Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:09 am BST

PDB ID	:	3U9S
Title	:	Crystal structure of P. aeruginosa 3-methylcrotonyl-CoA carboxylase (MCC) 750 kD holoenzyme, CoA complex
Authors	:	Huang, C.S.; Tong, L.
Deposited on	:	2011-10-19
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

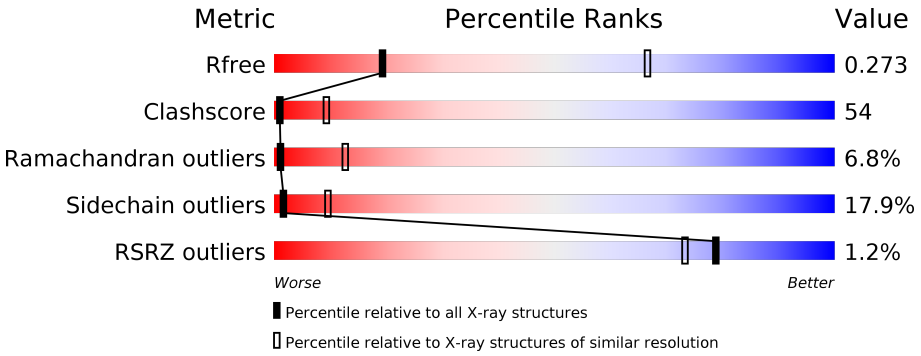
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	655	5% 27% 48% 17% • 5%
1	C	655	% 24% 44% 14% • 16%
1	E	655	25% 42% 16% • 16%
1	G	655	% 25% 42% 15% • 16%
1	I	655	% 23% 40% 12% • 24%
1	K	655	% 23% 38% 13% • 24%

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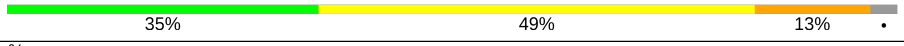
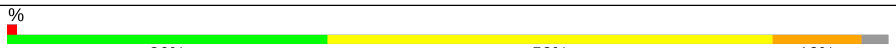
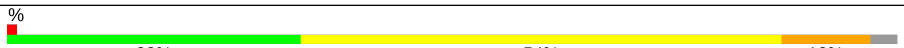
Mol	Chain	Length	Quality of chain
2	B	555	
2	D	555	
2	F	555	
2	H	555	
2	J	555	
2	L	555	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 49939 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 Methylcrotonyl-CoA carboxylase, alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	0	0
			4778	2978	892	886	22			
1	C	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	E	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	G	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	I	498	Total	C	N	O	S	0	0	0
			3853	2399	731	707	16			
1	K	497	Total	C	N	O	S	0	0	0
			3844	2393	729	706	16			

- Molecule 2 is a protein called Methylcrotonyl-CoA carboxylase, beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	D	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	F	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	H	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	J	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	L	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	EXPRESSION TAG	UNP Q9I1Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLY	-	EXPRESSION TAG	UNP Q9I297
B	10	SER	-	EXPRESSION TAG	UNP Q9I297
B	11	SER	-	EXPRESSION TAG	UNP Q9I297
B	12	HIS	-	EXPRESSION TAG	UNP Q9I297
B	13	HIS	-	EXPRESSION TAG	UNP Q9I297
B	14	HIS	-	EXPRESSION TAG	UNP Q9I297
B	15	HIS	-	EXPRESSION TAG	UNP Q9I297
B	16	HIS	-	EXPRESSION TAG	UNP Q9I297
B	17	HIS	-	EXPRESSION TAG	UNP Q9I297
B	18	SER	-	EXPRESSION TAG	UNP Q9I297
B	19	SER	-	EXPRESSION TAG	UNP Q9I297
B	20	GLY	-	EXPRESSION TAG	UNP Q9I297
B	21	LEU	-	EXPRESSION TAG	UNP Q9I297
B	22	VAL	-	EXPRESSION TAG	UNP Q9I297
B	23	PRO	-	EXPRESSION TAG	UNP Q9I297
B	24	ARG	-	EXPRESSION TAG	UNP Q9I297
B	25	GLY	-	EXPRESSION TAG	UNP Q9I297
B	26	SER	-	EXPRESSION TAG	UNP Q9I297
B	27	HIS	-	EXPRESSION TAG	UNP Q9I297
D	8	MET	-	EXPRESSION TAG	UNP Q9I297
D	9	GLY	-	EXPRESSION TAG	UNP Q9I297
D	10	SER	-	EXPRESSION TAG	UNP Q9I297
D	11	SER	-	EXPRESSION TAG	UNP Q9I297
D	12	HIS	-	EXPRESSION TAG	UNP Q9I297
D	13	HIS	-	EXPRESSION TAG	UNP Q9I297
D	14	HIS	-	EXPRESSION TAG	UNP Q9I297
D	15	HIS	-	EXPRESSION TAG	UNP Q9I297
D	16	HIS	-	EXPRESSION TAG	UNP Q9I297
D	17	HIS	-	EXPRESSION TAG	UNP Q9I297
D	18	SER	-	EXPRESSION TAG	UNP Q9I297
D	19	SER	-	EXPRESSION TAG	UNP Q9I297
D	20	GLY	-	EXPRESSION TAG	UNP Q9I297
D	21	LEU	-	EXPRESSION TAG	UNP Q9I297
D	22	VAL	-	EXPRESSION TAG	UNP Q9I297
D	23	PRO	-	EXPRESSION TAG	UNP Q9I297
D	24	ARG	-	EXPRESSION TAG	UNP Q9I297
D	25	GLY	-	EXPRESSION TAG	UNP Q9I297
D	26	SER	-	EXPRESSION TAG	UNP Q9I297
D	27	HIS	-	EXPRESSION TAG	UNP Q9I297
F	8	MET	-	EXPRESSION TAG	UNP Q9I297
F	9	GLY	-	EXPRESSION TAG	UNP Q9I297
F	10	SER	-	EXPRESSION TAG	UNP Q9I297

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Chain	Residue	Modelled	Actual	Comment	Reference
F	11	SER	-	EXPRESSION TAG	UNP Q9I297
F	12	HIS	-	EXPRESSION TAG	UNP Q9I297
F	13	HIS	-	EXPRESSION TAG	UNP Q9I297
F	14	HIS	-	EXPRESSION TAG	UNP Q9I297
F	15	HIS	-	EXPRESSION TAG	UNP Q9I297
F	16	HIS	-	EXPRESSION TAG	UNP Q9I297
F	17	HIS	-	EXPRESSION TAG	UNP Q9I297
F	18	SER	-	EXPRESSION TAG	UNP Q9I297
F	19	SER	-	EXPRESSION TAG	UNP Q9I297
F	20	GLY	-	EXPRESSION TAG	UNP Q9I297
F	21	LEU	-	EXPRESSION TAG	UNP Q9I297
F	22	VAL	-	EXPRESSION TAG	UNP Q9I297
F	23	PRO	-	EXPRESSION TAG	UNP Q9I297
F	24	ARG	-	EXPRESSION TAG	UNP Q9I297
F	25	GLY	-	EXPRESSION TAG	UNP Q9I297
F	26	SER	-	EXPRESSION TAG	UNP Q9I297
F	27	HIS	-	EXPRESSION TAG	UNP Q9I297
H	8	MET	-	EXPRESSION TAG	UNP Q9I297
H	9	GLY	-	EXPRESSION TAG	UNP Q9I297
H	10	SER	-	EXPRESSION TAG	UNP Q9I297
H	11	SER	-	EXPRESSION TAG	UNP Q9I297
H	12	HIS	-	EXPRESSION TAG	UNP Q9I297
H	13	HIS	-	EXPRESSION TAG	UNP Q9I297
H	14	HIS	-	EXPRESSION TAG	UNP Q9I297
H	15	HIS	-	EXPRESSION TAG	UNP Q9I297
H	16	HIS	-	EXPRESSION TAG	UNP Q9I297
H	17	HIS	-	EXPRESSION TAG	UNP Q9I297
H	18	SER	-	EXPRESSION TAG	UNP Q9I297
H	19	SER	-	EXPRESSION TAG	UNP Q9I297
H	20	GLY	-	EXPRESSION TAG	UNP Q9I297
H	21	LEU	-	EXPRESSION TAG	UNP Q9I297
H	22	VAL	-	EXPRESSION TAG	UNP Q9I297
H	23	PRO	-	EXPRESSION TAG	UNP Q9I297
H	24	ARG	-	EXPRESSION TAG	UNP Q9I297
H	25	GLY	-	EXPRESSION TAG	UNP Q9I297
H	26	SER	-	EXPRESSION TAG	UNP Q9I297
H	27	HIS	-	EXPRESSION TAG	UNP Q9I297
J	8	MET	-	EXPRESSION TAG	UNP Q9I297
J	9	GLY	-	EXPRESSION TAG	UNP Q9I297
J	10	SER	-	EXPRESSION TAG	UNP Q9I297
J	11	SER	-	EXPRESSION TAG	UNP Q9I297
J	12	HIS	-	EXPRESSION TAG	UNP Q9I297

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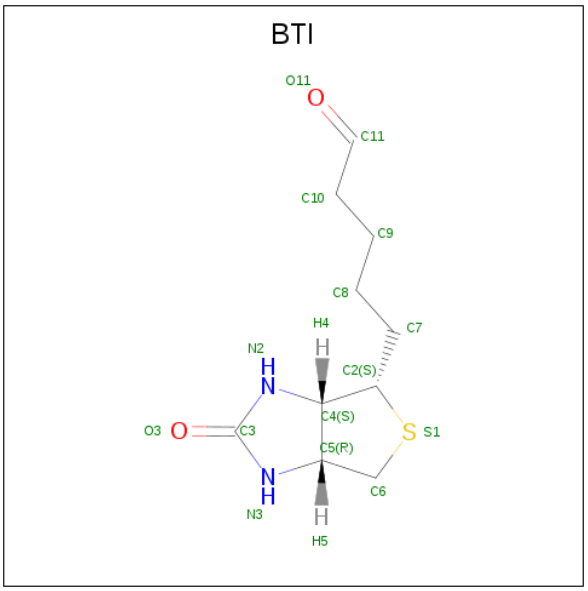
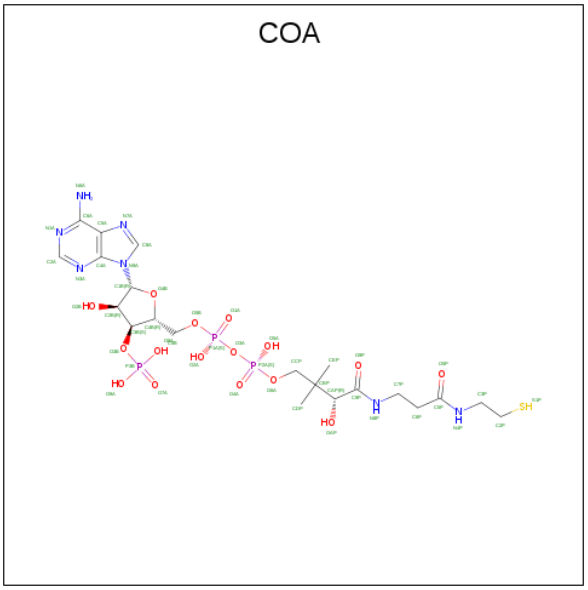
Chain	Residue	Modelled	Actual	Comment	Reference
J	13	HIS	-	EXPRESSION TAG	UNP Q9I297
J	14	HIS	-	EXPRESSION TAG	UNP Q9I297
J	15	HIS	-	EXPRESSION TAG	UNP Q9I297
J	16	HIS	-	EXPRESSION TAG	UNP Q9I297
J	17	HIS	-	EXPRESSION TAG	UNP Q9I297
J	18	SER	-	EXPRESSION TAG	UNP Q9I297
J	19	SER	-	EXPRESSION TAG	UNP Q9I297
J	20	GLY	-	EXPRESSION TAG	UNP Q9I297
J	21	LEU	-	EXPRESSION TAG	UNP Q9I297
J	22	VAL	-	EXPRESSION TAG	UNP Q9I297
J	23	PRO	-	EXPRESSION TAG	UNP Q9I297
J	24	ARG	-	EXPRESSION TAG	UNP Q9I297
J	25	GLY	-	EXPRESSION TAG	UNP Q9I297
J	26	SER	-	EXPRESSION TAG	UNP Q9I297
J	27	HIS	-	EXPRESSION TAG	UNP Q9I297
L	8	MET	-	EXPRESSION TAG	UNP Q9I297
L	9	GLY	-	EXPRESSION TAG	UNP Q9I297
L	10	SER	-	EXPRESSION TAG	UNP Q9I297
L	11	SER	-	EXPRESSION TAG	UNP Q9I297
L	12	HIS	-	EXPRESSION TAG	UNP Q9I297
L	13	HIS	-	EXPRESSION TAG	UNP Q9I297
L	14	HIS	-	EXPRESSION TAG	UNP Q9I297
L	15	HIS	-	EXPRESSION TAG	UNP Q9I297
L	16	HIS	-	EXPRESSION TAG	UNP Q9I297
L	17	HIS	-	EXPRESSION TAG	UNP Q9I297
L	18	SER	-	EXPRESSION TAG	UNP Q9I297
L	19	SER	-	EXPRESSION TAG	UNP Q9I297
L	20	GLY	-	EXPRESSION TAG	UNP Q9I297
L	21	LEU	-	EXPRESSION TAG	UNP Q9I297
L	22	VAL	-	EXPRESSION TAG	UNP Q9I297
L	23	PRO	-	EXPRESSION TAG	UNP Q9I297
L	24	ARG	-	EXPRESSION TAG	UNP Q9I297
L	25	GLY	-	EXPRESSION TAG	UNP Q9I297
L	26	SER	-	EXPRESSION TAG	UNP Q9I297
L	27	HIS	-	EXPRESSION TAG	UNP Q9I297

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	I	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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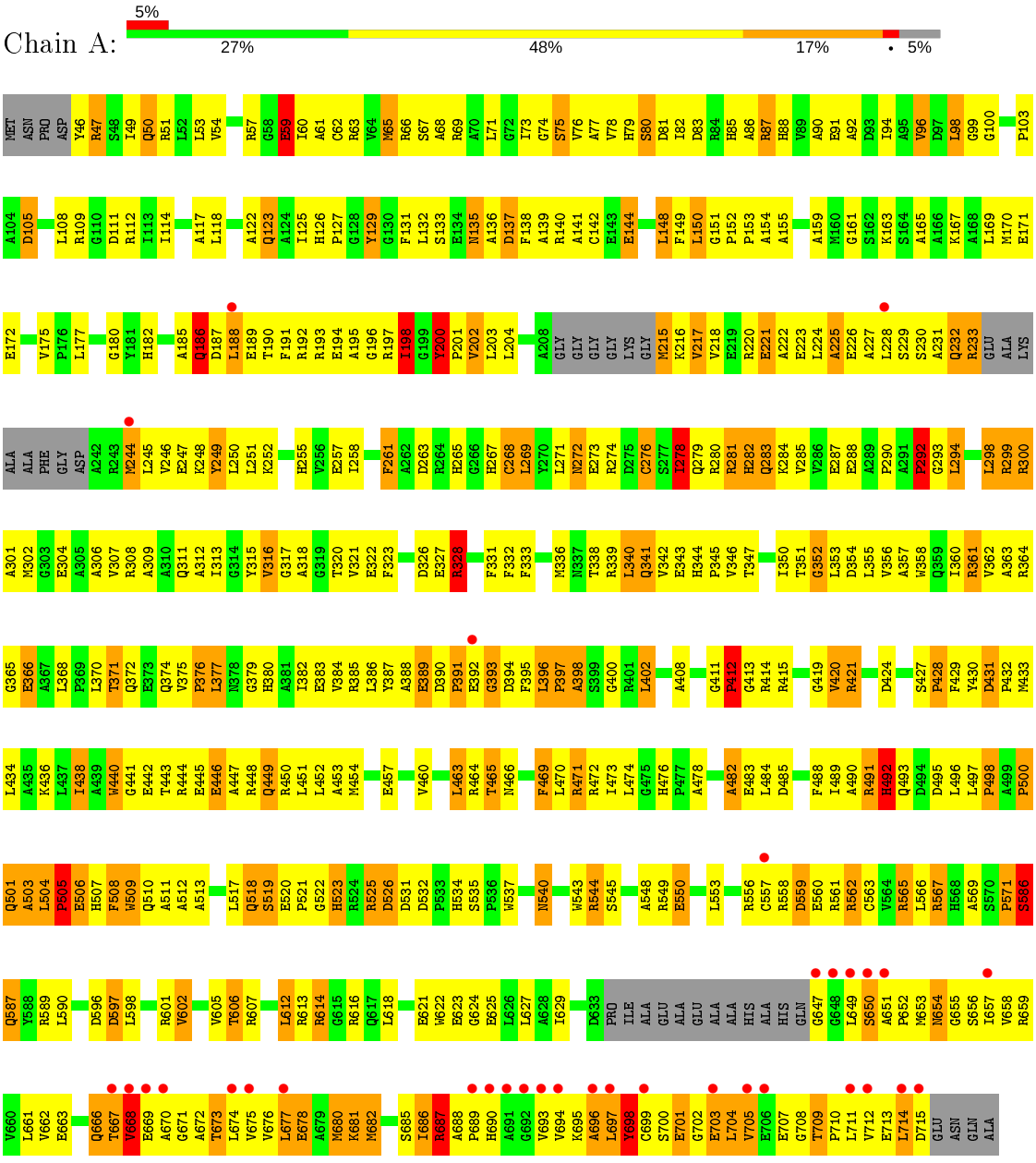
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

3 Residue-property plots (i)

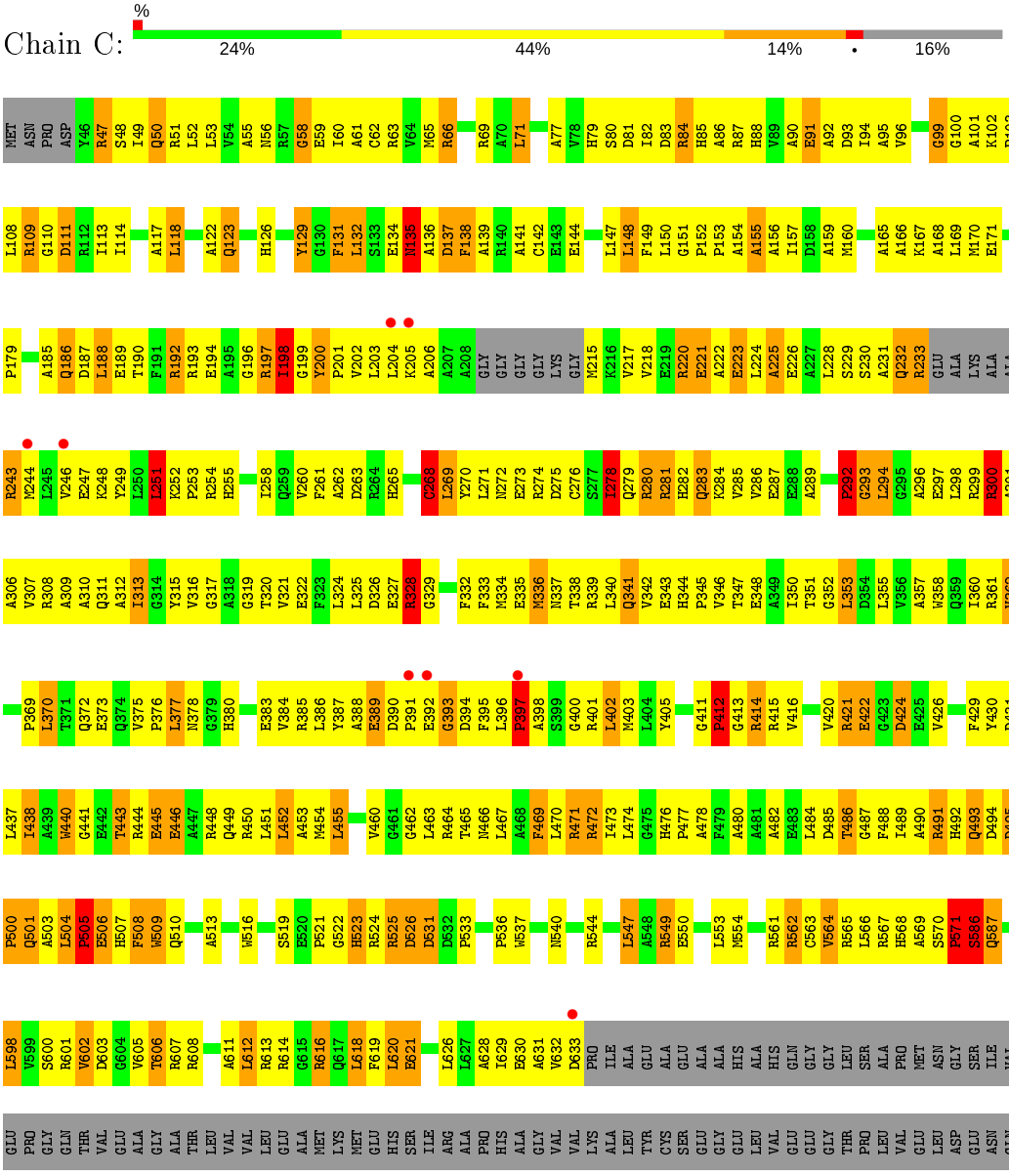
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit



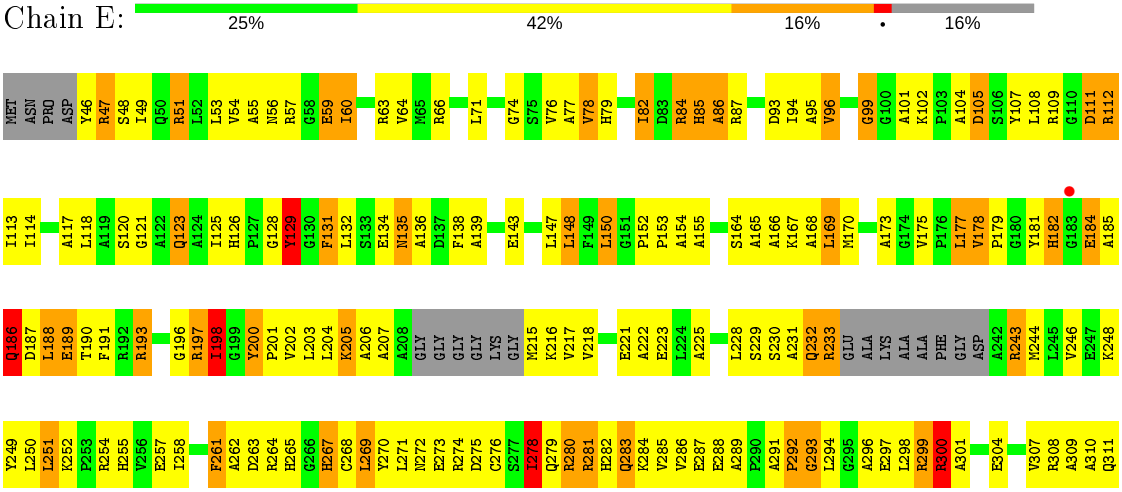
- Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

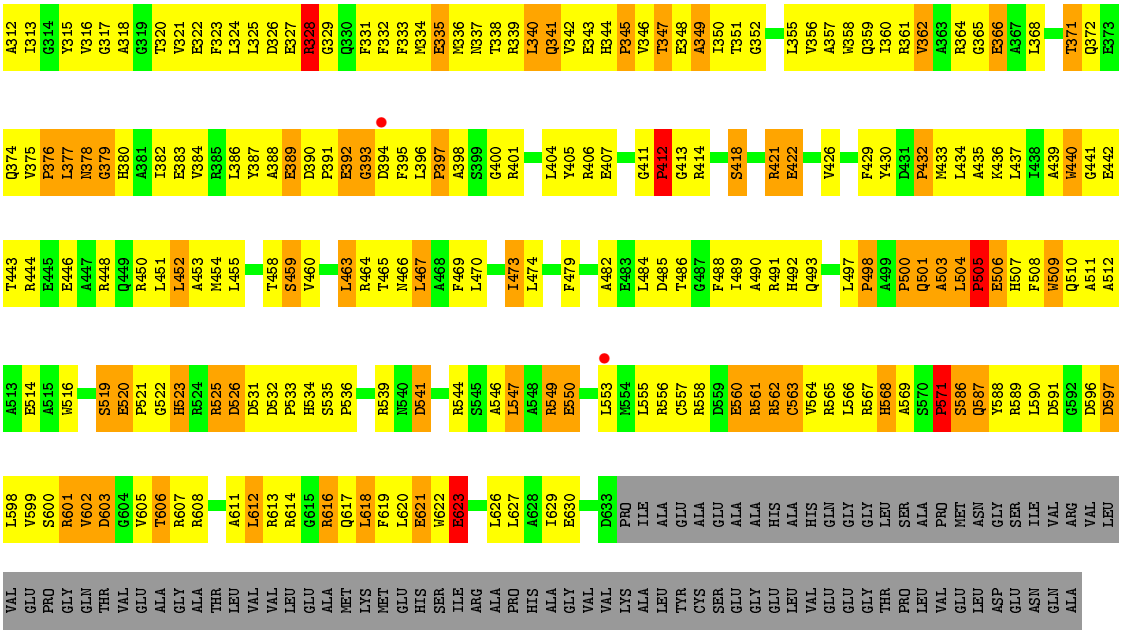
Chain C:



• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

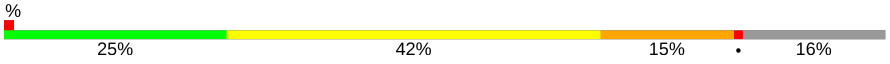
Chain E:

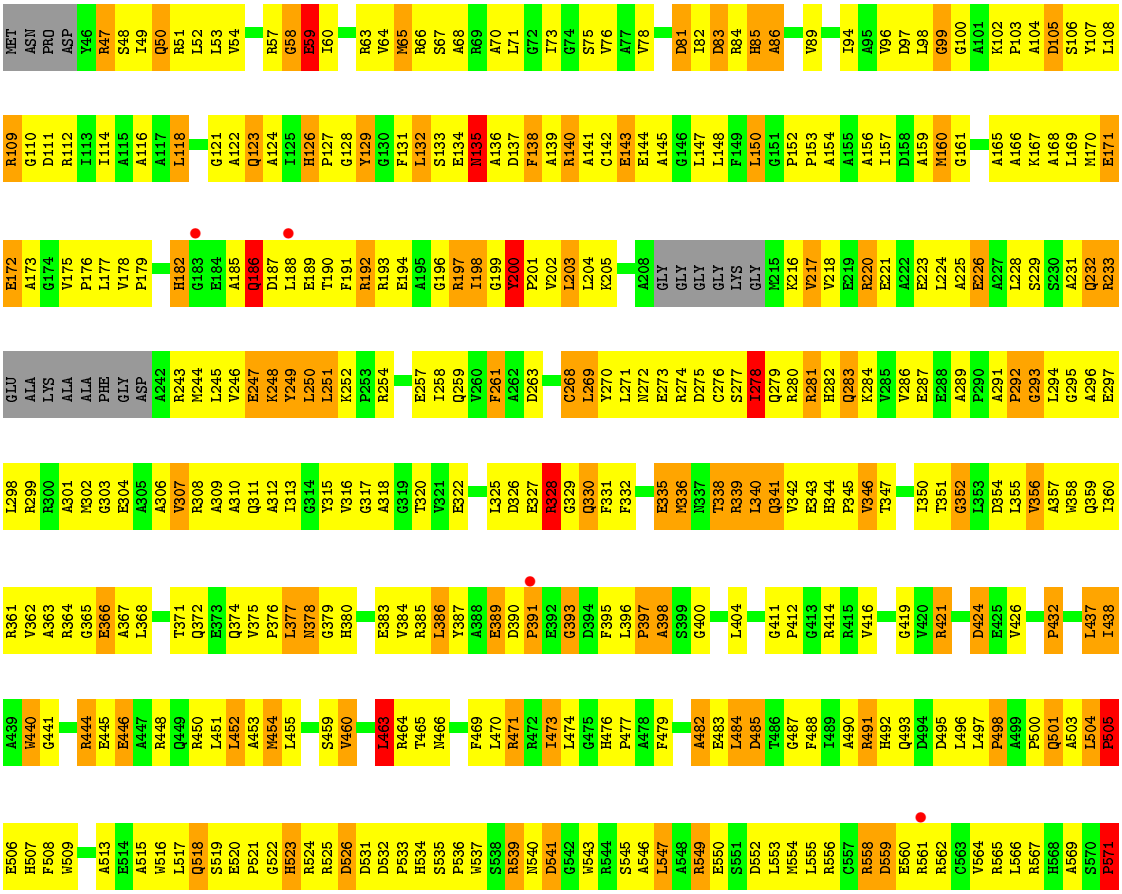


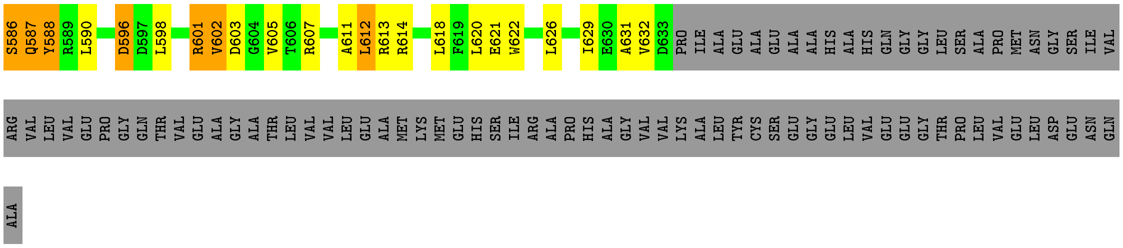


• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

Chain G:

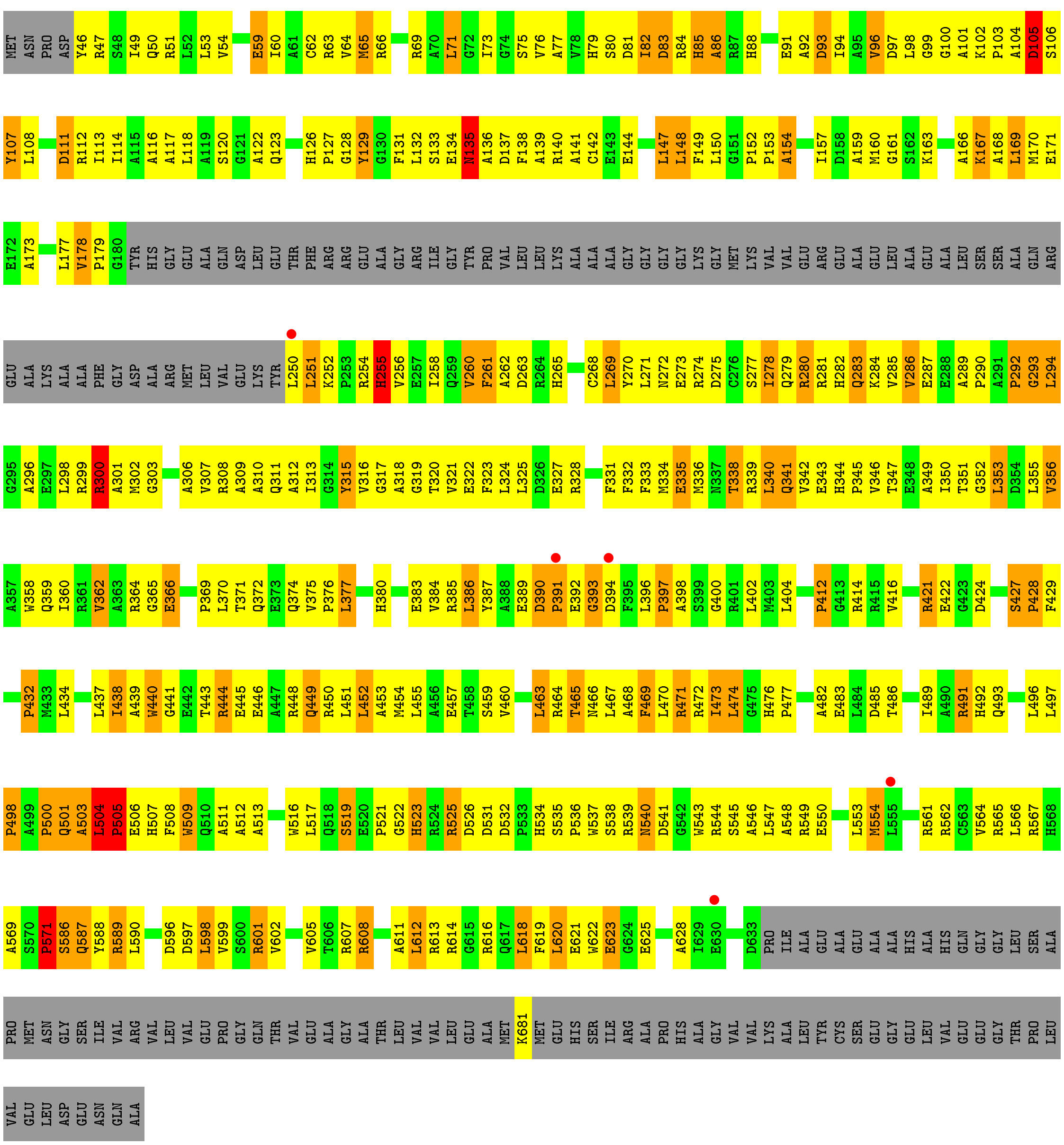






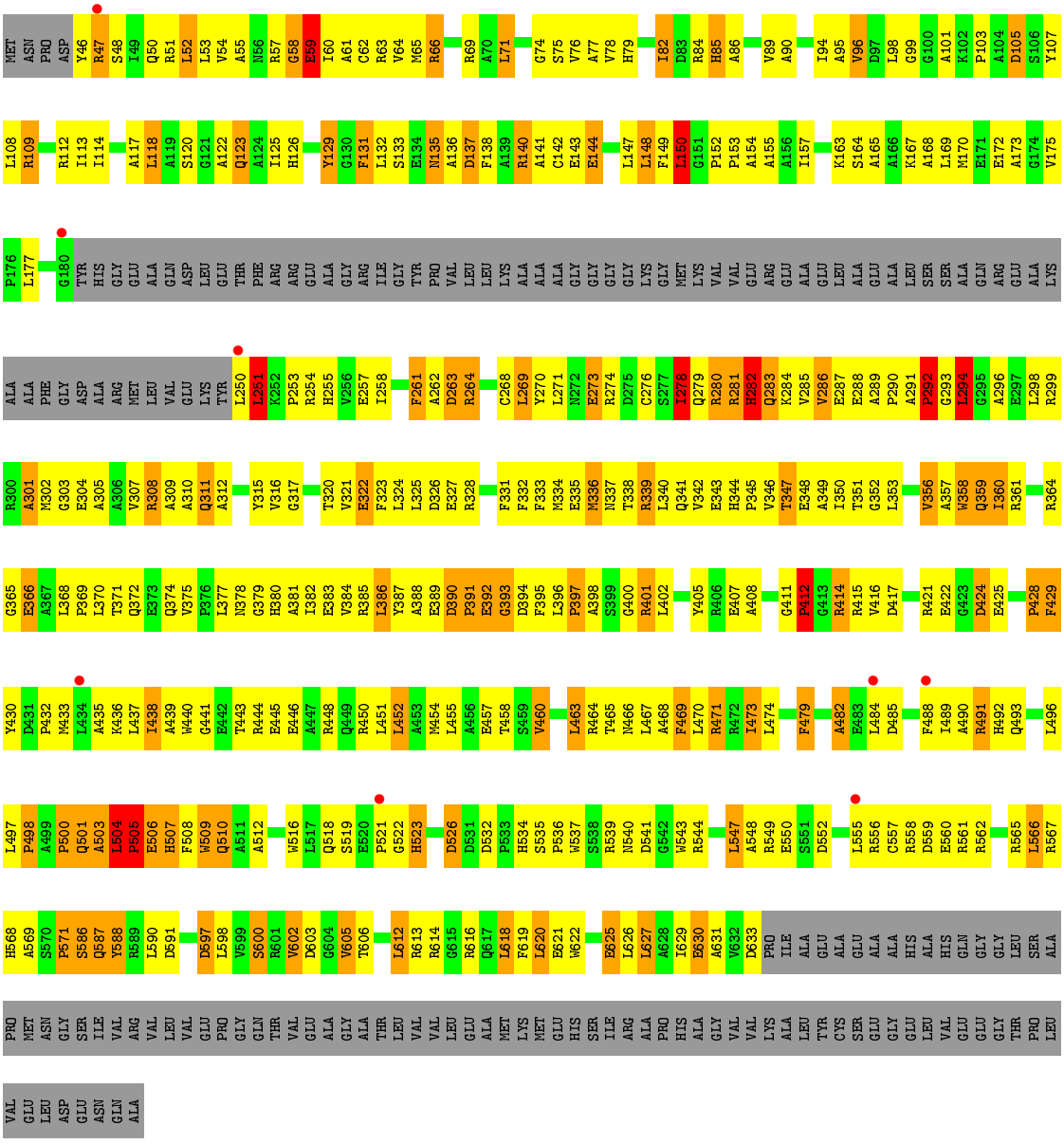
• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

Chain I:



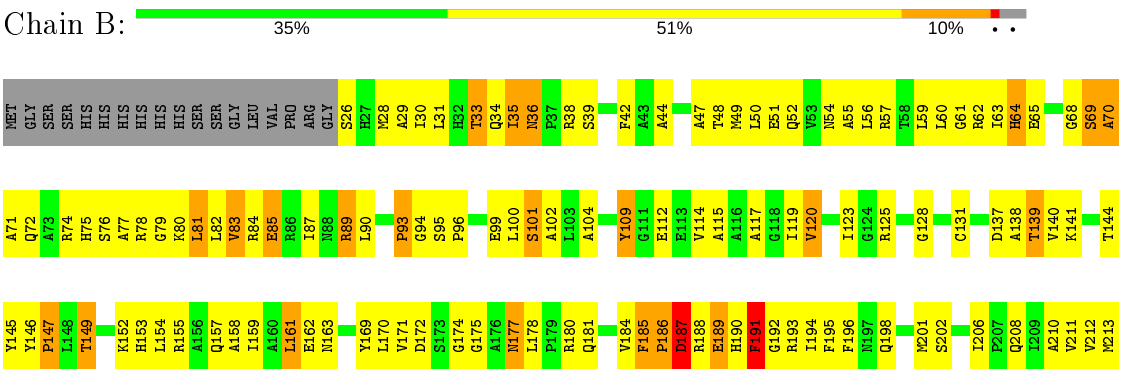
• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

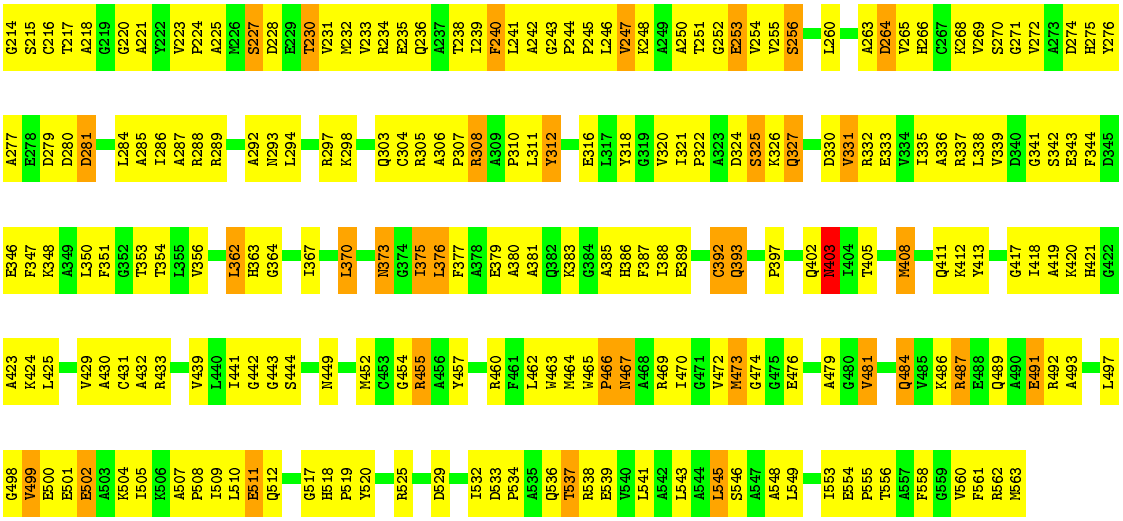
Chain K:

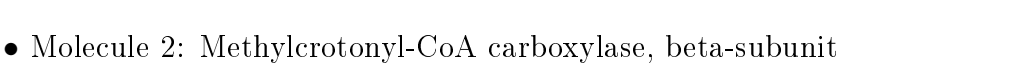


• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain B:

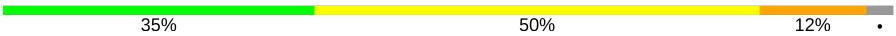


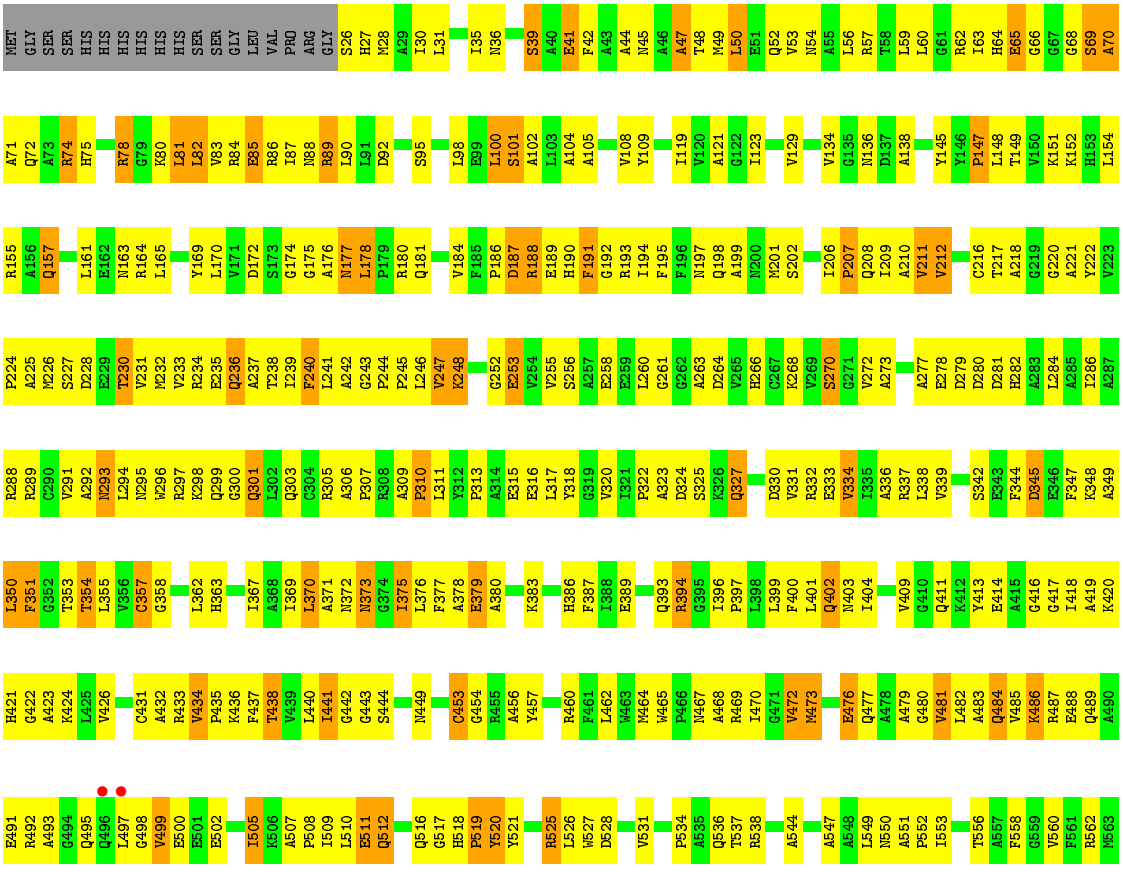


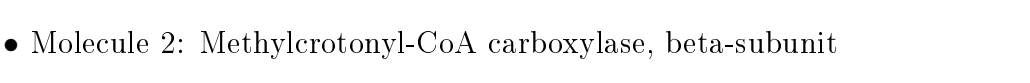


• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain D:

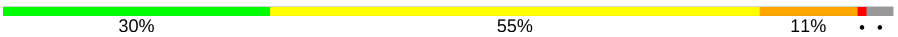


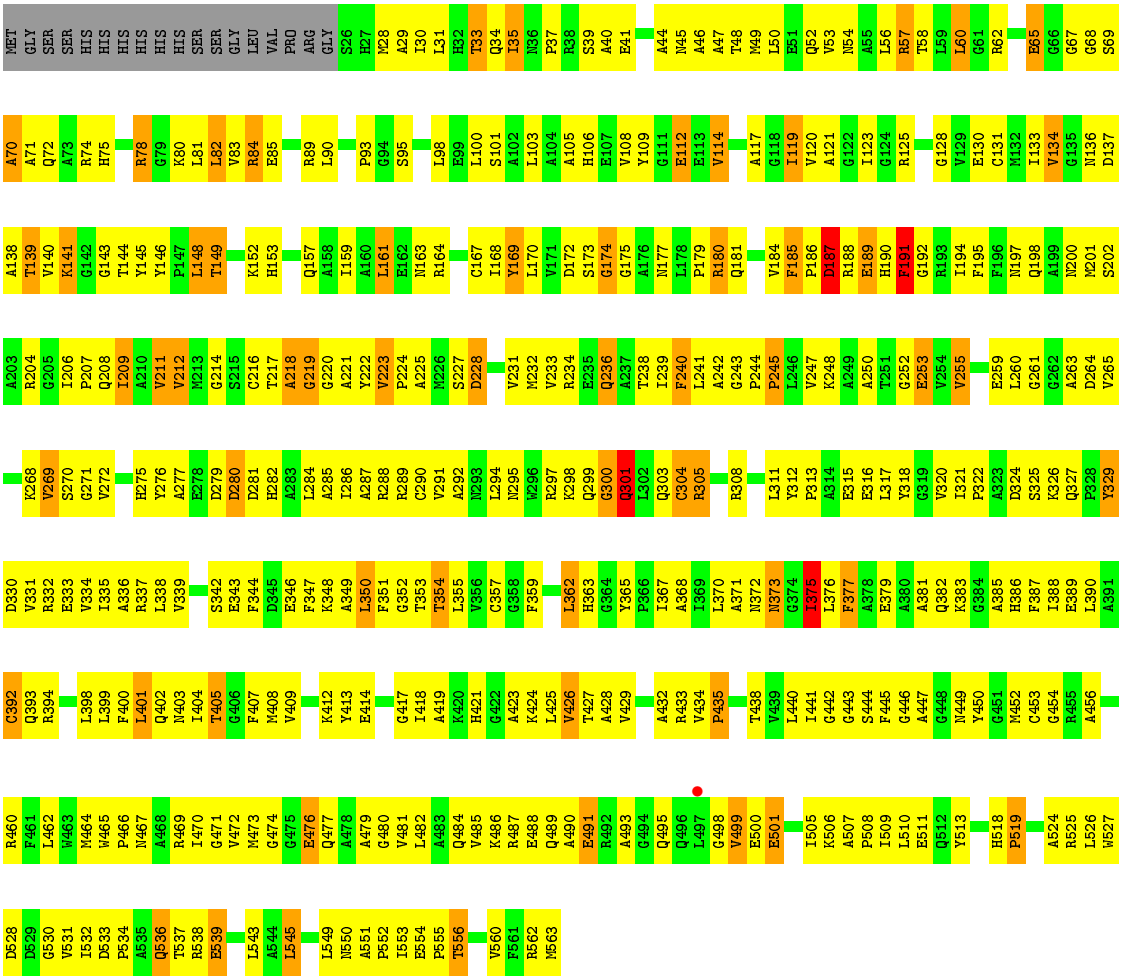




• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

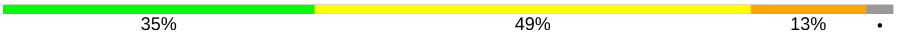
Chain F:

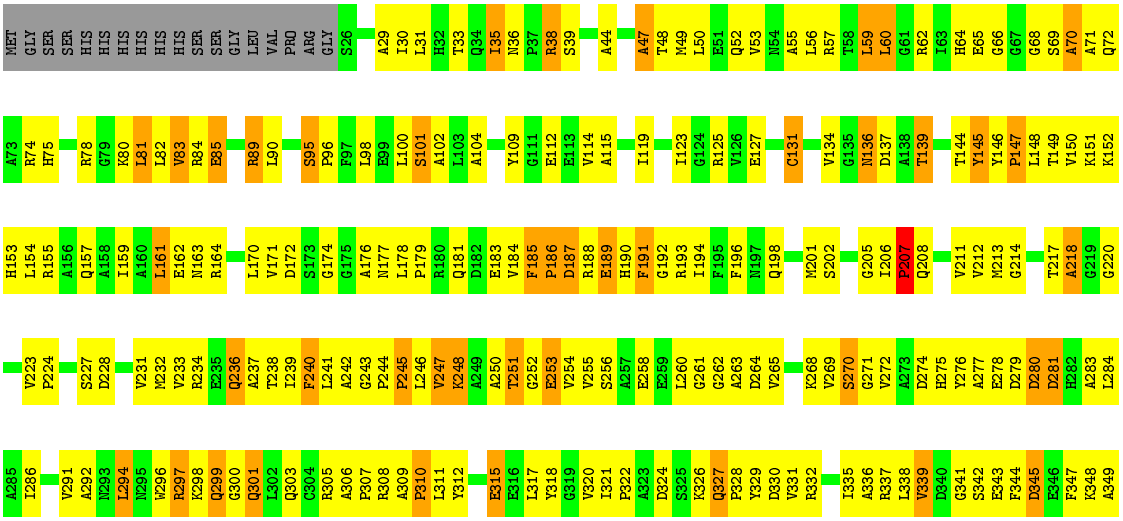


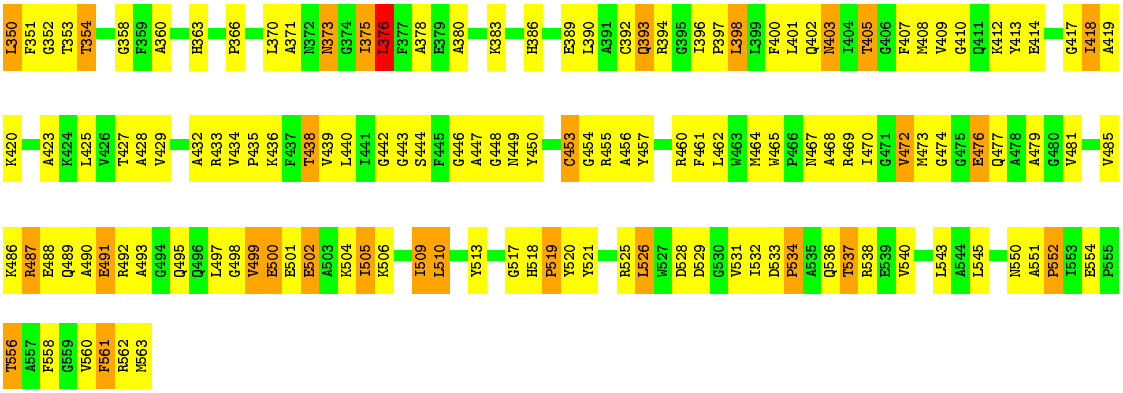


• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain H:

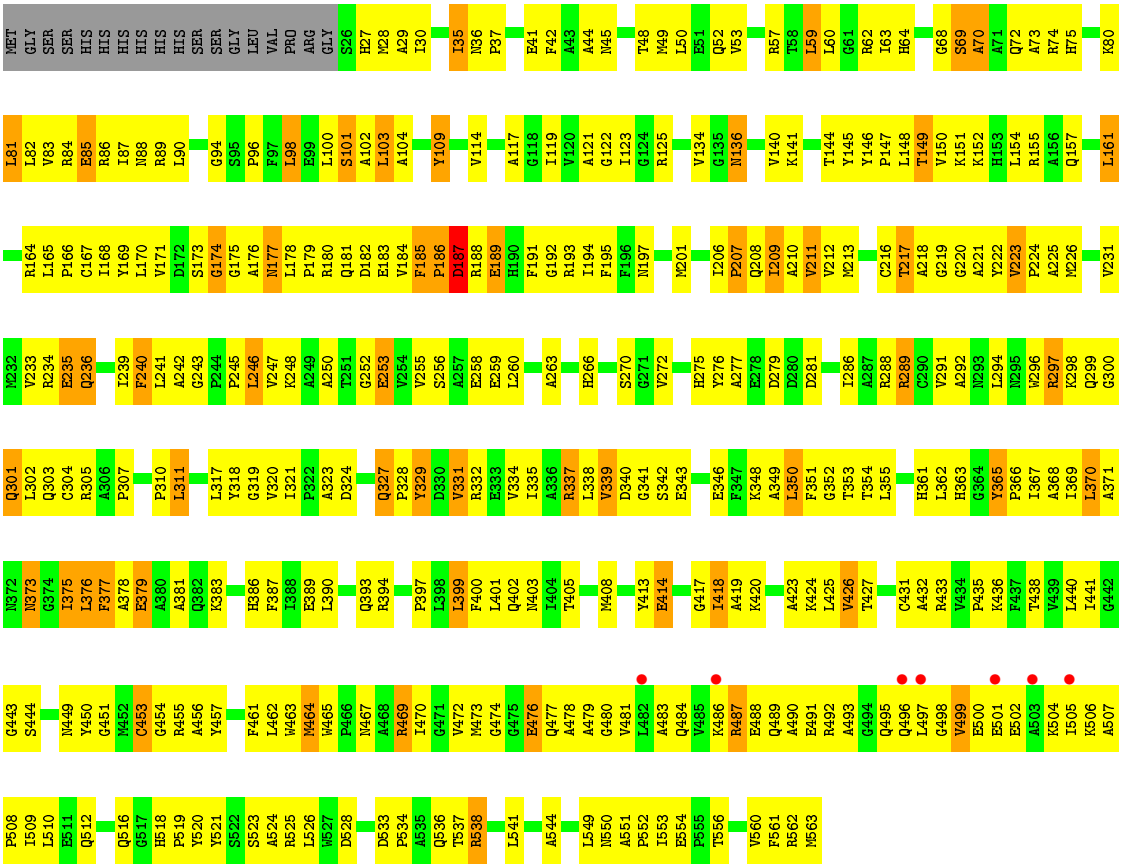






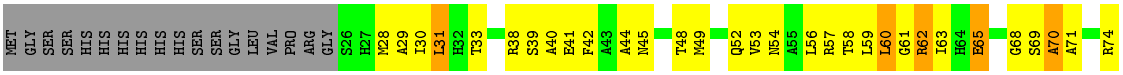
• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

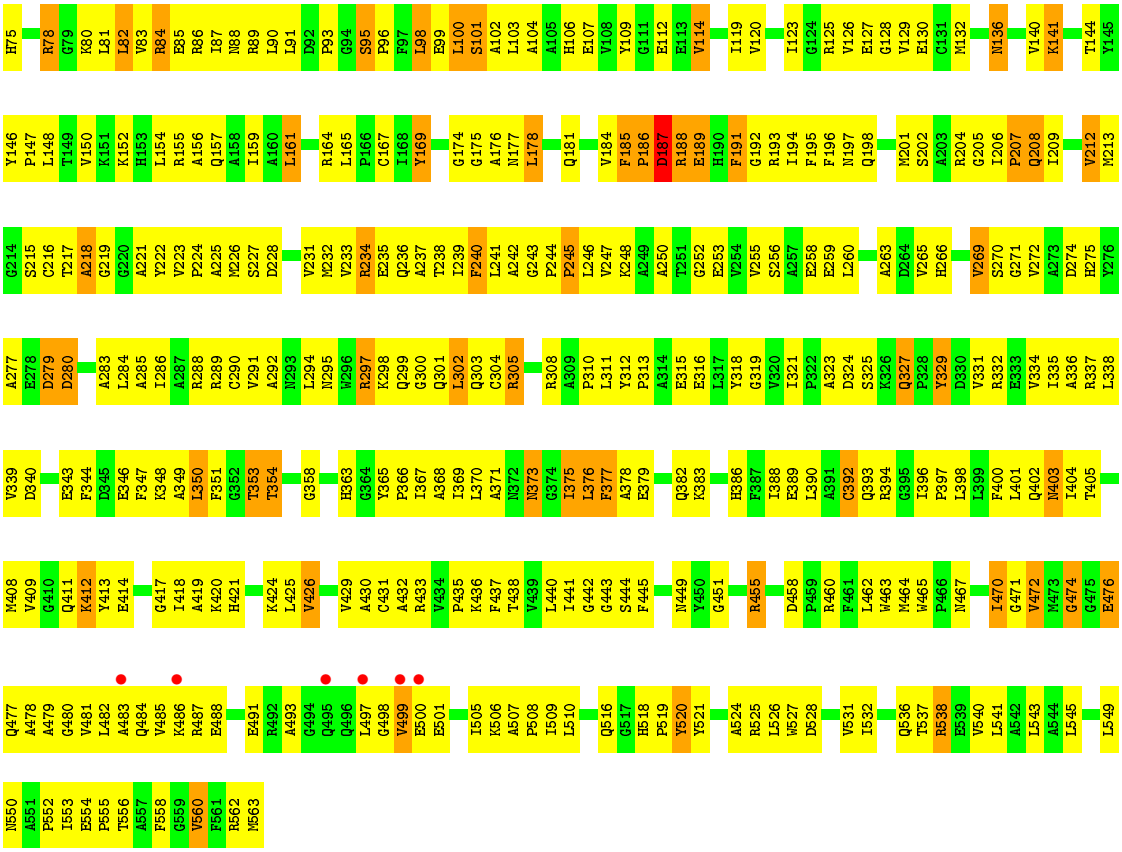
Chain J:



• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain L:




H75 R78 G79 K80 L81 L82 V83 R84 E85 R86 I87 N88 R89 L90 L91 D92 P93 G94 S95 P96 F97 L98 E99 L100 S101 A102 L103 A104 A105 H106 E107 V108 Y109 G111 E112 E113 V114 I119 V120 I123 G124 R125 V126 E127 G128 V129 E130 C131 M132 N136 V140 K141 T144 Y145
Y146 P147 L148 T149 V150 K151 K152 H153 L154 R155 A156 Q157 A158 I159 A160 L161 R164 L165 P166 C167 I168 Y169 G174 G175 A176 N177 L178 Q181 V184 F185 P186 D187 R188 E189 H190 F191 G192 R193 I194 F195 F196 N197 Q198 M201 S202 A203 R204 G205 I206 P207 Q208 I209 V212 M213
G214 S215 C216 T217 A218 G219 G220 A221 Y222 V223 P224 A225 M226 S227 D228 V231 M232 V233 R234 E235 Q236 A237 T238 I239 F240 L241 A242 G243 P244 P245 L246 V247 K248 A249 A250 T251 G252 E253 V254 V255 S256 A257 E258 E259 L260 A263 D264 V265 H266 V269 S270 G271 V272 A273 D274 H275 Y276
A277 E278 D279 D280 A283 L284 A285 I286 A287 R288 R289 C290 V291 A292 N293 L294 N295 W296 R297 K298 Q299 G300 Q301 L302 Q303 C304 R305 R308 A309 P310 L311 Y312 P313 A314 E315 E316 L317 Y318 G319 V320 I321 P322 A323 D324 S325 K326 Q327 P328 Y329 D330 V331 R332 E333 V334 I335 A336 R337 L338
V339 D340 E343 F344 D345 E346 F347 K348 A349 L350 F351 G352 T353 T354 G358 H363 G364 Y365 P366 I367 A368 I369 L370 A371 N372 N373 G374 I375 L376 F377 A378 E379 Q382 K383 H386 F387 I388 E389 L390 A391 C392 Q393 R394 G395 I396 P397 L398 L399 F400 L401 Q402 N403 I404 T405
M408 V409 G410 Q411 K412 Y413 E414 G417 I418 A419 K420 H421 K424 L425 V426 V429 A430 C431 A432 R433 V434 P435 K436 F437 T438 V439 L440 I441 G442 G443 S444 F445 N449 Y450 G451 R455 D458 P459 R460 F461 L462 W463 M464 W465 P466 N467 I470 G471 V472 M473 G474 G475 E476
Q477 A478 A479 G480 V481 L482 A483 Q484 V485 K486 R487 E488 E491 R492 A493 G494 Q495 Q496 L497 G498 V499 E500 E501 I505 K506 A507 P508 I509 L510 Q516 G517 H518 P519 Y520 V521 A524 R525 L526 W527 D528 V531 I532 Q536 T537 R538 E539 V540 L541 A542 L543 A544 L545 L549
N550 A551 P552 I553 E554 P555 T556 A557 F558 G559 V560 F561 R562 M563

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.51Å 255.34Å 152.67Å 90.00° 95.74° 90.00°	Depositor
Resolution (Å)	48.90 – 3.50 48.90 – 3.28	Depositor EDS
% Data completeness (in resolution range)	83.0 (48.90-3.50) 76.9 (48.90-3.28)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.292 0.213 , 0.273	Depositor DCC
R_{free} test set	6800 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.971	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 73.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	49939	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.68	0/4866	0.87	4/6581 (0.1%)
1	C	0.63	0/4362	0.86	3/5897 (0.1%)
1	E	0.65	1/4362 (0.0%)	0.85	3/5897 (0.1%)
1	G	0.65	0/4362	0.87	0/5897
1	I	0.66	0/3929	0.84	1/5315 (0.0%)
1	K	0.68	0/3921	0.85	2/5307 (0.0%)
2	B	0.67	0/4135	0.86	1/5605 (0.0%)
2	D	0.67	0/4135	0.86	3/5605 (0.1%)
2	F	0.64	0/4135	0.87	3/5605 (0.1%)
2	H	0.67	3/4135 (0.1%)	0.83	1/5605 (0.0%)
2	J	0.68	0/4135	0.87	2/5605 (0.0%)
2	L	0.67	0/4135	0.87	0/5605
All	All	0.66	4/50612 (0.0%)	0.86	23/68524 (0.0%)

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	E	0	1
1	G	0	2
1	I	0	1
2	B	0	1
2	H	0	1
2	J	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	131	CYS	CB-SG	-7.11	1.70	1.82
1	E	563	CYS	CB-SG	5.92	1.92	1.82
2	H	189	GLU	CB-CG	5.11	1.61	1.52
2	H	189	GLU	CG-CD	5.11	1.59	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	399	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	E	506	GLU	N-CA-C	-6.63	93.10	111.00
1	C	506	GLU	N-CA-C	-6.45	93.60	111.00
1	E	566	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	298	LEU	CA-CB-CG	-5.94	101.63	115.30
2	B	304	CYS	CA-CB-SG	5.52	123.94	114.00
2	J	246	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	294	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	251	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	396	LEU	CA-CB-CG	5.42	127.77	115.30
2	D	394	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	K	251	LEU	CA-CB-CG	5.39	127.70	115.30
1	I	506	GLU	N-CA-C	-5.36	96.53	111.00
1	E	379	GLY	N-CA-C	5.29	126.31	113.10
2	D	50	LEU	CA-CB-CG	5.25	127.36	115.30
2	F	148	LEU	CA-CB-CG	-5.24	103.24	115.30
2	F	401	LEU	CA-CB-CG	-5.21	103.31	115.30
2	H	60	LEU	CA-CB-CG	5.21	127.28	115.30
2	D	82	LEU	CA-CB-CG	-5.19	103.36	115.30
1	K	506	GLU	N-CA-C	-5.18	97.01	111.00
2	F	35	ILE	CB-CA-C	-5.10	101.40	111.60
1	A	506	GLU	N-CA-C	-5.09	97.25	111.00
1	C	199	GLY	N-CA-C	-5.08	100.39	113.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	698	TYR	Sidechain
2	B	109	TYR	Sidechain
1	E	129	TYR	Sidechain
1	G	129	TYR	Sidechain
1	G	588	TYR	Sidechain
2	H	145	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	I	129	TYR	Sidechain
2	J	109	TYR	Sidechain
2	J	365	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4778	0	4730	583	0
1	C	4280	0	4227	535	0
1	E	4280	0	4227	519	0
1	G	4280	0	4227	516	0
1	I	3853	0	3795	477	0
1	K	3844	0	3786	485	0
2	B	4051	0	4023	401	0
2	D	4051	0	4023	425	0
2	F	4051	0	4023	437	0
2	H	4051	0	4023	422	0
2	J	4051	0	4023	425	0
2	L	4051	0	4023	419	0
3	A	15	0	15	3	0
3	I	15	0	15	4	0
4	B	48	0	32	4	0
4	D	48	0	32	3	0
4	F	48	0	32	3	0
4	H	48	0	32	6	0
4	J	48	0	32	4	0
4	L	48	0	32	2	0
All	All	49939	0	49352	5408	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 54.

