C:344:VAL:HG22	2.40	0.52
1:A:252:LEU:HD22	1:A:255:PHE:HD2	1.74	0.52
1:C:294:ALA:HA	1:C:297:GLU:OE1	2.09	0.52
2:D:260:VAL:HG12	2:D:260:VAL:O	2.09	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
2:B:287:THR:C	2:B:289:PRO:HD2	2.29	0.52
1:C:152:LEU:O	1:C:156:ARG:HG2	2.09	0.52
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
1:C:68:VAL:HG21	1:C:118:VAL:HG21	1.91	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:59:ASN:ND2	2:D:60:LYS:H	2.07	0.52
1:A:30:ILE:CG1	1:A:31:GLN:N	2.70	0.52
2:D:140:SER:HA	2:D:171:VAL:H	1.74	0.52
1:A:172:TYR:HB3	1:A:205:ASP:H	1.75	0.52
2:B:103:TRP:O	2:B:104:ALA:C	2.48	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
1:C:307:PRO:HA	1:C:383:ALA:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:TRP:HZ3	1:C:428:LEU:HD22	1.71	0.52
1:C:71:GLU:OE2	4:C:502:GTP:O1B	2.28	0.52
2:D:239:THR:O	2:D:241:CYS:N	2.43	0.52
1:A:134:GLY:H	1:A:164:LYS:HG3	1.73	0.52
1:A:286:LEU:HD12	1:A:291:ILE:HG12	1.90	0.52
1:C:341:ILE:HG22	1:C:342:GLN:N	2.25	0.52
2:B:325:MET:HG2	2:B:355:VAL:HG11	1.91	0.52
2:B:69:ASP:CB	2:B:74:THR:HG23	2.39	0.52
1:A:139:HIS:CG	1:A:140:SER:N	2.77	0.52
1:A:401:LYS:O	1:A:402:ARG:CD	2.58	0.52
1:A:414:GLU:N	1:A:414:GLU:CD	2.64	0.52
2:B:132:LEU:HD11	2:B:135:PHE:CE2	2.45	0.52
2:B:399:PHE:HE2	2:B:404:PHE:HB3	1.74	0.52
1:C:139:HIS:O	1:C:140:SER:CB	2.58	0.52
1:C:101:ASN:C	1:C:185:TYR:OH	2.47	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:398:MET:C	1:C:400:ALA:H	2.13	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
2:D:93:VAL:HG23	2:D:95:GLY:N	2.25	0.52
2:B:51:VAL:HG22	2:B:245:PRO:HG2	1.90	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:405:LEU:C	2:B:405:LEU:HD22	2.30	0.52
2:D:197:ASN:O	2:D:198:THR:HB	2.08	0.52
2:D:2:ARG:HE	2:D:243:ARG:HD2	1.75	0.52
1:A:2:ARG:NH2	1:A:133:GLN:NE2	2.53	0.52
2:B:391:ILE:O	2:B:391:ILE:HG22	2.09	0.52
2:B:400:ARG:C	2:B:402:LYS:H	2.13	0.52
1:C:292:THR:OG1	1:C:292:THR:O	2.22	0.52
1:C:44:GLY:C	1:C:46:ASP:N	2.61	0.52
1:C:389:ALA:CB	1:C:429:GLU:OE2	2.58	0.52
1:A:115:ILE:O	1:A:119:LEU:HB2	2.09	0.51
1:A:221:ARG:H	1:A:221:ARG:CD	2.23	0.51
1:A:387:ALA:HB1	1:A:390:ARG:CZ	2.40	0.51
2:B:264:ARG:NH1	2:B:264:ARG:HG3	2.25	0.51
2:B:58:GLY:O	2:B:64:ARG:CZ	2.59	0.51
1:C:298:PRO:O	1:C:300:ASN:N	2.43	0.51
1:C:88:HIS:CB	1:C:91:GLN:HE22	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:ARG:HB2	2:D:374:SER:OG	2.10	0.51
2:D:397:ALA:O	2:D:398:MET:HB2	2.10	0.51
2:B:396:THR:HA	2:B:400:ARG:HB3	1.92	0.51
1:C:344:VAL:HG11	1:C:346:TRP:CE2	2.45	0.51
2:B:339:ASN:C	2:B:341:SER:N	2.60	0.51
1:C:44:GLY:HA3	1:C:47:ASP:HA	1.91	0.51
1:A:264:ARG:HH22	1:A:427:ALA:HB3	1.75	0.51
2:B:179:ASP:CB	2:B:182:VAL:HG23	2.37	0.51
2:B:198:THR:C	2:B:200:GLU:N	2.62	0.51
2:D:75:MET:O	2:D:76:ASP:O	2.27	0.51
1:A:285:GLN:C	1:A:286:LEU:HD23	2.31	0.51
2:B:249:ASN:CG	2:B:250:ALA:N	2.62	0.51
1:A:20:CYS:C	1:A:22:GLU:N	2.63	0.51
2:B:273:ALA:O	2:B:275:LEU:N	2.40	0.51
2:B:104:ALA:HB1	2:B:411:GLU:HB2	1.93	0.51
2:B:415:GLU:O	2:B:416:MET:O	2.28	0.51
1:C:388:TRP:CZ3	1:C:428:LEU:HD13	2.45	0.51
2:D:18:ALA:C	2:D:20:PHE:N	2.60	0.51
2:D:223:THR:HG23	2:D:225:GLY:N	2.25	0.51
2:B:357:ASP:CB	2:B:358:ILE:HD12	2.41	0.51
2:D:415:GLU:HG2	2:D:416:MET:H	1.75	0.51
1:C:322:ASP:HA	1:C:357:TYR:CD1	2.37	0.51
2:B:333:LEU:O	2:B:337:ASN:N	2.43	0.51
2:B:247:GLN:OE1	2:B:355:VAL:O	2.28	0.51
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
2:B:241:CYS:O	2:B:242:LEU:C	2.49	0.51
2:B:371:LEU:C	2:B:373:MET:H	2.14	0.51
2:B:5:VAL:HG22	2:B:64:ARG:HD3	1.92	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:202:PHE:CE1	1:A:378:LEU:HD22	2.42	0.51
2:B:7:ILE:HB	2:B:137:LEU:HA	1.91	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
2:D:154:ILE:HD11	2:D:168:THR:HG21	1.92	0.51
2:D:60:LYS:HD2	2:D:60:LYS:H	1.74	0.51
2:D:212:ILE:C	2:D:214:PHE:H	2.13	0.51
2:D:51:VAL:CG2	2:D:53:TYR:HB2	2.40	0.51
2:B:401:ARG:O	2:B:402:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PRO:HA	1:A:45:GLY:O	2.10	0.51
1:A:5:ILE:O	1:A:135:PHE:HA	2.10	0.51
2:D:318:VAL:O	2:D:318:VAL:HG12	2.11	0.51
2:B:24:ILE:HG22	2:B:24:ILE:O	2.10	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
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
1:C:413:MET:HE2	1:C:413:MET:H	1.75	0.51
1:C:78:VAL:HG11	1:C:92:LEU:CD2	2.39	0.51
2:D:179:ASP:HB2	2:D:182:VAL:N	2.25	0.51
2:D:400:ARG:C	2:D:402:LYS:N	2.63	0.51
2:D:59:ASN:CA	2:D:64:ARG:HH21	2.19	0.51
1:A:320:ARG:CB	1:A:374:ALA:HB3	2.37	0.51
1:A:288:VAL:HA	1:A:373:ARG:HD3	1.92	0.51
1:A:41:THR:O	1:A:42:ILE:HB	2.09	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
2:B:253:ARG:HG3	2:B:253:ARG:HH11	1.75	0.51
2:B:2:ARG:O	2:B:57:ALA:HB1	2.11	0.51
1:C:171:ILE:HA	1:C:204:VAL:HB	1.92	0.51
1:C:69:ASP:OD2	1:C:74:VAL:HG12	2.11	0.51
2:D:103:TRP:O	2:D:105:LYS:O	2.28	0.51
2:D:11:GLN:HG3	2:D:15:GLN:NE2	2.26	0.51
2:D:253:ARG:C	2:D:255:LEU:N	2.62	0.51
2:D:297:ASP:OD1	2:D:299:LYS:N	2.32	0.51
2:D:6:HIS:ND1	2:D:21:TRP:HZ2	2.09	0.51
2:D:51:VAL:C	2:D:53:TYR:N	2.64	0.51
1:A:293:ASN:C	1:A:296:PHE:H	2.14	0.51
3:E:90:UNK:O	3:E:91:UNK:O	2.29	0.51
1:A:101:ASN:C	1:A:101:ASN:HD22	2.14	0.51
1:A:16:ILE:O	1:A:17:GLY:C	2.49	0.51
2:B:372:LYS:O	2:B:373:MET:HG3	2.11	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
2:D:59:ASN:HB2	2:D:64:ARG:HE	1.74	0.51
2:B:212:ILE:C	2:B:214:PHE:H	2.13	0.51
1:A:423:GLU:O	1:A:426:ALA:HB3	2.11	0.51
2:B:162:PRO:O	2:B:163:ASP:C	2.47	0.51
2:B:90:ASP:OD1	2:B:91:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLU:HB3	1:C:221:ARG:CZ	2.40	0.51
1:C:215:ARG:NH2	1:C:300:ASN:HD21	2.07	0.51
1:C:405:VAL:O	1:C:409:VAL:HG23	2.11	0.51
2:D:158:ARG:O	2:D:159:GLU:C	2.49	0.51
2:D:179:ASP:HB3	2:D:182:VAL:H	1.73	0.51
2:D:241:CYS:O	2:D:242:LEU:C	2.50	0.51
2:D:264:ARG:O	2:D:265:LEU:O	2.29	0.51
2:D:283:TYR:CG	2:D:283:TYR:O	2.64	0.51
2:D:59:ASN:CA	2:D:60:LYS:HZ3	2.24	0.51
2:B:391:ILE:CD1	2:B:391:ILE:N	2.74	0.51
1:A:238:ILE:O	1:A:239:THR:C	2.48	0.51
2:D:86:ILE:H	2:D:88:ARG:CZ	2.24	0.51
1:C:38:SER:O	1:C:39:ASP:HB3	2.11	0.51
1:A:21:TRP:HA	1:A:24:TYR:HB2	1.93	0.51
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.93	0.51
2:B:79:ARG:HG3	2:B:88:ARG:HE	1.75	0.51
1:C:186:ASN:HD21	1:C:391:LEU:HD11	1.75	0.51
2:D:313:LEU:HD21	2:D:435:TYR:HD2	1.76	0.51
2:D:159:GLU:CD	3:E:82:UNK:CB	2.80	0.51
1:A:247:ALA:O	1:A:249:ASN:CG	2.49	0.51
1:C:247:ALA:O	1:C:249:ASN:CG	2.48	0.51
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
1:A:8:HIS:HE2	1:A:21:TRP:HE1	1.59	0.50
1:A:143:GLY:O	4:A:500:GTP:O3G	2.29	0.50
2:B:203:CYS:SG	2:B:384:ILE:HD11	2.52	0.50
1:C:5:ILE:CD1	1:C:125:LEU:HD22	2.41	0.50
2:D:186:ASN:HA	2:D:189:LEU:HD12	1.93	0.50
2:D:19:LYS:HZ2	2:D:82:PRO:HG3	1.76	0.50
1:C:239:THR:OG1	1:C:240:ALA:N	2.41	0.50
2:B:402:LYS:HE3	1:C:440:VAL:CG1	2.41	0.50
1:C:273:ALA:HB2	1:C:295:CYS:CA	2.41	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:368:LEU:N	1:A:368:LEU:HD12	2.26	0.50
2:B:395:PHE:CE2	2:B:418:PHE:O	2.64	0.50
1:C:75:ILE:CG1	1:C:75:ILE:O	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
2:B:277:SER:O	2:B:278:ARG:O	2.29	0.50
1:A:294:ALA:HA	1:A:297:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:UNK:O	3:E:5:UNK:C	2.59	0.50
2:B:154:ILE:C	2:B:156:LYS:N	2.64	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
2:B:93:VAL:HG23	2:B:94:PHE:N	2.25	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:HG12	1:C:260:VAL:O	2.10	0.50
1:C:381:THR:C	1:C:383:ALA:H	2.14	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:398:MET:C	2:D:400:ARG:N	2.65	0.50
1:A:333:ALA:O	1:A:336:LYS:N	2.43	0.50
2:D:308:ARG:HH21	2:D:342:TYR:HD1	1.48	0.50
1:C:311:LYS:HB2	1:C:344:VAL:HG22	1.92	0.50
1:C:341:ILE:N	1:C:341:ILE:HD12	2.26	0.50
1:A:363:VAL:HG22	1:A:367:ASP:OD2	2.10	0.50
1:C:25:CYS:SG	1:C:25:CYS:O	2.69	0.50
2:B:403:ALA:HB3	1:C:262:TYR:HE2	1.76	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
2:D:4:ILE:CD1	2:D:252:LEU:HD13	2.42	0.50
1:C:350:GLY:O	1:C:351:PHE:HD1	1.93	0.50
1:A:82:THR:HG22	1:A:83:TYR:H	1.76	0.50
1:A:38:SER:O	1:A:39:ASP:CB	2.59	0.50
1:C:317:LEU:HD23	1:C:377:MET:HB3	1.92	0.50
2:D:10:GLY:CA	2:D:146:GLY:HA3	2.41	0.50
1:A:152:LEU:O	1:A:156:ARG:HG2	2.10	0.50
2:B:133:GLN:HA	2:B:133:GLN:OE1	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
2:D:326:LYS:O	2:D:330:GLU:HG3	2.11	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: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
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
2:B:127:GLU:O	2:B:128:SER:C	2.50	0.50
2:B:158:ARG:CZ	2:B:197:ASN:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:140:SER:HA	2:B:171:VAL:H	1.76	0.50
1:A:181:VAL:HG23	1:A:404:PHE:HB2	1.93	0.50
1:A:344:VAL:CG1	1:A:346:TRP:NE1	2.73	0.50
1:A:413:MET:C	1:A:414:GLU:OE1	2.49	0.50
1:A:9:VAL:HA	1:A:68:VAL:O	2.12	0.50
1:A:74:VAL:HG13	1:A:75:ILE:N	2.27	0.50
2:B:115:VAL:HG23	2:B:149:MET:HE1	1.94	0.50
2:B:311:ARG:NH1	2:B:344:VAL:HA	2.26	0.50
2:B:266:HIS:ND1	2:B:432:TYR:CE1	2.79	0.50
1:C:190:THR:CA	1:C:193:THR:HG22	2.36	0.50
1:C:203:MET:HE1	1:C:388:TRP:HD1	1.76	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:284:ARG:HG3	2:D:284:ARG:HH11	1.77	0.50
2:D:2:ARG:NE	2:D:243:ARG:CD	2.72	0.50
1:A:332:ILE:HG23	1:A:351:PHE:CE2	2.46	0.50
2:B:400:ARG:C	2:B:402:LYS:N	2.62	0.50
1:A:258:ASN:HD22	1:A:258:ASN:H	1.52	0.50
1:A:40:LYS:HD2	1:A:41:THR:H	1.76	0.50
2:B:211:ASP:O	2:B:215:ARG:N	2.44	0.50
1:A:208:ALA:O	1:A:212:ILE:HG23	2.12	0.50
1:A:184:PRO:CG	1:A:399:TYR:CZ	2.93	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
1:C:103:TYR:O	1:C:104:ALA:C	2.47	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:77:GLU:C	1:C:83:TYR:HB2	2.32	0.50
2:D:311:ARG:HH11	2:D:344:VAL:HA	1.77	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
1:A:244:PHE:HE1	1:A:358:GLU:OE2	1.95	0.50
3:E:50:UNK:O	3:E:53:UNK:N	2.44	0.50
1:C:39:ASP:CG	1:C:40:LYS:N	2.62	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLY:CA	1:A:147:SER:HB3	2.42	0.50
1:A:9:VAL:HG21	1:A:150:THR:CG2	2.42	0.50
1:A:171:ILE:CD1	1:A:171:ILE:H	2.25	0.50
1:A:187:SER:C	1:A:189:LEU:H	2.15	0.50
1:A:194:THR:O	1:A:195:LEU:C	2.49	0.50
1:A:194:THR:O	1:A:196:GLU:N	2.45	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
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:194:THR:O	1:C:195:LEU:C	2.50	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
1:C:177:VAL:HG11	2:D:349:ASN:CB	2.42	0.50
2:D:241:CYS:SG	2:D:320:ARG:NH1	2.85	0.50
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.26	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
2:D:11:GLN:C	2:D:13:GLY:H	2.15	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
1:C:242:LEU:O	1:C:243:ARG:HG2	2.12	0.49
1:C:283:HIS:O	1:C:284:GLU:HB3	2.12	0.49
2:D:100:GLY:C	2:D:101:ASN:HD22	2.15	0.49
1:A:102:ASN:O	1:A:105:ARG:N	2.34	0.49
1:A:100:ALA:CA	1:A:105:ARG:HD2	2.41	0.49
1:A:174:ALA:CB	1:A:176:GLN:HG2	2.42	0.49
2:B:154:ILE:C	2:B:156:LYS:H	2.15	0.49
2:B:158:ARG:C	2:B:160:GLU:N	2.64	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:393:HIS:C	1:C:395:PHE:N	2.65	0.49
1:C:402:ARG:HD2	2:D:346:TRP:CE3	2.47	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:D:87:PHE:O	2:D:89:PRO:HD2	2.12	0.49
1:A:331:ALA:C	1:A:333:ALA:H	2.16	0.49
2:B:51:VAL:N	2:B:245:PRO:HB2	2.26	0.49
1:C:41:THR:O	1:C:42:ILE:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:HE3	1:A:197:HIS:NE2	2.27	0.49
1:A:381:THR:C	1:A:383:ALA:H	2.15	0.49
1:A:386:GLU:C	1:A:388:TRP:N	2.66	0.49
2:B:4:ILE:CD1	2:B:252:LEU:HD13	2.42	0.49
2:B:344:VAL:O	2:B:345:GLU:HB3	2.13	0.49
2:B:428:LEU:H	2:B:428:LEU:HD12	1.76	0.49
2:B:59:ASN:HB3	2:B:64:ARG:HB2	1.93	0.49
1:C:213:CYS:SG	1:C:217:LEU:CD2	2.99	0.49
2:D:107:HIS:ND1	2:D:107:HIS:O	2.46	0.49
2:D:114:LEU:O	2:D:115:VAL:C	2.49	0.49
2:D:2:ARG:CG	2:D:133:GLN:HE21	2.23	0.49
1:C:350:GLY:C	1:C:351:PHE:CD1	2.80	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
2:B:271:GLY:O	2:B:272:PHE:O	2.30	0.49
2:B:5:VAL:HA	2:B:64:ARG:HD2	1.93	0.49
1:C:414:GLU:CG	1:C:415:GLU:H	2.17	0.49
2:D:382:THR:HB	2:D:436:GLN:HG2	1.95	0.49
2:D:184:PRO:CB	2:D:399:PHE:CZ	2.95	0.49
2:D:424:ASN:O	2:D:427:ASP:HB2	2.12	0.49
2:D:79:ARG:O	2:D:79:ARG:HG2	2.13	0.49
2:B:398:MET:O	2:B:401:ARG:N	2.45	0.49
1:A:343:PHE:CD2	1:A:349:THR:HB	2.47	0.49
1:A:181:VAL:HG22	1:A:408:TYR:OH	2.12	0.49
2:B:295:MET:O	2:B:297:ASP:N	2.44	0.49
1:C:194:THR:O	1:C:196:GLU:N	2.45	0.49
1:C:264:ARG:HH22	1:C:427:ALA:HB3	1.78	0.49
1:C:202:PHE:CE1	1:C:378:LEU:HD22	2.43	0.49
1:C:93:ILE:HD13	1:C:118:VAL:HA	1.95	0.49
2:D:158:ARG:HB2	2:D:197:ASN:CB	2.31	0.49
2:D:71:GLU:CB	2:D:72:PRO:CD	2.90	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
2:B:189:LEU:O	2:B:192:HIS:ND1	2.38	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
2:D:259:MET:CE	2:D:316:ALA:HB2	2.42	0.49
1:A:238:ILE:O	1:A:242:LEU:HD12	2.12	0.49
3:E:25:UNK:O	3:E:27:UNK:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:CYS:C	1:A:22:GLU:H	2.16	0.49
1:C:37:PRO:HA	1:C:45:GLY:O	2.13	0.49
1:A:93:ILE:CD1	1:A:118:VAL:HA	2.42	0.49
1:A:217:LEU:HG	1:A:217:LEU:O	2.12	0.49
2:B:132:LEU:CB	2:B:164:ARG:HH21	2.15	0.49
2:B:395:PHE:CD2	2:B:422:GLU:OE1	2.66	0.49
2:B:59:ASN:CB	2:B:64:ARG:HE	2.25	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:7:ILE:HG21	1:C:122:ILE:CD1	2.42	0.49
2:D:174:SER:C	2:D:176:LYS:N	2.66	0.49
2:D:2:ARG:NH2	2:D:243:ARG:HA	2.28	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:168:GLU:HG3	1:A:201:ALA:CB	2.42	0.49
1:A:68:VAL:HG13	1:A:68:VAL:O	2.13	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
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:2:ARG:HH22	1:A:133:GLN:HE22	1.57	0.49
1:A:241:SER:CB	1:A:242:LEU:HD12	2.43	0.49
1:C:283:HIS:C	1:C:285:GLN:H	2.16	0.49
1:A:311:LYS:HB2	1:A:344:VAL:CG2	2.43	0.49
1:A:186:ASN:HD21	1:A:391:LEU:HD11	1.70	0.49
1:A:427:ALA:HA	1:A:430:LYS:CB	2.43	0.49
2:B:388:PHE:C	2:B:390:ARG:H	2.14	0.49
1:C:102:ASN:HB2	1:C:105:ARG:HB3	1.91	0.49
1:C:9:VAL:HG21	1:C:150:THR:HB	1.93	0.49
1:C:176:GLN:OE1	1:C:210:TYR:CE1	2.66	0.49
1:C:68:VAL:HG21	1:C:149:PHE:HE1	1.77	0.49
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.31	0.49
1:C:291:ILE:HG22	1:C:292:THR:N	2.28	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:395:PHE:C	1:A:397:LEU:N	2.63	0.49
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.93	0.49
2:B:149:MET:CE	2:B:152:LEU:HD23	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:O	2:B:159:GLU:C	2.51	0.49
2:B:242:LEU:O	2:B:243:ARG:HD3	2.12	0.49
2:B:133:GLN:NE2	2:B:252:LEU:CB	2.65	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:60:LYS:NZ	2:D:60:LYS:H	2.11	0.49
2:D:395:PHE:CE2	2:D:418:PHE:O	2.66	0.49
1:C:350:GLY:O	1:C:351:PHE:CD1	2.66	0.49
1:A:317:LEU:HD13	1:A:319:TYR:CE1	2.48	0.49
1:A:174:ALA:C	1:A:176:GLN:N	2.65	0.48
1:A:398:MET:C	1:A:400:ALA:H	2.14	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:185:TYR:O	1:C:186:ASN:C	2.51	0.48
2:D:344:VAL:CG2	2:D:345:GLU:N	2.76	0.48
2:D:106:GLY:O	2:D:149:MET:HA	2.13	0.48
2:D:154:ILE:C	2:D:156:LYS:N	2.65	0.48
2:D:204:ILE:HD13	2:D:231:VAL:HG13	1.94	0.48
2:D:8:GLN:O	2:D:67:LEU:HA	2.13	0.48
1:A:126:ALA:HB1	1:A:132:LEU:HD11	1.93	0.48
2:D:87:PHE:O	2:D:89:PRO:CD	2.61	0.48
1:A:256:GLN:HA	1:A:260:VAL:CG2	2.43	0.48
1:A:102:ASN:HB2	1:A:105:ARG:HB3	1.88	0.48
1:A:307:PRO:HA	1:A:383:ALA:HB3	1.95	0.48
1:A:428:LEU:C	1:A:430:LYS:N	2.66	0.48
2:B:102:ASN:HB3	2:B:105:LYS:CD	2.43	0.48
2:B:18:ALA:C	2:B:20:PHE:N	2.66	0.48
2:B:20:PHE:HZ	2:B:239:THR:HG21	1.78	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
2:B:283:TYR:C	2:B:285:ALA:H	2.16	0.48
1:C:303:VAL:HG21	1:C:384:ILE:HD11	1.94	0.48
2:D:313:LEU:O	2:D:314:THR:CG2	2.61	0.48
3:E:34:UNK:O	3:E:38:UNK:N	2.47	0.48
2:D:283:TYR:C	2:D:285:ALA:H	2.15	0.48
2:D:291:LEU:CD2	2:D:291:LEU:H	2.26	0.48
2:D:394:GLN:O	2:D:398:MET:CB	2.59	0.48
1:C:31:GLN:HB3	1:C:32:PRO:CD	2.37	0.48
1:A:294:ALA:HA	1:A:297:GLU:HB2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:PRO:CB	2:B:331:GLN:HE21	2.26	0.48
2:B:269:MET:SD	2:B:381:SER:HB3	2.54	0.48
1:C:174:ALA:CB	1:C:176:GLN:HG2	2.43	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:284:GLU:OE2	1:A:285:GLN:NE2	2.46	0.48
1:C:344:VAL:HG12	1:C:345:ASP:OD2	2.13	0.48
2:B:25:SER:HB3	2:B:369:ARG:HH22	1.79	0.48
1:A:179:THR:HB	1:A:182:VAL:HB	1.94	0.48
1:A:96:LYS:O	1:A:98:ASP:N	2.46	0.48
2:B:4:ILE:HG12	2:B:133:GLN:HG2	1.95	0.48
2:B:407:TRP:HE1	1:C:257:THR:HA	1.79	0.48
1:C:139:HIS:CG	1:C:140:SER:N	2.80	0.48
1:C:393:HIS:O	1:C:395:PHE:N	2.38	0.48