All (5408) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:LEU:HB3	1:C:505:PRO:HD2	1.23	1.17
1:G:200:TYR:CE1	1:G:221:GLU:HA	1.82	1.15
1:G:278:ILE:H	1:G:278:ILE:HD12	1.10	1.14
1:K:101:ALA:HB1	1:K:429:PHE:CE1	1.83	1.14
2:F:231:VAL:HG22	2:F:275:HIS:HB2	1.18	1.12
1:K:101:ALA:HB1	1:K:429:PHE:HE1	1.06	1.12
2:L:231:VAL:HG22	2:L:275:HIS:HB2	1.32	1.11
1:C:465:THR:HG22	1:C:467:LEU:H	1.13	1.11
1:I:605:VAL:HG12	1:K:96:VAL:HG12	1.26	1.11
1:A:396:LEU:HD12	1:A:464:ARG:HH12	1.15	1.11
2:D:217:THR:HG22	2:D:240:PHE:CE1	1.84	1.11
1:G:152:PRO:HD2	1:G:157:ILE:HD11	1.32	1.11
1:C:400:GLY:H	1:C:463:LEU:HD21	1.04	1.11
1:E:101:ALA:HB1	1:E:429:PHE:CE1	1.86	1.11
2:H:207:PRO:HG2	2:H:294:LEU:HD21	1.34	1.10
1:C:611:ALA:HB2	1:C:620:LEU:HD13	1.30	1.08
2:H:350:LEU:HD23	2:H:350:LEU:H	1.15	1.08
2:J:201:MET:HE3	2:J:208:GLN:HE22	1.13	1.08
2:J:495:GLN:HG2	2:J:496:GLN:H	1.16	1.08
2:D:217:THR:HG22	2:D:240:PHE:HE1	1.10	1.08
1:E:350:ILE:HA	1:E:440:TRP:HZ3	1.19	1.07
2:D:188:ARG:HH11	2:D:188:ARG:HB3	1.15	1.07
1:K:415:ARG:HD3	1:K:438:ILE:HD13	1.34	1.07
1:A:525:ARG:HH11	1:A:525:ARG:HB3	1.19	1.07
1:E:167:LYS:HE3	1:E:177:LEU:HD22	1.36	1.07
1:E:278:ILE:HD12	1:E:278:ILE:H	1.17	1.07
2:D:444:SER:HB3	2:D:470:ILE:HG13	1.29	1.07
2:H:291:VAL:HA	2:H:294:LEU:HD12	1.38	1.05
1:I:562:ARG:HH11	1:I:562:ARG:HB3	1.20	1.04
1:E:549:ARG:HH11	1:E:549:ARG:HG2	1.19	1.04
1:K:401:ARG:HH11	1:K:401:ARG:HB3	1.20	1.04
1:A:562:ARG:HH11	1:A:562:ARG:HB3	1.17	1.04
2:B:33:THR:HG23	2:B:35:ILE:H	1.20	1.04
1:G:605:VAL:HG12	1:I:96:VAL:HG13	1.36	1.04
1:I:599:VAL:HG22	1:I:608:ARG:HB3	1.37	1.04
1:K:47:ARG:HH11	1:K:47:ARG:HB2	1.20	1.04
2:L:375:ILE:HB	2:L:377:PHE:HE1	1.19	1.04
1:E:101:ALA:HB1	1:E:429:PHE:HE1	1.23	1.03
1:E:550:GLU:HG3	1:E:567:ARG:HD2	1.33	1.03
2:B:83:VAL:HG13	2:B:84:ARG:H	1.15	1.03
1:K:378:ASN:O	1:K:440:TRP:HH2	1.42	1.03
1:G:47:ARG:HB2	1:G:47:ARG:HH11	1.22	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:444:SER:HB2	2:H:470:ILE:HG13	1.41	1.02
1:C:278:ILE:H	1:C:278:ILE:HD12	1.17	1.02
2:F:375:ILE:HD12	2:F:375:ILE:H	1.20	1.02
1:A:383:GLU:HG3	1:A:438:ILE:HG23	1.42	1.01
2:L:538:ARG:HG3	2:L:538:ARG:HH11	1.26	1.01
1:G:153:PRO:HD3	1:G:316:VAL:HG23	1.43	1.00
1:A:232:GLN:HG2	1:A:233:ARG:NH1	1.76	1.00
2:H:161:LEU:HB2	2:H:201:MET:HE2	1.40	1.00
1:I:169:LEU:HD23	1:I:312:ALA:HB1	1.41	1.00
2:J:538:ARG:HH11	2:J:538:ARG:HG3	1.21	1.00
1:K:47:ARG:NH1	1:K:47:ARG:HB2	1.77	1.00
1:C:231:ALA:HB3	1:C:244:MET:SD	2.01	1.00
1:K:175:VAL:HG21	1:K:309:ALA:HB2	1.41	1.00
1:K:153:PRO:HD3	1:K:316:VAL:HG23	1.40	0.99
2:H:137:ASP:OD1	2:H:139:THR:HG23	1.62	0.99
1:G:251:LEU:HD22	1:G:328:ARG:HE	1.25	0.99
2:F:217:THR:HG22	2:F:240:PHE:HE1	1.24	0.99
1:G:175:VAL:HG21	1:G:309:ALA:HB2	1.43	0.99
2:F:137:ASP:HB3	2:F:140:VAL:HG23	1.45	0.99
1:I:278:ILE:H	1:I:278:ILE:HD12	1.24	0.99
2:L:403:ASN:ND2	2:L:442:GLY:HA3	1.78	0.99
1:K:66:ARG:HB2	1:K:66:ARG:HH11	1.26	0.99
2:B:137:ASP:HB3	2:B:140:VAL:HG23	1.43	0.98
1:E:304:GLU:O	1:E:307:VAL:HG12	1.62	0.98
1:G:185:ALA:CB	1:G:243:ARG:HG3	1.93	0.98
1:A:274:ARG:HH22	1:A:320:THR:HG21	1.29	0.98
1:A:544:ARG:HG2	1:A:544:ARG:HH11	1.25	0.98
2:B:82:LEU:H	2:B:82:LEU:HD12	1.29	0.98
1:E:251:LEU:H	1:E:251:LEU:HD12	1.26	0.98
2:H:375:ILE:HG22	2:H:376:LEU:H	1.26	0.97
1:I:596:ASP:OD1	1:I:612:LEU:HB3	1.64	0.97
1:E:562:ARG:HH11	1:E:562:ARG:HG2	1.26	0.97
1:G:63:ARG:HH21	1:G:356:VAL:HG23	1.28	0.97
1:E:53:LEU:HD13	1:E:117:ALA:HB2	1.47	0.97
1:C:232:GLN:H	1:C:233:ARG:NH2	1.63	0.97
1:E:505:PRO:HB3	1:E:507:HIS:HB2	1.47	0.97
1:C:203:LEU:HD23	1:C:205:LYS:NZ	1.79	0.97
1:C:285:VAL:HG12	1:C:286:VAL:HG23	1.47	0.97
1:E:465:THR:HG22	1:E:467:LEU:H	1.27	0.97
1:K:251:LEU:HD13	1:K:327:GLU:HB2	1.44	0.96
1:E:308:ARG:HH11	1:E:308:ARG:HG3	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:TYR:HB3	1:E:598:LEU:HD11	1.46	0.96
1:E:175:VAL:HG21	1:E:309:ALA:HB2	1.46	0.96
2:H:265:VAL:O	2:H:269:VAL:HB	1.66	0.96
1:I:550:GLU:HG2	1:I:567:ARG:HD2	1.46	0.96
2:L:189:GLU:CD	2:L:189:GLU:H	1.63	0.96
2:F:84:ARG:HG2	2:F:84:ARG:HH11	1.30	0.95
1:G:169:LEU:HD23	1:G:313:ILE:HG22	1.48	0.95
1:I:306:ALA:HB1	1:I:321:VAL:HG21	1.45	0.95
1:K:152:PRO:HG3	1:K:315:TYR:CZ	2.01	0.95
1:I:398:ALA:HB2	1:I:464:ARG:HE	1.30	0.95
1:A:200:TYR:CE1	1:A:221:GLU:HA	2.01	0.95
1:E:384:VAL:HG13	1:E:470:LEU:HD22	1.46	0.95
1:G:328:ARG:HG3	1:G:328:ARG:HH11	1.29	0.95
2:H:305:ARG:HH11	2:H:305:ARG:HB3	1.30	0.95
1:A:153:PRO:HD3	1:A:316:VAL:CG2	1.97	0.95
1:I:132:LEU:HD23	1:I:138:PHE:CD2	2.02	0.95
1:K:140:ARG:HB3	1:K:140:ARG:CZ	1.94	0.94
1:A:186:GLN:NE2	1:A:190:THR:H	1.65	0.94
1:A:278:ILE:H	1:A:278:ILE:HD12	1.31	0.94
1:A:186:GLN:HE22	1:A:190:THR:H	1.10	0.94
1:A:567:ARG:HH11	1:A:567:ARG:HG3	1.30	0.94
1:G:200:TYR:HE1	1:G:221:GLU:HA	1.28	0.94
2:L:350:LEU:H	2:L:350:LEU:HD23	1.29	0.94
2:B:444:SER:HB3	2:B:449:ASN:HD22	1.32	0.94
2:D:338:LEU:O	2:D:538:ARG:HD2	1.67	0.94
1:C:344:HIS:ND1	1:C:345:PRO:HD3	1.83	0.94
1:I:562:ARG:NH1	1:I:562:ARG:HB3	1.81	0.94
2:F:180:ARG:HG3	2:F:180:ARG:HH11	1.32	0.94
2:L:191:PHE:HD2	2:L:192:GLY:H	1.16	0.94
2:B:89:ARG:HG3	2:B:89:ARG:HH21	1.33	0.93
1:A:605:VAL:HG12	1:C:96:VAL:HG13	1.47	0.93
1:E:252:LYS:HE3	1:E:491:ARG:NH2	1.83	0.93
2:H:90:LEU:HB2	2:H:284:LEU:HD22	1.50	0.93
1:C:400:GLY:N	1:C:463:LEU:HD21	1.83	0.93
1:E:504:LEU:HB3	1:E:505:PRO:HD2	1.49	0.93
1:K:321:VAL:HG22	1:K:336:MET:HG3	1.48	0.93
2:D:311:LEU:HD12	2:D:342:SER:HB2	1.49	0.93
2:J:350:LEU:HD12	2:J:350:LEU:H	1.32	0.93
2:F:433:ARG:NH2	2:F:554:GLU:HG3	1.83	0.93
2:J:201:MET:HE3	2:J:208:GLN:NE2	1.83	0.93
1:A:671:GLY:O	1:A:687:ARG:HB3	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:469:ARG:HG2	2:J:469:ARG:HH21	1.34	0.92
1:K:304:GLU:HA	1:K:307:VAL:HG12	1.50	0.92
1:I:300:ARG:NH1	1:I:300:ARG:HB2	1.82	0.92
2:L:123:ILE:HD11	2:L:165:LEU:HD13	1.52	0.92
2:D:272:VAL:HG22	2:J:420:LYS:HB3	1.49	0.92
2:L:83:VAL:HG13	2:L:84:ARG:H	1.34	0.92
2:D:350:LEU:CD2	2:D:350:LEU:H	1.83	0.92
2:J:334:VAL:O	2:J:338:LEU:HD12	1.70	0.92
1:C:325:LEU:HD23	1:C:326:ASP:N	1.85	0.91
1:C:443:THR:HG23	1:C:446:GLU:HB2	1.51	0.91
2:B:83:VAL:HG13	2:B:84:ARG:N	1.84	0.91
2:L:518:HIS:ND1	2:L:519:PRO:HD2	1.85	0.91
2:B:487:ARG:HB3	2:B:497:LEU:HD22	1.51	0.91
2:B:33:THR:HB	2:B:312:TYR:CE2	2.06	0.91
2:D:464:MET:HE2	2:D:519:PRO:HG3	1.53	0.91
1:K:526:ASP:OD2	1:K:526:ASP:N	2.03	0.91
2:L:161:LEU:HD22	2:L:201:MET:HG2	1.52	0.91
1:A:586:SER:O	1:A:587:GLN:HB2	1.69	0.91
1:I:53:LEU:HD13	1:I:117:ALA:HB2	1.51	0.91
1:K:344:HIS:ND1	1:K:345:PRO:HD3	1.87	0.90
1:K:465:THR:HG22	1:K:467:LEU:H	1.34	0.90
1:A:186:GLN:HE21	1:A:187:ASP:H	0.96	0.90
1:G:559:ASP:O	1:G:560:GLU:HG3	1.70	0.90
1:A:653:MET:HG2	1:A:654:ASN:H	1.36	0.90
2:B:145:TYR:HD1	2:B:149:THR:HB	1.33	0.90
1:E:270:TYR:H	1:E:372:GLN:HE22	1.12	0.90
1:G:268:CYS:SG	1:G:307:VAL:HG23	2.12	0.90
2:J:119:ILE:HG23	2:J:152:LYS:HD3	1.52	0.90
2:B:518:HIS:ND1	2:B:519:PRO:HD2	1.86	0.90
1:K:270:TYR:H	1:K:372:GLN:HE22	1.12	0.90
1:E:400:GLY:H	1:E:463:LEU:HD11	1.35	0.89
1:G:328:ARG:HG3	1:G:328:ARG:NH1	1.83	0.89
2:D:350:LEU:HD23	2:D:350:LEU:H	1.34	0.89
1:G:185:ALA:HB3	1:G:243:ARG:HG3	1.52	0.89
2:H:297:ARG:HB2	2:L:303:GLN:HE21	1.38	0.89
1:C:504:LEU:HB3	1:C:505:PRO:CD	2.02	0.89
1:G:398:ALA:HB2	1:G:464:ARG:HE	1.36	0.89
2:J:117:ALA:O	2:J:149:THR:HG23	1.72	0.89
1:K:428:PRO:HG2	1:K:429:PHE:CD2	2.08	0.89
2:L:208:GLN:HA	2:L:208:GLN:HE21	1.38	0.89
2:L:375:ILE:HB	2:L:377:PHE:CE1	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:PHE:HB2	2:D:438:THR:HG23	1.55	0.89
2:F:212:VAL:HG23	2:F:231:VAL:O	1.73	0.89
2:J:81:LEU:HD22	2:J:85:GLU:HB3	1.54	0.88
1:C:270:TYR:H	1:C:372:GLN:HE22	1.20	0.88
2:D:188:ARG:HH11	2:D:188:ARG:CB	1.87	0.88
1:I:549:ARG:HG3	1:I:549:ARG:HH11	1.38	0.88
2:L:377:PHE:HD1	2:L:377:PHE:N	1.70	0.88
1:C:47:ARG:HH11	1:C:47:ARG:HB2	1.36	0.88
2:H:217:THR:HG22	2:H:240:PHE:HE1	1.36	0.88
2:J:233:VAL:HG13	2:J:279:ASP:HA	1.53	0.88
2:J:464:MET:HE2	2:J:519:PRO:HG3	1.55	0.88
1:E:232:GLN:HG2	1:E:233:ARG:NH1	1.87	0.88
2:J:231:VAL:HG22	2:J:275:HIS:HB2	1.55	0.88
1:C:49:ILE:CD1	1:C:364:ARG:HG2	2.03	0.88
2:F:217:THR:HG22	2:F:240:PHE:CE1	2.08	0.88
1:A:186:GLN:NE2	1:A:187:ASP:H	1.72	0.87
1:G:110:GLY:O	1:G:114:ILE:HG22	1.73	0.87
1:G:160:MET:HE2	1:G:313:ILE:HD13	1.57	0.87
2:J:495:GLN:HG2	2:J:496:GLN:N	1.89	0.87
1:C:505:PRO:HB3	1:C:507:HIS:HB2	1.53	0.87
1:A:398:ALA:HB2	1:A:464:ARG:HE	1.39	0.87
1:A:153:PRO:HD3	1:A:316:VAL:HG23	1.55	0.87
1:G:278:ILE:H	1:G:278:ILE:CD1	1.83	0.87
1:I:170:MET:CE	1:I:309:ALA:HB1	2.05	0.87
2:D:492:ARG:HH22	2:J:74:ARG:NH2	1.72	0.87
1:E:153:PRO:HD3	1:E:316:VAL:HG23	1.56	0.87
1:A:393:GLY:O	1:A:396:LEU:HG	1.75	0.87
1:C:53:LEU:HD13	1:C:117:ALA:HB2	1.57	0.86
1:C:203:LEU:HD23	1:C:205:LYS:HZ3	1.39	0.86
1:K:285:VAL:HG12	1:K:286:VAL:HG22	1.56	0.86
1:E:272:ASN:OD1	1:E:377:LEU:HD13	1.75	0.86
1:G:251:LEU:CD2	1:G:328:ARG:HE	1.87	0.86
2:L:440:LEU:HD12	2:L:464:MET:HE2	1.56	0.86
1:E:112:ARG:HG3	1:E:112:ARG:HH11	1.39	0.86
2:F:137:ASP:OD1	2:F:139:THR:HG23	1.76	0.86
2:L:33:THR:HB	2:L:312:TYR:CE2	2.10	0.86
1:A:62:CYS:O	1:A:66:ARG:HG3	1.75	0.86
2:B:210:ALA:HB3	2:B:230:THR:HG23	1.57	0.86
1:E:350:ILE:HA	1:E:440:TRP:CZ3	2.09	0.86
2:D:119:ILE:HG23	2:D:152:LYS:HD3	1.58	0.86
1:E:179:PRO:HB2	1:E:198:ILE:HG12	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:586:SER:O	1:G:587:GLN:HB2	1.73	0.86
1:K:69:ARG:HB2	1:K:69:ARG:NH1	1.91	0.86
1:A:202:VAL:HG23	1:A:248:LYS:HA	1.56	0.86
1:E:339:ARG:HG3	1:E:339:ARG:HH11	1.40	0.86
2:B:33:THR:HB	2:B:312:TYR:HE2	1.39	0.85
1:E:232:GLN:HG2	1:E:233:ARG:HH12	1.41	0.85
2:F:560:VAL:HG23	2:H:202:SER:OG	1.76	0.85
2:F:82:LEU:HD12	2:F:83:VAL:H	1.40	0.85
2:B:81:LEU:HD11	2:B:89:ARG:NH2	1.90	0.85
1:E:613:ARG:O	1:E:614:ARG:HD2	1.76	0.85
1:I:612:LEU:N	1:I:612:LEU:HD12	1.90	0.85
2:L:231:VAL:CG2	2:L:275:HIS:HB2	2.06	0.85
2:L:81:LEU:HD13	2:L:280:ASP:HB2	1.58	0.85
1:E:562:ARG:NH1	1:E:562:ARG:HG2	1.88	0.85
1:A:188:LEU:HD23	1:A:228:LEU:HD23	1.59	0.85
1:C:451:LEU:O	1:C:455:LEU:HD12	1.75	0.85
2:H:161:LEU:O	2:H:161:LEU:HD12	1.77	0.85
2:H:207:PRO:HG2	2:H:294:LEU:CD2	2.06	0.85
1:I:412:PRO:HB2	1:I:450:ARG:HD3	1.59	0.85
2:J:83:VAL:HG13	2:J:84:ARG:H	1.42	0.85
2:L:53:VAL:O	2:L:57:ARG:HG3	1.76	0.85
1:K:264:ARG:HH11	1:K:264:ARG:HB3	1.41	0.85
2:B:467:ASN:HD22	2:B:467:ASN:H	1.21	0.84
1:I:607:ARG:HB3	1:I:607:ARG:HH11	1.41	0.84
2:F:62:ARG:O	2:F:65:GLU:HB2	1.77	0.84
2:J:440:LEU:HD12	2:J:464:MET:HG3	1.57	0.84
2:H:171:VAL:HG23	2:H:212:VAL:HA	1.59	0.84
1:I:519:SER:HB2	1:I:613:ARG:HE	1.41	0.84
1:I:605:VAL:HG12	1:K:96:VAL:CG1	2.07	0.84
1:K:150:LEU:HD23	1:K:359:GLN:HB3	1.59	0.84
1:K:309:ALA:O	1:K:312:ALA:HB3	1.75	0.84
1:K:57:ARG:HD2	1:K:107:TYR:CE2	2.12	0.84
1:C:569:ALA:O	1:C:571:PRO:HD3	1.78	0.84
1:E:198:ILE:HG23	1:E:248:LYS:HG2	1.59	0.84
2:B:311:LEU:HD12	2:B:342:SER:HB2	1.60	0.84
2:L:497:LEU:HD21	2:L:505:ILE:HD12	1.60	0.84
1:K:150:LEU:CD2	1:K:359:GLN:HB3	2.07	0.84
1:A:490:ALA:O	1:A:493:GLN:HB2	1.77	0.83
1:A:53:LEU:HD22	1:A:117:ALA:HB2	1.60	0.83
2:D:400:PHE:HB2	2:D:438:THR:CG2	2.07	0.83
1:G:536:PRO:HB3	2:H:363:HIS:CE1	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:370:LEU:HD22	1:K:374:GLN:HB3	1.58	0.83
2:B:145:TYR:CD1	2:B:149:THR:HB	2.12	0.83
2:F:83:VAL:HG13	2:F:84:ARG:H	1.43	0.83
1:A:232:GLN:H	1:A:233:ARG:CZ	1.91	0.83
1:E:129:TYR:CE2	1:E:342:VAL:HA	2.13	0.83
1:E:300:ARG:NH1	1:E:300:ARG:HB2	1.93	0.83
1:G:380:HIS:NE2	1:G:444:ARG:HD2	1.94	0.83
2:L:525:ARG:HG3	2:L:525:ARG:HH11	1.42	0.83
2:J:444:SER:HB2	2:J:470:ILE:HG13	1.59	0.83
2:B:83:VAL:CG1	2:B:84:ARG:H	1.92	0.83
2:H:109:TYR:HE1	2:H:148:LEU:HD12	1.43	0.83
1:C:351:THR:OG1	1:C:352:GLY:N	2.07	0.83
2:D:230:THR:CG2	2:D:273:ALA:HA	2.08	0.83
1:G:251:LEU:HD22	1:G:328:ARG:NE	1.93	0.83
2:H:246:LEU:H	2:H:246:LEU:HD12	1.42	0.83
1:K:82:ILE:HD11	1:K:430:TYR:CE1	2.14	0.83
2:L:150:VAL:HG21	2:L:184:VAL:HG13	1.61	0.83
2:L:377:PHE:N	2:L:377:PHE:CD1	2.44	0.83
1:C:263:ASP:CB	1:C:362:VAL:HG12	2.09	0.83
2:D:164:ARG:HB3	2:D:551:ALA:HB2	1.61	0.83
2:D:41:GLU:O	2:D:44:ALA:HB3	1.78	0.83
1:G:496:LEU:O	1:G:497:LEU:HD23	1.79	0.83
2:H:231:VAL:CG2	2:H:275:HIS:HB2	2.08	0.83
1:A:269:LEU:HD12	1:A:375:VAL:HG22	1.61	0.82
1:A:396:LEU:HD12	1:A:464:ARG:NH1	1.93	0.82
1:A:203:LEU:HG	1:A:204:LEU:N	1.93	0.82
2:F:305:ARG:CB	2:F:305:ARG:HH11	1.92	0.82
2:H:299:GLN:HB2	2:H:552:PRO:HD3	1.61	0.82
1:I:588:TYR:HB3	1:I:598:LEU:HD11	1.60	0.82
1:K:386:LEU:HD21	1:K:467:LEU:HD13	1.60	0.82
1:A:268:CYS:SG	1:A:307:VAL:HG23	2.18	0.82
1:C:496:LEU:O	1:C:497:LEU:HD23	1.78	0.82
1:E:187:ASP:OD1	1:E:189:GLU:HB2	1.79	0.82
2:H:350:LEU:H	2:H:350:LEU:CD2	1.91	0.82
1:A:269:LEU:HD12	1:A:375:VAL:CG2	2.09	0.82
1:G:313:ILE:HD11	1:G:315:TYR:HD2	1.43	0.82
2:H:433:ARG:H	2:H:556:THR:HG23	1.44	0.82
1:C:607:ARG:HH11	1:C:607:ARG:HB2	1.44	0.82
2:H:317:LEU:HA	2:H:320:VAL:HG23	1.60	0.82
1:I:352:GLY:C	1:I:353:LEU:HD23	1.99	0.82
2:L:207:PRO:HG2	2:L:294:LEU:HD22	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:GLU:HG2	2:D:282:HIS:ND1	1.93	0.82
2:D:375:ILE:HG22	2:D:376:LEU:H	1.45	0.82
1:A:200:TYR:HE1	1:A:221:GLU:HA	1.44	0.82
1:A:695:LYS:HB2	1:A:715:ASP:HB3	1.61	0.82
2:B:191:PHE:HD2	2:B:192:GLY:H	1.28	0.82
1:E:285:VAL:HG12	1:E:286:VAL:HG23	1.60	0.82
1:E:490:ALA:O	1:E:493:GLN:HB2	1.80	0.82
1:G:186:GLN:NE2	1:G:190:THR:H	1.77	0.82
1:I:607:ARG:HG3	1:K:94:ILE:HG13	1.60	0.82
1:K:379:GLY:HA3	1:K:440:TRP:CZ2	2.15	0.82
1:C:108:LEU:HD23	1:C:132:LEU:CD1	2.09	0.82
1:C:611:ALA:CB	1:C:620:LEU:HD13	2.09	0.82
1:E:384:VAL:CG1	1:E:470:LEU:HD22	2.09	0.81
2:F:30:ILE:HD12	2:F:311:LEU:HD11	1.62	0.81
2:F:57:ARG:HG3	2:F:57:ARG:HH11	1.43	0.81
2:B:460:ARG:NH1	2:B:548:ALA:HB1	1.95	0.81
1:G:201:PRO:HG2	1:G:328:ARG:HH21	1.44	0.81
1:I:525:ARG:HH11	1:I:525:ARG:HB3	1.46	0.81
2:B:486:LYS:HG3	2:B:497:LEU:HD11	1.61	0.81
1:I:344:HIS:HB2	1:I:355:LEU:HD12	1.62	0.81
2:H:164:ARG:HD3	2:H:550:ASN:O	1.81	0.81
1:A:103:PRO:O	1:A:108:LEU:HD12	1.80	0.81
1:C:561:ARG:NH1	1:C:561:ARG:HB3	1.96	0.81
2:J:375:ILE:HD12	2:J:375:ILE:H	1.45	0.81
2:J:518:HIS:ND1	2:J:519:PRO:HD2	1.94	0.81
2:L:62:ARG:HG2	2:L:62:ARG:HH11	1.45	0.81
1:A:249:TYR:HD2	1:A:250:LEU:H	1.23	0.81
2:D:472:VAL:HG22	2:D:473:MET:HG2	1.62	0.81
1:I:73:ILE:HD11	1:I:364:ARG:HH22	1.46	0.81
1:K:469:PHE:O	1:K:473:ILE:HG22	1.81	0.81
1:K:539:ARG:HH21	2:L:363:HIS:CE1	1.99	0.81
1:A:562:ARG:HH11	1:A:562:ARG:CB	1.94	0.81
1:C:201:PRO:HD2	1:C:328:ARG:NH2	1.95	0.81
2:F:518:HIS:ND1	2:F:519:PRO:HD2	1.96	0.81
2:F:48:THR:O	2:F:52:GLN:HG3	1.80	0.81
1:K:350:ILE:HA	1:K:440:TRP:HZ3	1.44	0.81
2:B:420:LYS:HB3	2:L:272:VAL:HG22	1.60	0.80
2:D:230:THR:HG22	2:D:273:ALA:HA	1.63	0.80
1:G:232:GLN:HG2	1:G:233:ARG:NH1	1.95	0.80
1:K:53:LEU:HD13	1:K:117:ALA:HB2	1.62	0.80
1:A:442:GLU:OE2	1:A:446:GLU:HG2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ILE:HG23	1:C:488:PHE:HD2	1.44	0.80
1:E:251:LEU:HD12	1:E:251:LEU:N	1.96	0.80
2:J:444:SER:HB3	2:J:449:ASN:HD22	1.46	0.80
1:E:108:LEU:HA	1:E:132:LEU:HD21	1.63	0.80
2:F:490:ALA:O	2:F:495:GLN:HG3	1.80	0.80
1:I:476:HIS:ND1	1:I:477:PRO:HD2	1.97	0.80
1:A:292:PRO:HG2	1:A:484:LEU:HD11	1.63	0.80
2:F:161:LEU:HD22	2:F:201:MET:HG2	1.64	0.80
2:H:350:LEU:HD23	2:H:350:LEU:N	1.95	0.80
2:H:400:PHE:CE2	2:H:453:CYS:HB2	2.16	0.80
1:C:218:VAL:HA	1:C:223:GLU:OE2	1.81	0.80
2:H:35:ILE:HD12	2:H:320:VAL:HG13	1.61	0.80
2:L:54:ASN:HA	2:L:57:ARG:HD3	1.64	0.80
1:A:469:PHE:HZ	1:A:489:ILE:HD11	1.47	0.80
2:B:375:ILE:HG22	2:B:376:LEU:H	1.46	0.80
1:E:536:PRO:HB3	2:F:363:HIS:CE1	2.17	0.80
2:J:35:ILE:HD11	2:J:337:ARG:HH12	1.45	0.80
1:K:590:LEU:HD13	1:K:598:LEU:HD12	1.64	0.80
1:K:405:TYR:HB3	1:K:422:GLU:HB2	1.64	0.80
1:K:66:ARG:CB	1:K:66:ARG:HH11	1.94	0.80
1:A:492:HIS:ND1	1:A:492:HIS:N	2.29	0.80
2:B:439:VAL:HG22	2:B:463:TRP:HB2	1.63	0.80
1:G:257:GLU:O	1:G:273:GLU:HB2	1.82	0.80
1:K:490:ALA:O	1:K:493:GLN:HB2	1.82	0.80
2:B:138:ALA:HB2	2:B:172:ASP:OD2	1.80	0.80
1:C:186:GLN:NE2	1:C:190:THR:H	1.80	0.80
1:C:469:PHE:CE2	1:C:473:ILE:HD12	2.17	0.79
1:K:384:VAL:CG1	1:K:470:LEU:HD22	2.11	0.79
1:K:69:ARG:HH11	1:K:69:ARG:HB2	1.44	0.79
2:J:201:MET:CE	2:J:208:GLN:HE22	1.93	0.79
2:J:331:VAL:HB	2:J:373:ASN:ND2	1.97	0.79
1:G:150:LEU:HD23	1:G:363:ALA:HB2	1.64	0.79
1:I:73:ILE:HD11	1:I:364:ARG:NH2	1.96	0.79
2:J:375:ILE:HG22	2:J:376:LEU:H	1.47	0.79
2:J:538:ARG:HG3	2:J:538:ARG:NH1	1.90	0.79
1:A:681:LYS:HG2	3:A:801:BTI:O11	1.83	0.79
1:K:463:LEU:HD22	1:K:464:ARG:H	1.47	0.79
1:K:505:PRO:CB	1:K:507:HIS:HB2	2.13	0.79
1:A:278:ILE:HG21	1:A:473:ILE:HD11	1.64	0.79
1:C:81:ASP:O	1:C:84:ARG:HG2	1.81	0.79
2:H:172:ASP:OD1	2:H:214:GLY:HA3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:MET:HA	1:C:334:MET:CE	2.12	0.79
1:C:501:GLN:HE21	1:C:504:LEU:HD23	1.46	0.79
1:E:395:PHE:O	1:E:397:PRO:HD3	1.81	0.79
1:C:328:ARG:HG3	1:C:328:ARG:NH1	1.97	0.79
2:H:376:LEU:HD23	2:H:380:ALA:HB3	1.62	0.79
1:I:258:ILE:HD13	1:I:303:GLY:HA2	1.65	0.79
2:B:473:MET:HE1	2:L:246:LEU:HD21	1.63	0.79
2:D:299:GLN:CB	2:D:552:PRO:HD3	2.13	0.79
1:E:252:LYS:HE3	1:E:491:ARG:HH22	1.45	0.79
1:G:70:ALA:O	1:K:450:ARG:HD3	1.82	0.79
2:H:212:VAL:O	2:H:233:VAL:HG23	1.81	0.79
1:C:605:VAL:O	1:C:605:VAL:HG23	1.81	0.79
2:F:35:ILE:HD12	2:F:337:ARG:NH2	1.97	0.79
2:H:231:VAL:HG23	2:H:275:HIS:HB2	1.65	0.79
1:I:602:VAL:HG23	1:I:605:VAL:HG23	1.63	0.79
1:K:251:LEU:CD1	1:K:327:GLU:HB2	2.13	0.79
1:K:512:ALA:HB1	1:K:629:ILE:HD13	1.64	0.79
1:K:63:ARG:HA	1:K:66:ARG:HD3	1.65	0.79
1:C:294:LEU:CD1	1:C:299:ARG:HH12	1.96	0.79
1:C:607:ARG:CB	1:C:607:ARG:HH11	1.96	0.79
1:A:605:VAL:O	1:A:605:VAL:HG23	1.83	0.78
1:G:605:VAL:HG23	1:G:605:VAL:O	1.81	0.78
1:K:279:GLN:HE21	1:K:282:HIS:HA	1.46	0.78
1:K:463:LEU:CD2	1:K:464:ARG:H	1.94	0.78
1:C:450:ARG:O	1:C:453:ALA:HB3	1.83	0.78
2:F:81:LEU:HD12	2:F:280:ASP:HB3	1.64	0.78
1:C:108:LEU:HD23	1:C:132:LEU:HD13	1.63	0.78
2:D:217:THR:CG2	2:D:240:PHE:HE1	1.94	0.78
1:G:231:ALA:HB3	1:G:244:MET:HE3	1.64	0.78
2:J:332:ARG:HH11	2:J:332:ARG:HG3	1.47	0.78
2:L:193:ARG:HD2	2:L:196:PHE:HD2	1.47	0.78
1:A:682:MET:HA	2:F:326:LYS:HB3	1.66	0.78
2:H:305:ARG:NH1	2:H:305:ARG:HB3	1.99	0.78
1:I:279:GLN:O	1:I:489:ILE:HG21	1.81	0.78
2:J:300:GLY:HA3	2:J:549:LEU:HD23	1.64	0.78
1:I:255:HIS:CE1	1:I:322:GLU:HG2	2.18	0.78
1:G:186:GLN:HE22	1:G:190:THR:H	1.28	0.78
1:I:118:LEU:HD13	1:I:147:LEU:HD21	1.65	0.78
2:J:145:TYR:HD1	2:J:149:THR:HB	1.48	0.78
1:K:378:ASN:O	1:K:440:TRP:CH2	2.34	0.78
2:B:487:ARG:HB2	2:B:497:LEU:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:ILE:HD11	1:E:430:TYR:CE1	2.19	0.78
2:F:444:SER:HB2	2:F:470:ILE:HG13	1.64	0.78
1:I:473:ILE:HB	1:I:496:LEU:HD13	1.64	0.78
1:A:273:GLU:OE1	1:A:273:GLU:N	2.16	0.78
1:E:505:PRO:HB3	1:E:507:HIS:CB	2.14	0.78
1:K:109:ARG:HH11	1:K:109:ARG:HB3	1.48	0.78
1:A:186:GLN:HE21	1:A:187:ASP:N	1.80	0.78
2:B:346:GLU:OE1	2:B:356:VAL:HG13	1.82	0.78
1:E:150:LEU:HD22	1:E:359:GLN:HB3	1.66	0.78
2:H:311:LEU:HB2	2:H:342:SER:OG	1.84	0.78
2:B:467:ASN:N	2:B:467:ASN:HD22	1.82	0.77
1:E:264:ARG:HH11	1:E:264:ARG:HG2	1.49	0.77
2:H:307:PRO:HB3	2:H:363:HIS:HD2	1.47	0.77
1:K:274:ARG:HH11	1:K:347:THR:HB	1.49	0.77
1:K:46:TYR:HE1	1:K:366:GLU:HG3	1.47	0.77
2:B:425:LEU:O	2:B:429:VAL:HG23	1.83	0.77
1:C:251:LEU:HD11	1:C:328:ARG:HH21	1.50	0.77
1:C:334:MET:HA	1:C:334:MET:HE2	1.63	0.77
1:G:185:ALA:HB2	1:G:243:ARG:HG3	1.67	0.77
1:G:249:TYR:HD2	1:G:250:LEU:N	1.81	0.77
1:K:105:ASP:O	1:K:109:ARG:HD2	1.84	0.77
2:L:132:MET:HE3	2:L:156:ALA:O	1.85	0.77
2:L:365:TYR:HB2	2:L:545:LEU:HD13	1.65	0.77
2:B:117:ALA:O	2:B:149:THR:HG23	1.83	0.77
2:B:231:VAL:HG22	2:B:275:HIS:HB2	1.64	0.77
1:I:150:LEU:HD22	1:I:359:GLN:HB3	1.66	0.77
1:A:384:VAL:HG11	1:A:470:LEU:HD13	1.66	0.77
2:B:48:THR:O	2:B:52:GLN:HG3	1.85	0.77
1:C:294:LEU:HD11	1:C:299:ARG:HH12	1.49	0.77
2:D:389:GLU:HG2	2:H:560:VAL:HG13	1.66	0.77
1:A:380:HIS:NE2	1:A:444:ARG:HD2	1.99	0.77
1:C:53:LEU:HD13	1:C:117:ALA:CB	2.13	0.77
2:D:242:ALA:HB1	2:D:246:LEU:HD22	1.66	0.77
1:K:396:LEU:HD12	1:K:464:ARG:HH22	1.50	0.77
1:E:165:ALA:O	1:E:169:LEU:HD13	1.83	0.77
1:E:611:ALA:HB2	1:E:620:LEU:HD13	1.67	0.77
1:I:599:VAL:HG22	1:I:608:ARG:CB	2.14	0.77
1:G:203:LEU:HD12	1:G:204:LEU:N	2.00	0.77
2:H:198:GLN:HG2	2:H:208:GLN:OE1	1.85	0.77
2:H:498:GLY:O	2:H:500:GLU:N	2.17	0.77
1:K:567:ARG:HG3	1:K:567:ARG:HH11	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:VAL:HG21	1:A:674:LEU:CD2	2.15	0.77
1:E:616:ARG:O	1:E:616:ARG:HG3	1.84	0.77
2:J:41:GLU:O	2:J:44:ALA:HB3	1.84	0.77
1:A:525:ARG:HB3	1:A:525:ARG:NH1	2.00	0.77
1:C:228:LEU:HD23	1:C:229:SER:N	1.99	0.77
1:G:182:HIS:HB3	1:G:245:LEU:CD2	2.14	0.77
2:H:81:LEU:CD2	2:H:85:GLU:HB3	2.15	0.77
1:I:602:VAL:O	1:I:605:VAL:HG22	1.85	0.77
1:K:397:PRO:HB3	1:K:432:PRO:HG3	1.65	0.77
2:L:161:LEU:HD22	2:L:201:MET:CG	2.14	0.77
1:A:395:PHE:O	1:A:397:PRO:HD3	1.85	0.76
1:C:501:GLN:NE2	1:C:504:LEU:HD23	2.00	0.76
2:H:217:THR:HG22	2:H:240:PHE:CE1	2.20	0.76
2:J:469:ARG:NH2	2:J:469:ARG:HG2	1.99	0.76
1:A:232:GLN:HG2	1:A:233:ARG:HH11	1.48	0.76
1:C:504:LEU:CB	1:C:505:PRO:HD2	2.12	0.76
2:D:441:ILE:HG22	2:D:465:TRP:CD2	2.21	0.76
2:J:289:ARG:O	2:J:292:ALA:HB3	1.85	0.76
1:A:662:VAL:HG22	1:A:674:LEU:HA	1.67	0.76
1:A:53:LEU:HD12	1:A:76:VAL:O	1.84	0.76
1:C:300:ARG:NH1	1:C:300:ARG:HB2	1.99	0.76
1:C:503:ALA:O	1:C:504:LEU:O	2.02	0.76
2:F:117:ALA:O	2:F:149:THR:HG23	1.84	0.76
2:F:35:ILE:HD13	2:F:320:VAL:HG22	1.65	0.76
1:G:170:MET:SD	1:G:309:ALA:HB1	2.25	0.76
2:F:202:SER:OG	2:H:560:VAL:HG23	1.84	0.76
2:L:189:GLU:N	2:L:189:GLU:CD	2.32	0.76
2:H:275:HIS:HE1	2:L:347:PHE:HA	1.50	0.76
1:C:49:ILE:HD12	1:C:49:ILE:N	2.00	0.76
2:D:188:ARG:NH1	2:D:188:ARG:HB3	1.99	0.76
2:D:433:ARG:HG2	2:D:556:THR:HG23	1.67	0.76
2:F:390:LEU:O	2:F:394:ARG:HG3	1.85	0.76
2:L:74:ARG:NH2	2:L:78:ARG:HH12	1.83	0.76
2:B:155:ARG:O	2:B:159:ILE:HD13	1.85	0.76
1:I:278:ILE:HG21	1:I:473:ILE:HD11	1.67	0.76
1:A:544:ARG:HG2	1:A:544:ARG:NH1	1.94	0.76
1:C:383:GLU:HB2	1:C:438:ILE:HG23	1.67	0.76
2:D:89:ARG:HG3	2:D:89:ARG:HH21	1.51	0.76
2:B:101:SER:O	2:B:152:LYS:HE3	1.86	0.76
1:C:607:ARG:NH1	1:C:607:ARG:HB2	2.00	0.76
1:E:504:LEU:CB	1:E:505:PRO:HD2	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:526:ASP:N	1:G:526:ASP:OD2	2.18	0.76
2:H:440:LEU:HD12	2:H:464:MET:HE2	1.68	0.76
2:L:483:ALA:HB3	2:L:506:LYS:HE2	1.68	0.76
1:I:152:PRO:HG2	1:I:338:THR:HB	1.68	0.76
1:K:257:GLU:O	1:K:273:GLU:HB2	1.85	0.76
1:K:605:VAL:O	1:K:605:VAL:HG23	1.85	0.76
1:E:387:TYR:CE1	1:E:433:MET:HB2	2.20	0.76
1:G:204:LEU:CD2	1:G:246:VAL:HG22	2.15	0.76
2:F:272:VAL:HG22	2:H:420:LYS:HB3	1.66	0.76
1:K:350:ILE:HA	1:K:440:TRP:CZ3	2.20	0.76
1:K:619:PHE:HB3	1:K:626:LEU:HD11	1.67	0.76
1:K:536:PRO:HD3	2:L:363:HIS:CD2	2.20	0.76
1:C:50:GLN:HB2	1:C:123:GLN:NE2	2.01	0.75
2:D:54:ASN:HA	2:D:57:ARG:HG3	1.68	0.75
1:G:473:ILE:HB	1:G:496:LEU:HD13	1.66	0.75
2:J:75:HIS:HE1	2:J:80:LYS:HE2	1.50	0.75
1:C:285:VAL:HG12	1:C:286:VAL:CG2	2.15	0.75
1:C:390:ASP:OD1	1:C:393:GLY:HA3	1.87	0.75
1:E:188:LEU:HD23	1:E:228:LEU:HD23	1.68	0.75
2:F:355:LEU:O	2:F:383:LYS:HE2	1.86	0.75
2:H:57:ARG:HG3	2:H:57:ARG:HH11	1.49	0.75
2:J:402:GLN:NE2	2:J:449:ASN:HA	2.01	0.75
1:A:201:PRO:HD2	1:A:328:ARG:HH21	1.50	0.75
1:A:697:LEU:HB3	1:A:712:VAL:HG22	1.68	0.75
2:D:422:GLY:O	2:D:426:VAL:HG23	1.87	0.75
2:F:168:ILE:HA	2:F:209:ILE:HG22	1.66	0.75
2:F:376:LEU:HG	2:F:404:ILE:CD1	2.15	0.75
2:F:525:ARG:HH11	2:F:525:ARG:HG3	1.51	0.75
2:F:72:GLN:HG3	2:F:82:LEU:HD21	1.68	0.75
2:H:109:TYR:CE1	2:H:148:LEU:HD12	2.21	0.75
1:I:104:ALA:HA	1:I:108:LEU:HD12	1.67	0.75
1:I:340:LEU:HD11	1:I:356:VAL:HG23	1.67	0.75
2:J:375:ILE:HD12	2:J:375:ILE:N	2.00	0.75
1:A:705:VAL:HG21	1:A:711:LEU:HD21	1.68	0.75
1:C:611:ALA:HB2	1:C:620:LEU:CD1	2.14	0.75
1:G:350:ILE:HD12	1:G:377:LEU:HD13	1.68	0.75
2:J:161:LEU:CD1	2:J:201:MET:HG2	2.15	0.75
1:E:561:ARG:H	1:E:561:ARG:HD2	1.51	0.75
1:G:190:THR:HG23	1:G:193:ARG:HH21	1.52	0.75
1:I:269:LEU:HA	1:I:372:GLN:NE2	2.02	0.75
2:L:403:ASN:CG	2:L:442:GLY:HA3	2.06	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:441:ILE:HG22	2:L:465:TRP:CD2	2.22	0.75
1:G:150:LEU:CD2	1:G:363:ALA:HB2	2.16	0.75
2:L:299:GLN:OE1	2:L:552:PRO:HD3	1.86	0.75
1:C:395:PHE:O	1:C:397:PRO:HD3	1.86	0.75
1:E:278:ILE:HD11	1:E:484:LEU:HD23	1.69	0.75
2:F:161:LEU:HD22	2:F:201:MET:CG	2.17	0.75
1:G:254:ARG:HH12	1:G:293:GLY:H	1.32	0.75
1:A:666:GLN:O	1:A:693:VAL:HG13	1.87	0.74
1:E:170:MET:SD	1:E:309:ALA:HB1	2.27	0.74
2:F:218:ALA:O	2:F:221:ALA:HB3	1.87	0.74