1:C:427:ALA:HA	1:C:430:LYS:CB	2.43	0.48
1:C:77:GLU:OE2	1:C:83:TYR:CG	2.66	0.48
2:D:163:ASP:OD1	2:D:164:ARG:HG2	2.13	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:D:79:ARG:HA	2:D:84:GLY:CA	2.44	0.48
2:B:386:GLU:C	2:B:388:PHE:N	2.66	0.48
1:C:181:VAL:HG23	1:C:404:PHE:HB2	1.96	0.48
1:C:414:GLU:CA	1:C:417:GLU:HB2	2.44	0.48
1:C:101:ASN:CB	2:D:254:LYS:HD3	2.42	0.48
2:D:179:ASP:CB	2:D:182:VAL:HG23	2.41	0.48
2:D:90:ASP:OD1	2:D:91:ASN:ND2	2.47	0.48
1:C:244:PHE:HE1	1:C:358:GLU:OE2	1.97	0.48
2:D:51:VAL:HG22	2:D:245:PRO:HG2	1.96	0.48
1:A:283:HIS:C	1:A:285:GLN:H	2.16	0.48
1:C:274:PRO:HG3	1:C:373:ARG:O	2.13	0.48
2:D:279:GLY:O	2:D:281:GLN:N	2.47	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
2:B:181:VAL:C	2:B:184:PRO:HD2	2.34	0.48
2:D:103:TRP:O	2:D:104:ALA:C	2.52	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:B:402:LYS:CE	1:C:440:VAL:C	2.82	0.48
3:E:48:UNK:C	3:E:50:UNK:N	2.75	0.48
1:C:229:ARG:HB3	1:C:366:GLY:O	2.14	0.48
1:A:139:HIS:CD2	1:A:146:GLY:O	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:26:LEU:CG	1:A:361:THR:OG1	2.62	0.48
2:B:189:LEU:HA	2:B:192:HIS:CE1	2.48	0.48
2:B:284:ARG:HB3	2:B:287:THR:OG1	2.14	0.48
2:B:62:VAL:O	2:B:63:PRO:C	2.51	0.48
2:B:93:VAL:HG23	2:B:95:GLY:N	2.28	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:174:SER:C	2:D:176:LYS:H	2.16	0.48
2:D:284:ARG:HB2	2:D:290:GLU:OE1	2.14	0.48
2:D:400:ARG:C	2:D:402:LYS:H	2.17	0.48
2:B:397:ALA:O	2:B:398:MET:HB2	2.13	0.48
1:C:343:PHE:CD1	1:C:349:THR:HA	2.49	0.48
1:A:104:ALA:CA	1:A:108:TYR:HD2	2.23	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:23:LEU:C	1:A:25:CYS:N	2.67	0.48
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.27	0.48
2:B:182:VAL:CG1	2:B:182:VAL:O	2.53	0.48
1:C:103:TYR:CG	1:C:188:ILE:HD13	2.48	0.48
1:C:108:TYR:O	1:C:109:THR:C	2.52	0.48
2:D:350:ASN:C	2:D:350:ASN:HD22	2.17	0.48
2:D:383:ALA:C	2:D:385:GLN:N	2.67	0.48
2:B:212:ILE:HG21	2:B:230:LEU:HD21	1.96	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:D:84:GLY:HA2	2:D:88:ARG:HH21	1.78	0.48
1:A:286:LEU:O	1:A:287:SER:C	2.50	0.48
2:B:139:HIS:C	2:B:139:HIS:HD2	2.17	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
1:A:426:ALA:C	1:A:428:LEU:H	2.17	0.48
2:B:148:GLY:HA2	2:B:151:THR:HG22	1.95	0.48
2:B:293:GLN:C	2:B:295:MET:N	2.67	0.48
2:B:424:ASN:O	2:B:427:ASP:N	2.46	0.48
2:B:59:ASN:CA	2:B:64:ARG:HH21	2.23	0.48
1:C:218:ASP:CG	1:C:219:ILE:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASP:OD1	1:C:71:GLU:HG3	2.14	0.48
2:D:253:ARG:HG3	2:D:253:ARG:NH1	2.27	0.48
2:D:287:THR:C	2:D:289:PRO:HD2	2.34	0.48
2:D:62:VAL:CG2	2:D:62:VAL:O	2.62	0.48
1:C:289:ALA:HA	1:C:292:THR:HG23	1.95	0.48
1:A:101:ASN:CG	2:B:254:LYS:HD3	2.34	0.48
1:A:182:VAL:HG12	1:A:183:GLU:H	1.79	0.48
2:B:106:GLY:O	2:B:149:MET:HA	2.14	0.48
2:B:22:GLU:HG3	2:B:83:PHE:CE1	2.49	0.48
2:B:2:ARG:NH2	2:B:243:ARG:CA	2.76	0.48
2:B:297:ASP:OD1	2:B:299:LYS:N	2.36	0.48
1:C:180:ALA:O	1:C:182:VAL:N	2.47	0.48
1:C:212:ILE:C	1:C:214:ARG:H	2.17	0.48
2:D:262:PHE:HB3	2:D:263:PRO:CD	2.36	0.48
1:A:242:LEU:HB3	1:A:250:VAL:CG1	2.44	0.48
1:A:77:GLU:C	1:A:83:TYR:HB2	2.35	0.48
1:A:39:ASP:CG	1:A:40:LYS:N	2.60	0.48
1:C:296:PHE:HZ	1:C:317:LEU:HD21	1.79	0.48
1:A:326:LYS:HG2	1:A:326:LYS:O	2.13	0.48
1:A:311:LYS:CB	1:A:344:VAL:HG22	2.43	0.47
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
2:D:18:ALA:O	2:D:22:GLU:OE2	2.32	0.47
2:D:381:SER:C	2:D:383:ALA:H	2.16	0.47
1:A:164:LYS:CB	1:A:164:LYS:NZ	2.77	0.47
1:C:346:TRP:HZ2	1:C:435:VAL:HB	1.79	0.47
1:A:7:ILE:HG21	1:A:122:ILE:CD1	2.40	0.47
1:A:115:ILE:HG12	1:A:149:PHE:HE2	1.80	0.47
1:A:407:TRP:C	1:A:409:VAL:N	2.67	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:16:ILE:O	1:C:17:GLY:C	2.52	0.47
1:C:20:CYS:C	1:C:22:GLU:N	2.66	0.47
1:C:255:PHE:HD1	1:C:259:LEU:HD12	1.79	0.47
1:C:417:GLU:C	1:C:418:PHE:HD2	2.15	0.47
2:D:118:VAL:C	2:D:120:ASP:N	2.66	0.47
2:D:130:ASP:C	2:D:130:ASP:OD2	2.52	0.47
2:D:3:GLU:O	2:D:133:GLN:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:LYS:N	2:D:60:LYS:HZ3	2.12	0.47
1:C:284:GLU:OE2	1:C:285:GLN:NE2	2.46	0.47
1:A:46:ASP:O	1:A:47:ASP:C	2.52	0.47
1:A:355:ILE:N	1:A:355:ILE:CD1	2.76	0.47
1:A:294:ALA:C	1:A:296:PHE:N	2.67	0.47
1:C:296:PHE:CZ	1:C:317:LEU:HD21	2.48	0.47
1:A:174:ALA:C	1:A:176:GLN:H	2.18	0.47
1:A:209:ILE:H	1:A:209:ILE:CD1	2.28	0.47
1:A:426:ALA:C	1:A:428:LEU:N	2.67	0.47
2:B:14:ASN:O	2:B:18:ALA:N	2.47	0.47
2:B:200:GLU:CD	2:B:268:PHE:HE2	2.17	0.47
2:B:79:ARG:HG2	2:B:79:ARG:O	2.13	0.47
2:D:161:TYR:O	2:D:162:PRO:C	2.52	0.47
2:D:389:LYS:HA	2:D:392:SER:OG	2.14	0.47
1:C:243:ARG:NE	1:C:243:ARG:HA	2.29	0.47
1:C:128:GLN:HA	1:C:128:GLN:OE1	2.14	0.47
1:A:217:LEU:HD23	1:A:219:ILE:CD1	2.44	0.47
2:B:427:ASP:O	2:B:428:LEU:C	2.53	0.47
1:C:307:PRO:HA	1:C:383:ALA:CB	2.45	0.47
1:C:428:LEU:C	1:C:430:LYS:N	2.68	0.47
2:D:142:GLY:HA3	2:D:186:ASN:OD1	2.15	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
2:D:405:LEU:C	2:D:407:TRP:H	2.17	0.47
2:D:212:ILE:HG21	2:D:230:LEU:HD21	1.95	0.47
2:B:154:ILE:HD11	2:B:168:THR:HG21	1.96	0.47
2:B:144:GLY:HA3	2:B:185:TYR:OH	2.14	0.47
2:B:223:THR:HG23	2:B:225:GLY:H	1.79	0.47
2:B:206:ASN:ND2	2:B:227:LEU:CD2	2.71	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:408:TYR:HB2	1:C:418:PHE:HZ	1.79	0.47
1:C:426:ALA:C	1:C:428:LEU:N	2.67	0.47
2:D:315:VAL:HA	2:D:379:GLY:HA2	1.97	0.47
2:D:137:LEU:O	2:D:137:LEU:HG	2.15	0.47
2:D:255:LEU:HD21	2:D:259:MET:HG3	1.95	0.47
1:C:241:SER:HA	1:C:320:ARG:CZ	2.43	0.47
1:C:327:ASP:O	1:C:330:ALA:HB3	2.14	0.47
1:C:311:LYS:HD3	1:C:344:VAL:CG1	2.39	0.47
2:B:51:VAL:HG23	2:B:53:TYR:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:UNK:O	3:E:60:UNK:N	2.48	0.47
1:A:343:PHE:CG	1:A:349:THR:HB	2.49	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
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:O	2:B:176:LYS:N	2.47	0.47
2:B:179:ASP:HB2	2:B:182:VAL:N	2.29	0.47
2:B:178:SER:O	2:B:179:ASP:O	2.32	0.47
1:C:137:VAL:HG21	1:C:154:MET:CE	2.45	0.47
1:C:426:ALA:C	1:C:428:LEU:H	2.17	0.47
1:C:73:THR:HG23	1:C:74:VAL:H	1.79	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:202:TYR:HE1	2:D:378:ILE:HD12	1.76	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:B:100:GLY:C	2:B:101:ASN:HD22	2.18	0.47
2:B:286:LEU:CD1	2:B:371:LEU:O	2.63	0.47
1:C:179:THR:HG22	1:C:180:ALA:O	2.15	0.47
1:C:35:GLN:HE22	1:C:88:HIS:CG	2.32	0.47
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.49	0.47
2:B:154:ILE:HG23	2:B:197:ASN:HB3	1.97	0.47
2:B:282:GLN:C	2:B:285:ALA:H	2.17	0.47
1:C:190:THR:HG21	1:C:425:MET:SD	2.55	0.47
1:C:368:LEU:N	1:C:368:LEU:HD12	2.29	0.47
2:D:19:LYS:HA	2:D:22:GLU:CG	2.45	0.47
2:D:295:MET:HG2	2:D:377:PHE:HD2	1.79	0.47
2:D:1:MET:C	2:D:3:GLU:N	2.68	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:307:PRO:C	2:D:309:HIS:N	2.68	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
1:A:242:LEU:HD11	1:A:318:LEU:HG	1.97	0.47
1:C:312:TYR:O	1:C:344:VAL:HG23	2.14	0.47
1:C:286:LEU:O	1:C:287:SER:C	2.51	0.47
2:D:386:GLU:C	2:D:388:PHE:N	2.66	0.47
1:C:385:ALA:HB1	1:C:429:GLU:HG3	1.97	0.47
1:C:294:ALA:HA	1:C:297:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ALA:C	1:C:296:PHE:N	2.67	0.47
1:A:152:LEU:O	1:A:153:LEU:C	2.52	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
2:B:129:CYS:O	2:B:130:ASP:C	2.52	0.47
2:B:253:ARG:C	2:B:255:LEU:N	2.68	0.47
2:B:293:GLN:C	2:B:295:MET:H	2.17	0.47
1:C:23:LEU:O	1:C:26:LEU:CD1	2.63	0.47
1:C:401:LYS:O	1:C:402:ARG:NE	2.47	0.47
1:C:407:TRP:C	1:C:409:VAL:N	2.65	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:86:LEU:HD13	1:A:89:PRO:HD3	1.97	0.47
1:A:77:GLU:OE2	1:A:83:TYR:CG	2.68	0.47
1:A:314:ALA:O	1:A:315:CYS:HB3	2.15	0.47
1:A:306:ASP:HB3	1:A:386:GLU:OE1	2.15	0.47
2:B:174:SER:C	2:B:176:LYS:N	2.68	0.47
2:B:243:ARG:HD3	2:B:243:ARG:HA	1.47	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:256:GLN:HB3	1:C:260:VAL:CB	2.41	0.47
1:C:419:SER:O	1:C:422:ARG:HG2	2.14	0.47
1:C:9:VAL:HG21	1:C:150:THR:HG22	1.96	0.47
2:D:16:ILE:HD12	2:D:231:VAL:CG1	2.42	0.47
2:D:283:TYR:C	2:D:285:ALA:N	2.67	0.47
2:D:22:GLU:HG3	2:D:83:PHE:CE1	2.50	0.47
2:B:218:LYS:NZ	2:B:277:SER:HB3	2.29	0.47
1:C:243:ARG:NH1	1:C:250:VAL:HG13	2.19	0.47
1:A:274:PRO:HG3	1:A:373:ARG:O	2.14	0.47