1:A:525:ARG:CB	1:A:525:ARG:HH11	1.97	0.74
2:B:501:GLU:O	2:B:505:ILE:HG13	1.87	0.74
1:C:273:GLU:OE1	1:C:273:GLU:N	2.20	0.74
1:C:328:ARG:HG3	1:C:328:ARG:HH11	1.52	0.74
1:G:519:SER:HB3	1:G:613:ARG:HE	1.52	0.74
1:C:53:LEU:HD13	1:C:117:ALA:CA	2.17	0.74
2:J:35:ILE:HD11	2:J:337:ARG:NH1	2.02	0.74
1:A:440:TRP:C	1:A:440:TRP:CD1	2.60	0.74
1:C:233:ARG:HH11	1:C:233:ARG:HB3	1.52	0.74
1:C:315:TYR:OH	1:C:338:THR:HA	1.87	0.74
1:E:605:VAL:HG23	1:E:605:VAL:O	1.86	0.74
2:F:376:LEU:HG	2:F:404:ILE:HD11	1.67	0.74
2:H:375:ILE:HG22	2:H:376:LEU:N	2.03	0.74
2:H:476:GLU:HA	2:H:510:LEU:HD21	1.69	0.74
1:K:108:LEU:HD23	1:K:132:LEU:HD12	1.69	0.74
1:A:249:TYR:HD2	1:A:250:LEU:N	1.85	0.74
1:A:657:ILE:CD1	1:A:699:CYS:HB2	2.18	0.74
2:B:244:PRO:HA	2:B:247:VAL:HG12	1.69	0.74
1:C:135:ASN:OD1	1:C:135:ASN:O	2.05	0.74
1:G:204:LEU:HD23	1:G:246:VAL:HG22	1.69	0.74
1:G:519:SER:CB	1:G:613:ARG:HE	1.99	0.74
1:I:261:PHE:CE1	1:I:318:ALA:HB2	2.22	0.74
1:A:280:ARG:O	1:A:281:ARG:C	2.25	0.74
1:C:300:ARG:CZ	1:C:300:ARG:HB2	2.17	0.74
1:C:81:ASP:OD2	1:C:100:GLY:HA2	1.87	0.74
2:F:305:ARG:HH11	2:F:305:ARG:HB2	1.52	0.74
1:K:508:PHE:CZ	1:K:627:LEU:HD12	2.23	0.74
2:B:403:ASN:ND2	2:B:442:GLY:HA3	2.02	0.74
2:D:177:ASN:OD1	2:D:180:ARG:HG3	1.88	0.74
2:D:344:PHE:CZ	2:D:358:GLY:HA3	2.23	0.74
1:A:491:ARG:HB3	1:A:492:HIS:ND1	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:CD2	1:C:313:ILE:HG12	2.18	0.74
1:K:452:LEU:CD2	1:K:474:LEU:HB3	2.17	0.74
2:F:225:ALA:O	2:H:562:ARG:HD2	1.87	0.74
2:F:432:ALA:HA	2:F:556:THR:HG21	1.69	0.74
1:K:270:TYR:N	1:K:372:GLN:HE22	1.85	0.74
1:K:408:ALA:HB2	1:K:457:GLU:HB2	1.69	0.74
1:E:251:LEU:HD11	1:E:328:ARG:CZ	2.17	0.73
1:G:607:ARG:HB2	1:G:607:ARG:NH1	2.02	0.73
2:F:241:LEU:HB2	2:H:414:GLU:OE2	1.88	0.73
1:K:302:MET:HG2	1:K:331:PHE:CD1	2.23	0.73
2:D:53:VAL:HG21	2:D:318:TYR:HE1	1.53	0.73
2:F:469:ARG:HH21	2:F:469:ARG:HG2	1.51	0.73
1:I:169:LEU:HD23	1:I:312:ALA:CB	2.19	0.73
2:F:109:TYR:CZ	2:F:148:LEU:HD12	2.23	0.73
2:F:243:GLY:O	2:F:247:VAL:HG23	1.88	0.73
1:G:383:GLU:HB2	1:G:438:ILE:HG23	1.68	0.73
1:K:287:GLU:HG2	1:K:343:GLU:HG3	1.70	0.73
1:K:549:ARG:HH21	1:K:571:PRO:HA	1.51	0.73
1:G:53:LEU:HD11	1:G:78:VAL:CG1	2.18	0.73
1:I:504:LEU:CD2	1:I:505:PRO:HD2	2.18	0.73
1:K:152:PRO:HG3	1:K:315:TYR:CE1	2.24	0.73
1:K:304:GLU:HA	1:K:307:VAL:CG1	2.17	0.73
1:A:496:LEU:O	1:A:497:LEU:HD23	1.89	0.73
1:C:322:GLU:OE2	1:C:337:ASN:ND2	2.21	0.73
2:F:433:ARG:HH22	2:F:554:GLU:HG3	1.52	0.73
1:G:452:LEU:CD2	1:G:474:LEU:HB3	2.19	0.73
1:A:339:ARG:HH11	1:A:339:ARG:HG3	1.53	0.73
1:G:390:ASP:OD1	1:G:393:GLY:HA3	1.89	0.73
1:A:655:GLY:N	2:H:251:THR:HB	2.04	0.73
1:I:358:TRP:O	1:I:362:VAL:HG22	1.89	0.73
2:D:178:LEU:CD1	2:J:478:ALA:HB1	2.19	0.73
1:K:566:LEU:C	1:K:567:ARG:HD3	2.09	0.73
2:L:432:ALA:HA	2:L:556:THR:HG21	1.69	0.73
1:A:267:HIS:HB3	1:A:368:LEU:HD12	1.69	0.73
1:C:258:ILE:HD11	1:C:302:MET:HB3	1.70	0.73
2:F:375:ILE:CD1	2:F:375:ILE:H	1.94	0.73
1:E:47:ARG:HG3	1:E:48:SER:N	2.03	0.73
1:E:459:SER:HB3	1:E:621:GLU:OE1	1.89	0.73
1:G:169:LEU:CD2	1:G:313:ILE:HG22	2.19	0.73
1:I:278:ILE:H	1:I:278:ILE:CD1	2.00	0.73
1:I:280:ARG:HD3	1:I:280:ARG:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:550:GLU:HG2	1:K:567:ARG:NH1	2.03	0.73
1:I:491:ARG:HD2	1:I:492:HIS:CE1	2.23	0.73
2:J:490:ALA:HB1	2:J:495:GLN:OE1	1.88	0.73
1:K:505:PRO:HB2	1:K:507:HIS:HB2	1.68	0.73
1:K:543:TRP:HB3	2:L:96:PRO:HB3	1.71	0.73
1:C:232:GLN:N	1:C:233:ARG:NH2	2.36	0.73
2:D:507:ALA:N	2:D:508:PRO:HD2	2.03	0.73
1:E:541:ASP:HB2	1:E:549:ARG:NH2	2.04	0.73
1:K:108:LEU:HD23	1:K:132:LEU:CD1	2.19	0.73
1:A:220:ARG:HB2	1:A:223:GLU:HB3	1.70	0.72
2:B:246:LEU:HG	2:L:481:VAL:HG21	1.70	0.72
1:C:263:ASP:HB3	1:C:362:VAL:HG12	1.70	0.72
2:D:420:LYS:HG3	2:D:421:HIS:N	2.03	0.72
1:G:47:ARG:HG2	1:G:148:LEU:HD11	1.71	0.72
1:G:567:ARG:HH11	1:G:567:ARG:HG3	1.51	0.72
1:A:96:VAL:CG1	1:E:605:VAL:HG12	2.19	0.72
1:E:152:PRO:HG2	1:E:338:THR:HB	1.71	0.72
2:F:435:PRO:CD	2:F:553:ILE:HD12	2.19	0.72
1:G:395:PHE:O	1:G:397:PRO:HD3	1.89	0.72
1:I:601:ARG:HH11	1:I:601:ARG:HB3	1.53	0.72
2:D:472:VAL:HG11	2:J:181:GLN:CB	2.18	0.72
2:L:215:SER:HA	2:L:238:THR:OG1	1.89	0.72
1:C:350:ILE:HA	1:C:440:TRP:HZ3	1.54	0.72
1:C:586:SER:O	1:C:587:GLN:HB2	1.89	0.72
1:I:308:ARG:HG3	1:I:308:ARG:HH11	1.53	0.72
1:A:654:ASN:HB2	2:H:251:THR:OG1	1.89	0.72
1:I:261:PHE:CE2	1:I:358:TRP:HB3	2.24	0.72
2:J:484:GLN:HE21	2:J:484:GLN:HA	1.54	0.72
1:K:170:MET:SD	1:K:309:ALA:HB1	2.29	0.72
1:K:320:THR:HG21	1:K:341:GLN:HG3	1.71	0.72
2:L:234:ARG:HA	2:L:263:ALA:CB	2.19	0.72
2:L:82:LEU:H	2:L:82:LEU:HD12	1.54	0.72
1:A:503:ALA:O	1:A:504:LEU:O	2.08	0.72
2:B:71:ALA:HA	2:B:74:ARG:HB3	1.70	0.72
2:D:164:ARG:CB	2:D:551:ALA:HB2	2.18	0.72
2:D:379:GLU:OE1	2:D:379:GLU:N	2.23	0.72
1:E:569:ALA:O	1:E:571:PRO:HD3	1.89	0.72
1:G:313:ILE:HD11	1:G:315:TYR:CD2	2.25	0.72
2:L:81:LEU:HD21	2:L:89:ARG:NH2	2.04	0.72
2:B:212:VAL:HG21	2:B:239:ILE:HD11	1.71	0.72
1:C:188:LEU:HG	1:C:228:LEU:HD22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:THR:HG22	1:C:467:LEU:N	1.97	0.72
1:C:596:ASP:HB3	1:C:612:LEU:HD23	1.71	0.72
1:E:549:ARG:NH1	1:E:549:ARG:HG2	1.90	0.72
2:H:36:ASN:HD21	2:H:38:ARG:HD3	1.52	0.72
2:H:518:HIS:ND1	2:H:519:PRO:HD2	2.03	0.72
1:I:84:ARG:NH2	1:I:97:ASP:OD2	2.23	0.72
1:K:390:ASP:OD1	1:K:393:GLY:HA3	1.88	0.72
1:A:476:HIS:CE1	1:A:492:HIS:HD2	2.08	0.72
2:F:180:ARG:NH1	2:F:180:ARG:HG3	1.98	0.72
2:H:114:VAL:HG11	2:H:146:TYR:CZ	2.24	0.72
2:H:170:LEU:HD23	2:H:211:VAL:HB	1.72	0.72
1:I:421:ARG:HD3	1:I:424:ASP:OD2	1.90	0.72
1:I:54:VAL:O	1:I:54:VAL:HG12	1.89	0.72
2:J:438:THR:HB	2:J:462:LEU:HG	1.71	0.72
2:J:488:GLU:O	2:J:492:ARG:HG2	1.90	0.72
2:L:350:LEU:H	2:L:350:LEU:CD2	2.03	0.72
2:L:487:ARG:HG3	2:L:487:ARG:O	1.89	0.72
1:A:673:THR:HG21	1:A:676:VAL:HG22	1.72	0.72
1:A:96:VAL:HG13	1:E:605:VAL:HG12	1.70	0.72
1:G:326:ASP:OD1	1:G:328:ARG:HG2	1.89	0.72
1:G:504:LEU:HD13	1:G:622:TRP:HE1	1.55	0.72
1:K:401:ARG:NH1	1:K:401:ARG:HB3	2.00	0.72
1:A:150:LEU:CD2	1:A:363:ALA:HB2	2.19	0.72
1:E:525:ARG:HH11	1:E:525:ARG:HG2	1.55	0.72
1:I:346:VAL:O	1:I:349:ALA:HB3	1.89	0.72
2:L:53:VAL:HG12	2:L:57:ARG:HD2	1.72	0.72
1:A:351:THR:OG1	1:A:352:GLY:N	2.23	0.72
1:C:275:ASP:OD2	1:C:484:LEU:HD22	1.89	0.72
1:C:347:THR:O	1:C:351:THR:HG23	1.89	0.72
2:D:201:MET:HG2	2:D:206:ILE:HD12	1.70	0.72
2:D:351:PHE:CE2	2:D:379:GLU:HB3	2.24	0.72
1:E:467:LEU:HD12	1:E:467:LEU:O	1.90	0.72
1:I:251:LEU:HD11	1:I:328:ARG:NH2	2.03	0.72
1:I:505:PRO:CB	1:I:507:HIS:HB3	2.20	0.72
2:D:472:VAL:CG1	2:J:181:GLN:HB2	2.20	0.72
1:E:53:LEU:HD13	1:E:117:ALA:CB	2.19	0.71
2:J:119:ILE:CG2	2:J:152:LYS:HD3	2.18	0.71
1:C:186:GLN:HE22	1:C:190:THR:H	1.37	0.71
1:C:526:ASP:N	1:C:526:ASP:OD2	2.10	0.71
2:F:75:HIS:CE1	2:F:80:LYS:HE2	2.25	0.71
1:I:81:ASP:HB2	1:I:100:GLY:HA2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:486:LYS:HG2	2:J:505:ILE:HD12	1.70	0.71
1:C:320:THR:OG1	1:C:341:GLN:HG2	1.90	0.71
2:D:560:VAL:HG13	2:H:389:GLU:HB3	1.71	0.71
1:E:550:GLU:HG3	1:E:567:ARG:CD	2.16	0.71
1:E:516:TRP:CD2	1:E:555:LEU:HD21	2.25	0.71
2:F:231:VAL:HG22	2:F:275:HIS:CB	2.10	0.71
2:H:440:LEU:HD12	2:H:464:MET:HG3	1.72	0.71
2:H:498:GLY:C	2:H:500:GLU:H	1.93	0.71
2:L:218:ALA:O	2:L:221:ALA:HB3	1.91	0.71
2:B:194:ILE:HD12	2:B:194:ILE:N	2.03	0.71
1:C:198:ILE:HG23	1:C:248:LYS:HG2	1.72	0.71
1:C:50:GLN:H	1:C:123:GLN:HE21	1.39	0.71
1:G:393:GLY:O	1:G:396:LEU:HG	1.90	0.71
1:I:384:VAL:CG1	1:I:470:LEU:HD22	2.20	0.71
1:I:65:MET:HG3	1:I:75:SER:HB2	1.72	0.71
1:K:504:LEU:HD23	1:K:505:PRO:HD2	1.72	0.71
2:L:83:VAL:HG13	2:L:84:ARG:N	2.05	0.71
1:A:306:ALA:HB1	1:A:321:VAL:HG21	1.72	0.71
2:D:440:LEU:HB2	2:D:464:MET:HG3	1.70	0.71
1:G:473:ILE:HB	1:G:496:LEU:CD1	2.20	0.71
1:A:274:ARG:NH2	1:A:320:THR:HG21	2.04	0.71
1:C:613:ARG:O	1:C:614:ARG:HD2	1.90	0.71
1:E:553:LEU:O	1:E:564:VAL:HG22	1.89	0.71
1:K:54:VAL:CG1	1:K:64:VAL:HG11	2.20	0.71
1:E:218:VAL:O	1:E:218:VAL:HG23	1.89	0.71
1:E:261:PHE:CE1	1:E:318:ALA:HB2	2.26	0.71
1:E:344:HIS:ND1	1:E:345:PRO:HD3	2.05	0.71
1:E:525:ARG:NH1	1:E:525:ARG:HG2	2.03	0.71
2:H:417:GLY:C	2:H:419:ALA:H	1.94	0.71
1:C:287:GLU:OE2	1:C:287:GLU:N	2.24	0.71
1:C:440:TRP:CD1	1:C:440:TRP:C	2.64	0.71
1:C:61:ALA:O	1:C:65:MET:HB2	1.91	0.71
2:D:298:LYS:HE3	2:D:550:ASN:ND2	2.06	0.71
2:D:472:VAL:HG11	2:J:181:GLN:HB2	1.73	0.71
1:K:153:PRO:HD3	1:K:316:VAL:CG2	2.19	0.71
1:K:428:PRO:HG2	1:K:429:PHE:CE2	2.25	0.71
1:A:261:PHE:CD1	1:A:358:TRP:HE3	2.09	0.71
2:D:331:VAL:O	2:D:334:VAL:HG23	1.90	0.71
2:F:207:PRO:HG2	2:F:294:LEU:HD22	1.71	0.71
2:H:62:ARG:O	2:H:65:GLU:HB2	1.90	0.71
2:J:152:LYS:HA	2:J:526:LEU:HD21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:255:HIS:HE1	1:K:322:GLU:HG3	1.55	0.71
1:K:380:HIS:NE2	1:K:444:ARG:HG3	2.05	0.71
1:A:111:ASP:O	1:A:114:ILE:HG22	1.91	0.71
1:E:586:SER:O	1:E:587:GLN:HB2	1.90	0.71
1:I:270:TYR:H	1:I:372:GLN:HE22	1.39	0.71
1:I:504:LEU:HD23	1:I:505:PRO:HD2	1.71	0.71
1:I:681:LYS:HG2	3:I:801:BTI:O11	1.90	0.71
1:A:125:ILE:HD12	1:A:142:CYS:SG	2.31	0.70
1:A:344:HIS:ND1	1:A:345:PRO:HD3	2.06	0.70
1:I:144:GLU:HG2	1:I:144:GLU:O	1.90	0.70
1:A:152:PRO:HG2	1:A:338:THR:HB	1.73	0.70
1:A:384:VAL:CG2	1:A:451:LEU:HD21	2.20	0.70
1:A:567:ARG:NH1	1:A:567:ARG:HG3	1.99	0.70
1:C:372:GLN:O	1:C:375:VAL:HG22	1.90	0.70
1:E:275:ASP:OD2	1:E:484:LEU:HD22	1.91	0.70
1:E:315:TYR:OH	1:E:338:THR:HA	1.92	0.70
1:E:503:ALA:O	1:E:504:LEU:O	2.10	0.70
1:I:65:MET:HE1	1:I:92:ALA:HB2	1.73	0.70
2:D:49:MET:HG3	2:D:318:TYR:HD1	1.56	0.70
1:E:279:GLN:O	1:E:489:ILE:HG21	1.91	0.70
1:K:46:TYR:CE1	1:K:366:GLU:HG3	2.27	0.70
1:G:52:LEU:HD12	1:G:124:ALA:O	1.92	0.70
1:G:165:ALA:O	1:G:169:LEU:HD13	1.91	0.70
1:G:532:ASP:OD2	1:G:535:SER:HB2	1.91	0.70
1:A:562:ARG:NH1	1:A:562:ARG:HB3	2.00	0.70
2:D:299:GLN:HB2	2:D:552:PRO:HD3	1.72	0.70
1:E:200:TYR:O	1:E:202:VAL:N	2.24	0.70
1:E:390:ASP:OD1	1:E:464:ARG:HD2	1.90	0.70
2:H:405:THR:OG1	1:I:681:LYS:HG3	1.91	0.70
1:K:278:ILE:HD12	1:K:278:ILE:H	1.55	0.70
1:K:305:ALA:HA	1:K:308:ARG:HG3	1.73	0.70
1:G:218:VAL:HG11	1:G:224:LEU:HD13	1.74	0.70
1:G:280:ARG:O	1:G:281:ARG:C	2.30	0.70
1:G:588:TYR:HB3	1:G:598:LEU:HD11	1.72	0.70
2:H:533:ASP:HB3	2:H:536:GLN:HE21	1.57	0.70
1:I:444:ARG:HG2	1:I:444:ARG:HH11	1.55	0.70
1:I:586:SER:O	1:I:587:GLN:HB2	1.91	0.70
1:K:612:LEU:N	1:K:612:LEU:HD12	2.05	0.70
1:A:204:LEU:CD2	1:A:246:VAL:HG22	2.21	0.70
1:A:605:VAL:CG1	1:C:96:VAL:HG13	2.21	0.70
2:B:277:ALA:HB2	2:B:286:ILE:HD12	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLN:O	1:C:489:ILE:HG21	1.92	0.70
1:E:165:ALA:O	1:E:168:ALA:HB3	1.91	0.70
1:G:315:TYR:OH	1:G:338:THR:HA	1.92	0.70
1:I:150:LEU:HD21	1:I:359:GLN:O	1.92	0.70
1:I:452:LEU:HD23	1:I:474:LEU:HB3	1.74	0.70
1:I:608:ARG:HH22	1:K:90:ALA:HA	1.56	0.70
1:A:470:LEU:HA	1:A:473:ILE:HG22	1.73	0.70
1:G:517:LEU:HD22	1:G:553:LEU:HD11	1.74	0.70
2:H:444:SER:HB3	2:H:449:ASN:HD22	1.56	0.70
1:I:169:LEU:CD2	1:I:312:ALA:HB1	2.21	0.70
1:A:607:ARG:HG3	1:C:94:ILE:HG13	1.74	0.70
1:A:703:GLU:HG2	1:A:705:VAL:HG13	1.74	0.70
2:B:339:VAL:HG23	2:B:342:SER:HA	1.74	0.70
2:B:82:LEU:N	2:B:82:LEU:HD12	2.05	0.70
1:E:278:ILE:CD1	1:E:278:ILE:H	1.93	0.70
1:A:379:GLY:HA3	1:A:440:TRP:CH2	2.27	0.69
2:D:369:ILE:HG12	2:D:399:LEU:HD23	1.73	0.69
1:G:302:MET:HG2	1:G:331:PHE:CE2	2.26	0.69
1:G:440:TRP:CD1	1:G:440:TRP:C	2.65	0.69
2:B:84:ARG:HH11	2:B:84:ARG:HG2	1.57	0.69
1:E:308:ARG:HG3	1:E:308:ARG:NH1	2.05	0.69
1:E:152:PRO:HG3	1:E:315:TYR:CZ	2.27	0.69
2:F:83:VAL:HG13	2:F:84:ARG:N	2.05	0.69
1:G:503:ALA:HB2	1:G:560:GLU:OE1	1.92	0.69
2:H:201:MET:HG2	2:H:206:ILE:HB	1.74	0.69
2:H:315:GLU:CD	2:H:315:GLU:H	1.95	0.69
1:I:316:VAL:HG12	1:I:317:GLY:N	2.07	0.69
2:J:234:ARG:HA	2:J:263:ALA:CB	2.22	0.69
1:K:470:LEU:HA	1:K:473:ILE:CG2	2.22	0.69
1:K:448:ARG:HD3	1:K:474:LEU:O	1.92	0.69
1:K:496:LEU:O	1:K:497:LEU:HD23	1.90	0.69
1:A:200:TYR:O	1:A:202:VAL:N	2.25	0.69
1:A:384:VAL:HG23	1:A:451:LEU:HD21	1.74	0.69
2:D:315:GLU:N	2:D:315:GLU:OE1	2.24	0.69
1:E:118:LEU:CD1	1:E:147:LEU:HD21	2.22	0.69
2:L:81:LEU:HD13	2:L:280:ASP:CB	2.21	0.69
1:A:398:ALA:HB2	1:A:464:ARG:NE	2.08	0.69
1:A:384:VAL:CG1	1:A:470:LEU:HD13	2.22	0.69
2:H:350:LEU:N	2:H:350:LEU:CD2	2.54	0.69
1:I:607:ARG:HH11	1:I:607:ARG:CB	2.06	0.69
1:K:304:GLU:CA	1:K:307:VAL:HG12	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:TYR:HB3	1:C:422:GLU:HB2	1.74	0.69
1:E:300:ARG:NH1	1:E:300:ARG:CB	2.55	0.69
1:G:274:ARG:HH22	1:G:320:THR:HG21	1.57	0.69
2:H:375:ILE:CG2	2:H:376:LEU:H	2.00	0.69
2:B:188:ARG:N	2:L:455:ARG:HG3	2.08	0.69
1:A:261:PHE:CE2	1:A:318:ALA:HB2	2.28	0.69
1:A:470:LEU:HA	1:A:473:ILE:CG2	2.21	0.69
1:E:289:ALA:HB1	1:E:350:ILE:HD13	1.74	0.69
1:G:398:ALA:HB2	1:G:464:ARG:NE	2.07	0.69
1:I:278:ILE:CG2	1:I:489:ILE:HD13	2.22	0.69
2:J:441:ILE:O	2:J:441:ILE:HD12	1.93	0.69
1:K:153:PRO:O	1:K:157:ILE:HG13	1.92	0.69
1:K:393:GLY:O	1:K:396:LEU:HG	1.93	0.69
2:B:36:ASN:ND2	2:B:38:ARG:H	1.91	0.69
2:D:192:GLY:HA2	2:D:195:PHE:CD2	2.28	0.69
2:F:440:LEU:HD12	2:F:464:MET:HE2	1.75	0.69
2:J:83:VAL:HG13	2:J:84:ARG:HG3	1.73	0.69
2:L:538:ARG:NH1	2:L:538:ARG:HG3	1.99	0.69
1:A:698:TYR:N	1:A:698:TYR:CD2	2.60	0.69
2:B:297:ARG:HB3	2:B:297:ARG:HH11	1.57	0.69
2:B:465:TRP:HB3	2:B:467:ASN:ND2	2.07	0.69
1:C:386:LEU:HD12	1:C:434:LEU:HB2	1.74	0.69
1:C:47:ARG:HH11	1:C:47:ARG:CB	2.06	0.69
1:G:201:PRO:HG2	1:G:328:ARG:NH2	2.07	0.69
1:G:561:ARG:HH11	1:G:632:VAL:HG13	1.57	0.69
2:H:402:GLN:NE2	2:H:449:ASN:HA	2.07	0.69
2:H:326:LYS:NZ	1:I:681:LYS:HD3	2.08	0.69
1:K:616:ARG:O	1:K:630:GLU:HB2	1.93	0.69
2:L:368:ALA:HB3	2:L:398:LEU:HD23	1.73	0.69
2:B:144:THR:HG22	2:B:175:GLY:H	1.58	0.69
2:H:217:THR:CG2	2:H:240:PHE:HE1	2.03	0.69
1:I:547:LEU:HD23	1:I:547:LEU:N	2.07	0.69
1:A:543:TRP:HB3	2:B:96:PRO:HB3	1.73	0.69
2:D:464:MET:CE	2:D:519:PRO:HG3	2.21	0.69
1:E:189:GLU:OE1	1:E:189:GLU:HA	1.92	0.69
1:G:278:ILE:N	1:G:278:ILE:HD12	1.95	0.69
2:H:35:ILE:CD1	2:H:320:VAL:HG13	2.23	0.69
2:H:90:LEU:HD12	2:H:90:LEU:O	1.93	0.69
2:B:33:THR:HG23	2:B:35:ILE:N	2.03	0.69
1:E:108:LEU:HD23	1:E:132:LEU:CD2	2.22	0.69
2:F:200:ASN:HD22	2:F:204:ARG:NH2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:612:LEU:H	1:I:612:LEU:HD12	1.57	0.69
2:L:348:LYS:HB2	2:L:383:LYS:HE3	1.75	0.69
1:A:497:LEU:N	1:A:498:PRO:HD3	2.07	0.68
2:B:81:LEU:HD11	2:B:89:ARG:HH22	1.56	0.68
2:D:71:ALA:HA	2:D:74:ARG:HB3	1.74	0.68
1:G:304:GLU:HA	1:G:307:VAL:CG1	2.24	0.68
2:H:81:LEU:HD21	2:H:85:GLU:HB3	1.74	0.68
2:J:235:GLU:HA	2:J:258:GLU:OE1	1.92	0.68
2:J:377:PHE:N	2:J:377:PHE:CD1	2.61	0.68
2:B:511:GLU:HG3	2:B:512:GLN:N	2.08	0.68
1:C:287:GLU:HG2	1:C:343:GLU:HG3	1.74	0.68
1:E:587:GLN:HB3	1:E:588:TYR:HD1	1.56	0.68
1:G:114:ILE:O	1:G:118:LEU:HB2	1.94	0.68
1:I:380:HIS:CD2	1:I:444:ARG:HD2	2.29	0.68
1:A:616:ARG:O	1:A:616:ARG:HG3	1.91	0.68
1:C:280:ARG:O	1:C:281:ARG:C	2.32	0.68
1:E:270:TYR:H	1:E:372:GLN:NE2	1.88	0.68
1:E:400:GLY:H	1:E:463:LEU:CD1	2.06	0.68
1:E:623:GLU:N	1:E:623:GLU:CD	2.47	0.68
2:F:192:GLY:HA2	2:F:195:PHE:CD2	2.28	0.68
2:F:172:ASP:OD1	2:F:214:GLY:HA3	1.92	0.68
2:H:232:MET:CE	2:H:239:ILE:HG13	2.23	0.68
2:J:146:TYR:HE1	2:J:180:ARG:NH1	1.90	0.68
2:J:75:HIS:CE1	2:J:80:LYS:HE2	2.27	0.68
1:A:276:CYS:HB3	1:A:287:GLU:HG3	1.75	0.68
1:E:148:LEU:HD23	1:E:148:LEU:N	2.08	0.68
1:E:361:ARG:HH11	1:E:361:ARG:HG2	1.57	0.68
1:E:568:HIS:CD2	1:E:568:HIS:H	2.09	0.68
1:K:384:VAL:HG23	1:K:451:LEU:HD21	1.73	0.68
2:L:48:THR:O	2:L:52:GLN:HG3	1.92	0.68
2:L:74:ARG:HH21	2:L:78:ARG:HH12	1.40	0.68
1:C:107:TYR:O	1:C:132:LEU:HD21	1.93	0.68
1:C:353:LEU:N	1:C:353:LEU:HD23	2.09	0.68
1:C:452:LEU:HD23	1:C:474:LEU:HB3	1.76	0.68
1:E:390:ASP:CG	1:E:464:ARG:HD2	2.14	0.68
1:I:272:ASN:CG	1:I:377:LEU:HD22	2.14	0.68
1:I:300:ARG:CZ	1:I:300:ARG:HB2	2.24	0.68
1:I:504:LEU:HD23	1:I:505:PRO:CD	2.24	0.68
2:L:191:PHE:HD2	2:L:192:GLY:N	1.88	0.68
1:A:186:GLN:HE22	1:A:190:THR:N	1.88	0.68
2:D:233:VAL:HG13	2:D:279:ASP:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:LEU:CD2	1:E:368:LEU:HD13	2.23	0.68
1:G:545:SER:O	2:H:536:GLN:NE2	2.26	0.68
2:D:440:LEU:HD21	2:D:444:SER:HB2	1.75	0.68
1:E:270:TYR:N	1:E:372:GLN:HE22	1.90	0.68
2:F:501:GLU:O	2:F:505:ILE:HG13	1.94	0.68
1:G:469:PHE:CE1	1:G:497:LEU:HD21	2.28	0.68
1:I:278:ILE:N	1:I:278:ILE:HD12	2.05	0.68
1:I:339:ARG:NH1	1:I:341:GLN:HA	2.09	0.68
2:L:433:ARG:HH21	2:L:554:GLU:HG3	1.59	0.68
1:A:412:PRO:HB2	1:A:450:ARG:HD3	1.75	0.68
2:D:191:PHE:CD2	2:D:194:ILE:HD12	2.28	0.68
2:D:305:ARG:HH11	2:D:305:ARG:CB	2.07	0.68
1:G:315:TYR:CE2	1:G:338:THR:HG22	2.29	0.68
2:H:234:ARG:HD3	2:H:278:GLU:OE1	1.93	0.68
1:I:167:LYS:NZ	1:I:167:LYS:HB2	2.09	0.68
1:K:269:LEU:HD21	1:K:368:LEU:HD13	1.76	0.68
1:I:608:ARG:NH2	1:K:90:ALA:HA	2.09	0.68
1:A:150:LEU:HD23	1:A:363:ALA:HB2	1.76	0.68
1:A:252:LYS:HG2	1:A:485:ASP:HB3	1.75	0.68
1:E:504:LEU:O	1:E:505:PRO:O	2.12	0.68
2:H:71:ALA:HA	2:H:74:ARG:HB3	1.76	0.68
1:I:607:ARG:NH1	1:I:607:ARG:CB	2.57	0.68
1:K:439:ALA:HB3	1:K:451:LEU:HB2	1.74	0.68
1:E:547:LEU:N	1:E:547:LEU:HD23	2.09	0.67
1:G:341:GLN:OE1	1:G:342:VAL:HG23	1.93	0.67
2:J:441:ILE:C	2:J:441:ILE:HD12	2.13	0.67
1:K:357:ALA:HA	1:K:360:ILE:HD11	1.76	0.67
2:L:444:SER:HB2	2:L:470:ILE:HG13	1.76	0.67
1:A:169:LEU:HD23	1:A:313:ILE:HG22	1.74	0.67
1:A:537:TRP:CE2	2:B:543:LEU:HD22	2.29	0.67
1:C:82:ILE:HD11	1:C:430:TYR:CE1	2.28	0.67
2:D:481:VAL:HG12	2:J:245:PRO:HB2	1.77	0.67
1:E:132:LEU:HB3	1:E:138:PHE:CD2	2.30	0.67
2:F:173:SER:OG	2:F:174:GLY:N	2.23	0.67
2:F:84:ARG:NH1	2:F:84:ARG:HG2	2.06	0.67
1:G:607:ARG:HH11	1:G:607:ARG:CB	2.07	0.67
1:I:469:PHE:O	1:I:473:ILE:HG22	1.94	0.67
2:J:302:LEU:HD21	2:J:397:PRO:HD3	1.74	0.67
2:L:350:LEU:HD23	2:L:350:LEU:N	2.08	0.67
1:C:416:VAL:HG22	1:C:437:LEU:HD12	1.77	0.67
2:D:491:GLU:HA	2:D:495:GLN:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:THR:HG22	1:E:467:LEU:N	2.07	0.67
1:E:561:ARG:HH11	1:E:561:ARG:HG3	1.59	0.67
1:G:371:THR:OG1	1:G:374:GLN:HG3	1.95	0.67
2:H:164:ARG:HB2	2:H:551:ALA:HB2	1.75	0.67
2:H:207:PRO:CG	2:H:294:LEU:HD21	2.17	0.67
1:I:452:LEU:HD13	1:I:452:LEU:O	1.95	0.67
1:K:255:HIS:CE1	1:K:322:GLU:HG3	2.28	0.67
1:A:695:LYS:O	1:A:696:ALA:HB2	1.94	0.67
2:D:317:LEU:HD22	2:D:334:VAL:CG1	2.24	0.67
1:E:300:ARG:CZ	1:E:300:ARG:HB2	2.24	0.67
1:E:387:TYR:HE1	1:E:433:MET:HB2	1.59	0.67
1:G:114:ILE:HD11	1:G:145:ALA:HB3	1.75	0.67
1:I:605:VAL:HG23	1:I:605:VAL:O	1.94	0.67
2:J:233:VAL:CG1	2:J:279:ASP:HA	2.23	0.67
2:L:554:GLU:OE1	2:L:555:PRO:HD2	1.94	0.67
2:J:171:VAL:HG12	2:J:212:VAL:HG13	1.74	0.67
2:J:440:LEU:HD22	2:J:444:SER:OG	1.94	0.67
2:D:181:GLN:OE1	2:J:472:VAL:HG12	1.93	0.67
2:L:212:VAL:HG23	2:L:231:VAL:O	1.94	0.67
2:L:62:ARG:O	2:L:65:GLU:HB2	1.94	0.67
1:A:135:ASN:ND2	1:A:137:ASP:OD2	2.28	0.67
1:A:170:MET:SD	1:A:309:ALA:HB1	2.35	0.67
1:G:47:ARG:CB	1:G:47:ARG:HH11	2.03	0.67
2:H:75:HIS:HE1	2:H:80:LYS:HE2	1.59	0.67
1:I:391:PRO:HD3	1:I:465:THR:O	1.95	0.67
2:J:161:LEU:HD11	2:J:201:MET:HG2	1.75	0.67
2:J:81:LEU:HD11	2:J:89:ARG:NH2	2.09	0.67
2:B:189:GLU:N	2:B:189:GLU:OE1	2.28	0.67
1:C:200:TYR:OH	1:C:224:LEU:HD22	1.95	0.67
1:E:49:ILE:N	1:E:49:ILE:HD12	2.10	0.67
2:B:293:ASN:HB3	2:F:359:PHE:HD1	1.59	0.67
1:G:602:VAL:O	1:G:605:VAL:HG22	1.92	0.67
2:J:377:PHE:HA	2:J:418:ILE:HD11	1.77	0.67
2:J:525:ARG:HG3	2:J:525:ARG:HH11	1.59	0.67
1:K:264:ARG:CB	1:K:264:ARG:HH11	2.08	0.67
2:L:375:ILE:HD12	2:L:375:ILE:H	1.58	0.67
2:B:375:ILE:HG22	2:B:376:LEU:N	2.10	0.67
1:C:343:GLU:O	1:C:346:VAL:HG22	1.95	0.67
2:D:121:ALA:CB	2:D:134:VAL:HG22	2.24	0.67
1:E:104:ALA:HA	1:E:108:LEU:HD12	1.75	0.67
1:G:437:LEU:HD23	1:G:455:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:476:GLU:CA	2:H:510:LEU:HD21	2.25	0.67
1:I:251:LEU:HB2	1:I:327:GLU:HG3	1.74	0.67
2:B:155:ARG:NE	2:B:159:ILE:HD11	2.09	0.67
1:E:136:ALA:HB1	1:E:154:ALA:HB1	1.76	0.67
1:G:561:ARG:NH1	1:G:632:VAL:HG13	2.09	0.67
1:I:607:ARG:HG3	1:K:94:ILE:CG1	2.24	0.67
1:K:165:ALA:O	1:K:168:ALA:HB3	1.95	0.67
2:L:114:VAL:HG11	2:L:146:TYR:CE2	2.29	0.67
2:L:486:LYS:HG2	2:L:505:ILE:HD13	1.77	0.67
1:C:200:TYR:O	1:C:202:VAL:N	2.27	0.67
1:E:257:GLU:O	1:E:273:GLU:HB2	1.94	0.67
1:I:170:MET:HE3	1:I:309:ALA:HB1	1.75	0.67
1:A:129:TYR:CE2	1:A:342:VAL:HA	2.30	0.66
1:A:350:ILE:HD12	1:A:377:LEU:HD13	1.76	0.66
1:A:673:THR:CG2	1:A:676:VAL:HG22	2.25	0.66
1:C:598:LEU:HD23	1:C:598:LEU:O	1.95	0.66
1:E:201:PRO:HD2	1:E:328:ARG:NH2	2.10	0.66
1:G:452:LEU:HD22	1:G:474:LEU:HB3	1.76	0.66
1:G:99:GLY:HA3	1:G:105:ASP:O	1.95	0.66
1:I:277:SER:O	1:I:279:GLN:HG3	1.95	0.66
1:I:254:ARG:NH2	1:I:292:PRO:HB2	2.10	0.66
1:A:469:PHE:CZ	1:A:489:ILE:HD11	2.30	0.66
2:B:177:ASN:OD1	2:B:180:ARG:NH1	2.28	0.66
1:E:618:LEU:O	1:E:618:LEU:HD23	1.96	0.66
2:F:349:ALA:HB3	2:F:350:LEU:HD23	1.76	0.66
2:F:390:LEU:HD23	2:F:394:ARG:HH21	1.60	0.66
1:G:325:LEU:HD23	1:G:326:ASP:N	2.10	0.66
2:B:137:ASP:HB3	2:B:140:VAL:CG2	2.24	0.66
1:E:118:LEU:HD12	1:E:147:LEU:HD21	1.75	0.66
1:E:269:LEU:HB2	1:E:372:GLN:NE2	2.10	0.66
1:G:50:GLN:NE2	1:G:123:GLN:NE2	2.43	0.66
1:G:618:LEU:HD23	1:G:629:ILE:HD13	1.78	0.66
2:H:305:ARG:NH1	2:H:305:ARG:CB	2.58	0.66
2:H:345:ASP:OD2	2:H:345:ASP:N	2.27	0.66
1:I:412:PRO:CB	1:I:450:ARG:HD3	2.25	0.66
1:K:140:ARG:NH1	1:K:140:ARG:HB3	2.09	0.66
1:K:144:GLU:O	1:K:144:GLU:HG2	1.93	0.66
1:K:63:ARG:HD3	1:K:417:ASP:OD1	1.96	0.66
2:L:90:LEU:O	2:L:288:ARG:NH2	2.28	0.66
1:A:377:LEU:HG	1:A:377:LEU:O	1.94	0.66
1:A:649:LEU:HD11	1:A:689:PRO:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:PRO:O	1:C:501:GLN:HB3	1.95	0.66
2:D:379:GLU:H	2:D:379:GLU:CD	1.97	0.66
1:G:261:PHE:CE2	1:G:318:ALA:HB2	2.31	0.66
1:G:513:ALA:HB2	1:G:564:VAL:HG21	1.76	0.66
2:H:317:LEU:HA	2:H:320:VAL:CG2	2.24	0.66
1:I:280:ARG:O	1:I:281:ARG:C	2.32	0.66
2:J:487:ARG:HD2	2:J:502:GLU:OE1	1.95	0.66
2:D:433:ARG:HG3	2:D:433:ARG:HH11	1.60	0.66
2:D:520:TYR:N	2:D:520:TYR:HD2	1.94	0.66
2:F:80:LYS:HG2	2:F:236:GLN:OE1	1.94	0.66
2:H:269:VAL:HG12	2:H:270:SER:N	2.09	0.66
1:I:135:ASN:O	1:I:135:ASN:OD1	2.13	0.66
1:I:62:CYS:O	1:I:66:ARG:HG3	1.94	0.66
1:I:65:MET:HE3	1:I:92:ALA:HA	1.77	0.66
1:E:250:LEU:HD21	1:E:332:PHE:HE1	1.60	0.66
2:F:207:PRO:HG2	2:F:294:LEU:CD2	2.25	0.66
2:B:50:LEU:HD23	2:B:54:ASN:HD21	1.61	0.66
2:B:78:ARG:HH11	2:B:78:ARG:HG3	1.61	0.66
2:D:350:LEU:CD2	2:D:350:LEU:N	2.56	0.66
1:E:186:GLN:NE2	1:E:187:ASP:OD1	2.29	0.66
2:H:326:LYS:CE	1:I:681:LYS:HD3	2.26	0.66
2:J:270:SER:OG	2:J:272:VAL:HG23	1.95	0.66
2:J:476:GLU:CD	2:J:476:GLU:H	1.99	0.66
2:J:50:LEU:O	2:J:50:LEU:HD23	1.96	0.66
1:K:53:LEU:HD13	1:K:117:ALA:CB	2.26	0.66
1:C:251:LEU:HD11	1:C:328:ARG:NH2	2.10	0.66
1:C:384:VAL:CG1	1:C:470:LEU:HD13	2.26	0.66
1:E:469:PHE:O	1:E:473:ILE:HG22	1.96	0.66
2:F:377:PHE:H	2:F:377:PHE:HD1	1.42	0.66
2:F:377:PHE:N	2:F:377:PHE:CD1	2.63	0.66
1:I:51:ARG:HB2	1:I:122:ALA:HA	1.76	0.66
1:I:497:LEU:N	1:I:498:PRO:HD3	2.11	0.66
2:J:362:LEU:HB2	2:J:367:ILE:HD13	1.78	0.66
2:J:516:GLN:HA	2:J:521:TYR:CD2	2.30	0.66
1:K:357:ALA:HA	1:K:360:ILE:CD1	2.25	0.66
1:C:138:PHE:CD1	1:C:142:CYS:HB2	2.31	0.66
1:C:473:ILE:HA	1:C:496:LEU:HD21	1.76	0.66
1:E:519:SER:HB2	1:E:613:ARG:HE	1.60	0.66
1:G:335:GLU:HG3	1:G:336:MET:N	2.10	0.66
1:I:440:TRP:CD1	1:I:440:TRP:C	2.69	0.66
1:K:280:ARG:O	1:K:281:ARG:C	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:486:LYS:HG3	2:L:497:LEU:HD22	1.78	0.66
2:B:386:HIS:O	2:B:386:HIS:HD2	1.78	0.66
2:B:421:HIS:CE1	2:B:424:LYS:HZ2	2.14	0.66
1:K:396:LEU:O	1:K:398:ALA:N	2.29	0.66
1:K:401:ARG:HH11	1:K:401:ARG:CB	2.04	0.66
1:A:167:LYS:HE3	1:A:177:LEU:HD12	1.77	0.65
2:B:119:ILE:HG23	2:B:152:LYS:HD3	1.77	0.65
2:B:279:ASP:OD2	2:B:281:ASP:N	2.28	0.65
2:B:487:ARG:CB	2:B:497:LEU:HB2	2.26	0.65
2:B:84:ARG:HA	2:B:87:ILE:HD12	1.78	0.65
2:D:441:ILE:HG22	2:D:465:TRP:CE2	2.30	0.65
2:F:209:ILE:HD11	2:F:290:CYS:CB	2.26	0.65
1:K:76:VAL:HG11	1:K:120:SER:OG	1.95	0.65
1:A:269:LEU:HB2	1:A:372:GLN:NE2	2.11	0.65
2:B:193:ARG:NH1	2:B:196:PHE:CD2	2.64	0.65
2:D:53:VAL:O	2:D:57:ARG:HG3	1.97	0.65
2:F:311:LEU:HG	2:F:342:SER:HB2	1.77	0.65
2:J:191:PHE:CD2	2:J:194:ILE:HD13	2.31	0.65
2:J:49:MET:HG3	2:J:318:TYR:CD1	2.32	0.65
1:K:471:ARG:HH11	1:K:471:ARG:HB2	1.60	0.65
1:A:698:TYR:HD2	1:A:698:TYR:N	1.94	0.65
1:G:298:LEU:O	1:G:301:ALA:HB3	1.96	0.65
1:I:178:VAL:HG13	1:I:332:PHE:CB	2.25	0.65
1:I:284:LYS:HD3	1:I:343:GLU:OE1	1.97	0.65
1:I:427:SER:OG	1:I:428:PRO:HD2	1.97	0.65
1:I:532:ASP:OD2	2:J:365:TYR:OH	2.12	0.65
1:K:465:THR:HG22	1:K:467:LEU:N	2.08	0.65
1:K:99:GLY:HA3	1:K:105:ASP:O	1.97	0.65
2:L:123:ILE:CD1	2:L:165:LEU:HD13	2.26	0.65