1:C:311:LYS:CD	1:C:344:VAL:HG22	2.44	0.47
1:A:144:GLY:H	1:A:147:SER:HB3	1.76	0.47
1:A:206:ASN:O	1:A:207:GLU:C	2.53	0.47
1:A:209:ILE:HG22	1:A:227:LEU:HG	1.97	0.47
2:B:118:VAL:C	2:B:120:ASP:N	2.65	0.47
2:B:11:GLN:C	2:B:13:GLY:H	2.18	0.47
2:B:284:ARG:HG3	2:B:284:ARG:HH11	1.79	0.47
2:B:298:ALA:HB2	2:B:307:PRO:CD	2.45	0.47
1:A:177:VAL:HG11	2:B:349:ASN:CB	2.45	0.47
1:C:416:GLY:O	1:C:420:GLU:HB3	2.14	0.47
1:C:73:THR:HA	1:C:76:ASP:HB2	1.96	0.47
2:D:141:LEU:HG	2:D:170:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:ASN:O	2:D:189:LEU:HB2	2.15	0.47
2:D:320:ARG:CG	2:D:320:ARG:HH11	2.25	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:B:220:THR:HB	1:C:326:LYS:CE	2.45	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
2:D:203:CYS:SG	2:D:384:ILE:CD1	3.02	0.47
2:D:249:ASN:CG	2:D:250:ALA:N	2.68	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:265:ALA:O	1:A:266:HIS:O	2.33	0.46
1:A:264:ARG:O	1:A:266:HIS:ND1	2.48	0.46
1:A:362:VAL:O	1:A:370:LYS:NZ	2.48	0.46
1:A:185:TYR:CE1	1:A:408:TYR:HE1	2.33	0.46
2:B:191:VAL:CG1	2:B:191:VAL:O	2.58	0.46
2:D:238:VAL:HG22	2:D:376:THR:HG21	1.96	0.46
1:A:295:CYS:SG	1:A:377:MET:HE1	2.55	0.46
1:C:343:PHE:CG	1:C:349:THR:HB	2.50	0.46
2:B:402:LYS:HE3	1:C:440:VAL:C	2.35	0.46
1:C:273:ALA:HB2	1:C:295:CYS:HA	1.97	0.46
3:E:61:UNK:C	3:E:63:UNK:N	2.78	0.46
1:C:385:ALA:HB2	1:C:432:TYR:CD2	2.47	0.46
1:A:102:ASN:O	1:A:103:TYR:C	2.54	0.46
2:B:320:ARG:HH11	2:B:320:ARG:CG	2.25	0.46
1:C:172:TYR:CG	1:C:173:PRO:HD2	2.50	0.46
1:C:26:LEU:HG	1:C:361:THR:HB	1.97	0.46
2:D:3:GLU:HG2	2:D:58:GLY:O	2.15	0.46
2:D:401:ARG:O	2:D:402:LYS:HG3	2.15	0.46
2:D:63:PRO:C	2:D:65:ALA:N	2.67	0.46
1:A:393:HIS:C	1:A:395:PHE:N	2.68	0.46
1:A:402:ARG:NH1	2:B:346:TRP:CD2	2.83	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
2:B:305:CYS:O	2:B:306:ASP:C	2.53	0.46
2:B:75:MET:SD	2:B:79:ARG:CZ	3.02	0.46
1:C:68:VAL:O	1:C:68:VAL:HG13	2.14	0.46
1:C:9:VAL:CG2	1:C:9:VAL:O	2.63	0.46
2:D:313:LEU:O	2:D:314:THR:HG23	2.15	0.46
2:D:243:ARG:HA	2:D:243:ARG:HD3	1.52	0.46
2:D:60:LYS:CD	2:D:60:LYS:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:181:VAL:O	1:A:185:TYR:CD2	2.69	0.46
2:B:103:TRP:N	2:B:185:TYR:OH	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:101:ASN:OD1	2:D:254:LYS:CD	2.59	0.46
1:C:24:TYR:HA	1:C:26:LEU:CD1	2.46	0.46
2:D:350:ASN:ND2	2:D:350:ASN:N	2.62	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:243:ARG:NH1	1:A:250:VAL:CG1	2.72	0.46
1:A:275:VAL:CG1	1:A:275:VAL:O	2.63	0.46
1:C:273:ALA:HB2	1:C:295:CYS:CB	2.42	0.46
1:A:122:ILE:HG22	1:A:123:ARG:N	2.30	0.46
1:A:209:ILE:H	1:A:209:ILE:HD12	1.79	0.46
1:A:388:TRP:CZ3	1:A:428:LEU:HD13	2.50	0.46
2:B:124:LYS:O	2:B:124:LYS:HG3	2.15	0.46
2:B:405:LEU:C	2:B:407:TRP:H	2.18	0.46
1:C:386:GLU:C	1:C:388:TRP:N	2.68	0.46
1:C:398:MET:CE	1:C:399:TYR:HE1	2.29	0.46
2:D:350:ASN:H	2:D:350:ASN:ND2	2.13	0.46
2:D:322:ARG:NE	2:D:357:ASP:CB	2.74	0.46
1:C:344:VAL:CG1	1:C:345:ASP:N	2.75	0.46
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.51	0.46
2:B:320:ARG:HB3	2:B:320:ARG:CZ	2.45	0.46
2:B:60:LYS:HD2	2:B:60:LYS:H	1.79	0.46
2:B:73:GLY:O	2:B:78:VAL:HG21	2.16	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
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:287:SER:O	1:A:289:ALA:N	2.49	0.46
1:C:344:VAL:HG12	1:C:345:ASP:CG	2.36	0.46
1:A:112:LYS:HZ1	3:E:12:UNK:CB	2.29	0.46
1:A:218:ASP:CG	1:A:219:ILE:N	2.69	0.46
1:A:23:LEU:O	1:A:26:LEU:CD1	2.63	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
1:C:149:PHE:CD2	1:C:149:PHE:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:MET:CE	1:C:197:HIS:NE2	2.79	0.46
1:C:159:VAL:HG21	3:E:56:UNK:HA	1.98	0.46
2:D:18:ALA:O	2:D:21:TRP:N	2.46	0.46
2:D:378:ILE:O	2:D:378:ILE:HG22	2.16	0.46
1:C:245:ASP:O	1:C:249:ASN:OD1	2.33	0.46
1:A:341:ILE:N	1:A:341:ILE:HD12	2.30	0.46
1:A:398:MET:HB2	1:A:403:ALA:HB2	1.96	0.46
2:B:283:TYR:C	2:B:285:ALA:N	2.68	0.46
2:B:315:VAL:HA	2:B:379:GLY:HA2	1.98	0.46
2:B:383:ALA:C	2:B:385:GLN:N	2.68	0.46
2:B:194:LEU:HD12	2:B:428:LEU:HD21	1.97	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:20:CYS:C	1:C:22:GLU:H	2.19	0.46
2:D:174:SER:O	2:D:176:LYS:N	2.49	0.46
2:D:20:PHE:O	2:D:23:VAL:N	2.48	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:B:308:ARG:HG3	2:B:342:TYR:CZ	2.51	0.46
1:C:274:PRO:HB3	1:C:291:ILE:CD1	2.45	0.46
1:A:84:ARG:C	1:A:85:GLN:HG2	2.36	0.46
1:C:251:ASP:O	1:C:254:GLU:N	2.49	0.46
1:A:149:PHE:O	1:A:149:PHE:CD2	2.69	0.46
1:A:103:TYR:CD1	1:A:188:ILE:HD13	2.51	0.46
1:A:206:ASN:O	1:A:210:TYR:CD2	2.69	0.46
1:A:265:ALA:O	1:A:266:HIS:C	2.54	0.46
2:B:428:LEU:HD12	2:B:428:LEU:N	2.31	0.46
2:B:430:SER:O	2:B:431:GLU:C	2.54	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:238:VAL:HG21	2:D:378:ILE:HD11	1.98	0.46
2:D:215:ARG:CA	2:D:215:ARG:NE	2.78	0.46
2:B:398:MET:HG3	1:C:346:TRP:O	2.16	0.46
1:A:44:GLY:C	1:A:46:ASP:N	2.69	0.46
2:B:279:GLY:O	2:B:281:GLN:N	2.49	0.46
1:A:225:THR:HA	1:A:228:ASN:HB2	1.98	0.46
1:A:306:ASP:OD1	1:A:309:HIS:NE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:TYR:HD1	2:B:284:ARG:HH21	1.64	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
1:C:184:PRO:CG	1:C:399:TYR:CZ	2.98	0.46
2:D:122:VAL:CG1	2:D:123:ARG:N	2.78	0.46
2:D:259:MET:HE1	2:D:316:ALA:HB2	1.98	0.46
2:D:416:MET:HA	2:D:419:THR:OG1	2.16	0.46
1:C:331:ALA:O	1:C:335:ILE:HG23	2.15	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
1:C:42:ILE:HD12	1:C:43:GLY:H	1.81	0.46
1:A:21:TRP:N	1:A:21:TRP:CD1	2.84	0.45
1:A:210:TYR:CE2	1:A:227:LEU:CD2	2.98	0.45
1:A:276:ILE:CG1	1:A:282:TYR:CD2	2.98	0.45
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.35	0.45
2:B:287:THR:CB	2:B:289:PRO:HD2	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
1:C:419:SER:O	1:C:420:GLU:C	2.55	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
2:D:20:PHE:HZ	2:D:239:THR:HG21	1.81	0.45
2:D:290:GLU:HG2	2:D:294:GLN:HB2	1.97	0.45
1:A:242:LEU:O	1:A:250:VAL:HG12	2.16	0.45
1:A:36:MET:HE2	1:A:37:PRO:HD2	1.98	0.45
1:A:10:GLY:O	1:A:11:GLN:C	2.54	0.45
1:A:280:LYS:O	1:A:282:TYR:CD2	2.69	0.45
2:B:158:ARG:HB2	2:B:197:ASN:HD22	1.81	0.45
2:B:174:SER:C	2:B:176:LYS:H	2.19	0.45
2:B:208:ALA:HB2	2:B:304:ALA:CB	2.47	0.45
2:B:73:GLY:C	2:B:75:MET:H	2.20	0.45
2:B:81:GLY:N	2:B:82:PRO:HD2	2.32	0.45
1:C:102:ASN:O	1:C:103:TYR:C	2.53	0.45
1:C:206:ASN:O	1:C:210:TYR:CD2	2.69	0.45
1:C:398:MET:HE3	1:C:399:TYR:HE1	1.80	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
2:D:58:GLY:O	2:D:64:ARG:NH2	2.49	0.45
1:A:244:PHE:HD2	1:A:244:PHE:H	1.63	0.45
2:B:247:GLN:OE1	2:B:356:CYS:HA	2.16	0.45
2:B:211:ASP:O	2:B:215:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:CG1	1:A:75:ILE:N	2.78	0.45
2:B:313:LEU:O	2:B:314:THR:HG23	2.16	0.45
2:B:5:VAL:HG12	2:B:5:VAL:O	2.17	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
1:C:209:ILE:O	1:C:211:ASP:N	2.49	0.45
2:D:14:ASN:O	2:D:18:ALA:N	2.46	0.45
2:D:235:MET:O	2:D:239:THR:OG1	2.35	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: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
1:A:414:GLU:HA	1:A:417:GLU:HB2	1.98	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:5:ILE:O	1:C:136:SER:N	2.48	0.45
3:E:10:UNK:C	3:E:12:UNK:N	2.71	0.45
2:D:399:PHE:HE2	2:D:404:PHE:HB3	1.80	0.45
1:A:238:ILE:O	1:A:239:THR:O	2.35	0.45
2:D:276:THR:HG21	2:D:281:GLN:CB	2.47	0.45
1:A:143:GLY:O	1:A:144:GLY:C	2.55	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
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
2:B:60:LYS:CD	2:B:60:LYS:H	2.29	0.45
2:B:87:PHE:O	2:B:89:PRO:N	2.49	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:67:PHE:O	1:C:92:LEU:HA	2.16	0.45
2:D:284:ARG:O	2:D:285:ALA:C	2.54	0.45
2:D:2:ARG:O	2:D:2:ARG:HG2	2.17	0.45
1:C:380:ASN:O	1:C:380:ASN:CG	2.53	0.45
2:B:51:VAL:HG13	2:B:245:PRO:HB2	1.99	0.45
1:A:5:ILE:HG22	1:A:6:SER:N	2.31	0.45
1:A:108:TYR:O	1:A:109:THR:C	2.55	0.45
1:A:363:VAL:HG22	1:A:367:ASP:CG	2.36	0.45
1:A:398:MET:HE3	1:A:399:TYR:HE1	1.81	0.45
2:B:176:LYS:HD2	2:B:210:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:ASN:O	1:C:207:GLU:C	2.55	0.45
2:D:311:ARG:NE	2:D:436:GLN:O	2.50	0.45
2:D:234:THR:O	2:D:238:VAL:HG23	2.17	0.45
2:D:405:LEU:HD22	2:D:405:LEU:O	2.16	0.45