2:L:144:THR:HG22	2:L:175:GLY:H	1.61	0.65
1:C:129:TYR:CE2	1:C:342:VAL:HA	2.31	0.65
1:E:250:LEU:HD21	1:E:332:PHE:CE1	2.32	0.65
1:G:187:ASP:C	1:G:189:GLU:H	1.99	0.65
1:I:271:LEU:HA	1:I:375:VAL:HG11	1.78	0.65
2:J:486:LYS:HA	2:J:489:GLN:HE21	1.61	0.65
2:L:389:GLU:HG2	2:L:558:PHE:HE1	1.61	0.65
1:A:652:PRO:HD3	1:A:686:ILE:CG2	2.26	0.65
2:D:282:HIS:O	2:D:286:ILE:HG13	1.96	0.65
1:E:300:ARG:CB	1:E:300:ARG:HH11	2.10	0.65
1:G:169:LEU:O	1:G:173:ALA:HB2	1.95	0.65
1:G:304:GLU:HA	1:G:307:VAL:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:525:ARG:NH1	2:J:525:ARG:HG3	2.10	0.65
2:L:303:GLN:HA	2:L:303:GLN:OE1	1.97	0.65
1:A:308:ARG:HH11	1:A:308:ARG:HG3	1.60	0.65
2:B:560:VAL:HG13	2:J:389:GLU:HB3	1.78	0.65
1:C:495:ASP:OD2	1:C:495:ASP:N	2.29	0.65
1:E:321:VAL:O	1:E:321:VAL:HG12	1.96	0.65
1:E:405:TYR:HB3	1:E:422:GLU:HB2	1.79	0.65
1:E:512:ALA:HB1	1:E:629:ILE:HD13	1.78	0.65
2:H:349:ALA:HB3	2:H:350:LEU:CD2	2.27	0.65
1:I:141:ALA:HA	1:I:144:GLU:HB3	1.77	0.65
1:I:599:VAL:HG22	1:I:608:ARG:HD3	1.77	0.65
1:A:656:SER:OG	1:A:704:LEU:HD23	1.97	0.65
1:C:469:PHE:HZ	1:C:489:ILE:HD11	1.62	0.65
1:C:629:ILE:HD12	1:C:629:ILE:N	2.11	0.65
2:D:482:LEU:HD23	2:D:509:ILE:HG13	1.78	0.65
2:F:335:ILE:O	2:F:339:VAL:HG22	1.96	0.65
2:F:359:PHE:HE2	2:F:387:PHE:CE1	2.15	0.65
2:H:291:VAL:HA	2:H:294:LEU:CD1	2.22	0.65
2:H:378:ALA:H	2:H:418:ILE:HD11	1.62	0.65
1:K:273:GLU:OE2	1:K:291:ALA:N	2.30	0.65
1:A:383:GLU:HG3	1:A:438:ILE:CG2	2.22	0.65
1:A:559:ASP:O	1:A:560:GLU:HG3	1.97	0.65
2:B:270:SER:OG	2:B:272:VAL:HG23	1.96	0.65
1:E:123:GLN:O	1:E:148:LEU:HG	1.97	0.65
1:E:320:THR:HG21	1:E:341:GLN:HG3	1.78	0.65
1:E:522:GLY:O	1:E:523:HIS:HB2	1.96	0.65
1:G:503:ALA:O	1:G:504:LEU:O	2.14	0.65
2:H:207:PRO:HA	2:H:228:ASP:OD2	1.95	0.65
2:H:497:LEU:HD12	2:H:501:GLU:OE1	1.97	0.65
1:I:169:LEU:HD22	1:I:313:ILE:HG23	1.78	0.65
1:I:340:LEU:CD1	1:I:356:VAL:HG23	2.26	0.65
1:K:415:ARG:HG2	1:K:416:VAL:N	2.12	0.65
1:A:550:GLU:OE2	1:A:567:ARG:HD2	1.97	0.65
1:C:185:ALA:HB3	1:C:243:ARG:HB2	1.77	0.65
1:G:274:ARG:NH2	1:G:320:THR:HG21	2.12	0.65
1:G:380:HIS:CD2	1:G:444:ARG:HD2	2.31	0.65
1:I:344:HIS:N	1:I:345:PRO:CD	2.60	0.65
1:I:505:PRO:HB3	1:I:507:HIS:HB3	1.79	0.65
1:K:279:GLN:O	1:K:489:ILE:HG21	1.97	0.65
1:K:505:PRO:HB3	1:K:507:HIS:HB2	1.79	0.65
2:B:181:GLN:OE1	2:L:472:VAL:HG12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:LEU:HD13	2:B:201:MET:HG3	1.79	0.65
2:B:81:LEU:HD22	2:B:85:GLU:HB3	1.79	0.65
1:C:523:HIS:ND1	1:C:524:ARG:N	2.45	0.65
1:C:561:ARG:HH12	1:C:632:VAL:HG22	1.61	0.65
2:D:516:GLN:HA	2:D:521:TYR:CD2	2.32	0.65
2:J:191:PHE:HD2	2:J:192:GLY:H	1.44	0.65
1:E:339:ARG:HG3	1:E:339:ARG:NH1	2.12	0.64
1:E:63:ARG:O	1:E:63:ARG:NH1	2.30	0.64
2:F:375:ILE:HB	2:F:377:PHE:CE1	2.32	0.64
1:G:106:SER:OG	1:G:107:TYR:N	2.27	0.64
1:G:81:ASP:HB2	1:G:100:GLY:HA2	1.79	0.64
2:H:436:LYS:HD2	2:H:453:CYS:SG	2.37	0.64
1:I:108:LEU:HD23	1:I:132:LEU:CD1	2.27	0.64
1:I:569:ALA:O	1:I:571:PRO:HD3	1.98	0.64
2:J:194:ILE:HD12	2:J:194:ILE:H	1.61	0.64
1:A:204:LEU:O	1:A:215:MET:HA	1.96	0.64
2:B:250:ALA:O	2:B:252:GLY:N	2.30	0.64
2:B:375:ILE:H	2:B:375:ILE:HD12	1.62	0.64
2:D:101:SER:O	2:D:152:LYS:HE3	1.96	0.64
1:E:465:THR:HG22	1:E:466:ASN:N	2.11	0.64
2:F:234:ARG:HA	2:F:263:ALA:CB	2.27	0.64
2:F:209:ILE:HD11	2:F:290:CYS:HB3	1.77	0.64
2:F:473:MET:HE2	2:F:477:GLN:HB3	1.79	0.64
1:I:350:ILE:HD12	1:I:377:LEU:CD1	2.28	0.64
2:J:151:LYS:HG2	2:J:526:LEU:HD22	1.80	0.64
2:L:339:VAL:HG23	2:L:340:ASP:N	2.12	0.64
1:A:705:VAL:CG1	1:A:709:THR:HG21	2.27	0.64
2:B:109:TYR:OH	2:B:147:PRO:HB2	1.97	0.64
1:G:203:LEU:HD21	1:G:247:GLU:OE2	1.96	0.64
1:G:361:ARG:HG2	1:G:366:GLU:OE1	1.98	0.64
2:H:330:ASP:OD1	2:H:332:ARG:HG3	1.97	0.64
1:A:249:TYR:CD2	1:A:250:LEU:N	2.64	0.64
2:B:31:LEU:CD1	2:B:336:ALA:HB2	2.27	0.64
1:C:443:THR:CG2	1:C:446:GLU:HB2	2.25	0.64
1:C:451:LEU:CD2	1:C:474:LEU:HD11	2.28	0.64
1:E:384:VAL:CG1	1:E:470:LEU:HD13	2.26	0.64
2:F:417:GLY:C	2:F:419:ALA:H	2.01	0.64
1:G:444:ARG:HG2	1:G:444:ARG:HH11	1.61	0.64
2:H:163:ASN:OD1	2:H:460:ARG:HD2	1.98	0.64
2:J:355:LEU:HD21	2:J:370:LEU:CD2	2.27	0.64
2:J:375:ILE:CD1	2:J:375:ILE:H	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:C	1:A:567:ARG:HD3	2.18	0.64
1:A:654:ASN:C	2:H:251:THR:HB	2.18	0.64
1:C:384:VAL:HG11	1:C:470:LEU:HD13	1.79	0.64
1:E:99:GLY:HA3	1:E:105:ASP:O	1.97	0.64
1:G:51:ARG:HD3	1:G:121:GLY:C	2.18	0.64
2:H:159:ILE:HD13	2:H:461:PHE:CE2	2.32	0.64
2:H:303:GLN:NE2	2:J:297:ARG:HG3	2.12	0.64
1:K:152:PRO:HG2	1:K:338:THR:HB	1.80	0.64
1:K:257:GLU:C	1:K:258:ILE:HD12	2.18	0.64
2:L:74:ARG:HH21	2:L:78:ARG:NH1	1.95	0.64
1:A:601:ARG:HG2	1:A:606:THR:HB	1.78	0.64
1:C:522:GLY:O	1:C:523:HIS:HB2	1.96	0.64
2:D:121:ALA:HB2	2:D:134:VAL:HG22	1.80	0.64
2:D:199:ALA:HB1	2:J:427:THR:HG23	1.79	0.64
2:F:465:TRP:NE1	2:F:534:PRO:HA	2.13	0.64
1:G:328:ARG:CG	1:G:328:ARG:HH11	2.03	0.64
1:G:97:ASP:OD1	1:G:98:LEU:O	2.16	0.64
1:I:53:LEU:HD13	1:I:117:ALA:CB	2.26	0.64
2:J:331:VAL:HB	2:J:373:ASN:HD21	1.61	0.64
2:J:486:LYS:HD2	2:J:489:GLN:HE21	1.63	0.64
1:K:556:ARG:HD2	1:K:556:ARG:C	2.18	0.64
1:A:204:LEU:HD22	1:A:245:LEU:O	1.96	0.64
1:C:350:ILE:HD12	1:C:351:THR:CG2	2.28	0.64
1:C:562:ARG:HH11	1:C:562:ARG:HB3	1.62	0.64
2:D:372:ASN:ND2	2:D:404:ILE:HB	2.13	0.64
2:F:423:ALA:HA	2:F:426:VAL:HG23	1.80	0.64
2:F:498:GLY:O	2:F:500:GLU:N	2.30	0.64
2:F:81:LEU:HD12	2:F:280:ASP:CB	2.27	0.64
1:K:353:LEU:HD22	1:K:358:TRP:CH2	2.33	0.64
1:K:465:THR:HG22	1:K:466:ASN:N	2.13	0.64
2:L:127:GLU:OE1	2:L:127:GLU:HA	1.98	0.64
2:L:62:ARG:HG2	2:L:62:ARG:NH1	2.12	0.64
2:B:119:ILE:CG2	2:B:152:LYS:HD3	2.28	0.64
1:E:285:VAL:HG12	1:E:286:VAL:CG2	2.26	0.64
1:E:49:ILE:HD13	1:E:364:ARG:HG2	1.80	0.64
1:G:132:LEU:HD23	1:G:138:PHE:CE2	2.33	0.64
1:G:426:VAL:HG21	1:G:463:LEU:HD11	1.80	0.64
1:I:134:GLU:HG2	1:I:338:THR:OG1	1.98	0.64
1:I:503:ALA:O	1:I:504:LEU:O	2.14	0.64
1:I:522:GLY:O	1:I:523:HIS:HB2	1.97	0.64
2:J:240:PHE:CD2	2:J:260:LEU:HD23	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:286:VAL:HG21	1:K:473:ILE:HD11	1.80	0.64
1:C:393:GLY:O	1:C:396:LEU:HG	1.98	0.64
2:D:305:ARG:HH11	2:D:305:ARG:HB3	1.62	0.64
2:D:486:LYS:HG2	2:D:505:ILE:HD13	1.78	0.64
1:E:201:PRO:O	1:E:249:TYR:HB3	1.98	0.64
1:G:269:LEU:HD21	1:G:368:LEU:HD23	1.79	0.64
1:G:380:HIS:HE2	1:G:444:ARG:HD2	1.62	0.64
2:H:433:ARG:N	2:H:556:THR:HG23	2.11	0.64
1:I:255:HIS:HE1	1:I:322:GLU:HG2	1.63	0.64
1:I:476:HIS:CG	1:I:477:PRO:HD2	2.33	0.64
1:I:47:ARG:HE	1:I:148:LEU:HD21	1.62	0.64
1:K:398:ALA:HB2	1:K:464:ARG:HE	1.63	0.64
2:L:435:PRO:HD3	2:L:553:ILE:HG23	1.78	0.64
1:A:473:ILE:HB	1:A:496:LEU:HD13	1.79	0.64
2:B:393:GLN:HG2	2:B:393:GLN:O	1.98	0.64
2:B:89:ARG:HG3	2:B:89:ARG:NH2	2.05	0.64
1:C:294:LEU:HD12	1:C:294:LEU:O	1.98	0.64
2:H:438:THR:HG22	2:H:462:LEU:HG	1.80	0.64
1:K:503:ALA:O	1:K:504:LEU:O	2.16	0.64
2:L:465:TRP:HE3	2:L:467:ASN:HD21	1.43	0.64
1:C:274:ARG:HH22	1:C:320:THR:HG21	1.62	0.63
1:E:129:TYR:HE2	1:E:342:VAL:HA	1.59	0.63
2:F:53:VAL:CG1	2:F:57:ARG:NH1	2.61	0.63
1:K:339:ARG:NH1	1:K:341:GLN:OE1	2.31	0.63
1:K:361:ARG:HA	1:K:366:GLU:OE1	1.97	0.63
2:L:91:LEU:HD22	2:L:95:SER:OG	1.98	0.63
2:B:487:ARG:O	2:B:487:ARG:HG3	1.97	0.63
1:E:280:ARG:O	1:E:281:ARG:C	2.37	0.63
1:G:280:ARG:HH11	1:G:283:GLN:HE22	1.46	0.63
1:G:315:TYR:HE2	1:G:338:THR:HG22	1.63	0.63
1:G:497:LEU:N	1:G:498:PRO:HD3	2.13	0.63
2:H:476:GLU:OE2	2:H:477:GLN:N	2.32	0.63
1:I:63:ARG:NH1	1:I:63:ARG:O	2.30	0.63
2:J:109:TYR:HE2	2:J:147:PRO:HD2	1.63	0.63
2:J:121:ALA:CB	2:J:134:VAL:HG12	2.28	0.63
2:J:335:ILE:O	2:J:339:VAL:HG22	1.99	0.63
1:K:387:TYR:HB3	1:K:389:GLU:HG3	1.80	0.63
1:K:522:GLY:O	1:K:523:HIS:HB2	1.97	0.63
2:L:316:GLU:OE2	2:L:337:ARG:NH2	2.29	0.63
1:A:657:ILE:HD13	1:A:699:CYS:HB2	1.79	0.63
1:A:662:VAL:HG21	1:A:674:LEU:HD23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LYS:HZ1	1:C:247:GLU:HG2	1.63	0.63
1:E:201:PRO:HD2	1:E:328:ARG:HH21	1.63	0.63
1:E:567:ARG:HH11	1:E:567:ARG:HG3	1.63	0.63
1:E:404:LEU:CD1	1:E:612:LEU:HD13	2.28	0.63
2:F:248:LYS:HA	2:F:252:GLY:O	1.99	0.63
2:H:245:PRO:HB2	2:H:246:LEU:HD12	1.81	0.63
2:J:49:MET:HG3	2:J:318:TYR:HD1	1.61	0.63
1:K:47:ARG:HE	1:K:148:LEU:CD2	2.11	0.63
1:A:390:ASP:OD1	1:A:393:GLY:HA3	1.99	0.63
1:A:677:LEU:HD23	1:A:686:ILE:HD11	1.80	0.63
2:B:311:LEU:C	2:B:312:TYR:CD1	2.71	0.63
2:B:417:GLY:C	2:B:419:ALA:H	2.02	0.63
2:D:440:LEU:CD2	2:D:444:SER:HB2	2.29	0.63
2:D:484:GLN:HG3	2:D:485:VAL:N	2.13	0.63
1:G:132:LEU:HD23	1:G:138:PHE:CD2	2.34	0.63
1:I:300:ARG:HH11	1:I:300:ARG:HB2	1.63	0.63
1:I:549:ARG:HH11	1:I:549:ARG:CG	2.10	0.63
2:B:326:LYS:HZ1	2:B:405:THR:HG23	1.63	0.63
2:D:331:VAL:HG21	2:D:372:ASN:O	1.97	0.63
2:F:195:PHE:CE1	2:F:222:TYR:HB2	2.34	0.63
2:H:403:ASN:CG	2:H:442:GLY:HA3	2.19	0.63
1:K:441:GLY:HA2	1:K:450:ARG:NH2	2.13	0.63
1:A:220:ARG:HB2	1:A:223:GLU:CB	2.28	0.63
1:A:344:HIS:N	1:A:345:PRO:CD	2.62	0.63
2:D:105:ALA:HA	2:D:108:VAL:HG21	1.79	0.63
2:F:198:GLN:OE1	2:F:223:VAL:HG13	1.99	0.63
2:F:473:MET:CE	2:F:477:GLN:HB3	2.29	0.63
2:H:444:SER:HB2	2:H:470:ILE:CG1	2.25	0.63
2:H:49:MET:HE1	2:H:321:ILE:HG21	1.80	0.63
2:H:83:VAL:CG1	2:H:84:ARG:N	2.60	0.63
2:L:486:LYS:HE3	2:L:497:LEU:HD13	1.81	0.63
1:A:668:VAL:HG12	1:A:669:GLU:H	1.64	0.63
1:C:308:ARG:HG3	1:C:308:ARG:HH11	1.63	0.63
1:C:315:TYR:CE2	1:C:338:THR:HG22	2.33	0.63
2:D:230:THR:HG21	2:D:273:ALA:HA	1.80	0.63
1:E:82:ILE:HD11	1:E:430:TYR:HE1	1.64	0.63
1:G:218:VAL:HG11	1:G:224:LEU:CD1	2.28	0.63
1:K:105:ASP:C	1:K:109:ARG:HD2	2.18	0.63
1:K:401:ARG:HG3	1:K:425:GLU:OE2	1.99	0.63
1:K:605:VAL:O	1:K:605:VAL:CG2	2.47	0.63
2:L:289:ARG:O	2:L:292:ALA:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:HB2	1:A:100:GLY:HA2	1.80	0.63
1:A:652:PRO:HD3	1:A:686:ILE:HG21	1.81	0.63
2:B:31:LEU:HD12	2:B:336:ALA:HB2	1.80	0.63
1:C:278:ILE:HG23	1:C:488:PHE:CD2	2.32	0.63
2:D:119:ILE:CG2	2:D:152:LYS:HD3	2.27	0.63
1:E:153:PRO:HD3	1:E:316:VAL:CG2	2.29	0.63
1:G:271:LEU:HA	1:G:375:VAL:HG11	1.79	0.63
1:G:345:PRO:CB	1:G:438:ILE:HD13	2.29	0.63
1:G:490:ALA:O	1:G:493:GLN:HB2	1.99	0.63
2:H:193:ARG:NH1	2:H:196:PHE:CD2	2.67	0.63
2:B:29:ALA:O	2:B:343:GLU:HA	1.97	0.63
1:C:51:ARG:HB2	1:C:122:ALA:HA	1.81	0.63
1:C:47:ARG:NE	1:C:148:LEU:HD21	2.14	0.63
1:C:378:ASN:ND2	1:C:440:TRP:HH2	1.97	0.63
1:C:476:HIS:ND1	1:C:477:PRO:HD2	2.14	0.63
2:D:299:GLN:HB3	2:D:552:PRO:HD3	1.79	0.63
1:G:114:ILE:CD1	1:G:147:LEU:HD13	2.29	0.63
2:H:526:LEU:C	2:H:528:ASP:H	2.01	0.63
1:I:339:ARG:HH12	1:I:341:GLN:HA	1.64	0.63
1:I:386:LEU:HD21	1:I:467:LEU:CD1	2.29	0.63
2:J:248:LYS:O	2:J:248:LYS:HD2	1.99	0.63
1:K:455:LEU:CD1	1:K:474:LEU:HD12	2.29	0.63
1:A:365:GLY:O	1:A:366:GLU:O	2.17	0.62
2:B:312:TYR:HB2	2:B:337:ARG:HG2	1.81	0.62
1:C:350:ILE:HD12	1:C:351:THR:HG23	1.80	0.62
1:C:445:GLU:CD	1:C:448:ARG:NH2	2.52	0.62
1:E:254:ARG:HH22	1:E:293:GLY:H	1.46	0.62
1:E:274:ARG:HH11	1:E:347:THR:HB	1.64	0.62
1:I:250:LEU:HD21	1:I:332:PHE:CE1	2.34	0.62
2:J:317:LEU:HD22	2:J:334:VAL:HG13	1.81	0.62
1:K:269:LEU:HD12	1:K:375:VAL:HG21	1.79	0.62
1:A:345:PRO:HB3	1:A:438:ILE:CD1	2.30	0.62
2:B:192:GLY:HA2	2:B:195:PHE:CD2	2.34	0.62
1:C:274:ARG:HD3	1:C:347:THR:OG1	2.00	0.62
1:E:109:ARG:O	1:E:113:ILE:HG13	1.99	0.62
1:E:85:HIS:ND1	1:E:86:ALA:N	2.47	0.62
2:F:347:PHE:O	2:F:383:LYS:NZ	2.32	0.62
1:G:611:ALA:HB2	1:G:620:LEU:HD13	1.82	0.62
1:I:254:ARG:HH22	1:I:292:PRO:HB2	1.64	0.62
1:I:554:MET:HE3	1:I:554:MET:HA	1.82	0.62
2:L:464:MET:CE	2:L:470:ILE:HD12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:MET:HG2	2:B:318:TYR:HA	1.81	0.62
1:C:232:GLN:HG2	1:C:233:ARG:HH22	1.64	0.62
2:F:425:LEU:O	2:F:429:VAL:HG23	1.99	0.62
2:H:232:MET:HE3	2:H:239:ILE:HG13	1.80	0.62
1:K:136:ALA:HB1	1:K:154:ALA:HB1	1.81	0.62
2:L:197:ASN:O	2:L:201:MET:HG3	1.99	0.62
2:L:234:ARG:HG2	2:L:277:ALA:O	2.00	0.62
2:B:467:ASN:H	2:B:467:ASN:ND2	1.96	0.62
1:G:108:LEU:HD23	1:G:132:LEU:CD1	2.30	0.62
1:I:307:VAL:O	1:I:310:ALA:HB3	1.99	0.62
1:K:504:LEU:O	1:K:505:PRO:O	2.17	0.62
1:A:668:VAL:HG22	1:A:694:VAL:HG23	1.81	0.62
1:C:358:TRP:CZ2	1:C:369:PRO:HG2	2.34	0.62
1:E:264:ARG:NH1	1:E:264:ARG:HG2	2.12	0.62
1:E:358:TRP:O	1:E:362:VAL:HG22	2.00	0.62
1:E:269:LEU:HD23	1:E:368:LEU:HD13	1.80	0.62
1:G:63:ARG:NH2	1:G:356:VAL:HG23	2.07	0.62
1:G:397:PRO:HB3	1:G:432:PRO:HG3	1.80	0.62
1:G:391:PRO:HG3	1:G:466:ASN:HA	1.80	0.62
1:I:546:ALA:HB3	2:J:60:LEU:HD12	1.80	0.62
1:K:271:LEU:HD23	1:K:375:VAL:HG21	1.82	0.62
2:B:473:MET:CE	2:L:246:LEU:HD21	2.28	0.62
2:L:298:LYS:HE3	2:L:550:ASN:ND2	2.14	0.62
1:A:201:PRO:HD2	1:A:328:ARG:NH2	2.15	0.62
1:A:218:VAL:HG23	1:A:218:VAL:O	1.99	0.62
1:A:605:VAL:HG12	1:C:96:VAL:CG1	2.26	0.62
2:B:245:PRO:HB2	2:L:481:VAL:HG13	1.82	0.62
1:C:402:LEU:HD23	1:C:463:LEU:HD12	1.81	0.62
1:E:252:LYS:CE	1:E:491:ARG:HH22	2.13	0.62
1:E:525:ARG:CG	1:E:525:ARG:HH11	2.12	0.62
2:F:487:ARG:O	2:F:487:ARG:HG2	1.99	0.62
1:G:186:GLN:HE21	1:G:187:ASP:H	1.46	0.62
1:G:270:TYR:H	1:G:372:GLN:HE22	1.47	0.62
1:I:504:LEU:HD13	1:I:622:TRP:HE1	1.63	0.62
1:A:412:PRO:CB	1:A:450:ARG:HD3	2.29	0.62
1:A:663:GLU:HG2	1:A:666:GLN:NE2	2.14	0.62
1:C:352:GLY:C	1:C:353:LEU:HD23	2.20	0.62
1:I:285:VAL:HG12	1:I:286:VAL:HG22	1.81	0.62
2:L:123:ILE:HD11	2:L:165:LEU:CD1	2.25	0.62
1:C:294:LEU:CD1	1:C:299:ARG:NH1	2.63	0.62
1:C:66:ARG:CB	1:C:66:ARG:HH11	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:ARG:NH1	1:E:361:ARG:HG2	2.15	0.62
2:F:507:ALA:N	2:F:508:PRO:HD2	2.14	0.62
2:B:65:GLU:HG2	2:B:68:GLY:HA2	1.82	0.62
1:C:201:PRO:HD2	1:C:328:ARG:HH22	1.64	0.62
1:C:49:ILE:HD13	1:C:364:ARG:HG2	1.82	0.62
2:D:247:VAL:HG22	2:D:253:GLU:OE2	2.00	0.62
1:E:267:HIS:HB3	1:E:368:LEU:HD12	1.82	0.62
1:E:383:GLU:OE1	1:E:436:LYS:HG2	1.99	0.62
1:E:393:GLY:O	1:E:396:LEU:HG	2.00	0.62
1:E:503:ALA:HB2	1:E:560:GLU:OE1	1.99	0.62
2:H:417:GLY:C	2:H:419:ALA:N	2.48	0.62
1:I:613:ARG:O	1:I:614:ARG:HD2	2.00	0.62
2:J:72:GLN:O	2:J:75:HIS:HB3	1.99	0.62
1:K:129:TYR:CE2	1:K:342:VAL:HG13	2.35	0.62
1:K:567:ARG:NH1	1:K:567:ARG:HG3	2.09	0.62
2:L:305:ARG:HB2	2:L:305:ARG:CZ	2.29	0.62
1:C:186:GLN:HG2	1:C:187:ASP:OD2	2.00	0.62
2:D:138:ALA:HB2	2:D:172:ASP:OD2	2.00	0.62
2:D:272:VAL:O	2:D:272:VAL:HG12	2.00	0.62
2:D:68:GLY:O	2:D:70:ALA:N	2.32	0.62
1:I:46:TYR:HE1	1:I:364:ARG:HD3	1.65	0.62
2:J:45:ASN:OD1	2:J:323:ALA:N	2.33	0.62
1:K:270:TYR:CD1	1:K:372:GLN:NE2	2.68	0.62
1:K:82:ILE:HD11	1:K:430:TYR:HE1	1.62	0.62
2:B:481:VAL:HG13	2:L:245:PRO:CB	2.30	0.62
2:L:29:ALA:O	2:L:343:GLU:HA	1.99	0.62
1:C:384:VAL:CG1	1:C:470:LEU:HD22	2.30	0.61
1:E:152:PRO:HG3	1:E:315:TYR:CE1	2.35	0.61
2:F:145:TYR:CD1	2:F:149:THR:HB	2.35	0.61
2:F:554:GLU:HB3	2:F:555:PRO:HD2	1.82	0.61
2:H:191:PHE:HD2	2:H:192:GLY:H	1.48	0.61
1:I:269:LEU:CA	1:I:372:GLN:HE22	2.13	0.61
2:J:243:GLY:H	2:J:246:LEU:HD13	1.64	0.61
2:J:332:ARG:NH1	2:J:332:ARG:HG3	2.07	0.61
1:K:600:SER:OG	1:K:602:VAL:HG23	2.00	0.61
2:L:198:GLN:NE2	2:L:226:MET:O	2.32	0.61
1:A:391:PRO:HG3	1:A:466:ASN:HA	1.82	0.61
1:A:556:ARG:HG3	1:A:561:ARG:HB3	1.81	0.61
1:C:274:ARG:HG2	1:C:289:ALA:HB2	1.82	0.61
1:E:255:HIS:HE1	1:E:322:GLU:HG2	1.64	0.61
2:F:109:TYR:CE1	2:F:148:LEU:HD12	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:498:GLY:C	2:H:500:GLU:N	2.53	0.61
2:L:208:GLN:HE21	2:L:208:GLN:CA	2.11	0.61
1:A:221:GLU:HG3	1:A:222:ALA:N	2.14	0.61
1:A:271:LEU:O	1:A:272:ASN:HB2	1.99	0.61
1:A:709:THR:HG23	1:A:710:PRO:HD2	1.81	0.61
2:B:460:ARG:HH12	2:B:548:ALA:HB1	1.62	0.61
1:C:309:ALA:O	1:C:312:ALA:HB3	2.00	0.61
1:C:353:LEU:HD13	1:C:358:TRP:CZ2	2.35	0.61
1:C:357:ALA:O	1:C:361:ARG:HG3	2.00	0.61
1:C:561:ARG:NH1	1:C:632:VAL:HG22	2.16	0.61
2:D:244:PRO:HA	2:D:247:VAL:HG12	1.82	0.61
2:D:393:GLN:O	2:D:393:GLN:HG2	2.00	0.61
1:G:104:ALA:HA	1:G:108:LEU:HD12	1.81	0.61
2:H:68:GLY:O	2:H:70:ALA:N	2.33	0.61
1:I:169:LEU:O	1:I:173:ALA:HB2	1.99	0.61
1:I:471:ARG:HB2	1:I:471:ARG:HH11	1.65	0.61
1:K:285:VAL:HG12	1:K:286:VAL:CG2	2.27	0.61
1:K:379:GLY:HA3	1:K:440:TRP:CH2	2.35	0.61
2:L:525:ARG:NH1	2:L:525:ARG:HG3	2.12	0.61
1:A:50:GLN:HE21	1:A:123:GLN:NE2	1.99	0.61
1:A:613:ARG:HG2	1:A:614:ARG:N	2.15	0.61
2:D:119:ILE:HD11	2:D:134:VAL:CG1	2.31	0.61
1:E:232:GLN:CG	1:E:233:ARG:HH12	2.12	0.61
2:F:56:LEU:HG	2:F:60:LEU:HD12	1.81	0.61
2:H:465:TRP:HE3	2:H:467:ASN:HD21	1.48	0.61
2:H:521:TYR:CE1	2:H:525:ARG:CZ	2.83	0.61
2:H:164:ARG:CB	2:H:551:ALA:HB2	2.29	0.61
2:H:303:GLN:NE2	2:J:297:ARG:HD2	2.16	0.61
2:J:83:VAL:HG13	2:J:84:ARG:N	2.11	0.61
2:J:86:ARG:HD3	2:J:213:MET:SD	2.40	0.61
1:K:497:LEU:N	1:K:498:PRO:HD3	2.15	0.61
2:L:486:LYS:HG2	2:L:505:ILE:CD1	2.31	0.61
2:L:74:ARG:CZ	2:L:78:ARG:HH12	2.13	0.61
1:A:662:VAL:HG21	1:A:674:LEU:HD22	1.80	0.61
2:F:29:ALA:O	2:F:343:GLU:HA	2.01	0.61
1:I:111:ASP:O	1:I:114:ILE:HG22	2.01	0.61
1:I:613:ARG:HG2	1:I:614:ARG:N	2.14	0.61
2:J:59:LEU:O	2:J:59:LEU:HD12	1.99	0.61
2:L:390:LEU:O	2:L:394:ARG:HG3	2.00	0.61
2:L:476:GLU:HA	2:L:479:ALA:HB3	1.83	0.61
1:A:271:LEU:HA	1:A:375:VAL:HG11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:LEU:HD23	1:A:629:ILE:HD12	1.83	0.61
2:B:74:ARG:HG2	2:B:74:ARG:O	2.00	0.61
1:C:307:VAL:O	1:C:310:ALA:HB3	2.01	0.61
2:F:188:ARG:HA	2:H:456:ALA:HA	1.82	0.61
2:F:247:VAL:HG12	2:F:253:GLU:OE2	1.99	0.61
1:I:268:CYS:SG	1:I:307:VAL:HG22	2.41	0.61
1:I:328:ARG:NH1	1:I:328:ARG:HB2	2.16	0.61
2:J:486:LYS:HA	2:J:489:GLN:NE2	2.15	0.61
1:K:324:LEU:HB2	1:K:334:MET:SD	2.41	0.61
1:A:315:TYR:HE2	1:A:338:THR:HG22	1.65	0.61
1:A:54:VAL:HG11	1:A:61:ALA:HA	1.81	0.61
1:E:392:GLU:C	1:E:394:ASP:H	2.04	0.61
2:F:146:TYR:N	2:F:149:THR:OG1	2.34	0.61
2:F:563:MET:SD	2:L:424:LYS:HE3	2.40	0.61
1:G:513:ALA:HA	1:G:555:LEU:HD11	1.82	0.61
1:G:536:PRO:HB3	2:H:363:HIS:HE1	1.65	0.61
2:J:209:ILE:HG22	2:J:210:ALA:N	2.16	0.61
1:K:320:THR:O	1:K:336:MET:HG2	2.00	0.61
1:K:101:ALA:CB	1:K:429:PHE:HE1	1.98	0.61
2:L:403:ASN:HA	2:L:443:GLY:H	1.64	0.61
1:A:469:PHE:CD2	1:A:469:PHE:C	2.73	0.61
2:B:231:VAL:CG2	2:B:275:HIS:HB2	2.31	0.61
2:B:51:GLU:HA	2:B:54:ASN:HD22	1.65	0.61
2:B:75:HIS:CE1	2:B:80:LYS:HE2	2.35	0.61
1:C:263:ASP:OD1	1:C:265:HIS:HB2	2.00	0.61
1:C:294:LEU:HD13	1:C:299:ARG:NH1	2.15	0.61
1:E:273:GLU:OE2	1:E:291:ALA:N	2.34	0.61
1:E:328:ARG:HH11	1:E:328:ARG:HG3	1.65	0.61
1:E:101:ALA:HB1	1:E:429:PHE:CD1	2.36	0.61
2:F:194:ILE:O	2:F:198:GLN:HG3	2.01	0.61
1:G:200:TYR:O	1:G:202:VAL:N	2.34	0.61
1:G:448:ARG:HD3	1:G:474:LEU:O	2.00	0.61
1:G:612:LEU:HD12	1:G:612:LEU:O	1.99	0.61
1:K:269:LEU:CD2	1:K:368:LEU:HD13	2.31	0.61
1:K:307:VAL:O	1:K:310:ALA:HB3	2.01	0.61
2:B:87:ILE:CD1	2:B:120:VAL:HG11	2.31	0.61
2:B:403:ASN:HA	2:B:443:GLY:H	1.66	0.61
1:C:274:ARG:NH2	1:C:320:THR:HG21	2.16	0.61
2:D:376:LEU:HD23	2:D:380:ALA:HB3	1.82	0.61
1:E:131:PHE:HD1	1:E:131:PHE:H	1.47	0.61
1:E:344:HIS:N	1:E:345:PRO:CD	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ARG:HB2	1:G:122:ALA:HA	1.83	0.61
1:I:108:LEU:HD23	1:I:132:LEU:HD12	1.82	0.61
1:K:612:LEU:HD12	1:K:612:LEU:H	1.65	0.61
1:K:613:ARG:HG2	1:K:614:ARG:N	2.16	0.61
2:L:90:LEU:HB2	2:L:284:LEU:HD22	1.82	0.61
1:A:300:ARG:O	1:A:304:GLU:OE2	2.19	0.61
1:C:50:GLN:HB2	1:C:123:GLN:HE22	1.64	0.61
2:D:432:ALA:HA	2:D:556:THR:HG21	1.83	0.61
1:E:340:LEU:HG	1:E:359:GLN:NE2	2.16	0.61
2:F:359:PHE:CE2	2:F:387:PHE:CE1	2.89	0.61
2:F:399:LEU:HD12	2:F:400:PHE:N	2.16	0.61
1:I:328:ARG:CZ	1:I:328:ARG:HB2	2.31	0.61
1:K:66:ARG:CB	1:K:66:ARG:NH1	2.62	0.61
2:L:194:ILE:HD12	2:L:194:ILE:N	2.15	0.61
2:B:202:SER:HB2	2:L:560:VAL:HG23	1.83	0.60
2:B:561:PHE:CD2	2:J:563:MET:HE1	2.36	0.60
1:C:270:TYR:CD1	1:C:372:GLN:NE2	2.69	0.60
2:D:440:LEU:CD1	2:D:464:MET:HG3	2.31	0.60
1:E:602:VAL:O	1:E:602:VAL:HG12	2.00	0.60
1:G:389:GLU:HA	1:G:397:PRO:HA	1.82	0.60
1:G:71:LEU:CB	1:G:73:ILE:HD12	2.31	0.60
1:G:71:LEU:HB2	1:G:73:ILE:HD12	1.82	0.60
2:H:193:ARG:NH1	2:H:196:PHE:CE2	2.69	0.60
2:B:444:SER:CB	2:B:449:ASN:HD22	2.08	0.60
1:C:278:ILE:H	1:C:278:ILE:CD1	1.95	0.60
1:C:53:LEU:HD13	1:C:117:ALA:HA	1.82	0.60
2:D:109:TYR:OH	2:D:147:PRO:HB2	2.00	0.60
2:D:520:TYR:N	2:D:520:TYR:CD2	2.66	0.60
2:F:200:ASN:ND2	2:F:204:ARG:NH2	2.50	0.60
2:F:408:MET:HE3	2:F:409:VAL:H	1.65	0.60
2:F:498:GLY:C	2:F:500:GLU:H	2.05	0.60
1:G:249:TYR:HD2	1:G:250:LEU:H	1.49	0.60
1:G:283:GLN:NE2	1:G:389:GLU:OE1	2.32	0.60
1:G:396:LEU:O	1:G:398:ALA:N	2.33	0.60
2:H:258:GLU:OE2	2:H:262:GLY:HA3	2.00	0.60
2:H:270:SER:OG	2:H:272:VAL:HG23	2.00	0.60
2:H:400:PHE:CD2	2:H:453:CYS:HB2	2.35	0.60
1:I:54:VAL:HG21	1:I:64:VAL:CG1	2.31	0.60
2:J:462:LEU:HD23	2:J:463:TRP:N	2.16	0.60
1:A:543:TRP:O	1:A:544:ARG:NH1	2.34	0.60
1:C:549:ARG:NE	1:C:571:PRO:HG3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:300:GLY:O	2:D:301:GLN:HB2	2.00	0.60
1:E:112:ARG:HG3	1:E:112:ARG:NH1	2.12	0.60
1:E:269:LEU:HD23	1:E:269:LEU:H	1.65	0.60
1:E:320:THR:O	1:E:336:MET:HG2	2.01	0.60
2:F:484:GLN:HE22	2:F:487:ARG:NH1	1.98	0.60
1:G:379:GLY:HA3	1:G:440:TRP:CH2	2.37	0.60
1:I:505:PRO:HB2	1:I:507:HIS:HB3	1.82	0.60
2:J:351:PHE:O	2:J:383:LYS:HD2	2.01	0.60
1:K:269:LEU:HD12	1:K:375:VAL:CG2	2.32	0.60
1:A:196:GLY:O	1:A:198:ILE:N	2.34	0.60
1:A:304:GLU:O	1:A:307:VAL:HG12	2.00	0.60
1:A:267:HIS:CB	1:A:368:LEU:HD12	2.30	0.60
1:A:472:ARG:CZ	1:A:498:PRO:HD2	2.32	0.60
1:C:536:PRO:HB3	2:D:363:HIS:CD2	2.37	0.60
1:C:567:ARG:HG3	1:C:567:ARG:HH11	1.66	0.60
1:E:261:PHE:CZ	1:E:318:ALA:HB2	2.36	0.60
2:F:141:LYS:HE2	4:F:591:COA:O2B	2.01	0.60
1:G:250:LEU:HD12	1:G:250:LEU:H	1.66	0.60
1:G:47:ARG:HB2	1:G:47:ARG:NH1	2.06	0.60
1:G:618:LEU:O	1:G:629:ILE:HD12	2.01	0.60
2:H:30:ILE:HD13	2:H:343:GLU:HG2	1.81	0.60
2:H:500:GLU:HA	2:H:500:GLU:OE1	2.01	0.60
1:K:304:GLU:O	1:K:308:ARG:HG2	2.00	0.60
1:K:550:GLU:HG2	1:K:567:ARG:CZ	2.32	0.60
2:L:375:ILE:HG22	2:L:376:LEU:H	1.66	0.60
2:L:81:LEU:HD21	2:L:89:ARG:HH21	1.64	0.60
1:A:667:THR:HG22	1:A:667:THR:O	2.01	0.60
2:B:50:LEU:O	2:B:54:ASN:ND2	2.35	0.60
2:B:84:ARG:HG2	2:B:84:ARG:NH1	2.15	0.60
1:C:341:GLN:OE1	1:C:342:VAL:HG23	2.01	0.60
1:C:384:VAL:HG23	1:C:451:LEU:HD21	1.83	0.60
1:C:55:ALA:HB1	1:C:113:ILE:HD13	1.82	0.60
1:C:94:ILE:N	1:C:94:ILE:HD12	2.16	0.60
2:D:233:VAL:CG1	2:D:279:ASP:HA	2.31	0.60
2:D:28:MET:C	2:D:30:ILE:H	2.02	0.60
2:F:35:ILE:CD1	2:F:320:VAL:HG22	2.32	0.60
2:F:469:ARG:NH2	2:F:469:ARG:HG2	2.13	0.60
1:G:451:LEU:HA	1:G:454:MET:HG3	1.82	0.60
2:H:242:ALA:O	2:H:260:LEU:HD21	2.00	0.60
2:J:141:LYS:HZ1	2:J:177:ASN:HD21	1.50	0.60
2:J:164:ARG:HD3	2:J:550:ASN:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:294:LEU:CB	1:K:298:LEU:HD22	2.31	0.60
1:K:620:LEU:HD12	1:K:621:GLU:N	2.16	0.60
1:A:272:ASN:ND2	1:A:377:LEU:HD22	2.17	0.60
1:A:493:GLN:HE22	1:A:497:LEU:HB2	1.65	0.60
1:C:93:ASP:C	1:C:94:ILE:HD12	2.22	0.60
2:F:282:HIS:CE1	2:F:286:ILE:HD11	2.37	0.60
2:L:435:PRO:HG3	2:L:460:ARG:NH2	2.16	0.60
2:L:484:GLN:HG3	2:L:488:GLU:OE1	2.01	0.60
1:A:175:VAL:HG21	1:A:309:ALA:HB2	1.82	0.60
1:A:698:TYR:CE1	1:A:710:PRO:HB2	2.37	0.60
1:C:218:VAL:HG23	1:C:218:VAL:O	2.01	0.60
1:C:445:GLU:OE1	1:C:448:ARG:NH2	2.35	0.60
2:D:465:TRP:HB3	2:D:467:ASN:ND2	2.17	0.60
2:J:299:GLN:HB3	2:J:552:PRO:HD3	1.82	0.60
2:L:109:TYR:CE2	2:L:147:PRO:HD2	2.37	0.60
1:A:103:PRO:C	1:A:108:LEU:HD12	2.21	0.60
1:C:358:TRP:O	1:C:362:VAL:HG22	2.01	0.60
1:C:55:ALA:O	1:C:56:ASN:HB2	2.00	0.60
1:C:561:ARG:HB3	1:C:561:ARG:CZ	2.32	0.60
2:D:487:ARG:O	2:D:487:ARG:CG	2.49	0.60
1:E:197:ARG:O	1:E:198:ILE:HG13	2.02	0.60
2:F:191:PHE:HD2	2:F:192:GLY:H	1.47	0.60
2:F:507:ALA:HA	2:F:510:LEU:HD12	1.84	0.60
1:I:587:GLN:HB3	1:I:588:TYR:HD1	1.66	0.60
1:K:391:PRO:HD3	1:K:465:THR:O	2.02	0.60
1:C:304:GLU:HB3	1:C:308:ARG:NH2	2.17	0.60
1:C:387:TYR:HB2	1:C:466:ASN:ND2	2.17	0.60
1:E:169:LEU:N	1:E:169:LEU:HD12	2.17	0.60
1:I:148:LEU:N	1:I:148:LEU:HD23	2.17	0.60
1:I:587:GLN:OE1	1:I:587:GLN:HA	2.01	0.60
1:K:258:ILE:O	1:K:320:THR:HA	2.00	0.60
2:L:232:MET:HE3	2:L:239:ILE:HG13	1.84	0.60
2:F:114:VAL:HG11	2:F:146:TYR:CZ	2.37	0.60
2:F:338:LEU:HD21	2:F:537:THR:HB	1.82	0.60
1:G:607:ARG:NH1	1:G:607:ARG:CB	2.65	0.60
2:J:49:MET:CG	2:J:318:TYR:HD1	2.15	0.60
1:A:220:ARG:HG3	1:A:223:GLU:OE1	2.02	0.59
1:A:450:ARG:O	1:A:453:ALA:HB3	2.02	0.59
1:A:596:ASP:HB3	1:A:612:LEU:HB3	1.84	0.59
1:C:203:LEU:CD2	1:C:205:LYS:NZ	2.62	0.59
2:F:403:ASN:OD1	2:F:442:GLY:HA3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ARG:HD3	1:G:121:GLY:O	2.02	0.59
1:K:132:LEU:HD23	1:K:138:PHE:CD2	2.37	0.59
1:K:346:VAL:HG13	1:K:383:GLU:HB2	1.84	0.59
1:K:361:ARG:HG2	1:K:361:ARG:HH11	1.67	0.59
1:K:53:LEU:HD13	1:K:117:ALA:CA	2.32	0.59
1:K:559:ASP:O	1:K:560:GLU:HG3	2.02	0.59