2:D:59:ASN:HA	2:D:60:LYS:NZ	2.32	0.45
2:D:211:ASP:O	2:D:215:ARG:N	2.50	0.45
1:C:164:LYS:NZ	1:C:164:LYS:HB2	2.29	0.45
1:C:332:ILE:HG23	1:C:351:PHE:CE2	2.52	0.45
1:C:287:SER:O	1:C:289:ALA:N	2.50	0.45
2:D:140:SER:O	2:D:147:SER:OG	2.33	0.45
1:A:364:PRO:C	1:A:366:GLY:H	2.20	0.45
2:B:133:GLN:CG	2:B:252:LEU:HD22	2.47	0.45
1:C:16:ILE:HG22	1:C:17:GLY:H	1.79	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:327:ASP:O	1:A:330:ALA:HB3	2.16	0.45
1:C:371:VAL:HG12	1:C:372:GLN:H	1.81	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
1:A:417:GLU:C	1:A:418:PHE:HD2	2.17	0.45
2:B:102:ASN:HB3	2:B:105:LYS:CG	2.47	0.45
1:C:172:TYR:H	1:C:205:ASP:H	1.65	0.45
2:D:436:GLN:HE21	2:D:436:GLN:C	2.20	0.45
2:D:209:LEU:HD21	2:D:302:MET:HG3	1.98	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
1:A:155:GLU:OE2	1:A:196:GLU:HB3	2.17	0.45
2:B:298:ALA:HA	2:B:301:MET:CG	2.47	0.45
1:C:171:ILE:HG21	4:C:502:GTP:N3	2.32	0.45
1:C:396:ASP:O	1:C:400:ALA:HB3	2.17	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:C:326:LYS:HG2	1:C:326:LYS:O	2.16	0.45
2:D:85:GLN:HA	2:D:88:ARG:HG2	1.98	0.45
1:C:31:GLN:CB	1:C:32:PRO:CD	2.94	0.45
1:C:343:PHE:CD2	1:C:349:THR:HB	2.52	0.45
1:C:223:THR:O	1:C:226:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:N	1:A:171:ILE:CD1	2.78	0.45
1:A:346:TRP:CD1	1:A:346:TRP:N	2.74	0.45
2:B:115:VAL:HG21	2:B:152:LEU:CD2	2.47	0.45
2:B:126:SER:O	2:B:127:GLU:C	2.54	0.45
2:B:226:ASP:C	2:B:228:ASN:N	2.70	0.45
2:B:290:GLU:O	2:B:291:LEU:C	2.55	0.45
2:B:351:VAL:HG12	2:B:352:LYS:N	2.32	0.45
2:B:428:LEU:O	2:B:429:VAL:C	2.54	0.45
1:C:101:ASN:ND2	1:C:101:ASN:O	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:B:217:LEU:CG	2:B:218:LYS:N	2.75	0.45
1:A:351:PHE:HB3	1:A:352:LYS:H	1.63	0.45
1:C:433:GLU:C	1:C:435:VAL:N	2.69	0.45
1:A:83:TYR:O	1:A:84:ARG:HB2	2.17	0.45
1:A:255:PHE:CD1	1:A:259:LEU:HD12	2.52	0.45
3:E:3:UNK:C	3:E:5:UNK:N	2.80	0.45
2:B:115:VAL:CG1	2:B:156:LYS:HZ3	2.30	0.44
2:B:307:PRO:C	2:B:309:HIS:N	2.69	0.44
2:B:59:ASN:CA	2:B:60:LYS:HZ3	2.29	0.44
1:C:185:TYR:HA	1:C:188:ILE:CD1	2.33	0.44
1:C:256:GLN:C	1:C:258:ASN:H	2.19	0.44
2:D:115:VAL:CG1	2:D:156:LYS:HZ3	2.30	0.44
2:D:178:SER:O	2:D:179:ASP:O	2.35	0.44
1:A:284:GLU:O	1:A:285:GLN:CG	2.65	0.44
2:B:242:LEU:O	2:B:243:ARG:CD	2.64	0.44
1:C:86:LEU:HD13	1:C:89:PRO:HD3	1.99	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:C:163:LYS:C	1:C:164:LYS:HZ1	2.20	0.44
1:A:88:HIS:HA	1:A:89:PRO:HD2	1.87	0.44
2:B:51:VAL:O	2:B:53:TYR:N	2.50	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:24:TYR:HA	1:A:26:LEU:HD12	1.99	0.44
1:A:276:ILE:HD12	1:A:277:SER:H	1.79	0.44
1:A:9:VAL:O	1:A:9:VAL:CG2	2.66	0.44
2:B:184:PRO:CB	2:B:399:PHE:CZ	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:HA	2:B:290:GLU:CD	2.37	0.44
2:B:2:ARG:CZ	2:B:243:ARG:HD3	2.47	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:169:PHE:HE1	1:A:238:ILE:CD1	2.30	0.44
2:D:88:ARG:CB	2:D:89:PRO:HD3	2.34	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
1:A:420:GLU:OE1	1:A:420:GLU:C	2.54	0.44
2:B:298:ALA:HB2	2:B:307:PRO:HD2	2.00	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:363:VAL:HG22	1:C:367:ASP:OD2	2.18	0.44
1:C:413:MET:C	1:C:414:GLU:CD	2.76	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
1:A:164:LYS:NZ	1:A:164:LYS:N	2.60	0.44
1:C:380:ASN:OD1	1:C:380:ASN:O	2.35	0.44
2:B:308:ARG:NH2	2:B:342:TYR:CG	2.83	0.44
1:C:273:ALA:CB	1:C:295:CYS:HB2	2.45	0.44
2:B:138:THR:HG22	2:B:139:HIS:N	2.32	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:338:LYS:O	2:B:340:SER:N	2.43	0.44
2:B:4:ILE:N	2:B:58:GLY:HA2	2.33	0.44
1:C:188:ILE:HG13	1:C:188:ILE:H	1.62	0.44
2:B:407:TRP:HE1	1:C:257:THR:CA	2.31	0.44
1:C:428:LEU:C	1:C:430:LYS:H	2.21	0.44
1:C:67:PHE:O	1:C:75:ILE:HD11	2.17	0.44
1:C:7:ILE:O	1:C:7:ILE:HG13	2.18	0.44
2:D:344:VAL:O	2:D:346:TRP:CD1	2.70	0.44
1:C:96:LYS:HE3	1:C:96:LYS:HB2	1.77	0.44
2:D:95:GLY:O	2:D:96:GLN:HB3	2.18	0.44
2:D:97:SER:HG	2:D:110:GLU:CG	2.30	0.44
2:D:187:ALA:HB2	2:D:391:ILE:CG2	2.48	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:A:256:GLN:C	1:A:258:ASN:H	2.20	0.44
1:A:306:ASP:C	1:A:308:ARG:N	2.68	0.44
1:A:414:GLU:CG	1:A:415:GLU:H	2.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:CZ	2:B:243:ARG:CD	2.96	0.44
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.48	0.44
2:B:334:ASN:O	2:B:338:LYS:N	2.51	0.44
2:B:271:GLY:O	2:B:377:PHE:HB2	2.18	0.44
2:B:407:TRP:HE1	1:C:257:THR:N	2.15	0.44
2:B:12:CYS:HB2	5:B:501:GDP:PA	2.58	0.44
2:B:59:ASN:ND2	2:B:60:LYS:H	2.16	0.44
2:B:58:GLY:O	2:B:64:ARG:NH2	2.50	0.44
1:C:10:GLY:O	1:C:11:GLN:C	2.56	0.44
3:E:13:UNK:C	3:E:15:UNK:N	2.77	0.44
2:D:179:ASP:HB2	2:D:182:VAL:CB	2.47	0.44
1:C:340:THR:O	1:C:342:GLN:HG2	2.17	0.44
1:C:46:ASP:O	1:C:47:ASP:C	2.56	0.44
1:A:111:GLY:C	1:A:113:GLU:N	2.71	0.44
1:A:142:GLY:HA2	1:A:185:TYR:HB2	1.98	0.44
1:A:344:VAL:HG12	1:A:345:ASP:CG	2.38	0.44
2:B:103:TRP:O	2:B:105:LYS:N	2.50	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
2:B:182:VAL:HG11	5:B:501:GDP:O3'	2.17	0.44
1:C:227:LEU:CD1	1:C:227:LEU:N	2.81	0.44
1:C:259:LEU:HD21	1:C:378:LEU:CB	2.45	0.44
1:C:177:VAL:HG21	2:D:349:ASN:HB2	1.99	0.44
2:D:223:THR:C	2:D:225:GLY:H	2.20	0.44
2:D:358:ILE:HD12	2:D:358:ILE:N	2.21	0.44
1:C:312:TYR:H	1:C:312:TYR:HD1	1.65	0.44
3:E:71:UNK:O	3:E:74:UNK:N	2.51	0.44
1:A:305:CYS:C	1:A:386:GLU:OE1	2.56	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:306:ASP:C	1:C:308:ARG:N	2.69	0.44
1:C:277:SER:O	1:C:368:LEU:HB3	2.17	0.44
2:D:273:ALA:H	2:D:274:PRO:HD2	1.83	0.44
2:D:430:SER:O	2:D:431:GLU:C	2.56	0.44
2:D:51:VAL:HG23	2:D:53:TYR:HB2	1.99	0.44
1:A:289:ALA:HA	1:A:292:THR:HG23	1.96	0.44
1:C:288:VAL:HA	1:C:373:ARG:CD	2.47	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:ASP:HB2	2:B:182:VAL:CB	2.48	0.44
2:B:223:THR:C	2:B:225:GLY:H	2.20	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:152:LEU:O	1:C:153:LEU:C	2.55	0.44
1:C:206:ASN:CB	1:C:210:TYR:HE2	2.28	0.44
1:C:265:ALA:O	1:C:266:HIS:C	2.55	0.44
1:C:402:ARG:HG2	1:C:403:ALA:N	2.24	0.44
2:D:106:GLY:HA2	2:D:111:GLY:HA3	1.99	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:126:ALA:O	1:A:132:LEU:HD12	2.17	0.44
2:D:75:MET:SD	2:D:79:ARG:CZ	3.06	0.44
1:C:244:PHE:CZ	1:C:358:GLU:OE1	2.71	0.44
1:C:349:THR:OG1	1:C:349:THR:O	2.29	0.44
1:C:284:GLU:O	1:C:285:GLN:CG	2.65	0.44
1:A:411:GLU:O	1:A:411:GLU:OE2	2.36	0.43
2:B:223:THR:HG23	2:B:225:GLY:C	2.38	0.43
1:C:395:PHE:C	1:C:395:PHE:HD1	2.21	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:431:GLU:HA	2:D:434:GLN:HE21	1.83	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:A:67:PHE:O	1:A:92:LEU:HA	2.18	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: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:3:GLU:HG2	2:B:58:GLY:O	2.18	0.43
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.53	0.43
1:C:174:ALA:C	1:C:176:GLN:N	2.71	0.43
1:C:256:GLN:O	1:C:257:THR:C	2.57	0.43
1:C:171:ILE:HG21	4:C:502:GTP:HN22	1.82	0.43
1:C:91:GLN:HG2	1:C:92:LEU:CD1	2.47	0.43
2:D:133:GLN:NE2	2:D:252:LEU:CB	2.75	0.43
2:D:305:CYS:O	2:D:383:ALA:HB1	2.18	0.43
2:D:383:ALA:C	2:D:385:GLN:H	2.20	0.43
2:D:427:ASP:C	2:D:429:VAL:N	2.72	0.43
1:C:132:LEU:HB3	1:C:133:GLN:H	1.63	0.43
2:D:88:ARG:HA	2:D:91:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:VAL:N	2:D:245:PRO:CB	2.81	0.43
2:D:308:ARG:NH2	2:D:342:TYR:CB	2.81	0.43
2:B:333:LEU:O	2:B:336:GLN:HB3	2.18	0.43
1:C:3:GLU:HG3	1:C:3:GLU:O	2.18	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:284:ARG:HB2	2:B:290:GLU:OE1	2.17	0.43
2:D:198:THR:C	2:D:200:GLU:H	2.21	0.43
2:D:320:ARG:CG	2:D:320:ARG:NH1	2.80	0.43
1:C:328:VAL:O	1:C:330:ALA:N	2.52	0.43
1:C:33:ASP:O	1:C:34:GLY:C	2.57	0.43
2:B:139:HIS:O	2:B:170:SER:HA	2.17	0.43
1:C:229:ARG:HD2	1:C:366:GLY:HA3	1.99	0.43
1:A:174:ALA:HB1	1:A:176:GLN:HG2	2.01	0.43
1:A:203:MET:HE1	1:A:388:TRP:HD1	1.83	0.43
1:A:209:ILE:N	1:A:209:ILE:CD1	2.81	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:3:GLU:O	2:B:133:GLN:N	2.40	0.43
1:C:143:GLY:O	1:C:144:GLY:C	2.56	0.43
1:C:217:LEU:HD23	1:C:219:ILE:HD11	1.99	0.43
1:C:93:ILE:CD1	1:C:118:VAL:HA	2.48	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
1:A:88:HIS:O	1:A:90:GLU:N	2.51	0.43
1:A:371:VAL:CG1	1:A:372:GLN:H	2.32	0.43
1:C:371:VAL:HG11	1:C:373:ARG:O	2.18	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:205:ASP:OD2	1:A:205:ASP:C	2.56	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
1:C:187:SER:C	1:C:189:LEU:H	2.21	0.43
1:C:276:ILE:HG12	1:C:282:TYR:HD2	1.79	0.43
2:D:158:ARG:C	2:D:160:GLU:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:ASN:ND2	2:D:91:ASN:N	2.50	0.43
1:C:242:LEU:HD11	1:C:318:LEU:HG	2.00	0.43
1:C:27:GLU:CG	1:C:28:HIS:N	2.81	0.43
1:A:15:GLN:O	1:A:16:ILE:O	2.36	0.43
1:A:278:ALA:HA	1:A:282:TYR:OH	2.19	0.43
1:A:368:LEU:O	1:A:369:ALA:HB3	2.19	0.43
2:B:151:THR:HG21	2:B:189:LEU:HD21	1.99	0.43
2:B:18:ALA:O	2:B:21:TRP:N	2.51	0.43
1:C:403:ALA:C	1:C:405:VAL:H	2.22	0.43
2:D:63:PRO:C	2:D:65:ALA:H	2.20	0.43
1:A:36:MET:CE	1:A:37:PRO:HD2	2.48	0.43
2:D:193:GLN:HE21	2:D:193:GLN:HB3	1.66	0.43
1:A:179:THR:HG22	1:A:180:ALA:O	2.18	0.43
1:A:23:LEU:O	1:A:25:CYS:N	2.42	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
2:B:59:ASN:CG	2:B:60:LYS:HD2	2.39	0.43
1:C:179:THR:HB	1:C:182:VAL:HB	2.01	0.43
1:C:71:GLU:CD	4:C:502:GTP:O3G	2.57	0.43
2:D:343:PHE:HB3	2:D:350:ASN:OD1	2.17	0.43
2:D:180:THR:CB	2:D:404:PHE:CE1	2.97	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:353:THR:HG23	2:D:354:ALA:H	1.83	0.43
1:A:197:HIS:CG	1:A:198:SER:N	2.85	0.43
2:B:200:GLU:HG2	2:B:268:PHE:CE2	2.53	0.43
2:B:269:MET:HE2	2:B:269:MET:HB3	1.86	0.43
2:B:272:PHE:HB3	2:B:275:LEU:HD21	2.00	0.43
1:C:122:ILE:HG22	1:C:123:ARG:N	2.34	0.43
1:C:78:VAL:O	1:C:82:THR:CG2	2.63	0.43
2:D:208:ALA:O	2:D:212:ILE:HG13	2.19	0.43
1:A:256:GLN:HB3	1:A:260:VAL:CB	2.46	0.43
1:A:43:GLY:O	1:A:47:ASP:OD2	2.37	0.43
2:B:419:THR:O	2:B:423:SER:N	2.51	0.43
1:A:100:ALA:HA	1:A:105:ARG:CD	2.49	0.43
1:A:171:ILE:HA	1:A:204:VAL:HB	2.01	0.43
1:A:26:LEU:HD23	1:A:361:THR:OG1	2.18	0.43
1:A:395:PHE:C	1:A:397:LEU:H	2.20	0.43
1:A:409:VAL:HA	1:A:414:GLU:CD	2.32	0.43
1:A:428:LEU:C	1:A:430:LYS:H	2.22	0.43
2:B:59:ASN:CA	2:B:64:ARG:HE	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:VAL:C	1:C:411:GLU:N	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
2:D:92:PHE:CZ	2:D:117:SER:O	2.71	0.43
1:A:163:LYS:NZ	1:A:163:LYS:HB2	2.34	0.43
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.00	0.43
1:A:292:THR:O	1:A:292:THR:OG1	2.33	0.43
1:C:346:TRP:CE3	1:C:347:CYS:SG	3.12	0.43
1:A:77:GLU:HB3	1:A:83:TYR:HD2	1.76	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
2:B:276:THR:HG21	2:B:281:GLN:CG	2.49	0.43
1:C:294:ALA:C	1:C:296:PHE:H	2.22	0.43
1:A:229:ARG:NH1	1:A:229:ARG:HG3	2.34	0.43
2:D:10:GLY:HA3	2:D:146:GLY:HA3	1.99	0.43
1:A:100:ALA:HB1	1:A:105:ARG:HD2	2.00	0.43
1:A:185:TYR:O	1:A:186:ASN:C	2.56	0.43
2:B:132:LEU:O	2:B:164:ARG:NE	2.41	0.43
2:B:59:ASN:HA	2:B:60:LYS:NZ	2.33	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:60:LYS:HZ2	2:D:60:LYS:N	2.15	0.43
1:A:242:LEU:CG	1:A:318:LEU:HD11	2.47	0.43
2:B:402:LYS:HE3	1:C:440:VAL:HG12	1.99	0.43
1:A:181:VAL:HG13	1:A:185:TYR:CE2	2.53	0.42
1:A:189:LEU:C	1:A:189:LEU:HD13	2.40	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:273:ALA:HB3	2:B:274:PRO:HD3	2.01	0.42
2:B:286:LEU:CG	2:B:373:MET:HE3	2.44	0.42
2:B:88:ARG:O	2:B:91:ASN:ND2	2.52	0.42
1:C:217:LEU:CD2	1:C:219:ILE:HD11	2.49	0.42
2:D:311:ARG:HD3	2:D:311:ARG:H	1.84	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:312:TYR:CE2	2:D:377:PHE:CZ	3.06	0.42
2:D:211:ASP:O	2:D:215:ARG:HB2	2.19	0.42
2:D:389:LYS:C	2:D:392:SER:HG	2.22	0.42
2:D:86:ILE:H	2:D:88:ARG:NH2	2.17	0.42
1:A:39:ASP:OD2	1:A:40:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:ASP:N	2:B:211:ASP:OD1	2.52	0.42
3:E:14:UNK:C	3:E:16:UNK:N	2.81	0.42
1:A:306:ASP:N	1:A:307:PRO:HD3	2.33	0.42
2:B:283:TYR:CG	2:B:283:TYR:O	2.72	0.42
2:B:287:THR:OG1	2:B:290:GLU:CB	2.67	0.42
2:B:335:VAL:C	2:B:338:LYS:H	2.22	0.42
2:B:344:VAL:O	2:B:346:TRP:CD1	2.72	0.42
1:C:209:ILE:HG12	1:C:231:ILE:HD11	2.00	0.42
1:C:306:ASP:HB3	1:C:386:GLU:OE1	2.18	0.42
1:C:305:CYS:C	1:C:386:GLU:OE1	2.57	0.42
2:D:311:ARG:NH1	2:D:344:VAL:HA	2.35	0.42
2:D:200:GLU:CD	2:D:268:PHE:HE2	2.21	0.42
2:D:226:ASP:O	2:D:228:ASN:N	2.44	0.42
2:D:327:GLU:O	2:D:331:GLN:HB2	2.19	0.42
1:C:312:TYR:N	1:C:312:TYR:CD1	2.87	0.42
1:C:284:GLU:CG	1:C:285:GLN:HE21	2.22	0.42
1:C:273:ALA:HB3	1:C:291:ILE:HG23	2.01	0.42
3:E:75:UNK:C	3:E:77:UNK:N	2.78	0.42
1:A:46:ASP:O	1:A:47:ASP:O	2.37	0.42
2:D:52:TYR:CG	2:D:52:TYR:O	2.72	0.42
1:A:154:MET:C	1:A:156:ARG:N	2.70	0.42
2:B:2:ARG:HH21	2:B:243:ARG:HB3	1.84	0.42
1:C:119:LEU:HD22	1:C:156:ARG:CZ	2.49	0.42
1:C:264:ARG:HA	1:C:264:ARG:HD3	1.97	0.42
2:D:181:VAL:C	2:D:184:PRO:HD2	2.40	0.42
2:D:176:LYS:NZ	2:D:210:TYR:CG	2.84	0.42
2:D:312:TYR:HE2	2:D:377:PHE:CZ	2.37	0.42
2:B:212:ILE:O	2:B:217:LEU:HB3	2.19	0.42
1:A:242:LEU:CD2	1:A:318:LEU:HD21	2.33	0.42
2:B:322:ARG:CG	2:B:357:ASP:HA	2.33	0.42
2:D:395:PHE:CD2	2:D:422:GLU:OE1	2.71	0.42
1:C:31:GLN:OE1	1:C:32:PRO:HD3	2.19	0.42
1:A:284:GLU:CG	1:A:285:GLN:HE21	2.24	0.42
2:B:10:GLY:HA3	2:B:146:GLY:HA3	2.01	0.42
1:A:411:GLU:CA	1:A:411:GLU:OE2	2.68	0.42
2:B:97:SER:HG	2:B:110:GLU:CG	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:GLY:O	2:B:96:GLN:O	2.37	0.42
1:C:158:SER:HB3	1:C:166:LYS:HZ1	1.83	0.42
1:C:20:CYS:SG	1:C:232:GLY:HA2	2.59	0.42
2:D:4:ILE:HD11	2:D:252:LEU:HD13	2.00	0.42
2:D:84:GLY:C	2:D:85:GLN:HG2	2.39	0.42
2:D:322:ARG:CG	2:D:357:ASP:HA	2.34	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
1:A:311:LYS:CE	1:A:344:VAL:HA	2.50	0.42
1:A:412:GLY:HA2	1:A:413:MET:HE1	2.02	0.42
2:B:3:GLU:HB3	2:B:132:LEU:HA	2.01	0.42
2:B:174:SER:HB2	2:B:206:ASN:C	2.39	0.42
2:B:383:ALA:C	2:B:385:GLN:H	2.23	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:5:ILE:HG22	1:C:6:SER:N	2.34	0.42
1:C:83:TYR:O	1:C:84:ARG:HB2	2.20	0.42
3:E:30:UNK:O	3:E:31:UNK:C	2.67	0.42
2:D:165:ILE:HD13	2:D:199:ASP:OD1	2.18	0.42
1:C:332:ILE:HG23	1:C:351:PHE:CZ	2.55	0.42
1:A:291:ILE:CG2	1:A:375:VAL:HG21	2.44	0.42
1:C:286:LEU:HD12	1:C:291:ILE:CG1	2.48	0.42
1:A:339:ARG:CD	1:A:339:ARG:C	2.75	0.42
1:A:340:THR:C	1:A:341:ILE:HD12	2.40	0.42
1:C:44:GLY:O	1:C:46:ASP:N	2.52	0.42
1:A:349:THR:OG1	1:A:349:THR:O	2.31	0.42
1:A:305:CYS:O	1:A:306:ASP:HB2	2.19	0.42
1:A:73:THR:O	1:A:76:ASP:N	2.48	0.42
2:B:88:ARG:HA	2:B:91:ASN:ND2	2.35	0.42
1:C:111:GLY:C	1:C:113:GLU:N	2.73	0.42
1:C:190:THR:HA	1:C:193:THR:CG2	2.39	0.42
1:C:21:TRP:CD1	1:C:21:TRP:N	2.87	0.42
1:C:398:MET:CG	1:C:399:TYR:H	2.33	0.42
1:C:88:HIS:O	1:C:90:GLU:N	2.52	0.42
2:D:346:TRP:HZ2	2:D:435:TYR:HB3	1.85	0.42
2:D:126:SER:O	2:D:127:GLU:C	2.57	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:B:230:LEU:H	2:B:230:LEU:CD1	2.25	0.42
1:A:126:ALA:O	1:A:132:LEU:CD1	2.67	0.42
2:D:415:GLU:HG2	2:D:416:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:O	1:C:338:LYS:HG2	2.19	0.42
1:A:216:ASN:HB3	1:A:275:VAL:HG11	2.01	0.42
1:A:97:GLU:CD	1:A:97:GLU:H	2.23	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
2:B:350:ASN:HD22	2:B:350:ASN:C	2.21	0.42
2:B:415:GLU:HG2	2:B:416:MET:H	1.85	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:91:GLN:HE21	1:C:91:GLN:HB3	1.58	0.42
2:D:311:ARG:HB3	2:D:343:PHE:N	2.35	0.42
1:C:239:THR:O	1:C:243:ARG:HB2	2.19	0.42
1:A:286:LEU:HD12	1:A:291:ILE:CG1	2.49	0.42
1:A:209:ILE:CG2	1:A:213:CYS:HB2	2.47	0.42
2:B:123:ARG:C	2:B:125:GLU:N	2.72	0.42
2:B:178:SER:C	2:B:182:VAL:HB	2.35	0.42
2:B:350:ASN:N	2:B:350:ASN:ND2	2.67	0.42
1:C:405:VAL:CG2	1:C:405:VAL:O	2.68	0.42
1:C:413:MET:O	1:C:414:GLU:CB	2.66	0.42
2:D:224:TYR:O	2:D:228:ASN:HB2	2.20	0.42
2:D:320:ARG:HG2	2:D:320:ARG:NH1	2.32	0.42
2:D:88:ARG:HA	2:D:91:ASN:HD21	1.85	0.42
1:C:320:ARG:HH21	1:C:356:ASN:ND2	2.18	0.42
1:C:431:ASP:C	1:C:433:GLU:H	2.23	0.42
2:D:269:MET:HG2	2:D:384:ILE:HB	2.01	0.42
1:A:294:ALA:C	1:A:296:PHE:H	2.23	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:6:HIS:HD2	2:B:136:GLN:OE1	2.03	0.42
1:C:192:HIS:C	1:C:194:THR:H	2.23	0.42
1:C:88:HIS:HA	1:C:89:PRO:HD2	1.84	0.42
2:D:102:ASN:HD22	2:D:105:LYS:H	1.62	0.42
2:B:333:LEU:HG	2:B:337:ASN:HD21	1.82	0.42
1:C:229:ARG:HG3	1:C:229:ARG:NH1	2.33	0.42
1:A:312:TYR:HD1	1:A:312:TYR:H	1.67	0.42
1:A:208:ALA:HB2	1:A:302:MET:O	2.20	0.42
2:B:1:MET:C	2:B:3:GLU:N	2.73	0.42
2:B:224:TYR:C	2:B:226:ASP:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:HIS:HE2	1:C:21:TRP:HE1	1.66	0.42