2:L:365:TYR:CB	2:L:545:LEU:HD13	2.30	0.59
2:L:438:THR:HG22	2:L:462:LEU:HG	1.83	0.59
1:A:257:GLU:O	1:A:273:GLU:HB2	2.02	0.59
1:A:602:VAL:O	1:A:605:VAL:HG22	2.01	0.59
1:A:652:PRO:CD	1:A:686:ILE:HG12	2.32	0.59
1:A:80:SER:OG	1:A:81:ASP:N	2.33	0.59
2:B:191:PHE:HD2	2:B:192:GLY:N	1.99	0.59
2:B:35:ILE:HD11	2:B:337:ARG:NH1	2.17	0.59
1:C:455:LEU:O	1:C:471:ARG:NH1	2.34	0.59
2:D:317:LEU:HD22	2:D:334:VAL:HG12	1.84	0.59
1:E:63:ARG:NH1	1:E:356:VAL:HG21	2.17	0.59
1:G:178:VAL:HG22	1:G:332:PHE:CD1	2.37	0.59
1:I:104:ALA:HA	1:I:108:LEU:CD1	2.32	0.59
1:I:350:ILE:HD12	1:I:377:LEU:HD11	1.84	0.59
1:I:398:ALA:HB2	1:I:464:ARG:NE	2.10	0.59
2:L:218:ALA:O	2:L:221:ALA:CB	2.49	0.59
1:A:180:GLY:HA2	1:A:198:ILE:HD11	1.85	0.59
1:A:255:HIS:CE1	1:A:322:GLU:HG2	2.38	0.59
2:B:193:ARG:HD2	2:B:196:PHE:HD2	1.66	0.59
1:C:169:LEU:HD21	1:C:313:ILE:HG12	1.84	0.59
1:G:536:PRO:HG2	2:H:543:LEU:HD23	1.84	0.59
1:I:167:LYS:O	1:I:171:GLU:HB2	2.01	0.59
1:I:298:LEU:O	1:I:301:ALA:HB3	2.03	0.59
1:I:302:MET:HA	1:I:331:PHE:CE1	2.36	0.59
1:K:273:GLU:OE1	1:K:299:ARG:NH1	2.35	0.59
1:A:504:LEU:O	1:A:505:PRO:O	2.20	0.59
2:B:234:ARG:HA	2:B:263:ALA:CB	2.31	0.59
1:C:188:LEU:H	1:C:188:LEU:HD12	1.67	0.59
2:D:119:ILE:HD11	2:D:134:VAL:HG13	1.85	0.59
2:D:562:ARG:HG3	2:D:562:ARG:HH11	1.67	0.59
2:F:234:ARG:HA	2:F:263:ALA:HB3	1.85	0.59
2:F:270:SER:OG	2:F:271:GLY:N	2.33	0.59
2:L:208:GLN:HA	2:L:208:GLN:NE2	2.13	0.59
2:B:217:THR:HG22	2:B:240:PHE:CE1	2.37	0.59
1:C:489:ILE:HG23	1:C:490:ALA:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ARG:NH1	1:C:63:ARG:O	2.35	0.59
2:F:218:ALA:O	2:F:221:ALA:CB	2.50	0.59
2:F:525:ARG:HG3	2:F:525:ARG:NH1	2.17	0.59
2:H:354:THR:HG21	2:H:375:ILE:HB	1.85	0.59
1:I:277:SER:HB3	1:I:485:ASP:O	2.01	0.59
1:I:549:ARG:HG3	1:I:549:ARG:NH1	2.14	0.59
2:J:486:LYS:HG2	2:J:505:ILE:CD1	2.31	0.59
2:J:507:ALA:HA	2:J:510:LEU:HD12	1.85	0.59
2:L:414:GLU:HA	2:L:418:ILE:HG22	1.83	0.59
1:A:288:GLU:HB3	1:A:382:ILE:HG12	1.85	0.59
1:A:540:ASN:C	1:A:540:ASN:HD22	2.06	0.59
1:C:452:LEU:CD2	1:C:474:LEU:HB3	2.32	0.59
2:D:305:ARG:NH1	2:D:305:ARG:CB	2.66	0.59
2:D:82:LEU:HD12	2:D:82:LEU:N	2.18	0.59
2:F:486:LYS:HG2	2:F:505:ILE:HD13	1.84	0.59
2:H:476:GLU:H	2:H:476:GLU:CD	2.04	0.59
2:H:52:GLN:O	2:H:55:ALA:HB3	2.03	0.59
1:I:397:PRO:HB3	1:I:432:PRO:HG3	1.85	0.59
1:I:513:ALA:CB	1:I:564:VAL:HG11	2.33	0.59
1:K:152:PRO:CG	1:K:315:TYR:CZ	2.83	0.59
1:K:395:PHE:O	1:K:397:PRO:HD3	2.03	0.59
2:D:486:LYS:HA	2:D:486:LYS:HE3	1.84	0.59
1:E:108:LEU:HD23	1:E:132:LEU:HD22	1.85	0.59
1:E:365:GLY:O	1:E:366:GLU:O	2.21	0.59
1:G:76:VAL:HG13	1:G:94:ILE:HB	1.85	0.59
1:I:294:LEU:HD11	1:I:299:ARG:HH12	1.68	0.59
1:I:540:ASN:C	1:I:540:ASN:HD22	2.06	0.59
2:J:375:ILE:HG22	2:J:376:LEU:N	2.17	0.59
1:K:491:ARG:HD2	1:K:492:HIS:CE1	2.38	0.59
2:L:464:MET:HE1	2:L:470:ILE:HD12	1.83	0.59
2:B:109:TYR:CD2	2:B:146:TYR:HD1	2.21	0.59
2:B:444:SER:HB3	2:B:449:ASN:ND2	2.12	0.59
1:C:99:GLY:HA3	1:C:105:ASP:O	2.02	0.59
1:E:607:ARG:HG3	1:E:607:ARG:HH11	1.68	0.59
1:I:315:TYR:OH	1:I:338:THR:HA	2.02	0.59
1:I:392:GLU:C	1:I:394:ASP:H	2.06	0.59
2:J:509:ILE:HD13	2:J:512:GLN:OE1	2.01	0.59
2:L:350:LEU:CD2	2:L:350:LEU:N	2.65	0.59
2:L:49:MET:HE1	2:L:467:ASN:HB3	1.85	0.59
2:B:109:TYR:CE2	2:B:147:PRO:HD2	2.38	0.59
2:B:223:VAL:O	2:B:227:SER:OG	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:O	2:B:288:ARG:NH2	2.36	0.59
2:B:331:VAL:HG12	2:B:373:ASN:CG	2.23	0.59
2:D:345:ASP:OD1	2:F:289:ARG:NE	2.33	0.59
2:D:508:PRO:HG2	2:D:509:ILE:H	1.67	0.59
1:E:76:VAL:HG11	1:E:120:SER:OG	2.03	0.59
1:E:509:TRP:CZ3	1:E:562:ARG:HB2	2.38	0.59
2:F:245:PRO:CB	2:H:481:VAL:HG13	2.32	0.59
2:F:412:LYS:HE3	2:F:413:TYR:CE1	2.38	0.59
2:F:435:PRO:HD3	2:F:553:ILE:HG23	1.83	0.59
2:F:491:GLU:C	2:F:493:ALA:H	2.05	0.59
1:G:385:ARG:HB3	1:G:387:TYR:HE1	1.68	0.59
1:G:549:ARG:CG	1:G:549:ARG:HH11	2.16	0.59
2:H:533:ASP:CB	2:H:536:GLN:HE21	2.15	0.59
1:I:351:THR:OG1	1:I:352:GLY:N	2.36	0.59
1:I:504:LEU:HB3	1:I:505:PRO:HD2	1.84	0.59
1:K:169:LEU:O	1:K:173:ALA:HB2	2.03	0.59
1:K:279:GLN:HB2	1:K:283:GLN:O	2.02	0.59
1:K:452:LEU:HD21	1:K:474:LEU:HB3	1.83	0.59
1:A:482:ALA:O	1:A:484:LEU:N	2.30	0.59
1:A:512:ALA:HB1	1:A:629:ILE:HD13	1.85	0.59
1:A:676:VAL:HG13	1:A:685:SER:OG	2.03	0.59
1:C:465:THR:HG22	1:C:466:ASN:N	2.17	0.59
2:D:349:ALA:HB3	2:D:350:LEU:HD22	1.85	0.59
2:H:300:GLY:O	2:H:301:GLN:HB2	2.02	0.59
1:G:534:HIS:HB3	2:H:307:PRO:CG	2.33	0.59
2:J:141:LYS:NZ	2:J:177:ASN:HD21	2.00	0.59
2:J:311:LEU:HD12	2:J:341:GLY:O	2.03	0.59
2:J:35:ILE:CD1	2:J:320:VAL:HG22	2.33	0.59
1:K:271:LEU:HA	1:K:375:VAL:HG11	1.84	0.59
1:A:697:LEU:CB	1:A:712:VAL:HG22	2.32	0.58
1:C:389:GLU:HG2	1:C:397:PRO:HG3	1.85	0.58
2:D:331:VAL:H	2:D:373:ASN:HD21	1.50	0.58
1:G:416:VAL:HG22	1:G:437:LEU:HD12	1.85	0.58
1:G:53:LEU:HD11	1:G:78:VAL:HG13	1.83	0.58
2:H:297:ARG:HB2	2:L:303:GLN:NE2	2.14	0.58
2:H:48:THR:O	2:H:52:GLN:HG3	2.03	0.58
2:L:167:CYS:HB2	2:L:208:GLN:NE2	2.18	0.58
2:D:248:LYS:HA	2:D:252:GLY:O	2.03	0.58
1:E:553:LEU:HB2	1:E:564:VAL:CG2	2.34	0.58
2:F:441:ILE:HG22	2:F:465:TRP:CD2	2.38	0.58
1:G:274:ARG:HH22	1:G:320:THR:CG2	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:ARG:HH11	1:G:308:ARG:HG3	1.68	0.58
2:J:512:GLN:O	2:J:516:GLN:HG3	2.04	0.58
1:K:396:LEU:HD12	1:K:464:ARG:NH2	2.19	0.58
2:L:155:ARG:O	2:L:159:ILE:HD12	2.03	0.58
2:B:481:VAL:HG13	2:L:245:PRO:HB3	1.86	0.58
1:C:272:ASN:CG	1:C:377:LEU:HD22	2.23	0.58
1:C:508:PHE:O	1:C:510:GLN:N	2.37	0.58
1:C:516:TRP:CZ2	1:C:631:ALA:HB2	2.38	0.58
1:C:570:SER:OG	1:C:570:SER:O	2.21	0.58
2:F:300:GLY:HA3	2:F:549:LEU:HD23	1.85	0.58
1:G:187:ASP:O	1:G:189:GLU:N	2.36	0.58
1:I:315:TYR:HE2	1:I:336:MET:CE	2.15	0.58
2:J:191:PHE:HA	2:J:194:ILE:HD11	1.84	0.58
2:J:390:LEU:O	2:J:394:ARG:HG3	2.03	0.58
2:J:89:ARG:HH21	2:J:89:ARG:HG3	1.67	0.58
1:K:470:LEU:O	1:K:473:ILE:HG23	2.03	0.58
2:L:234:ARG:HA	2:L:263:ALA:HB3	1.85	0.58
2:L:247:VAL:O	2:L:250:ALA:HB3	2.03	0.58
1:A:444:ARG:O	1:A:447:ALA:HB3	2.02	0.58
2:D:151:LYS:HG2	2:D:526:LEU:HD13	1.86	0.58
1:E:358:TRP:HA	1:E:361:ARG:HD2	1.84	0.58
1:G:223:GLU:O	1:G:223:GLU:HG2	2.02	0.58
1:G:567:ARG:NH1	1:G:567:ARG:HG3	2.15	0.58
2:H:153:HIS:ND1	2:H:194:ILE:HD13	2.18	0.58
1:A:654:ASN:HB2	2:H:251:THR:CB	2.34	0.58
2:H:398:LEU:HD12	2:H:434:VAL:CG2	2.33	0.58
1:I:274:ARG:HD3	1:I:346:VAL:CG2	2.34	0.58
1:I:46:TYR:CE1	1:I:364:ARG:HD3	2.37	0.58
1:I:623:GLU:OE1	1:I:623:GLU:HA	2.03	0.58
1:I:71:LEU:HD23	1:I:71:LEU:O	2.03	0.58
2:J:324:ASP:O	2:J:327:GLN:HB2	2.04	0.58
1:A:298:LEU:O	1:A:301:ALA:HB3	2.04	0.58
1:A:65:MET:HG3	1:A:75:SER:CB	2.33	0.58
1:A:53:LEU:HD12	1:A:76:VAL:HB	1.85	0.58
2:B:50:LEU:CD2	2:B:54:ASN:HD21	2.16	0.58
1:G:108:LEU:HD23	1:G:132:LEU:HD13	1.86	0.58
1:G:189:GLU:OE1	1:G:193:ARG:HD3	2.03	0.58
2:D:516:GLN:OE1	2:J:181:GLN:NE2	2.35	0.58
2:J:533:ASP:HB3	2:J:536:GLN:HE21	1.68	0.58
2:J:302:LEU:HD12	2:J:549:LEU:HD11	1.86	0.58
2:L:239:ILE:O	2:L:266:HIS:NE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ARG:HH22	2:B:343:GLU:CD	2.06	0.58
2:B:33:THR:HG23	2:B:34:GLN:N	2.19	0.58
2:B:78:ARG:HG3	2:B:78:ARG:NH1	2.18	0.58
2:D:264:ASP:OD2	2:D:268:LYS:HE3	2.04	0.58
1:E:232:GLN:O	1:E:233:ARG:HG2	2.02	0.58
2:F:440:LEU:HD12	2:F:464:MET:CE	2.32	0.58
2:H:170:LEU:CD2	2:H:211:VAL:HB	2.33	0.58
2:H:476:GLU:CD	2:H:476:GLU:N	2.57	0.58
2:H:50:LEU:O	2:H:50:LEU:HD23	2.04	0.58
1:I:65:MET:HE3	1:I:92:ALA:CA	2.34	0.58
1:A:136:ALA:O	1:A:137:ASP:C	2.41	0.58
1:C:274:ARG:NH1	1:C:347:THR:OG1	2.26	0.58
1:C:360:ILE:O	1:C:364:ARG:HD2	2.03	0.58
2:D:305:ARG:NH1	2:D:305:ARG:HB2	2.19	0.58
2:D:418:ILE:O	2:D:418:ILE:HG13	2.03	0.58
1:E:108:LEU:HD23	1:E:132:LEU:HD21	1.86	0.58
1:E:109:ARG:HD3	1:E:112:ARG:NH2	2.18	0.58
2:F:57:ARG:HG3	2:F:57:ARG:NH1	2.17	0.58
1:G:199:GLY:O	1:G:201:PRO:N	2.36	0.58
1:G:501:GLN:HE21	1:G:504:LEU:HG	1.69	0.58
1:G:550:GLU:HG3	1:G:567:ARG:HD2	1.85	0.58
2:H:243:GLY:C	2:H:245:PRO:HD2	2.23	0.58
2:H:33:THR:HB	2:H:312:TYR:CE2	2.38	0.58
2:J:521:TYR:CE1	2:J:525:ARG:NH2	2.71	0.58
1:K:250:LEU:HD21	1:K:332:PHE:HE1	1.69	0.58
1:K:258:ILE:HD12	1:K:258:ILE:N	2.19	0.58
1:K:294:LEU:HB3	1:K:298:LEU:HD22	1.85	0.58
1:K:437:LEU:HD22	1:K:455:LEU:HD23	1.86	0.58
1:K:587:GLN:C	1:K:588:TYR:HD1	2.07	0.58
1:A:51:ARG:HB2	1:A:122:ALA:HA	1.85	0.58
2:B:155:ARG:O	2:B:159:ILE:CD1	2.51	0.58
2:B:484:GLN:HA	2:B:484:GLN:HE21	1.69	0.58
2:D:151:LYS:HE3	2:D:526:LEU:HB2	1.86	0.58
1:G:280:ARG:NH1	1:G:389:GLU:OE1	2.36	0.58
1:G:201:PRO:CG	1:G:328:ARG:HH21	2.15	0.58
2:H:449:ASN:OD1	2:H:454:GLY:HA3	2.03	0.58
1:I:386:LEU:HD21	1:I:467:LEU:HD12	1.85	0.58
1:K:268:CYS:SG	1:K:307:VAL:HG23	2.43	0.58
1:K:388:ALA:HB3	1:K:432:PRO:HB2	1.85	0.58
2:B:279:ASP:C	2:B:279:ASP:OD2	2.42	0.58
1:C:271:LEU:O	1:C:272:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASN:OD1	1:C:377:LEU:HD22	2.04	0.58
2:D:444:SER:OG	2:D:449:ASN:ND2	2.37	0.58
1:E:255:HIS:CE1	1:E:322:GLU:HG2	2.38	0.58
1:E:341:GLN:OE1	1:E:342:VAL:HG23	2.04	0.58
2:H:268:LYS:HE3	2:L:350:LEU:HD12	1.85	0.58
2:H:324:ASP:O	2:H:327:GLN:HB2	2.03	0.58
2:H:327:GLN:OE1	2:H:328:PRO:HD2	2.03	0.58
2:J:195:PHE:CE1	2:J:222:TYR:HB2	2.39	0.58
2:J:218:ALA:O	2:J:221:ALA:HB3	2.04	0.58
1:K:393:GLY:O	1:K:396:LEU:CG	2.52	0.58
1:A:99:GLY:HA3	1:A:105:ASP:O	2.03	0.58
2:D:195:PHE:CE1	2:D:222:TYR:HB2	2.39	0.58
2:D:242:ALA:CB	2:D:246:LEU:HD22	2.34	0.58
2:D:370:LEU:HD11	2:D:387:PHE:HD2	1.68	0.58
1:E:299:ARG:O	1:E:301:ALA:N	2.37	0.58
1:E:562:ARG:HH11	1:E:562:ARG:CG	2.06	0.58
1:E:611:ALA:HB2	1:E:620:LEU:CD1	2.33	0.58
2:F:247:VAL:HG13	2:H:409:VAL:HG23	1.83	0.58
1:G:59:GLU:OE1	1:G:129:TYR:OH	2.22	0.58
1:I:466:ASN:O	1:I:470:LEU:HG	2.04	0.58
1:I:465:THR:HG22	1:I:467:LEU:H	1.69	0.58
1:I:607:ARG:NH1	1:I:607:ARG:HB3	2.14	0.58
2:J:48:THR:O	2:J:52:GLN:HG3	2.04	0.58
2:L:404:ILE:HG23	2:L:404:ILE:O	2.04	0.58
1:A:299:ARG:O	1:A:301:ALA:N	2.37	0.57
2:B:159:ILE:H	2:B:159:ILE:HD12	1.68	0.57
2:B:232:MET:HE2	2:B:263:ALA:HA	1.86	0.57
2:B:33:THR:HG23	2:B:35:ILE:HG13	1.84	0.57
2:D:351:PHE:O	2:D:383:LYS:HD2	2.04	0.57
2:B:293:ASN:HB3	2:F:359:PHE:CD1	2.39	0.57
2:F:331:VAL:H	2:F:373:ASN:HD21	1.52	0.57
2:F:417:GLY:C	2:F:419:ALA:N	2.53	0.57
2:H:432:ALA:HA	2:H:556:THR:HG21	1.84	0.57
2:J:28:MET:HE3	1:K:633:ASP:OD1	2.03	0.57
2:L:195:PHE:CE1	2:L:222:TYR:HB2	2.39	0.57
2:J:303:GLN:NE2	2:L:297:ARG:HB2	2.18	0.57
1:A:274:ARG:HH22	1:A:320:THR:CG2	2.09	0.57
1:A:279:GLN:O	1:A:489:ILE:HG21	2.04	0.57
1:A:653:MET:HG2	1:A:654:ASN:N	2.13	0.57
2:D:237:ALA:O	2:D:238:THR:HG23	2.04	0.57
2:F:31:LEU:HD21	2:F:344:PHE:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:ARG:HH21	2:F:89:ARG:HG3	1.69	0.57
1:G:170:MET:SD	1:G:309:ALA:CB	2.90	0.57
1:I:306:ALA:HB1	1:I:321:VAL:CG2	2.29	0.57
1:K:539:ARG:HH21	2:L:363:HIS:HE1	1.51	0.57
2:L:302:LEU:HD22	2:L:366:PRO:HG2	1.85	0.57
1:A:300:ARG:CZ	1:A:304:GLU:OE1	2.52	0.57
1:A:493:GLN:NE2	1:A:497:LEU:HB2	2.19	0.57
1:A:504:LEU:HD13	1:A:622:TRP:HE1	1.68	0.57
1:A:525:ARG:HD2	2:B:125:ARG:HH21	1.69	0.57
2:B:95:SER:HB2	2:B:125:ARG:HB2	1.86	0.57
1:C:101:ALA:HB1	1:C:429:PHE:CE1	2.39	0.57
1:C:333:PHE:CE1	1:C:335:GLU:HA	2.38	0.57
1:C:94:ILE:HG22	1:C:95:ALA:N	2.20	0.57
1:G:445:GLU:CD	1:G:448:ARG:NH2	2.58	0.57
1:G:515:ALA:HB2	1:G:598:LEU:HD22	1.86	0.57
1:I:270:TYR:N	1:I:372:GLN:HE22	2.01	0.57
2:J:102:ALA:C	2:J:104:ALA:H	2.07	0.57
4:J:591:COA:H122	4:J:591:COA:O1A	2.04	0.57
1:K:78:VAL:HB	1:K:98:LEU:HD21	1.86	0.57
2:L:346:GLU:HG2	2:L:349:ALA:HA	1.86	0.57
2:L:375:ILE:N	2:L:375:ILE:HD12	2.18	0.57
2:L:351:PHE:O	2:L:383:LYS:HD2	2.02	0.57
2:L:42:PHE:HA	2:L:45:ASN:HD22	1.69	0.57
1:A:361:ARG:CG	1:A:361:ARG:HH11	2.16	0.57
1:C:344:HIS:HB2	1:C:355:LEU:HD12	1.86	0.57
1:C:561:ARG:NH1	1:C:561:ARG:CB	2.66	0.57
1:C:605:VAL:CG2	1:C:605:VAL:O	2.50	0.57
2:D:62:ARG:O	2:D:65:GLU:HB2	2.03	0.57
2:F:90:LEU:HB2	2:F:284:LEU:HD22	1.86	0.57
2:F:41:GLU:O	2:F:44:ALA:HB3	2.04	0.57
1:G:258:ILE:HD12	1:G:306:ALA:HB2	1.86	0.57
1:G:263:ASP:OD2	1:G:367:ALA:HA	2.04	0.57
1:G:302:MET:HG2	1:G:331:PHE:CD2	2.40	0.57
1:I:300:ARG:HH11	1:I:300:ARG:CB	2.16	0.57
1:I:428:PRO:HG2	1:I:429:PHE:CD1	2.39	0.57
1:K:279:GLN:NE2	1:K:282:HIS:HA	2.19	0.57
1:A:195:ALA:HB1	1:A:200:TYR:HE2	1.69	0.57
2:B:397:PRO:HG2	2:B:545:LEU:HD21	1.85	0.57
1:E:298:LEU:O	1:E:301:ALA:HB3	2.04	0.57
1:E:546:ALA:O	2:F:57:ARG:NE	2.31	0.57
2:F:33:THR:HG22	2:F:312:TYR:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:ALA:O	1:G:168:ALA:HB3	2.04	0.57
1:G:474:LEU:HD23	1:G:479:PHE:CE1	2.39	0.57
2:H:44:ALA:O	2:H:47:ALA:HB3	2.04	0.57
2:J:491:GLU:HA	2:J:495:GLN:O	2.04	0.57
1:A:302:MET:HG2	1:A:331:PHE:CD2	2.40	0.57
2:D:211:VAL:HG13	2:D:231:VAL:HB	1.85	0.57
1:E:437:LEU:CD2	1:E:455:LEU:HD23	2.34	0.57
1:E:47:ARG:HH11	1:E:47:ARG:HB2	1.69	0.57
2:F:484:GLN:HE22	2:F:487:ARG:CZ	2.17	0.57
1:G:611:ALA:HB2	1:G:620:LEU:CD1	2.34	0.57
2:F:185:PHE:CE2	2:H:472:VAL:HA	2.40	0.57
2:H:485:VAL:CG2	2:H:486:LYS:N	2.68	0.57
1:K:516:TRP:HA	1:K:618:LEU:HD13	1.86	0.57
2:L:30:ILE:HD12	2:L:311:LEU:HD11	1.87	0.57
2:B:347:PHE:O	2:B:348:LYS:C	2.42	0.57
2:B:89:ARG:CG	2:B:89:ARG:HH21	2.14	0.57
2:D:50:LEU:HD23	2:D:54:ASN:ND2	2.19	0.57
1:E:531:ASP:HB3	2:F:298:LYS:HB2	1.87	0.57
2:F:435:PRO:CG	2:F:553:ILE:HD12	2.34	0.57
1:I:167:LYS:HB2	1:I:167:LYS:HZ2	1.68	0.57
1:I:278:ILE:HG23	1:I:489:ILE:HD13	1.86	0.57
1:I:607:ARG:NH1	1:I:607:ARG:HB2	2.20	0.57
1:K:305:ALA:CA	1:K:308:ARG:HG3	2.34	0.57
1:K:536:PRO:O	1:K:539:ARG:HG2	2.05	0.57
2:L:305:ARG:CZ	2:L:305:ARG:CB	2.82	0.57
2:L:305:ARG:HB3	2:L:305:ARG:NH1	2.19	0.57
1:A:347:THR:O	1:A:351:THR:HG23	2.05	0.57
2:B:245:PRO:CB	2:L:481:VAL:HG13	2.34	0.57
2:B:52:GLN:O	2:B:55:ALA:HB3	2.05	0.57
1:C:243:ARG:O	1:C:243:ARG:HG2	2.04	0.57
1:C:544:ARG:HH21	2:D:88:ASN:ND2	2.03	0.57
1:E:47:ARG:HG3	1:E:48:SER:H	1.69	0.57
1:E:500:PRO:O	1:E:501:GLN:HB3	2.05	0.57
1:E:563:CYS:SG	1:E:565:ARG:NH2	2.78	0.57
2:F:180:ARG:CG	2:F:180:ARG:HH11	2.12	0.57
2:F:255:VAL:HG22	2:F:259:GLU:OE1	2.04	0.57
1:G:109:ARG:HB3	1:G:109:ARG:HH11	1.69	0.57
1:G:135:ASN:OD1	1:G:135:ASN:O	2.22	0.57
1:G:176:PRO:C	1:G:177:LEU:HD23	2.25	0.57
1:G:228:LEU:HG	1:G:229:SER:N	2.18	0.57
1:G:385:ARG:HB3	1:G:387:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:315:GLU:CD	2:H:315:GLU:N	2.58	0.57
1:I:365:GLY:O	1:I:366:GLU:O	2.22	0.57
1:I:69:ARG:NH2	1:I:91:GLU:O	2.38	0.57
1:I:99:GLY:HA3	1:I:105:ASP:O	2.04	0.57
1:K:105:ASP:N	1:K:105:ASP:OD2	2.32	0.57
2:L:161:LEU:CD2	2:L:201:MET:HG2	2.29	0.57
1:A:195:ALA:HB1	1:A:200:TYR:CE2	2.40	0.57
1:C:220:ARG:HB2	1:C:223:GLU:HB3	1.86	0.57
1:C:325:LEU:HD23	1:C:326:ASP:H	1.68	0.57
2:F:330:ASP:OD1	2:F:332:ARG:HB2	2.05	0.57
1:G:220:ARG:HB2	1:G:223:GLU:HB3	1.87	0.57
1:G:550:GLU:CG	1:G:567:ARG:HD2	2.34	0.57
1:G:587:GLN:HA	1:G:587:GLN:OE1	2.04	0.57
2:H:476:GLU:OE2	2:H:477:GLN:HG2	2.04	0.57
2:H:56:LEU:O	2:H:56:LEU:HD12	2.05	0.57
1:I:269:LEU:CA	1:I:372:GLN:NE2	2.67	0.57
1:I:504:LEU:CB	1:I:505:PRO:HD2	2.34	0.57
2:J:144:THR:HG21	4:J:591:COA:C5A	2.35	0.57
1:K:251:LEU:HD22	1:K:327:GLU:OE2	2.04	0.57
1:A:377:LEU:CG	1:A:377:LEU:O	2.51	0.57
1:A:675:VAL:HG11	1:A:711:LEU:HD13	1.85	0.57
1:C:141:ALA:HA	1:C:144:GLU:HB3	1.86	0.57
1:C:114:ILE:CD1	1:C:147:LEU:HD12	2.35	0.57
1:C:287:GLU:HG2	1:C:343:GLU:CG	2.35	0.57
1:E:223:GLU:HG2	1:E:223:GLU:O	2.04	0.57
1:E:248:LYS:HE3	1:E:328:ARG:HH12	1.70	0.57
2:F:241:LEU:HD12	2:H:418:ILE:HG23	1.87	0.57
2:F:386:HIS:O	2:F:390:LEU:HD12	2.05	0.57
1:G:205:LYS:HE2	1:G:245:LEU:HD13	1.87	0.57
1:G:365:GLY:O	1:G:366:GLU:O	2.22	0.57
2:H:485:VAL:HG23	2:H:486:LYS:N	2.20	0.57
2:H:521:TYR:O	2:H:525:ARG:HG3	2.05	0.57
1:I:107:TYR:HB2	1:I:131:PHE:CE1	2.40	0.57
1:I:289:ALA:HB1	1:I:350:ILE:HD13	1.87	0.57
1:I:374:GLN:O	1:I:376:PRO:HD3	2.03	0.57
1:I:549:ARG:CG	1:I:549:ARG:NH1	2.67	0.57
2:J:185:PHE:N	2:J:186:PRO:HD2	2.20	0.57
2:J:379:GLU:H	2:J:379:GLU:CD	2.08	0.57
1:K:321:VAL:HG22	1:K:336:MET:CG	2.29	0.57
2:B:265:VAL:O	2:B:269:VAL:HB	2.05	0.56
2:D:449:ASN:OD1	2:D:454:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:GLN:HG3	1:E:190:THR:OG1	2.05	0.56
1:E:276:CYS:HB2	1:E:284:LYS:NZ	2.20	0.56
1:E:404:LEU:HD13	1:E:612:LEU:HD13	1.86	0.56
2:F:146:TYR:N	2:F:149:THR:HG1	2.03	0.56
2:F:331:VAL:HA	2:F:334:VAL:HG23	1.87	0.56
2:F:308:ARG:HH22	2:F:343:GLU:HG3	1.69	0.56
1:I:269:LEU:HA	1:I:372:GLN:HE22	1.70	0.56
1:I:504:LEU:O	1:I:505:PRO:O	2.23	0.56
1:K:500:PRO:O	1:K:501:GLN:HB3	2.05	0.56
2:L:235:GLU:HA	2:L:258:GLU:OE1	2.03	0.56
2:L:311:LEU:HB2	2:L:312:TYR:CE1	2.40	0.56
2:L:54:ASN:O	2:L:58:THR:HG23	2.05	0.56
1:A:563:CYS:SG	1:A:565:ARG:NH2	2.77	0.56
2:B:193:ARG:NH1	2:B:196:PHE:CE2	2.74	0.56
2:B:457:TYR:N	2:B:457:TYR:CD2	2.71	0.56
2:D:45:ASN:OD1	2:D:323:ALA:N	2.38	0.56
1:E:561:ARG:H	1:E:561:ARG:CD	2.18	0.56
2:F:334:VAL:O	2:F:338:LEU:HD12	2.05	0.56
1:G:445:GLU:CD	1:G:448:ARG:HH21	2.08	0.56
1:G:469:PHE:CD1	1:G:497:LEU:HD21	2.40	0.56
2:H:246:LEU:N	2:H:246:LEU:HD12	2.18	0.56
2:H:400:PHE:CD2	2:H:453:CYS:CB	2.88	0.56
2:H:521:TYR:CD1	2:H:525:ARG:NH1	2.72	0.56
1:I:299:ARG:O	1:I:301:ALA:N	2.38	0.56
1:I:47:ARG:HH21	1:I:148:LEU:HD22	1.70	0.56
2:J:334:VAL:O	2:J:338:LEU:CD1	2.50	0.56
2:J:498:GLY:O	2:J:500:GLU:N	2.38	0.56
2:J:523:SER:HA	2:J:528:ASP:OD2	2.06	0.56
1:K:109:ARG:NH1	1:K:109:ARG:HB3	2.18	0.56
1:K:302:MET:HG2	1:K:331:PHE:CE1	2.40	0.56
1:A:231:ALA:HA	1:A:233:ARG:HH22	1.71	0.56
1:A:269:LEU:H	1:A:269:LEU:HD23	1.69	0.56
1:C:384:VAL:CG2	1:C:451:LEU:HD21	2.34	0.56
1:C:415:ARG:HD3	1:C:438:ILE:CD1	2.35	0.56
2:D:462:LEU:HD23	2:D:462:LEU:C	2.25	0.56
2:D:48:THR:O	2:D:52:GLN:HG3	2.04	0.56
2:D:62:ARG:HG2	2:D:62:ARG:HH11	1.71	0.56
1:E:169:LEU:H	1:E:169:LEU:CD1	2.19	0.56
2:F:433:ARG:H	2:F:556:THR:HG23	1.71	0.56
2:F:82:LEU:HD12	2:F:83:VAL:N	2.16	0.56
1:G:96:VAL:HG11	1:G:116:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:469:PHE:CE2	1:G:473:ILE:HG21	2.41	0.56
1:I:77:ALA:HB1	1:I:88:HIS:HD2	1.70	0.56
2:L:388:ILE:O	2:L:392:CYS:HB2	2.05	0.56
1:A:469:PHE:HD2	1:A:469:PHE:C	2.08	0.56
2:B:217:THR:HG22	2:B:240:PHE:HE1	1.71	0.56
1:C:516:TRP:O	1:C:519:SER:OG	2.23	0.56
1:C:536:PRO:HB3	2:D:363:HIS:NE2	2.19	0.56
2:D:476:GLU:OE2	2:D:477:GLN:N	2.38	0.56
1:E:378:ASN:O	1:E:440:TRP:CH2	2.58	0.56
1:E:613:ARG:HG2	1:E:614:ARG:N	2.21	0.56
1:K:387:TYR:CE2	1:K:433:MET:HB2	2.40	0.56
2:L:191:PHE:HE2	2:L:195:PHE:CZ	2.23	0.56
1:A:251:LEU:HD11	1:A:328:ARG:CZ	2.36	0.56
1:A:345:PRO:HB3	1:A:438:ILE:HD13	1.87	0.56
2:B:170:LEU:HD22	2:B:211:VAL:HB	1.86	0.56
1:C:188:LEU:HG	1:C:228:LEU:CD2	2.35	0.56
1:C:613:ARG:O	1:C:614:ARG:CD	2.53	0.56
1:E:508:PHE:HB2	1:E:622:TRP:CE2	2.41	0.56
2:F:109:TYR:OH	2:F:148:LEU:HD12	2.06	0.56
2:F:219:GLY:C	2:F:221:ALA:H	2.08	0.56
2:F:435:PRO:CD	2:F:553:ILE:HG23	2.34	0.56
1:G:326:ASP:OD1	1:G:327:GLU:N	2.38	0.56
1:G:150:LEU:HD21	1:G:363:ALA:CB	2.36	0.56
1:I:96:VAL:HG21	1:I:116:ALA:HB1	1.86	0.56
1:I:341:GLN:OE1	1:I:342:VAL:HG23	2.06	0.56
1:I:531:ASP:OD2	2:J:298:LYS:HB2	2.05	0.56
2:J:464:MET:CE	2:J:519:PRO:HG3	2.33	0.56
1:K:400:GLY:H	1:K:463:LEU:HD11	1.70	0.56
1:K:54:VAL:HG11	1:K:64:VAL:HG11	1.85	0.56
1:K:54:VAL:HG13	1:K:64:VAL:HG11	1.85	0.56
2:L:421:HIS:HA	2:L:424:LYS:HD2	1.87	0.56
1:A:169:LEU:CD2	1:A:313:ILE:HG22	2.36	0.56
2:F:84:ARG:CG	2:F:84:ARG:HH11	2.11	0.56
1:G:141:ALA:HA	1:G:144:GLU:HB3	1.87	0.56
1:G:259:GLN:OE1	1:G:320:THR:HG22	2.05	0.56
1:G:270:TYR:CE2	1:G:303:GLY:HA3	2.40	0.56
2:H:440:LEU:CD1	2:H:464:MET:HE2	2.34	0.56
2:H:447:ALA:H	3:I:801:BTI:HN3	1.52	0.56
2:J:476:GLU:OE2	2:J:477:GLN:HG3	2.06	0.56
2:J:521:TYR:CE1	2:J:525:ARG:CZ	2.89	0.56
1:K:590:LEU:HD13	1:K:598:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:HG3	1:A:315:TYR:CZ	2.40	0.56
1:A:204:LEU:HD22	1:A:246:VAL:HG22	1.88	0.56
1:A:663:GLU:HG3	1:A:666:GLN:HB2	1.87	0.56
2:B:218:ALA:O	2:B:221:ALA:HB3	2.05	0.56
2:B:498:GLY:O	2:B:500:GLU:N	2.38	0.56
1:C:373:GLU:N	1:C:373:GLU:OE1	2.36	0.56
1:C:378:ASN:ND2	1:C:440:TRP:CH2	2.74	0.56
2:D:278:GLU:HG2	2:D:282:HIS:CE1	2.39	0.56
2:D:476:GLU:HA	2:D:510:LEU:HD21	1.86	0.56
1:E:185:ALA:O	1:E:186:GLN:O	2.24	0.56
1:E:397:PRO:HB3	1:E:432:PRO:HG3	1.87	0.56
2:F:362:LEU:HD12	2:F:367:ILE:HD13	1.88	0.56
1:G:138:PHE:CE1	1:G:142:CYS:HB2	2.40	0.56
1:G:543:TRP:HB3	2:H:96:PRO:HB3	1.88	0.56
2:H:349:ALA:HB3	2:H:350:LEU:HD22	1.88	0.56
1:I:289:ALA:O	1:I:350:ILE:HG21	2.05	0.56
2:J:185:PHE:H	2:J:186:PRO:HD2	1.69	0.56
2:J:484:GLN:HA	2:J:484:GLN:NE2	2.19	0.56
2:D:202:SER:OG	2:J:560:VAL:HG23	2.06	0.56
2:J:68:GLY:O	2:J:70:ALA:N	2.39	0.56
1:K:602:VAL:O	1:K:602:VAL:HG12	2.06	0.56
2:L:313:PRO:HB2	2:L:316:GLU:HG3	1.88	0.56
1:A:431:ASP:C	1:A:431:ASP:OD2	2.44	0.56
1:A:607:ARG:HB3	1:A:607:ARG:HH11	1.70	0.56
2:B:402:GLN:OE1	2:B:452:MET:HB2	2.05	0.56
2:B:246:LEU:HD11	4:B:591:COA:O5P	2.06	0.56
1:C:278:ILE:HD11	1:C:484:LEU:CD2	2.35	0.56
1:C:387:TYR:H	1:C:466:ASN:ND2	2.03	0.56
1:C:562:ARG:HH11	1:C:562:ARG:CB	2.19	0.56
1:C:516:TRP:CH2	1:C:631:ALA:HB2	2.40	0.56
1:E:328:ARG:NH1	1:E:328:ARG:HG3	2.19	0.56
2:F:119:ILE:HG21	2:F:149:THR:HG22	1.87	0.56
2:F:440:LEU:HB2	2:F:464:MET:HG3	1.88	0.56
1:G:281:ARG:HH21	1:G:395:PHE:HD2	1.53	0.56
1:I:251:LEU:O	1:I:327:GLU:HG2	2.05	0.56
1:K:51:ARG:HB2	1:K:122:ALA:HA	1.87	0.56
1:K:250:LEU:HD21	1:K:332:PHE:CE1	2.41	0.56
2:L:53:VAL:HG12	2:L:57:ARG:CD	2.36	0.56
1:A:81:ASP:HB3	1:A:100:GLY:O	2.05	0.56
1:A:429:PHE:O	1:A:430:TYR:CD2	2.59	0.56
2:B:109:TYR:HE2	2:B:147:PRO:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:TYR:N	2:B:149:THR:OG1	2.39	0.56
2:B:248:LYS:CG	2:B:254:VAL:HG22	2.36	0.56
2:B:248:LYS:HA	2:B:252:GLY:O	2.06	0.56
1:C:170:MET:HE1	1:C:309:ALA:HB1	1.87	0.56
2:D:234:ARG:HA	2:D:263:ALA:CB	2.36	0.56
2:D:562:ARG:HG3	2:D:562:ARG:NH1	2.20	0.56
1:E:607:ARG:NH1	1:E:607:ARG:HG3	2.21	0.56
2:F:389:GLU:OE2	2:L:560:VAL:HG12	2.05	0.56
1:G:345:PRO:HB2	1:G:438:ILE:HD13	1.87	0.56
2:H:234:ARG:HA	2:H:263:ALA:CB	2.36	0.56
2:J:49:MET:HG2	2:J:318:TYR:HA	1.88	0.56
1:A:345:PRO:CB	1:A:438:ILE:HD13	2.36	0.56
1:A:672:ALA:O	1:A:674:LEU:HG	2.06	0.56
2:B:159:ILE:N	2:B:159:ILE:HD12	2.21	0.56
2:B:417:GLY:C	2:B:419:ALA:N	2.57	0.56
1:C:175:VAL:O	1:C:177:LEU:HD12	2.06	0.56
1:C:342:VAL:HG11	1:C:385:ARG:CZ	2.36	0.56
1:E:263:ASP:HA	1:E:362:VAL:HG12	1.86	0.56
1:E:519:SER:HB2	1:E:613:ARG:NE	2.21	0.56
1:G:269:LEU:CD2	1:G:368:LEU:HD23	2.35	0.56
1:G:378:ASN:O	1:G:440:TRP:CZ3	2.59	0.56
1:G:488:PHE:CD2	1:G:488:PHE:C	2.79	0.56
2:H:213:MET:HE2	2:H:280:ASP:HA	1.88	0.56
2:H:233:VAL:CG1	2:H:279:ASP:HA	2.36	0.56
1:K:251:LEU:HG	1:K:328:ARG:NH1	2.20	0.56
2:B:178:LEU:HD12	2:L:482:LEU:HD13	1.87	0.56
1:A:384:VAL:CG1	1:A:470:LEU:HD22	2.36	0.56
1:A:695:LYS:O	1:A:695:LYS:HG2	2.04	0.56
2:B:119:ILE:HD11	2:B:153:HIS:ND1	2.21	0.56
2:D:484:GLN:HG2	2:J:245:PRO:HB3	1.88	0.56
1:G:384:VAL:HB	1:G:470:LEU:HD13	1.87	0.56
2:H:412:LYS:HG3	2:H:413:TYR:N	2.21	0.56
1:G:537:TRP:CE2	2:H:543:LEU:HD22	2.41	0.56
2:J:305:ARG:HH21	2:J:361:HIS:CG	2.24	0.56
2:J:449:ASN:OD1	2:J:454:GLY:HA3	2.05	0.56
2:J:444:SER:CB	2:J:470:ILE:HG13	2.34	0.56
2:L:164:ARG:HG2	2:L:164:ARG:O	2.06	0.56
2:L:462:LEU:C	2:L:462:LEU:HD23	2.26	0.56
1:A:497:LEU:N	1:A:498:PRO:CD	2.69	0.55
1:C:47:ARG:NH1	1:C:47:ARG:CB	2.69	0.55
1:C:49:ILE:CD1	1:C:364:ARG:CG	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:PRO:HG3	2:D:239:ILE:HD13	1.88	0.55
1:E:596:ASP:HB3	1:E:612:LEU:HD23	1.88	0.55
1:G:50:GLN:HE21	1:G:123:GLN:NE2	2.03	0.55
2:J:121:ALA:HB2	2:J:134:VAL:HG12	1.87	0.55
2:J:243:GLY:N	2:J:246:LEU:HD13	2.20	0.55
2:B:194:ILE:CD1	2:B:194:ILE:N	2.68	0.55
1:E:150:LEU:CD2	1:E:359:GLN:HB3	2.34	0.55
1:E:388:ALA:HB2	1:E:434:LEU:HD11	1.89	0.55
1:G:52:LEU:HD22	1:G:360:ILE:HD11	1.87	0.55
1:G:611:ALA:CB	1:G:620:LEU:HD13	2.37	0.55
2:H:244:PRO:N	2:H:245:PRO:CD	2.69	0.55
2:H:291:VAL:CA	2:H:294:LEU:HD12	2.26	0.55
1:I:302:MET:HG2	1:I:331:PHE:CG	2.40	0.55
1:I:65:MET:CE	1:I:92:ALA:HB2	2.36	0.55
2:J:340:ASP:OD2	2:J:538:ARG:NH2	2.38	0.55
1:K:408:ALA:HB1	1:K:457:GLU:OE1	2.05	0.55
1:K:440:TRP:C	1:K:440:TRP:CD1	2.79	0.55
1:A:346:VAL:HG12	1:A:383:GLU:HB2	1.88	0.55
2:B:247:VAL:HG22	2:B:253:GLU:OE2	2.07	0.55
2:B:467:ASN:N	2:B:467:ASN:ND2	2.52	0.55
1:C:260:VAL:HG22	1:C:319:GLY:O	2.06	0.55
2:D:71:ALA:CB	2:D:74:ARG:HD3	2.36	0.55
2:D:83:VAL:HG13	2:D:84:ARG:H	1.71	0.55
2:F:331:VAL:O	2:F:334:VAL:HG23	2.07	0.55
2:F:357:CYS:SG	2:F:370:LEU:HD23	2.46	0.55
1:I:469:PHE:HD1	1:I:497:LEU:HD21	1.70	0.55
2:D:193:ARG:NH1	2:J:456:ALA:O	2.36	0.55
2:L:193:ARG:O	2:L:193:ARG:HG3	2.05	0.55