1:C:269:LEU:C	1:C:269:LEU:CD1	2.84	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
2:D:104:ALA:HB1	2:D:411:GLU:HB2	2.02	0.42
1:C:321:GLY:CA	1:C:358:GLU:O	2.68	0.42
2:D:69:ASP:HB3	2:D:74:THR:HG23	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
2:B:122:VAL:CG1	2:B:123:ARG:N	2.82	0.41
2:B:1:MET:C	2:B:3:GLU:H	2.20	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
2:D:60:LYS:HZ3	2:D:60:LYS:H	1.68	0.41
1:A:182:VAL:HA	1:A:185:TYR:HD2	1.86	0.41
1:A:181:VAL:O	1:A:184:PRO:HG2	2.20	0.41
1:A:403:ALA:C	1:A:405:VAL:H	2.23	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:161:TYR:O	1:C:162:GLY:C	2.59	0.41
1:C:168:GLU:O	1:C:168:GLU:HG3	2.20	0.41
1:C:215:ARG:HG2	1:C:216:ASN:N	2.36	0.41
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.49	0.41
1:A:245:ASP:O	1:A:249:ASN:OD1	2.37	0.41
1:C:242:LEU:CG	1:C:318:LEU:HD11	2.50	0.41
1:A:33:ASP:O	1:A:34:GLY:C	2.59	0.41
3:E:16:UNK:O	3:E:20:UNK:N	2.53	0.41
1:A:214:ARG:HG3	1:A:214:ARG:O	2.20	0.41
2:B:165:ILE:HG13	2:B:253:ARG:HG2	2.02	0.41
2:B:291:LEU:H	2:B:291:LEU:CD2	2.32	0.41
2:D:121:VAL:O	2:D:121:VAL:HG12	2.20	0.41
2:D:286:LEU:HA	2:D:290:GLU:CD	2.40	0.41
2:D:214:PHE:CE2	2:D:215:ARG:NE	2.88	0.41
1:C:163:LYS:NZ	1:C:163:LYS:HB2	2.34	0.41
1:A:237:SER:C	1:A:241:SER:CB	2.88	0.41
2:D:73:GLY:O	2:D:78:VAL:HG21	2.20	0.41
1:C:312:TYR:N	1:C:312:TYR:HD1	2.17	0.41
1:C:38:SER:O	1:C:39:ASP:CB	2.68	0.41
1:C:42:ILE:HA	1:C:42:ILE:HD12	1.87	0.41
1:A:5:ILE:O	1:A:136:SER:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:HD2	1:A:315:CYS:HB2	1.84	0.41
1:A:117:LEU:O	1:A:121:ARG:HB2	2.21	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:395:PHE:CE1	2:B:399:PHE:CD1	3.08	0.41
2:B:404:PHE:CD2	2:B:404:PHE:O	2.69	0.41
1:C:10:GLY:O	1:C:12:ALA:N	2.54	0.41
1:C:363:VAL:HG22	1:C:367:ASP:CG	2.41	0.41
1:C:69:ASP:CG	1:C:71:GLU:H	2.23	0.41
2:D:132:LEU:HD22	2:D:164:ARG:CG	2.48	0.41
2:D:283:TYR:O	2:D:284:ARG:HB2	2.20	0.41
2:D:3:GLU:OE2	2:D:130:ASP:CB	2.60	0.41
2:D:218:LYS:NZ	2:D:278:ARG:CB	2.80	0.41
2:D:208:ALA:HB2	2:D:304:ALA:CB	2.51	0.41
1:A:35:GLN:HE22	1:A:88:HIS:CD2	2.38	0.41
1:A:30:ILE:HG13	1:A:31:GLN:H	1.81	0.41
1:C:253:THR:OG1	1:C:254:GLU:N	2.53	0.41
2:B:215:ARG:NE	2:B:215:ARG:CA	2.80	0.41
1:C:317:LEU:HD23	1:C:377:MET:HB2	2.00	0.41
1:A:229:ARG:HB3	1:A:366:GLY:O	2.20	0.41
1:A:3:GLU:O	1:A:3:GLU:HG3	2.19	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:191:VAL:HG21	2:B:421:ALA:CB	2.28	0.41
2:B:313:LEU:C	2:B:314:THR:HG23	2.41	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:121:ARG:O	1:C:122:ILE:C	2.57	0.41
1:C:139:HIS:HB3	1:C:170:SER:CA	2.44	0.41
2:B:407:TRP:NE1	1:C:257:THR:HA	2.34	0.41
2:D:176:LYS:HD2	2:D:210:TYR:CE1	2.55	0.41
2:D:223:THR:HG23	2:D:225:GLY:C	2.41	0.41
2:D:265:LEU:HB2	2:D:266:HIS:H	1.58	0.41
2:D:335:VAL:C	2:D:338:LYS:H	2.23	0.41
2:B:190:SER:O	2:B:425:MET:HB2	2.21	0.41
1:A:27:GLU:OE1	1:A:28:HIS:CE1	2.73	0.41
1:A:105:ARG:HG3	1:A:411:GLU:HG3	2.03	0.41
1:A:180:ALA:HB3	2:B:258:ASN:ND2	2.36	0.41
1:A:409:VAL:C	1:A:411:GLU:N	2.73	0.41
1:A:419:SER:O	1:A:420:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:HD3	2:B:197:ASN:HD22	1.73	0.41
2:B:351:VAL:O	2:B:352:LYS:HG3	2.21	0.41
2:B:427:ASP:C	2:B:429:VAL:N	2.73	0.41
1:C:144:GLY:O	1:C:145:THR:C	2.59	0.41
1:C:174:ALA:HB2	1:C:206:ASN:CB	2.50	0.41
1:C:395:PHE:C	1:C:397:LEU:H	2.23	0.41
1:C:416:GLY:C	1:C:418:PHE:H	2.19	0.41
1:C:228:ASN:ND2	4:C:502:GTP:O6	2.53	0.41
1:C:84:ARG:C	1:C:85:GLN:HG2	2.41	0.41
2:D:115:VAL:HG11	2:D:156:LYS:HZ3	1.80	0.41
2:D:115:VAL:HG23	2:D:149:MET:HE1	2.02	0.41
2:D:154:ILE:HG23	2:D:166:MET:HE3	2.03	0.41
2:D:320:ARG:HE	2:D:360:PRO:HG3	1.85	0.41
2:D:372:LYS:HA	2:D:372:LYS:HE2	2.02	0.41
2:D:97:SER:HG	2:D:110:GLU:CD	2.23	0.41
1:A:238:ILE:N	1:A:241:SER:CB	2.84	0.41
1:A:167:LEU:HD13	1:A:252:LEU:HD11	2.03	0.41
2:D:333:LEU:O	2:D:336:GLN:HB3	2.20	0.41
1:A:139:HIS:O	1:A:140:SER:CB	2.68	0.41
1:A:24:TYR:HA	1:A:26:LEU:CD1	2.50	0.41
1:A:409:VAL:HG22	1:A:414:GLU:CD	2.40	0.41
2:B:103:TRP:HB2	2:B:185:TYR:CE2	2.56	0.41
2:B:103:TRP:H	2:B:408:TYR:HE1	1.69	0.41
2:B:236:SER:C	2:B:238:VAL:H	2.24	0.41
2:B:4:ILE:HD13	2:B:252:LEU:HD13	2.03	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:313:LEU:HD21	2:B:435:TYR:CD2	2.54	0.41
2:D:103:TRP:HE1	2:D:151:THR:HG21	1.85	0.41
2:D:102:ASN:N	2:D:185:TYR:OH	2.53	0.41
2:D:289:PRO:HA	2:D:292:THR:OG1	2.21	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
2:D:73:GLY:C	2:D:75:MET:H	2.24	0.41
1:A:317:LEU:HA	1:A:377:MET:HB2	2.02	0.41
1:A:251:ASP:OD2	1:A:252:LEU:N	2.54	0.41
2:B:310:GLY:HA3	2:B:436:GLN:HG2	2.03	0.41
1:A:197:HIS:O	1:A:198:SER:OG	2.35	0.41
1:A:344:VAL:HG12	1:A:345:ASP:H	1.83	0.41
2:B:102:ASN:HD22	2:B:105:LYS:H	1.58	0.41
2:B:271:GLY:C	2:B:272:PHE:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:GLY:O	2:B:96:GLN:HB3	2.21	0.41
1:C:142:GLY:HA2	1:C:185:TYR:HB2	2.03	0.41
1:C:255:PHE:O	1:C:259:LEU:HB2	2.21	0.41
2:D:176:LYS:O	2:D:177:VAL:HB	2.21	0.41
2:D:59:ASN:CG	2:D:60:LYS:HD2	2.41	0.41
1:A:335:ILE:O	1:A:336:LYS:C	2.59	0.41
1:A:335:ILE:CG1	1:A:336:LYS:N	2.77	0.41
1:A:30:ILE:HD12	1:A:30:ILE:C	2.40	0.41
2:D:267:PHE:N	2:D:267:PHE:CD2	2.89	0.41
1:A:343:PHE:CD1	1:A:349:THR:HA	2.55	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:388:TRP:HZ3	1:A:428:LEU:HD22	1.82	0.41
2:B:232:SER:C	2:B:234:THR:H	2.22	0.41
2:B:76:ASP:HB2	2:B:77:SER:H	1.46	0.41
1:C:306:ASP:N	1:C:307:PRO:HD3	2.35	0.41
1:C:9:VAL:HG21	1:C:150:THR:CB	2.51	0.41
1:A:184:PRO:CB	1:A:399:TYR:CE2	3.04	0.41
1:A:311:LYS:HD3	1:A:344:VAL:CB	2.51	0.41
1:A:365:GLY:O	1:A:368:LEU:HD12	2.20	0.41
1:A:398:MET:CG	1:A:399:TYR:H	2.34	0.41
1:A:413:MET:C	1:A:414:GLU:CD	2.80	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:384:ILE:O	2:B:384:ILE:HG12	2.20	0.41
2:B:63:PRO:C	2:B:65:ALA:N	2.74	0.41
2:B:404:PHE:HZ	1:C:257:THR:O	2.04	0.41
2:D:158:ARG:NH1	2:D:197:ASN:OD1	2.54	0.41
2:D:226:ASP:C	2:D:228:ASN:N	2.74	0.41
2:D:16:ILE:CD1	2:D:231:VAL:CG1	2.99	0.41
2:D:103:TRP:H	2:D:408:TYR:HE1	1.68	0.41
2:D:8:GLN:O	2:D:68:VAL:N	2.54	0.41
2:D:88:ARG:O	2:D:91:ASN:ND2	2.54	0.41
2:D:51:VAL:HG22	2:D:245:PRO:CB	2.51	0.41
1:A:273:ALA:HB2	1:A:295:CYS:CB	2.51	0.41
1:C:311:LYS:HB2	1:C:344:VAL:CG2	2.50	0.41
2:B:51:VAL:HG22	2:B:245:PRO:CB	2.51	0.41
1:C:371:VAL:CG1	1:C:372:GLN:N	2.82	0.41
1:A:339:ARG:O	1:A:339:ARG:HD2	2.21	0.41
2:B:247:GLN:HG2	2:B:355:VAL:HB	2.03	0.41
2:B:52:TYR:CG	2:B:52:TYR:O	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:398:MET:HE2	1:A:399:TYR:CE1	2.56	0.41
2:B:103:TRP:C	2:B:105:LYS:N	2.74	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:19:LYS:HA	2:B:22:GLU:CG	2.51	0.41
2:B:407:TRP:CZ2	1:C:256:GLN:CB	2.91	0.41
1:C:108:TYR:HB3	1:C:413:MET:HE3	2.03	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: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
2:B:325:MET:CG	2:B:355:VAL:HG11	2.51	0.41
2:B:25:SER:HB3	2:B:369:ARG:NH2	2.34	0.41
1:A:128:GLN:OE1	1:A:128:GLN:HA	2.21	0.41
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.40
1:A:431:ASP:C	1:A:433:GLU:H	2.22	0.40
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
2:D:350:ASN:C	2:D:351:VAL:CG2	2.89	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:253:ARG:C	2:D:255:LEU:H	2.22	0.40
1:C:164:LYS:NZ	1:C:164:LYS:N	2.69	0.40
1:A:244:PHE:CE1	1:A:358:GLU:OE2	2.74	0.40
1:C:320:ARG:N	1:C:374:ALA:O	2.49	0.40
1:A:295:CYS:SG	1:A:295:CYS:O	2.78	0.40
1:A:269:LEU:HD11	1:A:301:GLN:HB3	2.03	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
1:A:72:PRO:HB3	1:A:94:THR:HG1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:NH1	1:C:214:ARG:HG3	2.35	0.40
1:C:362:VAL:HG12	1:C:363:VAL:N	2.36	0.40
1:C:405:VAL:HG22	1:C:405:VAL:O	2.20	0.40
2:D:346:TRP:CZ2	2:D:435:TYR:HB3	2.57	0.40
2:D:123:ARG:C	2:D:125:GLU:N	2.74	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
1:A:175:PRO:HB2	1:A:207:GLU:OE2	2.22	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
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:179:ASP:CB	2:D:181:VAL:HG12	2.42	0.40
2:D:144:GLY:N	2:D:185:TYR:CZ	2.89	0.40
2:D:427:ASP:O	2:D:428:LEU:C	2.59	0.40
2:D:429:VAL:O	2:D:433:GLN:HG2	2.22	0.40
1:A:132:LEU:HB3	1:A:133:GLN:H	1.66	0.40