1:A:448:ARG:HD3	1:A:474:LEU:O	2.07	0.55
1:A:504:LEU:HB3	1:A:505:PRO:HD2	1.87	0.55
1:A:519:SER:HB2	1:A:613:ARG:HE	1.71	0.55
1:A:589:ARG:HG2	1:A:590:LEU:H	1.70	0.55
1:A:65:MET:HE1	1:A:88:HIS:O	2.06	0.55
1:C:448:ARG:HG2	1:C:474:LEU:HD22	1.88	0.55
1:C:561:ARG:CB	1:C:561:ARG:HH11	2.19	0.55
1:C:596:ASP:CB	1:C:612:LEU:HD23	2.35	0.55
2:D:50:LEU:HD23	2:D:50:LEU:O	2.07	0.55
2:F:362:LEU:HD12	2:F:367:ILE:CD1	2.37	0.55
1:G:200:TYR:OH	1:G:224:LEU:HD23	2.05	0.55
1:G:607:ARG:HB3	1:G:607:ARG:HH11	1.71	0.55
1:G:613:ARG:O	1:G:614:ARG:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:231:VAL:HG22	2:H:275:HIS:HB2	1.88	0.55
2:H:476:GLU:HA	2:H:510:LEU:CD2	2.36	0.55
1:I:525:ARG:CB	1:I:525:ARG:HH11	2.16	0.55
2:J:479:ALA:O	2:J:506:LYS:HE2	2.06	0.55
2:L:288:ARG:HG2	2:L:288:ARG:HH21	1.71	0.55
2:L:435:PRO:HG3	2:L:460:ARG:HH22	1.71	0.55
2:B:239:ILE:O	2:B:266:HIS:CE1	2.59	0.55
1:C:398:ALA:HB2	1:C:464:ARG:NE	2.21	0.55
1:E:308:ARG:HH11	1:E:308:ARG:CG	2.11	0.55
1:C:446:GLU:OE1	1:E:71:LEU:HD22	2.07	0.55
2:F:398:LEU:CD1	2:F:434:VAL:HG21	2.35	0.55
1:I:449:GLN:OE1	1:K:364:ARG:NH2	2.40	0.55
1:I:79:HIS:HD2	1:I:80:SER:O	1.89	0.55
1:K:504:LEU:HD23	1:K:505:PRO:CD	2.35	0.55
2:B:386:HIS:CD2	2:B:386:HIS:O	2.59	0.55
1:C:47:ARG:HE	1:C:148:LEU:HD21	1.72	0.55
1:E:108:LEU:HA	1:E:132:LEU:CD2	2.34	0.55
2:F:189:GLU:OE1	2:F:189:GLU:N	2.30	0.55
2:F:388:ILE:HD11	2:F:429:VAL:HG22	1.89	0.55
1:G:182:HIS:HB3	1:G:245:LEU:HD21	1.89	0.55
2:H:427:THR:HB	2:H:561:PHE:HE2	1.71	0.55
2:J:170:LEU:HD23	2:J:211:VAL:CG2	2.36	0.55
2:J:420:LYS:HE3	2:J:563:MET:O	2.07	0.55
1:K:169:LEU:N	1:K:169:LEU:HD12	2.22	0.55
1:K:429:PHE:CD2	1:K:429:PHE:N	2.71	0.55
1:K:66:ARG:HB2	1:K:66:ARG:NH1	2.08	0.55
1:A:427:SER:OG	1:A:428:PRO:HD2	2.07	0.55
1:A:491:ARG:C	1:A:493:GLN:H	2.10	0.55
1:A:534:HIS:O	2:B:363:HIS:HE1	1.90	0.55
2:B:264:ASP:OD1	2:B:276:TYR:HE1	1.90	0.55
2:B:89:ARG:HD2	2:B:281:ASP:OD1	2.06	0.55
1:C:513:ALA:HB2	1:C:564:VAL:HG11	1.89	0.55
2:D:371:ALA:HB2	2:D:401:LEU:HD12	1.89	0.55
2:D:375:ILE:HG22	2:D:376:LEU:N	2.18	0.55
1:E:300:ARG:HB3	1:E:300:ARG:HH11	1.71	0.55
1:G:103:PRO:O	1:G:108:LEU:HD12	2.06	0.55
1:I:278:ILE:HG22	1:I:489:ILE:HD13	1.88	0.55
1:I:531:ASP:HB3	2:J:298:LYS:HB2	1.88	0.55
2:J:173:SER:OG	2:J:174:GLY:N	2.39	0.55
2:J:191:PHE:HA	2:J:194:ILE:CD1	2.37	0.55
1:A:361:ARG:HH11	1:A:361:ARG:HG2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:C	1:A:394:ASP:H	2.10	0.55
1:A:532:ASP:O	1:A:535:SER:HB2	2.07	0.55
2:B:157:GLN:HB3	2:B:201:MET:HE1	1.89	0.55
1:C:263:ASP:HB3	1:C:362:VAL:CG1	2.35	0.55
1:C:170:MET:CE	1:C:309:ALA:HB1	2.36	0.55
2:D:191:PHE:CE2	2:D:194:ILE:HD12	2.42	0.55
1:E:276:CYS:HB2	1:E:284:LYS:HZ2	1.72	0.55
1:E:401:ARG:HH11	1:E:401:ARG:HG2	1.71	0.55
2:F:121:ALA:HB2	2:F:134:VAL:HG13	1.89	0.55
2:F:412:LYS:HG3	2:F:413:TYR:N	2.22	0.55
1:G:364:ARG:HD2	1:G:366:GLU:OE1	2.07	0.55
1:G:426:VAL:HG21	1:G:463:LEU:CD1	2.36	0.55
1:I:47:ARG:HH11	1:I:47:ARG:HB2	1.71	0.55
1:I:47:ARG:HE	1:I:148:LEU:CD2	2.20	0.55
1:K:163:LYS:HE2	1:K:167:LYS:NZ	2.22	0.55
1:K:448:ARG:HG2	1:K:474:LEU:HD22	1.89	0.55
1:K:586:SER:O	1:K:587:GLN:HB2	2.06	0.55
2:L:167:CYS:HB2	2:L:208:GLN:HE22	1.72	0.55
1:A:302:MET:HG2	1:A:331:PHE:CE2	2.42	0.55
1:A:647:GLY:N	1:A:714:LEU:HB2	2.22	0.55
1:A:671:GLY:HA2	1:A:688:ALA:H	1.71	0.55
2:B:418:ILE:HG13	2:B:418:ILE:O	2.07	0.55
1:C:328:ARG:HH11	1:C:328:ARG:CG	2.19	0.55
1:C:549:ARG:HD3	1:C:568:HIS:O	2.07	0.55
2:D:164:ARG:HG2	2:D:164:ARG:O	2.05	0.55
2:D:192:GLY:HA2	2:D:195:PHE:HD2	1.68	0.55
2:D:498:GLY:O	2:D:500:GLU:N	2.40	0.55
1:E:621:GLU:HG3	1:E:626:LEU:HB2	1.88	0.55
1:G:153:PRO:HD2	1:G:156:ALA:HB3	1.89	0.55
2:H:344:PHE:CZ	2:H:358:GLY:HA3	2.42	0.55
2:J:161:LEU:HD13	2:J:201:MET:HG2	1.87	0.55
2:D:178:LEU:HD12	2:J:478:ALA:HB1	1.88	0.55
1:K:320:THR:CG2	1:K:341:GLN:HG3	2.36	0.55
1:K:506:GLU:O	1:K:507:HIS:C	2.45	0.55
1:K:519:SER:HB2	1:K:613:ARG:HE	1.72	0.55
1:C:134:GLU:O	1:C:135:ASN:HB3	2.07	0.55
2:D:303:GLN:HE21	2:F:297:ARG:HB2	1.71	0.55
1:E:307:VAL:O	1:E:310:ALA:HB3	2.07	0.55
1:G:150:LEU:CD2	1:G:359:GLN:O	2.55	0.55
1:G:201:PRO:CG	1:G:328:ARG:NH2	2.70	0.55
2:H:211:VAL:O	2:H:211:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:275:HIS:CE1	2:L:347:PHE:HA	2.36	0.55
1:I:263:ASP:HB3	1:I:362:VAL:HG12	1.88	0.55
1:I:273:GLU:OE1	1:I:273:GLU:N	2.40	0.55
2:J:533:ASP:O	2:J:534:PRO:C	2.45	0.55
2:J:538:ARG:HH11	2:J:538:ARG:CG	2.05	0.55
1:K:65:MET:SD	1:K:75:SER:HB3	2.47	0.55
1:C:225:ALA:O	1:C:228:LEU:HB3	2.07	0.54
1:C:601:ARG:HE	1:C:606:THR:HG23	1.71	0.54
2:D:498:GLY:C	2:D:500:GLU:H	2.10	0.54
1:E:357:ALA:O	1:E:361:ARG:HG3	2.08	0.54
1:E:350:ILE:HD12	1:E:377:LEU:CD1	2.37	0.54
1:E:541:ASP:HB2	1:E:549:ARG:HH21	1.70	0.54
1:K:254:ARG:HH22	1:K:292:PRO:HB2	1.71	0.54
1:K:61:ALA:O	1:K:65:MET:HB2	2.07	0.54
1:A:217:VAL:CG2	1:A:249:TYR:HD1	2.20	0.54
1:C:169:LEU:HD23	1:C:313:ILE:HG12	1.87	0.54
1:C:278:ILE:HD11	1:C:484:LEU:HD21	1.89	0.54
1:C:613:ARG:HG2	1:C:614:ARG:N	2.23	0.54
2:D:317:LEU:HD22	2:D:334:VAL:HG13	1.89	0.54
1:E:516:TRP:CG	1:E:555:LEU:HD11	2.42	0.54
2:F:138:ALA:HB2	2:F:172:ASP:OD2	2.07	0.54
2:F:187:ASP:OD2	2:H:151:LYS:NZ	2.32	0.54
1:I:328:ARG:CB	1:I:328:ARG:NH1	2.70	0.54
2:J:201:MET:CE	2:J:208:GLN:NE2	2.62	0.54
2:J:164:ARG:CB	2:J:551:ALA:HB2	2.37	0.54
1:K:384:VAL:HG13	1:K:470:LEU:HD22	1.87	0.54
2:L:441:ILE:HG22	2:L:465:TRP:CE3	2.42	0.54
1:A:463:LEU:CD2	1:A:464:ARG:H	2.21	0.54
1:C:375:VAL:O	1:C:375:VAL:HG23	2.08	0.54
2:D:469:ARG:HD2	2:D:517:GLY:O	2.07	0.54
1:E:384:VAL:HG11	1:E:470:LEU:HD13	1.89	0.54
1:E:558:ARG:HD2	1:E:560:GLU:OE2	2.07	0.54
2:F:245:PRO:HB3	2:H:481:VAL:HG13	1.88	0.54
2:H:59:LEU:O	2:H:59:LEU:HD12	2.07	0.54
1:I:302:MET:HG2	1:I:331:PHE:CD1	2.43	0.54
2:J:141:LYS:HG3	2:J:141:LYS:O	2.07	0.54
1:K:108:LEU:HA	1:K:132:LEU:HD11	1.88	0.54
1:K:47:ARG:HE	1:K:148:LEU:HD21	1.71	0.54
2:L:103:LEU:O	2:L:524:ALA:HA	2.07	0.54
2:L:402:GLN:HE22	2:L:449:ASN:ND2	2.05	0.54
2:L:74:ARG:NE	2:L:78:ARG:HH12	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:83:VAL:CG1	2:L:84:ARG:H	2.16	0.54
1:A:109:ARG:NE	1:A:112:ARG:NH2	2.56	0.54
1:A:251:LEU:HD12	1:A:326:ASP:OD2	2.08	0.54
1:A:681:LYS:NZ	2:F:474:GLY:H	2.05	0.54
1:A:85:HIS:NE2	1:A:424:ASP:OD1	2.40	0.54
1:C:509:TRP:CZ2	1:C:562:ARG:HG3	2.43	0.54
2:D:402:GLN:HE22	2:D:444:SER:CB	2.20	0.54
1:E:262:ALA:O	1:E:362:VAL:HG11	2.08	0.54
1:G:218:VAL:HG21	1:G:224:LEU:HD13	1.89	0.54
1:G:391:PRO:HD3	1:G:465:THR:O	2.07	0.54
2:H:274:ASP:OD1	2:L:348:LYS:HE2	2.07	0.54
1:I:307:VAL:CG1	1:I:307:VAL:O	2.56	0.54
1:I:589:ARG:HG2	1:I:590:LEU:H	1.71	0.54
1:K:172:GLU:OE2	1:K:172:GLU:O	2.24	0.54
2:L:144:THR:HG21	4:L:591:COA:C5A	2.38	0.54
1:A:71:LEU:O	1:A:71:LEU:HD23	2.06	0.54
2:B:225:ALA:O	2:L:562:ARG:HD2	2.07	0.54
2:B:56:LEU:O	2:B:60:LEU:HG	2.08	0.54
1:C:129:TYR:CD2	1:C:342:VAL:HA	2.43	0.54
1:E:605:VAL:O	1:E:605:VAL:CG2	2.54	0.54
2:F:325:SER:HB3	2:F:326:LYS:NZ	2.23	0.54
1:G:362:VAL:CG2	1:G:363:ALA:N	2.71	0.54
2:H:247:VAL:HG22	2:H:253:GLU:OE2	2.07	0.54
2:J:103:LEU:O	2:J:524:ALA:HA	2.07	0.54
2:J:161:LEU:HD13	2:J:201:MET:SD	2.48	0.54
2:J:491:GLU:C	2:J:493:ALA:H	2.09	0.54
2:L:444:SER:HB3	2:L:449:ASN:HD22	1.72	0.54
1:A:446:GLU:O	1:A:450:ARG:HB2	2.08	0.54
1:A:681:LYS:HG3	1:A:681:LYS:O	2.06	0.54
2:B:375:ILE:HG21	2:B:408:MET:HB2	1.90	0.54
2:B:465:TRP:HB3	2:B:467:ASN:HD21	1.70	0.54
2:B:420:LYS:HE3	2:B:563:MET:O	2.06	0.54
1:C:165:ALA:O	1:C:168:ALA:HB3	2.08	0.54
1:C:254:ARG:HH12	1:C:293:GLY:H	1.56	0.54
1:A:446:GLU:OE1	1:C:71:LEU:HD21	2.08	0.54
2:D:233:VAL:HG13	2:D:279:ASP:CA	2.38	0.54
2:D:339:VAL:CG2	2:D:342:SER:HA	2.37	0.54
2:D:89:ARG:NH2	2:D:89:ARG:HG3	2.19	0.54
1:E:587:GLN:HB3	1:E:588:TYR:CD1	2.40	0.54
2:F:408:MET:O	2:F:418:ILE:HD13	2.08	0.54
1:G:186:GLN:HE22	1:G:189:GLU:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:119:ILE:CG2	2:H:152:LYS:HD3	2.38	0.54
1:K:270:TYR:H	1:K:372:GLN:NE2	1.94	0.54
2:L:98:LEU:HD21	2:L:463:TRP:HZ2	1.71	0.54
1:A:280:ARG:HG2	1:A:280:ARG:O	2.07	0.54
1:A:496:LEU:C	1:A:498:PRO:HD3	2.27	0.54
2:B:271:GLY:O	2:F:348:LYS:NZ	2.33	0.54
1:E:129:TYR:CD2	1:E:342:VAL:HA	2.43	0.54
1:E:169:LEU:N	1:E:169:LEU:CD1	2.71	0.54
1:E:450:ARG:O	1:E:453:ALA:HB3	2.07	0.54
2:F:233:VAL:HG11	2:F:236:GLN:NE2	2.23	0.54
1:G:607:ARG:HG3	1:I:94:ILE:HG12	1.89	0.54
2:J:90:LEU:HD21	2:J:168:ILE:HD13	1.89	0.54
2:J:234:ARG:HA	2:J:263:ALA:HB3	1.87	0.54
2:J:277:ALA:HB2	2:J:286:ILE:HD12	1.90	0.54
2:J:366:PRO:O	2:J:397:PRO:HD2	2.08	0.54
1:K:175:VAL:CG2	1:K:309:ALA:HB2	2.27	0.54
1:K:69:ARG:CB	1:K:69:ARG:HH11	2.18	0.54
1:A:136:ALA:HB1	1:A:154:ALA:HB1	1.90	0.54
1:A:414:ARG:HB2	1:A:454:MET:SD	2.48	0.54
1:A:689:PRO:O	1:A:690:HIS:ND1	2.40	0.54
1:E:114:ILE:O	1:E:118:LEU:HB2	2.07	0.54
1:E:187:ASP:C	1:E:189:GLU:H	2.11	0.54
1:E:188:LEU:CD2	1:E:228:LEU:HD23	2.38	0.54
1:E:271:LEU:O	1:E:272:ASN:HB2	2.08	0.54
1:E:392:GLU:O	1:E:394:ASP:N	2.41	0.54
2:F:362:LEU:HD21	2:F:538:ARG:HG3	1.90	0.54
2:J:432:ALA:HA	2:J:556:THR:HG21	1.88	0.54
1:K:365:GLY:O	1:K:366:GLU:O	2.26	0.54
2:L:136:ASN:OD1	2:L:136:ASN:N	2.41	0.54
2:L:429:VAL:CG1	2:L:430:ALA:N	2.70	0.54
2:L:87:ILE:N	2:L:87:ILE:HD12	2.23	0.54
1:A:313:ILE:HD11	1:A:315:TYR:HD2	1.72	0.54
2:B:212:VAL:O	2:B:233:VAL:HG23	2.08	0.54
2:D:487:ARG:NH2	2:D:502:GLU:OE2	2.41	0.54
1:E:114:ILE:HD11	1:E:138:PHE:CE1	2.43	0.54
1:E:611:ALA:CB	1:E:620:LEU:HD13	2.36	0.54
2:F:153:HIS:ND1	2:F:194:ILE:HD13	2.23	0.54
2:F:184:VAL:O	2:F:191:PHE:HB2	2.08	0.54
2:F:44:ALA:O	2:F:47:ALA:HB3	2.07	0.54
2:F:57:ARG:CG	2:F:57:ARG:HH11	2.16	0.54
1:G:331:PHE:O	1:G:332:PHE:CD2	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:LEU:HD12	4:H:591:COA:N6A	2.22	0.54
2:J:141:LYS:HZ1	2:J:177:ASN:ND2	2.06	0.54
1:K:391:PRO:HG3	1:K:466:ASN:HA	1.89	0.54
1:K:587:GLN:C	1:K:588:TYR:CD1	2.81	0.54
1:A:170:MET:SD	1:A:309:ALA:CB	2.96	0.54
2:B:423:ALA:HB1	2:L:226:MET:HG3	1.89	0.54
1:C:200:TYR:O	1:C:202:VAL:HG12	2.07	0.54
1:C:397:PRO:HB3	1:C:432:PRO:HG3	1.89	0.54
1:E:504:LEU:HB3	1:E:505:PRO:CD	2.31	0.54
2:F:388:ILE:HG21	2:F:428:ALA:HB1	1.90	0.54
2:F:74:ARG:HG2	2:F:74:ARG:O	2.07	0.54
1:G:156:ALA:O	1:G:159:ALA:HB3	2.08	0.54
1:I:505:PRO:HB3	1:I:507:HIS:CB	2.37	0.54
1:I:509:TRP:CH2	1:I:562:ARG:HG3	2.43	0.54
1:K:351:THR:OG1	1:K:352:GLY:N	2.41	0.54
1:K:415:ARG:CD	1:K:438:ILE:HD13	2.23	0.54
1:K:590:LEU:HD12	1:K:597:ASP:O	2.07	0.54
1:A:513:ALA:CB	1:A:566:LEU:HD21	2.39	0.53
1:A:79:HIS:HD2	1:A:80:SER:O	1.91	0.53
2:B:154:LEU:HD23	2:B:157:GLN:NE2	2.22	0.53
1:C:505:PRO:CB	1:C:507:HIS:HB2	2.34	0.53
1:E:270:TYR:CD1	1:E:372:GLN:NE2	2.76	0.53
1:E:378:ASN:O	1:E:440:TRP:HH2	1.91	0.53
2:H:335:ILE:O	2:H:339:VAL:HG22	2.08	0.53
2:H:425:LEU:O	2:H:429:VAL:HG23	2.09	0.53
2:J:272:VAL:HG12	2:J:272:VAL:O	2.07	0.53
1:K:508:PHE:HB2	1:K:622:TRP:CE2	2.42	0.53
1:A:290:PRO:HD2	1:A:380:HIS:ND1	2.23	0.53
2:B:381:ALA:HB1	2:B:425:LEU:HB2	1.90	0.53
1:C:443:THR:HG23	1:C:446:GLU:H	1.73	0.53
1:E:258:ILE:O	1:E:320:THR:HA	2.07	0.53
1:E:418:SER:HB2	1:E:435:ALA:HB2	1.89	0.53
1:E:278:ILE:HG21	1:E:473:ILE:HD11	1.89	0.53
1:E:600:SER:O	1:E:606:THR:HA	2.08	0.53
1:G:448:ARG:HG3	1:G:479:PHE:CE1	2.43	0.53
1:G:487:GLY:O	1:G:490:ALA:HB3	2.08	0.53
1:I:621:GLU:HG3	1:I:625:GLU:O	2.08	0.53
1:I:60:ILE:O	1:I:64:VAL:HG12	2.08	0.53
2:J:145:TYR:CD2	2:J:191:PHE:HE1	2.26	0.53
2:J:329:TYR:OH	2:J:441:ILE:HD13	2.07	0.53
2:L:332:ARG:HH22	2:L:353:THR:HG22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:OE2	1:A:448:ARG:NH2	2.41	0.53
2:B:421:HIS:HA	2:B:424:LYS:HE3	1.90	0.53
1:C:148:LEU:HD23	1:C:148:LEU:N	2.23	0.53
1:C:203:LEU:HD23	1:C:205:LYS:HZ2	1.67	0.53
1:C:350:ILE:HA	1:C:440:TRP:CZ3	2.39	0.53
1:E:440:TRP:CD1	1:E:440:TRP:C	2.81	0.53
2:F:192:GLY:HA2	2:F:195:PHE:HD2	1.72	0.53
1:G:559:ASP:C	1:G:560:GLU:HG3	2.28	0.53
1:I:106:SER:O	1:I:108:LEU:N	2.41	0.53
1:I:343:GLU:C	1:I:345:PRO:HD2	2.28	0.53
1:I:414:ARG:HB3	1:I:454:MET:SD	2.48	0.53
1:K:384:VAL:HG11	1:K:470:LEU:HD22	1.88	0.53
2:B:56:LEU:HG	2:B:60:LEU:HD11	1.91	0.53
1:C:108:LEU:HD23	1:C:132:LEU:HD11	1.88	0.53
1:C:547:LEU:HD23	1:C:547:LEU:N	2.23	0.53
1:E:520:GLU:O	1:E:522:GLY:N	2.41	0.53
2:F:313:PRO:HB2	2:F:316:GLU:HG3	1.89	0.53
2:F:375:ILE:N	2:F:375:ILE:HD12	2.05	0.53
2:F:484:GLN:O	2:F:488:GLU:HG3	2.08	0.53
2:H:36:ASN:ND2	2:H:38:ARG:HD3	2.23	0.53
2:J:298:LYS:HD3	2:J:550:ASN:HA	1.89	0.53
2:J:414:GLU:OE1	2:J:414:GLU:HA	2.07	0.53
2:J:499:VAL:HG12	2:J:499:VAL:O	2.08	0.53
2:L:192:GLY:HA2	2:L:195:PHE:CD2	2.43	0.53
2:L:445:PHE:HA	2:L:471:GLY:O	2.08	0.53
2:B:289:ARG:O	2:B:292:ALA:HB3	2.09	0.53
2:B:326:LYS:NZ	2:B:405:THR:HG23	2.23	0.53
1:C:131:PHE:HB3	1:C:132:LEU:HD22	1.90	0.53
1:C:388:ALA:HB3	1:C:432:PRO:HB2	1.91	0.53
2:D:400:PHE:HB2	2:D:438:THR:HG22	1.86	0.53
1:E:489:ILE:HG23	1:E:490:ALA:N	2.24	0.53
2:H:306:ALA:O	2:H:308:ARG:HG3	2.08	0.53
2:H:502:GLU:O	2:H:502:GLU:HG2	2.08	0.53
1:I:49:ILE:N	1:I:49:ILE:HD12	2.22	0.53
2:J:109:TYR:N	2:J:109:TYR:CD1	2.77	0.53
2:J:465:TRP:HB3	2:J:467:ASN:ND2	2.24	0.53
1:K:129:TYR:CD2	1:K:342:VAL:HA	2.44	0.53
1:K:108:LEU:HA	1:K:132:LEU:CD1	2.39	0.53
1:K:344:HIS:CE1	1:K:345:PRO:HD3	2.43	0.53
1:K:358:TRP:HD1	1:K:361:ARG:HD2	1.72	0.53
1:K:613:ARG:O	1:K:614:ARG:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ARG:NH1	1:A:361:ARG:CG	2.72	0.53
2:D:431:CYS:HB2	2:D:558:PHE:HD2	1.74	0.53
2:F:57:ARG:CG	2:F:57:ARG:NH1	2.72	0.53
2:F:78:ARG:HH22	2:H:492:ARG:NH1	2.06	0.53
2:H:57:ARG:NH1	2:H:57:ARG:HG3	2.16	0.53
1:I:491:ARG:C	1:I:493:GLN:H	2.11	0.53
1:A:172:GLU:OE2	1:A:172:GLU:O	2.26	0.53
1:A:292:PRO:HG2	1:A:484:LEU:CD1	2.38	0.53
1:A:360:ILE:O	1:A:364:ARG:HG3	2.08	0.53
1:C:197:ARG:O	1:C:198:ILE:HG13	2.09	0.53
1:C:178:VAL:HG22	1:C:332:PHE:HB3	1.89	0.53
2:F:376:LEU:HG	2:F:404:ILE:HD13	1.89	0.53
1:G:271:LEU:O	1:G:272:ASN:HB2	2.07	0.53
2:H:378:ALA:H	2:H:418:ILE:CD1	2.21	0.53
1:K:140:ARG:CZ	1:K:140:ARG:CB	2.79	0.53
1:K:405:TYR:HD1	1:K:460:VAL:HG13	1.73	0.53
1:K:55:ALA:HB1	1:K:113:ILE:HD13	1.89	0.53
2:L:155:ARG:NE	2:L:159:ILE:HD11	2.24	0.53
1:A:545:SER:O	2:B:536:GLN:NE2	2.28	0.53
1:A:586:SER:O	1:A:587:GLN:CB	2.48	0.53
2:D:224:PRO:CG	2:D:239:ILE:HD13	2.38	0.53
1:E:181:TYR:CD1	1:E:182:HIS:N	2.76	0.53
1:E:444:ARG:NH2	1:E:479:PHE:CE1	2.77	0.53
2:F:67:GLY:N	2:F:139:THR:OG1	2.35	0.53
1:G:232:GLN:HG2	1:G:233:ARG:CZ	2.39	0.53
1:I:611:ALA:HB2	1:I:620:LEU:HD13	1.90	0.53
2:J:123:ILE:HD13	2:J:165:LEU:HD11	1.91	0.53
2:J:417:GLY:C	2:J:419:ALA:N	2.61	0.53
2:L:520:TYR:H	2:L:520:TYR:HD2	1.57	0.53
1:A:191:PHE:CE2	1:A:228:LEU:HD11	2.44	0.53
1:A:391:PRO:HD3	1:A:465:THR:O	2.08	0.53
1:A:380:HIS:CD2	1:A:444:ARG:HD2	2.44	0.53
2:B:85:GLU:OE1	2:B:85:GLU:HA	2.09	0.53
1:C:478:ALA:CB	1:C:488:PHE:HE1	2.21	0.53
2:D:188:ARG:HH11	2:D:188:ARG:CG	2.22	0.53
2:D:45:ASN:OD1	2:D:322:PRO:HA	2.08	0.53
1:E:251:LEU:H	1:E:251:LEU:CD1	2.10	0.53
1:E:63:ARG:HH12	1:E:356:VAL:HG21	1.73	0.53
2:F:192:GLY:HA3	2:H:450:TYR:CZ	2.44	0.53
2:F:65:GLU:O	2:F:72:GLN:NE2	2.41	0.53
1:G:516:TRP:CD1	1:G:553:LEU:HD22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:MET:HG3	1:G:75:SER:CB	2.38	0.53
2:H:521:TYR:CE1	2:H:525:ARG:NH1	2.77	0.53
2:J:145:TYR:CD1	2:J:149:THR:HB	2.37	0.53
2:J:178:LEU:HG	4:J:591:COA:H61A	1.73	0.53
2:J:461:PHE:CD1	2:J:544:ALA:HB1	2.44	0.53
1:K:278:ILE:HG23	1:K:488:PHE:HD2	1.73	0.53
1:K:567:ARG:HD3	1:K:567:ARG:N	2.24	0.53
2:L:425:LEU:HD21	2:L:451:GLY:O	2.09	0.53
2:L:536:GLN:O	2:L:540:VAL:HG23	2.08	0.53
1:A:76:VAL:HG13	1:A:94:ILE:HB	1.91	0.53
1:C:296:ALA:O	1:C:300:ARG:HG2	2.09	0.53
2:D:437:PHE:HE1	2:D:544:ALA:HB1	1.74	0.53
2:H:109:TYR:OH	2:H:147:PRO:HB2	2.09	0.53
2:H:213:MET:HA	2:H:233:VAL:CG2	2.39	0.53
1:I:103:PRO:O	1:I:108:LEU:HD12	2.09	0.53
2:L:334:VAL:HG12	2:L:338:LEU:HD11	1.91	0.53
1:A:138:PHE:CE1	1:A:142:CYS:HB2	2.44	0.52
1:A:694:VAL:HG11	1:A:697:LEU:HD22	1.91	0.52
1:C:47:ARG:O	1:C:364:ARG:HB3	2.08	0.52
1:C:421:ARG:HG2	1:C:424:ASP:OD2	2.09	0.52
1:C:451:LEU:HD23	1:C:474:LEU:HD11	1.90	0.52
1:C:508:PHE:O	1:C:509:TRP:C	2.47	0.52
1:E:550:GLU:HA	1:E:567:ARG:CD	2.39	0.52
2:F:484:GLN:HE22	2:F:487:ARG:NH2	2.07	0.52
1:G:152:PRO:CD	1:G:157:ILE:HD11	2.22	0.52
1:G:194:GLU:C	1:G:196:GLY:N	2.60	0.52
1:G:254:ARG:NH2	1:G:292:PRO:HD2	2.22	0.52
1:G:344:HIS:N	1:G:345:PRO:CD	2.73	0.52
1:G:482:ALA:O	1:G:484:LEU:HD12	2.09	0.52
1:G:508:PHE:HA	1:G:622:TRP:CZ3	2.44	0.52
2:H:390:LEU:O	2:H:394:ARG:HG3	2.09	0.52
1:I:517:LEU:HD11	2:J:94:GLY:HA3	1.90	0.52
2:L:288:ARG:NH2	2:L:288:ARG:HG2	2.24	0.52
1:A:203:LEU:O	1:A:204:LEU:HD23	2.07	0.52
1:A:304:GLU:HA	1:A:307:VAL:HG12	1.91	0.52
1:A:150:LEU:HD21	1:A:363:ALA:CB	2.38	0.52
1:A:506:GLU:HA	1:A:506:GLU:OE1	2.09	0.52
2:B:230:THR:OG1	2:L:562:ARG:NH2	2.41	0.52
1:C:201:PRO:O	1:C:249:TYR:HB3	2.09	0.52
2:F:402:GLN:HE22	2:F:449:ASN:HA	1.72	0.52
2:H:49:MET:CE	2:H:321:ILE:HG21	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:211:VAL:CG1	2:J:231:VAL:HB	2.39	0.52
1:K:52:LEU:HD11	1:K:126:HIS:HB2	1.90	0.52
1:A:309:ALA:O	1:A:312:ALA:HB3	2.09	0.52
2:B:312:TYR:N	2:B:312:TYR:CD1	2.77	0.52
2:B:83:VAL:HG13	2:B:84:ARG:HG3	1.92	0.52
2:D:324:ASP:O	2:D:327:GLN:HB2	2.09	0.52
2:D:400:PHE:CB	2:D:438:THR:CG2	2.83	0.52
2:D:82:LEU:H	2:D:82:LEU:HD12	1.72	0.52
1:E:486:THR:HG22	1:E:486:THR:O	2.09	0.52
2:F:157:GLN:NE2	2:F:197:ASN:HB2	2.25	0.52
2:F:354:THR:HG22	2:F:375:ILE:N	2.24	0.52
1:G:152:PRO:HG2	1:G:338:THR:HB	1.91	0.52
1:G:519:SER:HB2	1:G:613:ARG:HE	1.72	0.52
1:I:251:LEU:HD21	1:I:328:ARG:HH22	1.74	0.52
2:J:462:LEU:HD23	2:J:462:LEU:C	2.29	0.52
2:J:473:MET:HE2	2:J:477:GLN:HB3	1.92	0.52
2:L:59:LEU:HD22	2:L:520:TYR:CE1	2.44	0.52
1:A:678:GLU:O	1:A:678:GLU:CD	2.48	0.52
2:B:201:MET:HB3	2:B:208:GLN:HE21	1.72	0.52
1:C:308:ARG:HG3	1:C:308:ARG:NH1	2.24	0.52
2:F:352:GLY:HA3	2:F:379:GLU:HB3	1.90	0.52
1:G:404:LEU:CD2	1:G:612:LEU:HD11	2.40	0.52
2:H:309:ALA:O	2:H:310:PRO:O	2.27	0.52
2:H:30:ILE:HG22	2:H:31:LEU:N	2.24	0.52
2:H:81:LEU:HD23	2:H:82:LEU:H	1.75	0.52
1:I:400:GLY:H	1:I:463:LEU:HD11	1.75	0.52
2:J:486:LYS:HD2	2:J:489:GLN:NE2	2.24	0.52
1:A:268:CYS:O	1:A:307:VAL:HG21	2.09	0.52
1:A:153:PRO:CD	1:A:316:VAL:HG23	2.36	0.52
2:B:231:VAL:CG2	2:B:286:ILE:HG21	2.40	0.52
2:B:82:LEU:H	2:B:82:LEU:CD1	2.09	0.52
1:C:485:ASP:OD2	1:C:487:GLY:N	2.37	0.52
2:D:397:PRO:HA	2:D:434:VAL:CG2	2.39	0.52
2:D:44:ALA:O	2:D:47:ALA:HB3	2.09	0.52
2:D:431:CYS:O	2:D:556:THR:HG23	2.10	0.52
1:E:598:LEU:HD12	1:E:599:VAL:N	2.24	0.52
2:F:289:ARG:O	2:F:292:ALA:HB3	2.09	0.52
1:G:152:PRO:HB2	1:G:157:ILE:HG12	1.92	0.52
1:G:196:GLY:O	1:G:198:ILE:N	2.41	0.52
1:G:523:HIS:ND1	1:G:524:ARG:N	2.58	0.52
2:F:181:GLN:OE1	2:H:472:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:438:ILE:N	1:I:438:ILE:HD12	2.24	0.52
1:I:562:ARG:HH11	1:I:562:ARG:CB	2.08	0.52
1:I:618:LEU:C	1:I:618:LEU:HD12	2.29	0.52
2:L:102:ALA:C	2:L:104:ALA:H	2.11	0.52
2:L:114:VAL:HG12	2:L:140:VAL:CG1	2.39	0.52
2:L:114:VAL:HG11	2:L:146:TYR:CZ	2.44	0.52
2:L:277:ALA:HB2	2:L:286:ILE:CD1	2.40	0.52
1:A:165:ALA:O	1:A:169:LEU:HD13	2.09	0.52
1:A:556:ARG:HH11	1:A:556:ARG:HG2	1.74	0.52
1:C:465:THR:CG2	1:C:466:ASN:N	2.72	0.52
2:B:303:GLN:NE2	2:D:297:ARG:HB2	2.25	0.52
1:E:470:LEU:HA	1:E:473:ILE:CG2	2.40	0.52
1:E:491:ARG:HD2	1:E:492:HIS:CE1	2.45	0.52
2:F:526:LEU:C	2:F:528:ASP:H	2.10	0.52
2:F:71:ALA:HA	2:F:74:ARG:HB3	1.90	0.52
1:G:504:LEU:O	1:G:505:PRO:O	2.28	0.52
2:H:234:ARG:HA	2:H:263:ALA:HB3	1.92	0.52
1:I:154:ALA:HA	1:I:157:ILE:HD12	1.91	0.52
1:K:269:LEU:HD23	1:K:269:LEU:N	2.24	0.52
2:L:155:ARG:HE	2:L:159:ILE:HD11	1.74	0.52
1:A:346:VAL:CG2	1:A:347:THR:N	2.72	0.52
1:C:69:ARG:HB3	1:C:69:ARG:HH11	1.74	0.52
2:D:313:PRO:HD2	2:D:316:GLU:OE1	2.10	0.52
1:E:547:LEU:CD2	1:E:547:LEU:N	2.73	0.52
1:E:531:ASP:OD2	2:F:298:LYS:HG3	2.10	0.52
2:F:339:VAL:HG23	2:F:342:SER:HA	1.90	0.52
2:F:476:GLU:HA	2:F:479:ALA:HB3	1.92	0.52
2:H:279:ASP:C	2:H:279:ASP:OD2	2.48	0.52
2:J:211:VAL:HG13	2:J:231:VAL:HB	1.89	0.52
2:J:29:ALA:O	2:J:343:GLU:HA	2.09	0.52
2:J:381:ALA:HA	2:J:425:LEU:HD22	1.92	0.52
1:K:135:ASN:HD21	1:K:138:PHE:HB2	1.74	0.52
2:L:109:TYR:OH	2:L:147:PRO:HB2	2.08	0.52
1:A:444:ARG:HG2	1:A:444:ARG:NH1	2.24	0.52
2:B:432:ALA:HA	2:B:556:THR:HG21	1.91	0.52
2:D:239:ILE:O	2:D:266:HIS:NE2	2.39	0.52
2:D:252:GLY:O	2:D:253:GLU:HB3	2.09	0.52
2:D:481:VAL:HG12	2:J:245:PRO:CB	2.39	0.52
1:E:169:LEU:HD23	1:E:313:ILE:HG22	1.91	0.52
1:C:605:VAL:HG12	1:E:96:VAL:CG1	2.39	0.52
2:F:508:PRO:O	2:F:511:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:VAL:HG23	1:G:249:TYR:HD1	1.74	0.52
2:H:171:VAL:CG2	2:H:212:VAL:HA	2.36	0.52
2:D:472:VAL:HG12	2:J:181:GLN:HB2	1.92	0.52
1:K:408:ALA:CB	1:K:457:GLU:HB2	2.37	0.52
2:L:265:VAL:O	2:L:269:VAL:HG23	2.09	0.52
2:L:338:LEU:HD22	2:L:537:THR:HG22	1.92	0.52
1:A:605:VAL:O	1:A:605:VAL:CG2	2.56	0.52
2:B:201:MET:HB3	2:B:208:GLN:NE2	2.25	0.52
1:C:251:LEU:CD2	1:C:328:ARG:HE	2.23	0.52
1:C:395:PHE:C	1:C:397:PRO:HD3	2.30	0.52
2:D:324:ASP:HB3	2:D:327:GLN:HB2	1.91	0.52
1:E:396:LEU:O	1:E:398:ALA:N	2.43	0.52
2:F:74:ARG:NH2	2:F:78:ARG:NH1	2.58	0.52
1:G:302:MET:HG2	1:G:331:PHE:CZ	2.44	0.52
2:H:231:VAL:HG11	2:H:283:ALA:HB1	1.92	0.52
1:I:391:PRO:HG2	1:I:468:ALA:HB3	1.91	0.52
2:J:300:GLY:O	2:J:301:GLN:HB2	2.10	0.52
1:K:123:GLN:O	1:K:148:LEU:HG	2.10	0.52
1:K:302:MET:HG2	1:K:331:PHE:CG	2.45	0.52
1:C:203:LEU:HG	1:C:204:LEU:N	2.25	0.52
1:C:252:LYS:CG	1:C:485:ASP:HB3	2.40	0.52
2:F:449:ASN:OD1	2:F:454:GLY:HA3	2.11	0.52
2:F:54:ASN:O	2:F:58:THR:HG23	2.10	0.52
2:H:220:GLY:O	2:H:224:PRO:HD2	2.10	0.52
2:H:75:HIS:CE1	2:H:80:LYS:HE2	2.43	0.52
1:I:344:HIS:N	1:I:345:PRO:HD3	2.25	0.52
1:I:623:GLU:OE1	1:I:623:GLU:CA	2.58	0.52
2:J:297:ARG:HB3	2:J:297:ARG:NH1	2.25	0.52
1:K:455:LEU:HD12	1:K:474:LEU:HD12	1.90	0.52
1:A:217:VAL:HG21	1:A:249:TYR:CD1	2.45	0.51
1:A:622:TRP:O	1:A:622:TRP:CD1	2.63	0.51
2:B:274:ASP:OD1	2:F:348:LYS:HE2	2.10	0.51
2:B:449:ASN:OD1	2:B:454:GLY:HA3	2.09	0.51
2:B:75:HIS:C	2:B:77:ALA:N	2.64	0.51
1:C:469:PHE:HE2	1:C:473:ILE:HD12	1.68	0.51
2:D:351:PHE:HE2	2:D:379:GLU:HB3	1.75	0.51
1:G:78:VAL:HB	1:G:98:LEU:HD21	1.92	0.51
1:I:269:LEU:HB3	1:I:372:GLN:NE2	2.25	0.51
1:I:54:VAL:HG21	1:I:64:VAL:HG13	1.92	0.51
2:H:303:GLN:NE2	2:J:297:ARG:CD	2.73	0.51
1:K:537:TRP:HB3	2:L:125:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:402:GLN:HE22	2:L:449:ASN:HD22	1.58	0.51
1:A:201:PRO:CD	1:A:328:ARG:HH21	2.19	0.51
1:A:358:TRP:CH2	1:A:370:LEU:HD12	2.45	0.51
1:C:278:ILE:N	1:C:278:ILE:HD12	2.03	0.51
1:C:152:PRO:HG2	1:C:338:THR:HB	1.91	0.51
1:C:339:ARG:HH11	1:C:339:ARG:HG3	1.74	0.51
2:D:211:VAL:CG1	2:D:231:VAL:HB	2.39	0.51
2:D:362:LEU:HD23	2:D:362:LEU:C	2.29	0.51
1:E:278:ILE:HG23	1:E:488:PHE:CD2	2.45	0.51
2:F:185:PHE:CD2	2:H:472:VAL:HA	2.45	0.51
2:F:398:LEU:HD12	2:F:398:LEU:N	2.25	0.51
1:G:446:GLU:HG3	1:I:71:LEU:HD21	1.91	0.51
1:G:508:PHE:O	1:G:509:TRP:C	2.48	0.51
2:H:407:PHE:CE1	2:H:447:ALA:HB3	2.45	0.51
1:I:599:VAL:CG2	1:I:608:ARG:HD3	2.41	0.51
2:J:369:ILE:HG12	2:J:399:LEU:HD23	1.92	0.51
2:L:82:LEU:HD12	2:L:82:LEU:N	2.24	0.51
1:C:289:ALA:O	1:C:350:ILE:HG21	2.10	0.51
1:C:175:VAL:HG21	1:C:309:ALA:HB2	1.92	0.51
1:C:319:GLY:HA2	1:C:339:ARG:O	2.10	0.51
2:D:289:ARG:O	2:D:292:ALA:HB3	2.10	0.51
2:D:339:VAL:HG22	2:D:342:SER:HA	1.91	0.51
2:D:472:VAL:CG1	2:J:181:GLN:CB	2.83	0.51
2:F:347:PHE:O	2:F:348:LYS:C	2.47	0.51
1:G:189:GLU:HG3	1:G:190:THR:N	2.24	0.51
1:G:47:ARG:HG3	1:G:48:SER:N	2.25	0.51
2:H:248:LYS:HA	2:H:252:GLY:O	2.10	0.51
2:H:392:CYS:SG	2:H:556:THR:HG21	2.50	0.51
1:I:380:HIS:NE2	1:I:444:ARG:HD2	2.24	0.51
2:J:36:ASN:HD22	2:J:37:PRO:HD2	1.74	0.51
2:J:424:LYS:NZ	2:J:562:ARG:O	2.43	0.51
2:J:87:ILE:HG22	2:J:88:ASN:N	2.26	0.51
1:K:63:ARG:NH2	1:K:356:VAL:CG2	2.73	0.51
1:A:283:GLN:NE2	1:A:389:GLU:OE1	2.44	0.51
1:A:339:ARG:NH1	1:A:339:ARG:HG3	2.23	0.51
1:A:360:ILE:O	1:A:360:ILE:HG22	2.10	0.51
1:A:150:LEU:CD2	1:A:363:ALA:CB	2.88	0.51
2:D:386:HIS:O	2:D:386:HIS:HD2	1.93	0.51
1:E:229:SER:O	1:E:231:ALA:N	2.42	0.51
1:E:350:ILE:HD12	1:E:377:LEU:HD11	1.92	0.51
1:E:533:PRO:C	1:E:535:SER:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:408:MET:HG3	2:F:413:TYR:CE2	2.45	0.51
1:G:114:ILE:HD11	1:G:145:ALA:CB	2.40	0.51
1:G:202:VAL:CG2	1:G:247:GLU:O	2.59	0.51
2:H:339:VAL:HG11	2:H:360:ALA:CB	2.40	0.51
2:H:378:ALA:N	2:H:418:ILE:HD11	2.25	0.51
2:H:532:ILE:O	2:H:534:PRO:HD3	2.10	0.51
1:I:104:ALA:CA	1:I:108:LEU:HD12	2.37	0.51
1:I:274:ARG:NH1	1:I:347:THR:OG1	2.40	0.51
1:I:390:ASP:OD1	1:I:393:GLY:HA3	2.09	0.51