1:A:322:ASP:OD1	1:A:357:TYR:O	2.39	0.40
1:A:380:ASN:CG	1:A:380:ASN:O	2.60	0.40
2:B:172:VAL:CG1	2:B:173:PRO:HD2	2.42	0.40
1:A:142:GLY:O	1:A:182:VAL:HG22	2.20	0.40
1:A:181:VAL:HG13	1:A:408:TYR:HH	1.86	0.40
1:A:187:SER:C	1:A:189:LEU:N	2.74	0.40
1:A:145:THR:CB	4:A:500:GTP:PG	3.10	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: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:174:ALA:C	1:C:176:GLN:H	2.25	0.40
1:C:184:PRO:HB2	1:C:399:TYR:CE2	2.56	0.40
2:D:350:ASN:O	2:D:351:VAL:HG22	2.21	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:62:VAL:O	2:D:63:PRO:C	2.59	0.40
1:A:79:ARG:HD3	1:A:86:LEU:HD11	2.04	0.40
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.04	0.40
2:D:308:ARG:NH2	2:D:339:ASN:CB	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:21:UNK:O	3:E:24:UNK:CA	2.69	0.40
2:B:436:GLN:C	2:B:436:GLN:HE21	2.23	0.40
1:A:221:ARG:H	1:A:221:ARG:NE	2.20	0.40
1:A:313:MET:HE2	1:A:346:TRP:HH2	1.87	0.40
1:A:402:ARG:O	1:A:405:VAL:HG12	2.21	0.40
2:B:117:SER:O	2:B:120:ASP:HB2	2.21	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:144:GLY:N	2:B:185:TYR:CZ	2.90	0.40
2:B:258:ASN:OD1	2:B:352:LYS:HD2	2.21	0.40
2:B:88:ARG:HA	2:B:91:ASN:HD21	1.87	0.40
1:C:115:ILE:CD1	1:C:156:ARG:HG3	2.34	0.40
2:D:290:GLU:O	2:D:291:LEU:C	2.59	0.40
1:A:317:LEU:CD2	1:A:377:MET:HB3	2.50	0.40
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.39	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	2
1	C	419/451 (93%)	219 (52%)	114 (27%)	86 (20%)	0	2
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	2

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	278 (78%)	76 (22%)	1	10
1	C	354/377 (94%)	279 (79%)	75 (21%)	1	11
2	B	347/381 (91%)	274 (79%)	73 (21%)	1	11
2	D	347/381 (91%)	270 (78%)	77 (22%)	1	10
All	All	1402/1516 (92%)	1101 (78%)	301 (22%)	1	10

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	16	ILE
1	A	23	LEU
1	A	25	CYS
1	A	30	ILE
1	A	32	PRO

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Mol	Chain	Res	Type
1	A	40	LYS
1	A	46	ASP
1	A	47	ASP
1	A	71	GLU
1	A	73	THR
1	A	77	GLU
1	A	83	TYR
1	A	86	LEU
1	A	87	PHE
1	A	91	GLN
1	A	92	LEU
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	164	LYS
1	A	179	THR
1	A	181	VAL
1	A	182	VAL
1	A	196	GLU
1	A	197	HIS
1	A	199	ASP
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	250	VAL
1	A	252	LEU
1	A	255	PHE
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

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Mol	Chain	Res	Type
1	A	285	GLN
1	A	292	THR
1	A	295	CYS
1	A	297	GLU
1	A	302	MET
1	A	309	HIS
1	A	316	CYS
1	A	318	LEU
1	A	322	ASP
1	A	335	ILE
1	A	336	LYS
1	A	345	ASP
1	A	346	TRP
1	A	349	THR
1	A	356	ASN
1	A	373	ARG
1	A	376	CYS
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	425	MET
1	A	428	LEU
1	A	431	ASP
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	88	ARG
2	B	91	ASN
2	B	113	GLU
2	B	119	LEU
2	B	128	SER
2	B	136	GLN
2	B	139	HIS

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Mol	Chain	Res	Type
2	B	149	MET
2	B	157	ILE
2	B	158	ARG
2	B	160	GLU
2	B	163	ASP
2	B	167	ASN
2	B	168	THR
2	B	180	THR
2	B	185	TYR
2	B	186	ASN
2	B	192	HIS
2	B	193	GLN
2	B	194	LEU
2	B	201	THR
2	B	203	CYS
2	B	211	ASP
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	252	LEU
2	B	253	ARG
2	B	254	LYS
2	B	255	LEU
2	B	265	LEU
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	350	ASN

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Mol	Chain	Res	Type
2	B	352	LYS
2	B	377	PHE
2	B	380	ASN
2	B	388	PHE
2	B	395	PHE
2	B	401	ARG
2	B	404	PHE
2	B	405	LEU
2	B	407	TRP
2	B	409	THR
2	B	414	ASP
2	B	416	MET
2	B	419	THR
2	B	424	ASN
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	83	TYR
1	C	86	LEU
1	C	87	PHE
1	C	91	GLN
1	C	101	ASN
1	C	105	ARG
1	C	115	ILE
1	C	125	LEU
1	C	130	THR
1	C	141	PHE
1	C	150	THR
1	C	164	LYS

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Mol	Chain	Res	Type
1	C	175	PRO
1	C	179	THR
1	C	181	VAL
1	C	182	VAL
1	C	196	GLU
1	C	197	HIS
1	C	199	ASP
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	255	PHE
1	C	258	ASN
1	C	267	PHE
1	C	269	LEU
1	C	275	VAL
1	C	279	GLU
1	C	282	TYR
1	C	285	GLN
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	336	LYS
1	C	345	ASP
1	C	346	TRP
1	C	349	THR
1	C	356	ASN
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

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Mol	Chain	Res	Type
1	C	414	GLU
1	C	418	PHE
1	C	420	GLU
1	C	425	MET
1	C	428	LEU
1	C	431	ASP
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	88	ARG
2	D	91	ASN
2	D	94	PHE
2	D	113	GLU
2	D	119	LEU
2	D	128	SER
2	D	136	GLN
2	D	139	HIS
2	D	149	MET
2	D	157	ILE
2	D	158	ARG
2	D	160	GLU
2	D	163	ASP
2	D	167	ASN
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	203	CYS
2	D	218	LYS
2	D	228	ASN
2	D	239	THR
2	D	244	PHE
2	D	245	PRO

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Mol	Chain	Res	Type
2	D	249	ASN
2	D	251	ASP
2	D	252	LEU
2	D	253	ARG
2	D	254	LYS
2	D	255	LEU
2	D	265	LEU
2	D	278	ARG
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	377	PHE
2	D	380	ASN
2	D	381	SER
2	D	382	THR
2	D	388	PHE
2	D	395	PHE
2	D	398	MET
2	D	401	ARG
2	D	404	PHE
2	D	405	LEU
2	D	407	TRP
2	D	409	THR
2	D	414	ASP
2	D	416	MET
2	D	419	THR
2	D	424	ASN
2	D	425	MET
2	D	426	ASN
2	D	436	GLN

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Mol	Chain	Res	Type
2	D	437	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	102	ASN
1	A	133	GLN
1	A	176	GLN
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	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	85	GLN
2	B	91	ASN
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	426	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

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Mol	Chain	Res	Type
1	C	176	GLN
1	C	186	ASN
1	C	256	GLN
1	C	258	ASN
1	C	285	GLN
1	C	300	ASN
1	C	301	GLN
1	C	356	ASN
2	D	6	HIS
2	D	8	GLN
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	133	GLN
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	349	ASN
2	D	350	ASN
2	D	380	ASN
2	D	426	ASN
2	D	433	GLN
2	D	434	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	500	-	25,34,34	1.48	4 (16%)	34,54,54	2.14	5 (14%)
5	GDP	B	501	-	23,30,30	1.72	4 (17%)	30,47,47	2.45	6 (20%)
4	GTP	C	502	-	25,34,34	1.55	3 (12%)	34,54,54	2.22	6 (17%)
5	GDP	D	503	-	23,30,30	1.56	3 (13%)	30,47,47	2.18	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	500	-	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3
4	GTP	C	502	-	-	0/18/38/38	0/3/3/3
5	GDP	D	503	-	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	O4'-C1'	-3.12	1.37	1.41
5	D	503	GDP	PA-O2A	-2.23	1.45	1.54
4	A	500	GTP	PA-O2A	-2.20	1.45	1.54
5	B	501	GDP	PA-O2A	-2.15	1.45	1.54
4	A	500	GTP	O5'-C5'	-2.11	1.36	1.44
4	C	502	GTP	O4'-C1'	2.06	1.43	1.41
5	D	503	GDP	C2-N1	2.16	1.39	1.35
4	A	500	GTP	C2-N1	2.49	1.39	1.35
5	B	501	GDP	C2-N1	3.08	1.40	1.35
4	C	502	GTP	C2-N1	3.21	1.41	1.35
4	A	500	GTP	C6-N1	4.53	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	GTP	C6-N1	4.97	1.42	1.33
5	D	503	GDP	C6-N1	5.33	1.43	1.33
5	B	501	GDP	C6-N1	5.60	1.43	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C5-C6-N1	-8.42	112.08	123.59
5	D	503	GDP	C5-C6-N1	-7.99	112.67	123.59
4	C	502	GTP	C5-C6-N1	-7.92	112.76	123.59
4	A	500	GTP	C5-C6-N1	-7.76	112.99	123.59
5	B	501	GDP	C4'-O4'-C1'	-4.77	104.48	109.72
4	A	500	GTP	O3A-PA-O5'	-3.28	94.25	102.94
4	A	500	GTP	N3-C2-N1	-3.25	122.50	127.44
5	B	501	GDP	N3-C2-N1	-3.13	122.68	127.44
4	C	502	GTP	N3-C2-N1	-3.13	122.68	127.44
4	C	502	GTP	O3A-PA-O5'	-3.07	94.79	102.94
5	D	503	GDP	N3-C2-N1	-2.69	123.35	127.44
5	B	501	GDP	C6-C5-C4	-2.68	117.69	120.90
4	A	500	GTP	C6-C5-C4	-2.67	117.71	120.90
5	D	503	GDP	C6-C5-C4	-2.59	117.80	120.90
4	C	502	GTP	C6-C5-C4	-2.57	117.83	120.90
5	B	501	GDP	O3A-PA-O5'	-2.34	96.72	102.94
4	C	502	GTP	PA-O3A-PB	3.39	142.26	132.73
5	D	503	GDP	C6-N1-C2	6.46	124.91	115.94
4	A	500	GTP	C6-N1-C2	6.50	124.97	115.94
4	C	502	GTP	C6-N1-C2	6.52	124.98	115.94
5	B	501	GDP	C6-N1-C2	6.86	125.46	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

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



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.