1:I:543:TRP:HB3	2:J:96:PRO:HB3	1.92	0.51
1:K:392:GLU:C	1:K:394:ASP:H	2.14	0.51
1:K:489:ILE:HG23	1:K:490:ALA:N	2.26	0.51
2:L:152:LYS:HA	2:L:526:LEU:HD21	1.93	0.51
1:A:186:GLN:NE2	1:A:187:ASP:N	2.50	0.51
1:A:255:HIS:HE1	1:A:322:GLU:HG2	1.75	0.51
1:A:346:VAL:CG1	1:A:383:GLU:HB2	2.41	0.51
2:B:248:LYS:HG2	2:B:254:VAL:HG22	1.92	0.51
1:C:156:ALA:O	1:C:159:ALA:HB3	2.10	0.51
1:C:405:TYR:HD1	1:C:460:VAL:HG13	1.76	0.51
1:C:47:ARG:HG3	1:C:48:SER:N	2.24	0.51
1:E:280:ARG:HD3	1:E:283:GLN:NE2	2.26	0.51
2:F:484:GLN:NE2	2:F:487:ARG:NH1	2.58	0.51
1:G:134:GLU:O	1:G:135:ASN:HB3	2.10	0.51
1:G:354:ASP:OD2	1:G:357:ALA:HB2	2.11	0.51
1:I:444:ARG:CG	1:I:444:ARG:HH11	2.23	0.51
1:I:509:TRP:CD2	1:I:562:ARG:HD3	2.45	0.51
2:J:171:VAL:CG1	2:J:212:VAL:HG13	2.41	0.51
2:J:467:ASN:H	2:J:467:ASN:ND2	2.09	0.51
2:J:483:ALA:HB3	2:J:506:LYS:HE3	1.91	0.51
1:K:164:SER:OG	1:K:165:ALA:N	2.43	0.51
2:L:294:LEU:O	2:L:295:ASN:C	2.45	0.51
1:A:221:GLU:CG	1:A:222:ALA:N	2.74	0.51
1:A:508:PHE:O	1:A:510:GLN:N	2.44	0.51
1:A:590:LEU:HD12	1:A:597:ASP:O	2.10	0.51
2:B:500:GLU:O	2:B:504:LYS:HD3	2.11	0.51
1:C:344:HIS:CG	1:C:345:PRO:HD3	2.44	0.51
1:C:497:LEU:N	1:C:498:PRO:HD3	2.25	0.51
1:C:71:LEU:HD23	1:C:71:LEU:O	2.11	0.51
2:D:487:ARG:HA	2:D:497:LEU:HD13	1.91	0.51
2:D:526:LEU:C	2:D:528:ASP:H	2.14	0.51
2:F:433:ARG:N	2:F:556:THR:HG23	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:378:ASN:O	1:G:440:TRP:HZ3	1.94	0.51
2:H:161:LEU:HD22	2:H:201:MET:HG3	1.93	0.51
2:H:486:LYS:HG2	2:H:505:ILE:CD1	2.40	0.51
2:J:217:THR:HG22	2:J:240:PHE:HE1	1.76	0.51
2:J:486:LYS:HG3	2:J:497:LEU:HD22	1.93	0.51
1:K:143:GLU:HA	1:K:147:LEU:O	2.10	0.51
2:L:347:PHE:CE2	2:L:348:LYS:HG2	2.45	0.51
1:A:187:ASP:OD1	1:A:189:GLU:N	2.44	0.51
1:A:269:LEU:HD23	1:A:368:LEU:HD13	1.93	0.51
1:A:273:GLU:HG2	1:A:274:ARG:N	2.25	0.51
1:A:695:LYS:O	1:A:696:ALA:CB	2.58	0.51
2:B:231:VAL:HG21	2:B:286:ILE:CG2	2.41	0.51
2:B:284:LEU:O	2:B:287:ALA:HB3	2.10	0.51
2:B:533:ASP:HB3	2:B:536:GLN:HE21	1.76	0.51
2:B:89:ARG:CG	2:B:89:ARG:NH2	2.70	0.51
1:C:138:PHE:CE1	1:C:142:CYS:HB2	2.45	0.51
1:C:563:CYS:SG	1:C:565:ARG:NH2	2.83	0.51
1:G:114:ILE:HD11	1:G:147:LEU:HD13	1.93	0.51
1:G:249:TYR:CD2	1:G:250:LEU:N	2.69	0.51
2:H:457:TYR:N	2:H:457:TYR:CD2	2.78	0.51
2:D:389:GLU:CG	2:H:560:VAL:HG13	2.39	0.51
2:J:435:PRO:HD3	2:J:553:ILE:HG23	1.92	0.51
1:K:140:ARG:NH1	1:K:140:ARG:CB	2.72	0.51
1:K:304:GLU:O	1:K:307:VAL:HG12	2.10	0.51
1:K:357:ALA:O	1:K:361:ARG:HG3	2.11	0.51
2:B:479:ALA:HB2	2:B:509:ILE:CG2	2.40	0.51
1:C:522:GLY:O	1:C:523:HIS:CB	2.57	0.51
2:D:192:GLY:HA3	2:J:450:TYR:CZ	2.46	0.51
1:E:387:TYR:HB2	1:E:466:ASN:ND2	2.25	0.51
2:F:45:ASN:OD1	2:F:322:PRO:HA	2.10	0.51
1:G:231:ALA:HB3	1:G:244:MET:CE	2.36	0.51
2:H:191:PHE:HD2	2:H:192:GLY:N	2.09	0.51
2:J:299:GLN:HG2	2:J:552:PRO:HB3	1.93	0.51
2:L:298:LYS:HG2	2:L:550:ASN:HA	1.92	0.51
1:A:148:LEU:N	1:A:148:LEU:HD23	2.25	0.51
1:C:299:ARG:O	1:C:301:ALA:N	2.44	0.51
1:C:344:HIS:CE1	1:C:345:PRO:HD3	2.46	0.51
1:C:348:GLU:OE1	1:C:415:ARG:NH1	2.40	0.51
1:C:387:TYR:C	1:C:389:GLU:H	2.14	0.51
1:C:101:ALA:HB1	1:C:429:PHE:CD1	2.46	0.51
2:D:216:CYS:SG	2:D:220:GLY:O	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:403:ASN:HA	2:D:443:GLY:H	1.76	0.51
2:D:457:TYR:CD2	2:D:457:TYR:N	2.79	0.51
2:D:486:LYS:HG2	2:D:505:ILE:CD1	2.41	0.51
2:F:217:THR:CG2	2:F:240:PHE:HE1	2.10	0.51
2:F:331:VAL:HG21	2:F:371:ALA:HB1	1.92	0.51
1:G:150:LEU:CD2	1:G:363:ALA:CB	2.85	0.51
1:G:320:THR:HG21	1:G:341:GLN:HB2	1.93	0.51
1:G:473:ILE:CB	1:G:496:LEU:HD13	2.39	0.51
2:H:246:LEU:H	2:H:246:LEU:CD1	2.18	0.51
2:H:298:LYS:HE3	2:H:550:ASN:ND2	2.26	0.51
1:I:251:LEU:HD11	1:I:328:ARG:HH22	1.72	0.51
1:I:497:LEU:N	1:I:498:PRO:CD	2.74	0.51
1:I:602:VAL:HG23	1:I:605:VAL:O	2.11	0.51
2:J:299:GLN:CG	2:J:552:PRO:HD3	2.40	0.51
2:L:441:ILE:HG22	2:L:465:TRP:CE2	2.46	0.51
1:C:252:LYS:HG3	1:C:485:ASP:HB3	1.92	0.51
1:C:62:CYS:HB3	1:C:91:GLU:OE1	2.11	0.51
2:D:258:GLU:HG3	2:D:258:GLU:O	2.10	0.51
2:D:440:LEU:HD12	2:D:464:MET:HG3	1.91	0.51
2:F:192:GLY:HA3	2:H:450:TYR:CE1	2.46	0.51
2:F:216:CYS:HB3	2:F:239:ILE:HA	1.91	0.51
2:F:346:GLU:HG3	2:F:357:CYS:O	2.11	0.51
1:G:179:PRO:O	1:G:248:LYS:HB2	2.10	0.51
1:G:251:LEU:O	1:G:252:LYS:C	2.50	0.51
1:G:448:ARG:HG3	1:G:479:PHE:HE1	1.74	0.51
2:H:420:LYS:O	2:H:423:ALA:HB3	2.10	0.51
1:I:159:ALA:C	1:I:161:GLY:H	2.14	0.51
2:J:189:GLU:O	2:J:189:GLU:CD	2.50	0.51
1:K:307:VAL:O	1:K:311:GLN:NE2	2.44	0.51
2:L:132:MET:HE1	2:L:156:ALA:HA	1.93	0.51
2:L:308:ARG:NH2	2:L:343:GLU:OE1	2.44	0.51
1:A:194:GLU:C	1:A:196:GLY:N	2.63	0.50
1:A:278:ILE:H	1:A:278:ILE:CD1	2.06	0.50
1:A:320:THR:HG21	1:A:341:GLN:HB2	1.93	0.50
1:A:508:PHE:O	1:A:509:TRP:C	2.48	0.50
1:A:65:MET:CE	1:A:88:HIS:O	2.58	0.50
1:A:78:VAL:HB	1:A:98:LEU:HD21	1.94	0.50
2:B:326:LYS:NZ	2:B:405:THR:CG2	2.74	0.50
1:C:431:ASP:OD1	1:C:432:PRO:HD2	2.11	0.50
2:D:59:LEU:O	2:D:63:ILE:HG13	2.11	0.50
1:E:437:LEU:HD23	1:E:455:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:108:VAL:HG11	2:F:148:LEU:CD1	2.40	0.50
1:G:411:GLY:H	1:G:414:ARG:HG3	1.76	0.50
1:I:289:ALA:HA	1:I:290:PRO:C	2.30	0.50
2:J:171:VAL:O	2:J:171:VAL:HG12	2.09	0.50
1:K:76:VAL:HA	1:K:94:ILE:O	2.10	0.50
2:L:147:PRO:HA	2:L:184:VAL:HG22	1.93	0.50
1:A:263:ASP:HB3	1:A:362:VAL:HG12	1.92	0.50
2:D:357:CYS:SG	2:D:370:LEU:HG	2.51	0.50
2:D:53:VAL:O	2:D:57:ARG:CG	2.59	0.50
1:E:541:ASP:CB	1:E:549:ARG:NH2	2.74	0.50
2:F:247:VAL:O	2:F:250:ALA:HB3	2.12	0.50
1:G:51:ARG:CD	1:G:121:GLY:O	2.59	0.50
1:G:437:LEU:HD23	1:G:455:LEU:CD2	2.41	0.50
1:K:324:LEU:HB3	1:K:334:MET:CE	2.41	0.50
1:K:353:LEU:HD22	1:K:358:TRP:CZ2	2.47	0.50
1:K:466:ASN:ND2	1:K:470:LEU:HD11	2.26	0.50
1:A:258:ILE:O	1:A:320:THR:HA	2.10	0.50
2:B:33:THR:CG2	2:B:35:ILE:HG13	2.40	0.50
1:E:167:LYS:HE3	1:E:177:LEU:CD2	2.24	0.50
1:E:193:ARG:HG2	1:E:193:ARG:HH11	1.76	0.50
1:E:323:PHE:CE1	1:E:331:PHE:HD1	2.30	0.50
1:E:541:ASP:CB	1:E:549:ARG:HH21	2.25	0.50
1:E:614:ARG:HB2	1:E:619:PHE:HE1	1.77	0.50
2:F:83:VAL:CG1	2:F:84:ARG:H	2.20	0.50
1:G:135:ASN:ND2	1:G:137:ASP:OD2	2.44	0.50
1:G:328:ARG:HB2	1:G:330:GLN:OE1	2.11	0.50
2:H:317:LEU:CA	2:H:320:VAL:HG23	2.37	0.50
2:H:472:VAL:HG22	2:H:473:MET:HG2	1.94	0.50
1:I:315:TYR:HD1	1:I:316:VAL:N	2.09	0.50
1:I:54:VAL:O	1:I:54:VAL:CG1	2.59	0.50
2:J:191:PHE:HD2	2:J:192:GLY:N	2.08	0.50
2:J:234:ARG:C	2:J:235:GLU:HG2	2.31	0.50
2:J:252:GLY:O	2:J:253:GLU:O	2.29	0.50
2:J:179:PRO:CD	4:J:591:COA:H2A	2.40	0.50
1:K:315:TYR:OH	1:K:338:THR:HA	2.12	0.50
1:K:411:GLY:O	1:K:412:PRO:C	2.49	0.50
1:K:516:TRP:CD2	1:K:555:LEU:HD21	2.47	0.50
1:K:54:VAL:HG11	1:K:61:ALA:HA	1.93	0.50
2:B:187:ASP:O	2:B:190:HIS:HB2	2.11	0.50
2:B:87:ILE:HD11	2:B:120:VAL:CG1	2.42	0.50
2:D:440:LEU:HD13	2:D:464:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:ALA:O	1:G:350:ILE:HG21	2.11	0.50
2:H:403:ASN:ND2	2:H:442:GLY:HA3	2.27	0.50
1:I:285:VAL:HG12	1:I:286:VAL:CG2	2.41	0.50
1:I:254:ARG:HH22	1:I:293:GLY:H	1.59	0.50
2:J:484:GLN:HE21	2:J:484:GLN:CA	2.18	0.50
2:J:59:LEU:O	2:J:63:ILE:HG13	2.11	0.50
1:K:613:ARG:O	1:K:614:ARG:CD	2.59	0.50
1:A:427:SER:OG	1:A:428:PRO:N	2.45	0.50
1:C:292:PRO:HG2	1:C:484:LEU:CD1	2.42	0.50
2:D:161:LEU:HD12	2:D:161:LEU:O	2.11	0.50
2:D:417:GLY:C	2:D:419:ALA:N	2.64	0.50
2:D:488:GLU:O	2:D:492:ARG:HG2	2.11	0.50
1:E:263:ASP:HA	1:E:362:VAL:CG1	2.41	0.50
1:E:380:HIS:CE1	1:E:444:ARG:HD2	2.47	0.50
1:E:555:LEU:HD22	1:E:629:ILE:HG22	1.94	0.50
2:D:26:SER:CB	2:F:289:ARG:NH1	2.75	0.50
2:F:498:GLY:C	2:F:500:GLU:N	2.64	0.50
2:F:90:LEU:HD12	2:F:288:ARG:HG3	1.92	0.50
1:G:400:GLY:H	1:G:463:LEU:HD21	1.77	0.50
2:H:277:ALA:HB2	2:H:286:ILE:HD12	1.92	0.50
1:I:258:ILE:CD1	1:I:303:GLY:HA2	2.38	0.50
2:J:206:ILE:O	2:J:206:ILE:HG22	2.12	0.50
1:K:280:ARG:HG3	1:K:395:PHE:CD2	2.46	0.50
2:L:157:GLN:NE2	2:L:197:ASN:CB	2.75	0.50
2:L:255:VAL:HG13	2:L:259:GLU:OE1	2.11	0.50
2:B:50:LEU:HD23	2:B:54:ASN:ND2	2.26	0.50
1:C:276:CYS:CB	1:C:284:LYS:HD3	2.42	0.50
2:F:485:VAL:HA	2:F:488:GLU:OE1	2.12	0.50
1:G:140:ARG:NH1	1:G:144:GLU:OE2	2.44	0.50
1:G:605:VAL:CG2	1:G:605:VAL:O	2.53	0.50
1:G:460:VAL:O	1:G:626:LEU:HD23	2.11	0.50
1:I:299:ARG:C	1:I:301:ALA:N	2.65	0.50
2:D:78:ARG:HH22	2:J:492:ARG:HH22	1.59	0.50
1:K:129:TYR:O	1:K:129:TYR:HD1	1.94	0.50
1:K:107:TYR:HB2	1:K:131:PHE:CE1	2.46	0.50
2:L:321:ILE:HD13	2:L:329:TYR:CE2	2.47	0.50
2:L:426:VAL:O	2:L:429:VAL:HG12	2.11	0.50
1:A:204:LEU:HD21	1:A:246:VAL:HG22	1.93	0.50
1:A:281:ARG:HH21	1:A:395:PHE:HD2	1.60	0.50
1:C:77:ALA:O	1:C:95:ALA:HA	2.11	0.50
2:D:161:LEU:HB2	2:D:201:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:521:TYR:CD1	2:D:525:ARG:NH1	2.80	0.50
1:C:544:ARG:HH21	2:D:88:ASN:HD21	1.58	0.50
1:E:351:THR:OG1	1:E:352:GLY:N	2.45	0.50
1:E:440:TRP:CG	1:E:441:GLY:N	2.79	0.50
1:G:177:LEU:HD23	1:G:177:LEU:N	2.26	0.50
2:H:317:LEU:O	2:H:318:TYR:C	2.49	0.50
1:I:103:PRO:C	1:I:108:LEU:HD12	2.31	0.50
1:I:178:VAL:HG13	1:I:332:PHE:HB3	1.93	0.50
2:J:109:TYR:CE2	2:J:147:PRO:HD2	2.45	0.50
1:K:141:ALA:HA	1:K:144:GLU:OE2	2.11	0.50
1:K:441:GLY:HA2	1:K:450:ARG:HH21	1.75	0.50
1:K:50:GLN:HB2	1:K:123:GLN:OE1	2.11	0.50
1:A:299:ARG:C	1:A:301:ALA:N	2.65	0.50
2:B:35:ILE:HD12	2:B:337:ARG:NH2	2.26	0.50
2:B:362:LEU:HD21	2:B:541:LEU:HB2	1.94	0.50
2:B:87:ILE:HD11	2:B:120:VAL:HG11	1.93	0.50
1:C:263:ASP:C	1:C:265:HIS:H	2.15	0.50
2:D:331:VAL:HG11	2:D:371:ALA:HB1	1.93	0.50
2:D:487:ARG:HG3	2:D:487:ARG:O	2.12	0.50
2:F:393:GLN:HG2	2:F:393:GLN:O	2.10	0.50
2:F:487:ARG:CG	2:F:487:ARG:O	2.58	0.50
2:H:272:VAL:O	2:H:272:VAL:HG12	2.11	0.50
2:F:242:ALA:HB2	2:H:409:VAL:HG11	1.93	0.50
1:I:469:PHE:HA	1:I:472:ARG:HE	1.76	0.50
2:J:518:HIS:CD2	2:J:520:TYR:H	2.29	0.50
1:A:59:GLU:HB3	1:A:419:GLY:N	2.26	0.50
1:A:699:CYS:HA	1:A:703:GLU:OE1	2.11	0.50
2:B:36:ASN:OD1	2:B:39:SER:N	2.45	0.50
2:B:466:PRO:HD3	2:B:532:ILE:O	2.12	0.50
1:C:135:ASN:O	1:C:135:ASN:CG	2.50	0.50
2:D:154:LEU:HA	2:D:157:GLN:HG3	1.94	0.50
2:D:457:TYR:N	2:D:457:TYR:HD2	2.08	0.50
1:E:131:PHE:HD1	1:E:131:PHE:N	2.09	0.50
1:E:139:ALA:O	1:E:143:GLU:HB2	2.11	0.50
1:E:346:VAL:HG13	1:E:383:GLU:HB2	1.94	0.50
2:F:324:ASP:OD1	2:F:324:ASP:C	2.50	0.50
2:F:476:GLU:OE2	2:F:477:GLN:N	2.45	0.50
1:G:205:LYS:CE	1:G:245:LEU:HD13	2.41	0.50
2:F:241:LEU:HD12	2:H:418:ILE:CG2	2.41	0.50
1:I:107:TYR:O	1:I:113:ILE:HD11	2.12	0.50
1:I:299:ARG:C	1:I:301:ALA:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:352:GLY:O	1:I:353:LEU:HD23	2.11	0.50
1:I:392:GLU:O	1:I:394:ASP:N	2.44	0.50
2:J:375:ILE:O	2:J:376:LEU:HB2	2.12	0.50
1:K:412:PRO:CB	1:K:450:ARG:HH11	2.25	0.50
1:K:557:CYS:O	1:K:558:ARG:C	2.50	0.50
1:K:618:LEU:O	1:K:618:LEU:HD23	2.11	0.50
1:K:508:PHE:HB2	1:K:622:TRP:CZ2	2.47	0.50
1:K:63:ARG:HH22	1:K:356:VAL:HG23	1.77	0.50
2:L:324:ASP:O	2:L:327:GLN:HB2	2.12	0.50
2:L:87:ILE:H	2:L:87:ILE:HD12	1.76	0.50
1:A:569:ALA:O	1:A:571:PRO:HD3	2.12	0.49
1:A:76:VAL:HG13	1:A:94:ILE:CG2	2.41	0.49
2:B:240:PHE:CE1	2:B:243:GLY:HA2	2.47	0.49
1:C:269:LEU:HD13	1:C:375:VAL:CG1	2.42	0.49
2:D:397:PRO:HA	2:D:434:VAL:HG23	1.94	0.49
1:E:264:ARG:C	1:E:265:HIS:HD2	2.16	0.49
2:F:372:ASN:ND2	2:F:404:ILE:HD13	2.27	0.49
2:F:46:ALA:O	2:F:50:LEU:HB2	2.13	0.49
2:F:487:ARG:HH11	2:F:487:ARG:CB	2.25	0.49
1:G:160:MET:CE	1:G:313:ILE:HG21	2.42	0.49
1:G:446:GLU:O	1:G:450:ARG:HB2	2.12	0.49
1:G:81:ASP:C	1:G:83:ASP:H	2.15	0.49
1:I:274:ARG:HG2	1:I:289:ALA:HB2	1.94	0.49
2:L:194:ILE:N	2:L:194:ILE:CD1	2.74	0.49
1:A:257:GLU:OE1	1:A:343:GLU:OE2	2.30	0.49
1:A:445:GLU:O	1:A:449:GLN:HB2	2.12	0.49
1:A:677:LEU:HD21	1:A:711:LEU:HD11	1.94	0.49
1:A:702:GLY:O	1:A:704:LEU:HG	2.12	0.49
2:B:213:MET:HE2	2:B:280:ASP:HA	1.93	0.49
1:C:149:PHE:CE1	1:C:151:GLY:HA3	2.47	0.49
1:C:553:LEU:HD12	1:C:566:LEU:HD11	1.93	0.49
1:E:297:GLU:O	1:E:300:ARG:HG3	2.13	0.49
2:F:525:ARG:O	2:F:526:LEU:HB2	2.12	0.49
2:F:298:LYS:HE3	2:F:550:ASN:ND2	2.27	0.49
1:G:159:ALA:C	1:G:161:GLY:H	2.15	0.49
1:G:339:ARG:HG3	1:G:340:LEU:O	2.12	0.49
1:I:289:ALA:CB	1:I:350:ILE:HD13	2.41	0.49
2:J:189:GLU:C	2:J:189:GLU:CD	2.71	0.49
1:K:132:LEU:HD23	1:K:138:PHE:CE2	2.46	0.49
1:K:63:ARG:NH1	1:K:356:VAL:HG21	2.26	0.49
1:K:516:TRP:HA	1:K:618:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ARG:HG3	1:A:549:ARG:HH11	1.77	0.49
1:A:613:ARG:O	1:A:614:ARG:HD3	2.11	0.49
2:B:44:ALA:O	2:B:47:ALA:HB3	2.12	0.49
2:D:163:ASN:OD1	2:D:460:ARG:NH1	2.43	0.49
2:D:418:ILE:HG23	2:D:419:ALA:N	2.26	0.49
2:D:66:GLY:C	2:D:68:GLY:H	2.16	0.49
2:D:71:ALA:HB1	2:D:74:ARG:HD3	1.93	0.49
1:E:550:GLU:HA	1:E:567:ARG:HD3	1.94	0.49
2:F:294:LEU:O	2:F:295:ASN:C	2.50	0.49
2:F:301:GLN:HE21	2:F:301:GLN:HA	1.77	0.49
2:F:476:GLU:O	2:F:480:GLY:N	2.45	0.49
1:G:569:ALA:O	1:G:571:PRO:HD3	2.12	0.49
2:H:205:GLY:O	2:H:207:PRO:HD3	2.13	0.49
2:H:403:ASN:HA	2:H:443:GLY:H	1.76	0.49
1:I:308:ARG:HG3	1:I:308:ARG:NH1	2.22	0.49
2:J:242:ALA:O	2:J:260:LEU:HD21	2.13	0.49
1:K:253:PRO:HB2	1:K:324:LEU:HG	1.93	0.49
1:K:321:VAL:HA	1:K:336:MET:HG2	1.94	0.49
1:K:407:GLU:HA	1:K:458:THR:HG22	1.93	0.49
2:L:538:ARG:CG	2:L:538:ARG:NH1	2.70	0.49
1:A:496:LEU:C	1:A:497:LEU:HD23	2.32	0.49
1:A:501:GLN:HE21	1:A:504:LEU:HG	1.77	0.49
1:C:320:THR:HG21	1:C:341:GLN:HB2	1.94	0.49
1:C:365:GLY:O	1:C:366:GLU:O	2.30	0.49
1:C:50:GLN:OE1	1:C:50:GLN:N	2.45	0.49
1:E:333:PHE:CE1	1:E:335:GLU:HA	2.48	0.49
1:E:516:TRP:O	1:E:519:SER:OG	2.25	0.49
1:E:532:ASP:O	1:E:535:SER:HB2	2.13	0.49
1:E:63:ARG:HG3	1:E:63:ARG:NH1	2.28	0.49
2:F:225:ALA:O	2:H:562:ARG:CD	2.59	0.49
2:F:264:ASP:OD2	2:F:268:LYS:HE3	2.12	0.49
2:F:311:LEU:CG	2:F:342:SER:HB2	2.41	0.49
1:G:220:ARG:HE	1:G:220:ARG:HA	1.77	0.49
1:G:287:GLU:HG2	1:G:343:GLU:HG3	1.95	0.49
1:G:519:SER:HB2	1:G:613:ARG:HH21	1.78	0.49
1:G:546:ALA:HB3	2:H:60:LEU:HD12	1.93	0.49
1:G:54:VAL:HG12	1:G:54:VAL:O	2.13	0.49
2:J:538:ARG:CG	2:J:538:ARG:NH1	2.66	0.49
1:K:125:ILE:HG13	1:K:147:LEU:HD13	1.92	0.49
2:L:248:LYS:HA	2:L:252:GLY:O	2.11	0.49
2:L:74:ARG:HH21	2:L:78:ARG:NH2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASP:O	1:A:191:PHE:HB2	2.13	0.49
1:A:508:PHE:CE1	1:A:627:LEU:HD12	2.48	0.49
2:B:431:CYS:O	2:B:433:ARG:HG2	2.12	0.49
2:D:272:VAL:O	2:D:272:VAL:CG1	2.59	0.49
1:E:101:ALA:CB	1:E:429:PHE:HE1	2.10	0.49
1:E:49:ILE:CD1	1:E:49:ILE:N	2.74	0.49
2:F:284:LEU:O	2:F:287:ALA:HB3	2.13	0.49
1:I:47:ARG:NH1	1:I:47:ARG:HB2	2.26	0.49
1:I:496:LEU:O	1:I:497:LEU:HD23	2.12	0.49
1:A:261:PHE:CD1	1:A:358:TRP:CE3	2.96	0.49
2:B:81:LEU:HD11	2:B:89:ARG:HH21	1.77	0.49
1:C:403:MET:CE	1:C:462:GLY:HA3	2.43	0.49
2:D:157:GLN:O	2:D:201:MET:HE1	2.12	0.49
2:D:201:MET:CG	2:D:206:ILE:HD12	2.41	0.49
2:D:347:PHE:HA	2:F:275:HIS:HE1	1.76	0.49
2:D:441:ILE:HG22	2:D:465:TRP:CE3	2.48	0.49
1:E:131:PHE:CD1	1:E:131:PHE:N	2.81	0.49
1:E:107:TYR:HB3	1:E:131:PHE:HD2	1.78	0.49
1:E:389:GLU:HA	1:E:397:PRO:HA	1.94	0.49
1:E:440:TRP:CD1	1:E:441:GLY:N	2.80	0.49
2:F:250:ALA:O	2:F:252:GLY:N	2.45	0.49
1:G:217:VAL:CG2	1:G:249:TYR:HD1	2.25	0.49
2:H:123:ILE:HA	2:H:131:CYS:O	2.12	0.49
1:I:384:VAL:HG13	1:I:470:LEU:HD22	1.95	0.49
1:I:79:HIS:CD2	1:I:80:SER:O	2.66	0.49
2:J:176:ALA:O	2:J:178:LEU:N	2.46	0.49
2:J:377:PHE:CA	2:J:418:ILE:HD11	2.41	0.49
2:J:473:MET:CE	2:J:477:GLN:HB3	2.43	0.49
2:J:50:LEU:C	2:J:50:LEU:HD23	2.33	0.49
1:K:466:ASN:HD21	1:K:470:LEU:HD11	1.78	0.49
1:A:513:ALA:HB1	1:A:566:LEU:HD21	1.94	0.49
2:B:247:VAL:HG23	2:L:409:VAL:HG23	1.94	0.49
1:C:344:HIS:N	1:C:345:PRO:CD	2.76	0.49
1:C:619:PHE:CE2	1:C:628:ALA:HB2	2.47	0.49
2:D:232:MET:O	2:D:277:ALA:HB3	2.12	0.49
1:E:125:ILE:CD1	1:E:147:LEU:HD13	2.42	0.49
1:E:465:THR:CG2	1:E:467:LEU:H	2.11	0.49
1:E:46:TYR:CE1	1:E:364:ARG:HB3	2.47	0.49
1:E:56:ASN:ND2	1:E:60:ILE:HG21	2.27	0.49
1:G:103:PRO:C	1:G:108:LEU:HD12	2.33	0.49
1:G:261:PHE:CZ	1:G:318:ALA:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:PHE:CD1	1:G:358:TRP:CE3	2.99	0.49
2:H:444:SER:CB	2:H:449:ASN:HD22	2.25	0.49
1:I:333:PHE:CE1	1:I:335:GLU:HA	2.48	0.49
1:I:102:LYS:HD3	1:I:429:PHE:HD2	1.78	0.49
2:J:408:MET:HG2	2:J:413:TYR:CD1	2.47	0.49
2:J:536:GLN:O	2:J:537:THR:C	2.49	0.49
1:K:101:ALA:HB1	1:K:429:PHE:CD1	2.45	0.49
2:L:429:VAL:HG13	2:L:430:ALA:N	2.28	0.49
1:A:589:ARG:O	1:A:598:LEU:HD12	2.12	0.49
1:A:63:ARG:NH2	1:A:356:VAL:HG23	2.27	0.49
1:A:671:GLY:HA2	1:A:688:ALA:N	2.28	0.49
2:B:185:PHE:H	2:B:186:PRO:HD2	1.78	0.49
1:C:269:LEU:CD2	1:C:370:LEU:O	2.61	0.49
1:C:446:GLU:O	1:C:450:ARG:HB2	2.12	0.49
1:C:491:ARG:HD2	1:C:492:HIS:CE1	2.48	0.49
2:D:440:LEU:CB	2:D:464:MET:HG3	2.42	0.49
1:E:251:LEU:HD11	1:E:328:ARG:NH2	2.27	0.49
2:F:338:LEU:HD21	2:F:537:THR:CG2	2.42	0.49
1:G:168:ALA:O	1:G:171:GLU:HB2	2.13	0.49
1:G:198:ILE:O	1:G:248:LYS:NZ	2.40	0.49
1:G:534:HIS:HB3	2:H:307:PRO:HG2	1.94	0.49
2:H:305:ARG:HH11	2:H:305:ARG:CB	2.08	0.49
2:H:335:ILE:HD13	2:H:344:PHE:CE1	2.47	0.49
2:H:520:TYR:CD2	2:H:520:TYR:N	2.80	0.49
1:I:114:ILE:HD11	1:I:142:CYS:HA	1.94	0.49
1:I:389:GLU:O	1:I:390:ASP:HB2	2.12	0.49
1:I:82:ILE:HG13	1:I:83:ASP:OD1	2.13	0.49
2:J:36:ASN:HD22	2:J:37:PRO:CD	2.25	0.49
2:J:476:GLU:CD	2:J:476:GLU:N	2.66	0.49
1:K:278:ILE:H	1:K:278:ILE:CD1	2.19	0.49
1:K:383:GLU:HG2	1:K:384:VAL:N	2.28	0.49
1:A:278:ILE:HG23	1:A:488:PHE:HD2	1.78	0.49
1:A:353:LEU:HD13	1:A:358:TRP:CH2	2.48	0.49
1:A:607:ARG:NH1	1:A:607:ARG:CB	2.76	0.49
2:B:100:LEU:HD22	2:B:529:ASP:HB3	1.94	0.49
2:B:324:ASP:O	2:B:327:GLN:HB2	2.13	0.49
2:B:554:GLU:OE2	2:B:555:PRO:HD2	2.13	0.49
1:C:200:TYR:OH	1:C:224:LEU:CD2	2.59	0.49
2:D:119:ILE:O	2:D:119:ILE:HG23	2.12	0.49
1:E:107:TYR:HB2	1:E:131:PHE:CE2	2.48	0.49
1:E:123:GLN:CD	1:E:123:GLN:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:ARG:NH1	1:E:549:ARG:CG	2.69	0.49
1:E:55:ALA:O	1:E:56:ASN:HB2	2.13	0.49
3:A:801:BTI:O3	2:F:407:PHE:HD1	1.96	0.49
2:F:435:PRO:HG2	2:F:553:ILE:HD12	1.94	0.49
2:F:74:ARG:HH22	2:F:78:ARG:NH1	2.10	0.49
1:G:138:PHE:C	1:G:138:PHE:CD1	2.85	0.49
1:G:344:HIS:ND1	1:G:345:PRO:HD3	2.27	0.49
2:H:154:LEU:HD23	2:H:157:GLN:NE2	2.27	0.49
2:F:242:ALA:CB	2:H:409:VAL:HG11	2.42	0.49
2:J:463:TRP:HH2	2:J:544:ALA:HB2	1.78	0.49
1:K:274:ARG:HG2	1:K:289:ALA:HB2	1.95	0.49
1:K:320:THR:HG21	1:K:341:GLN:CG	2.41	0.49
1:K:408:ALA:H	1:K:458:THR:CG2	2.26	0.49
1:K:588:TYR:N	1:K:588:TYR:CD1	2.81	0.49
2:L:347:PHE:CZ	2:L:348:LYS:HG2	2.48	0.49
2:L:378:ALA:O	2:L:379:GLU:C	2.49	0.49
2:L:74:ARG:HH21	2:L:78:ARG:HH22	1.60	0.49
1:A:354:ASP:CG	1:A:357:ALA:HB2	2.34	0.49
1:A:548:ALA:O	1:A:550:GLU:OE1	2.31	0.49
1:A:612:LEU:HD12	1:A:612:LEU:O	2.13	0.49
2:B:170:LEU:CD2	2:B:211:VAL:HB	2.43	0.49
2:B:75:HIS:HE1	2:B:80:LYS:HE2	1.78	0.49
1:C:154:ALA:O	1:C:155:ALA:C	2.51	0.49
1:C:478:ALA:HB1	1:C:488:PHE:HE1	1.78	0.49
1:C:618:LEU:O	1:C:618:LEU:HG	2.09	0.49
2:D:491:GLU:C	2:D:493:ALA:H	2.15	0.49
2:D:487:ARG:HD3	2:D:497:LEU:HB2	1.94	0.49
1:E:296:ALA:O	1:E:300:ARG:HG2	2.13	0.49
1:E:434:LEU:N	1:E:434:LEU:HD12	2.27	0.49
1:E:384:VAL:HG12	1:E:470:LEU:HD13	1.95	0.49
1:E:596:ASP:CG	1:E:612:LEU:HD23	2.33	0.49
1:E:557:CYS:HB2	1:E:629:ILE:HG12	1.95	0.49
2:H:102:ALA:C	2:H:104:ALA:H	2.14	0.49
1:A:654:ASN:OD1	2:H:251:THR:HG21	2.13	0.49
2:H:162:GLU:OE1	2:H:460:ARG:HA	2.13	0.49
1:I:289:ALA:HA	1:I:290:PRO:O	2.13	0.49
1:I:353:LEU:HD23	1:I:353:LEU:N	2.28	0.49
1:K:400:GLY:H	1:K:463:LEU:CD1	2.26	0.49
2:L:244:PRO:N	2:L:245:PRO:CD	2.76	0.49
1:A:699:CYS:HA	1:A:703:GLU:CD	2.34	0.48
2:B:161:LEU:HB2	2:B:201:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:GLN:O	2:B:411:GLN:NE2	2.46	0.48
1:C:221:GLU:HG3	1:C:222:ALA:N	2.28	0.48
1:C:549:ARG:CG	1:C:549:ARG:HH11	2.26	0.48
1:E:280:ARG:HH11	1:E:389:GLU:CD	2.16	0.48
2:F:354:THR:CG2	2:F:375:ILE:N	2.76	0.48
2:H:335:ILE:O	2:H:339:VAL:CG2	2.61	0.48
2:H:339:VAL:CG1	2:H:360:ALA:HB1	2.43	0.48
2:H:449:ASN:ND2	2:H:470:ILE:HD11	2.28	0.48
2:J:141:LYS:NZ	2:J:177:ASN:ND2	2.59	0.48
2:J:207:PRO:HG2	2:J:294:LEU:HD13	1.95	0.48
1:K:269:LEU:HB2	1:K:372:GLN:NE2	2.28	0.48
2:L:185:PHE:HB3	2:L:186:PRO:CD	2.43	0.48
2:L:191:PHE:CD2	2:L:192:GLY:N	2.74	0.48
2:L:233:VAL:HG13	2:L:279:ASP:HA	1.95	0.48
2:B:137:ASP:OD1	2:B:139:THR:HG23	2.12	0.48
2:B:30:ILE:HD13	2:B:343:GLU:HG2	1.94	0.48
2:B:375:ILE:O	2:B:376:LEU:HB2	2.13	0.48
1:C:476:HIS:CG	1:C:477:PRO:HD2	2.48	0.48
1:C:549:ARG:CZ	1:C:571:PRO:HG3	2.43	0.48
2:D:68:GLY:O	2:D:69:SER:C	2.52	0.48
1:E:520:GLU:C	1:E:522:GLY:H	2.17	0.48
2:F:331:VAL:O	2:F:334:VAL:N	2.41	0.48
2:F:479:ALA:HB1	2:F:506:LYS:CG	2.43	0.48
1:G:197:ARG:O	1:G:198:ILE:HG13	2.13	0.48
1:G:534:HIS:HB3	2:H:307:PRO:HG3	1.93	0.48
2:H:394:ARG:HB2	2:H:396:ILE:HD12	1.95	0.48
2:H:413:TYR:O	2:H:418:ILE:HB	2.13	0.48
2:H:432:ALA:HA	2:H:556:THR:CG2	2.43	0.48
2:H:562:ARG:NH1	2:H:562:ARG:HG3	2.27	0.48
1:I:618:LEU:HG	1:I:618:LEU:O	2.13	0.48
2:J:197:ASN:O	2:J:201:MET:HG3	2.12	0.48
2:J:371:ALA:HB2	2:J:401:LEU:HD12	1.94	0.48
1:K:389:GLU:HA	1:K:397:PRO:HA	1.94	0.48
1:A:261:PHE:CZ	1:A:318:ALA:HB2	2.49	0.48
1:A:400:GLY:H	1:A:463:LEU:HD11	1.78	0.48
2:B:193:ARG:HD2	2:B:196:PHE:CD2	2.47	0.48
1:C:315:TYR:HE2	1:C:338:THR:HG22	1.76	0.48
1:C:470:LEU:O	1:C:473:ILE:HG22	2.14	0.48
1:C:602:VAL:HG12	1:C:602:VAL:O	2.13	0.48
1:C:83:ASP:HB3	1:C:86:ALA:HB2	1.94	0.48
2:F:141:LYS:O	2:F:141:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:485:VAL:HG11	4:H:591:COA:OAP	2.13	0.48
2:F:71:ALA:O	2:F:74:ARG:HB3	2.13	0.48
1:G:299:ARG:C	1:G:301:ALA:N	2.67	0.48
1:G:258:ILE:CD1	1:G:306:ALA:HB2	2.43	0.48
1:G:469:PHE:HE1	1:G:497:LEU:HD21	1.75	0.48
1:I:65:MET:HG3	1:I:75:SER:CB	2.43	0.48
2:J:166:PRO:HD3	2:J:296:TRP:CZ2	2.48	0.48
2:J:355:LEU:HD21	2:J:370:LEU:HD23	1.93	0.48
2:J:440:LEU:CD1	2:J:464:MET:HG3	2.37	0.48
2:J:470:ILE:HG23	2:J:470:ILE:O	2.13	0.48
1:K:79:HIS:CD2	1:K:84:ARG:HA	2.47	0.48
2:L:482:LEU:HD23	2:L:509:ILE:HG13	1.94	0.48
1:A:298:LEU:HG	1:A:298:LEU:O	2.12	0.48
1:A:491:ARG:HB3	1:A:492:HIS:CE1	2.49	0.48
1:A:659:ARG:HG2	1:A:676:VAL:HB	1.95	0.48
1:C:231:ALA:CB	1:C:244:MET:SD	2.90	0.48
1:C:389:GLU:HA	1:C:397:PRO:HA	1.95	0.48
1:C:411:GLY:O	1:C:412:PRO:C	2.51	0.48
2:D:218:ALA:O	2:D:221:ALA:HB3	2.14	0.48
2:D:316:GLU:CB	2:D:337:ARG:HE	2.27	0.48
2:D:86:ARG:HA	2:D:284:LEU:HD11	1.93	0.48
1:E:165:ALA:O	1:E:169:LEU:CD1	2.59	0.48
2:F:300:GLY:O	2:F:301:GLN:HB2	2.14	0.48
2:F:533:ASP:HB3	2:F:536:GLN:HE21	1.79	0.48
1:G:85:HIS:NE2	1:G:424:ASP:OD1	2.47	0.48
2:H:469:ARG:HH21	2:H:469:ARG:HG2	1.78	0.48
1:I:255:HIS:ND1	1:I:255:HIS:C	2.67	0.48
2:J:414:GLU:OE1	2:J:414:GLU:CA	2.61	0.48
2:J:521:TYR:O	2:J:525:ARG:NH1	2.47	0.48
1:K:380:HIS:CD2	1:K:444:ARG:HG3	2.48	0.48
1:K:536:PRO:HD3	2:L:363:HIS:HD2	1.75	0.48
1:K:61:ALA:HA	1:K:64:VAL:HG12	1.95	0.48
2:L:86:ARG:HD3	2:L:213:MET:SD	2.54	0.48
1:A:138:PHE:C	1:A:138:PHE:CD1	2.87	0.48
1:A:537:TRP:CD2	2:B:543:LEU:HD22	2.49	0.48
2:B:83:VAL:CG1	2:B:84:ARG:N	2.55	0.48
2:D:431:CYS:HB2	2:D:558:PHE:CD2	2.48	0.48
2:D:476:GLU:H	2:D:476:GLU:CD	2.17	0.48
1:E:320:THR:CG2	1:E:341:GLN:HG3	2.43	0.48
1:G:536:PRO:HB3	2:H:363:HIS:ND1	2.26	0.48
1:I:254:ARG:O	1:I:256:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:350:LEU:CD1	2:J:350:LEU:H	2.03	0.48
2:L:470:ILE:HG22	2:L:470:ILE:O	2.13	0.48
2:L:83:VAL:O	2:L:87:ILE:CD1	2.62	0.48
1:A:284:LYS:NZ	1:A:341:GLN:NE2	2.61	0.48
1:A:345:PRO:HG2	1:A:436:LYS:HE2	1.94	0.48
2:B:297:ARG:NH1	2:B:297:ARG:HB3	2.26	0.48
2:B:65:GLU:O	2:B:72:GLN:NE2	2.47	0.48
1:C:49:ILE:HD13	1:C:364:ARG:CG	2.42	0.48
1:C:505:PRO:HB3	1:C:507:HIS:CB	2.36	0.48
2:F:279:ASP:OD2	2:F:279:ASP:N	2.44	0.48
1:G:345:PRO:HB3	1:G:438:ILE:HD13	1.95	0.48
1:I:532:ASP:OD2	1:I:535:SER:HB2	2.13	0.48
1:I:602:VAL:HG23	1:I:605:VAL:CG2	2.40	0.48
1:I:519:SER:CB	1:I:613:ARG:HE	2.19	0.48
1:I:54:VAL:HG21	1:I:64:VAL:HG11	1.95	0.48
2:J:119:ILE:O	2:J:119:ILE:HG23	2.14	0.48
2:J:386:HIS:O	2:J:386:HIS:HD2	1.96	0.48
2:L:154:LEU:HD21	2:L:194:ILE:HD12	1.95	0.48
1:A:200:TYR:CD1	1:A:221:GLU:HA	2.45	0.48
2:B:232:MET:CE	2:B:263:ALA:HA	2.44	0.48
2:D:289:ARG:HA	2:D:289:ARG:HD2	1.62	0.48
2:D:35:ILE:HD12	2:D:320:VAL:HG22	1.95	0.48
2:D:479:ALA:HB2	2:D:509:ILE:CG2	2.44	0.48
1:E:109:ARG:CD	1:E:112:ARG:NH2	2.76	0.48
1:E:263:ASP:OD2	1:E:267:HIS:HB2	2.14	0.48
2:F:408:MET:CE	2:F:409:VAL:H	2.27	0.48
1:G:279:GLN:HB2	1:G:283:GLN:O	2.14	0.48
1:G:507:HIS:HB3	1:G:622:TRP:HH2	1.77	0.48
2:H:248:LYS:HG2	2:H:254:VAL:HG22	1.95	0.48
1:I:85:HIS:ND1	1:I:86:ALA:N	2.62	0.48
2:D:199:ALA:CB	2:J:427:THR:HG23	2.42	0.48
1:K:474:LEU:HA	1:K:479:PHE:HD1	1.79	0.48
1:K:54:VAL:HG11	1:K:64:VAL:CG1	2.43	0.48
2:L:402:GLN:NE2	2:L:444:SER:OG	2.45	0.48
1:A:269:LEU:CD2	1:A:368:LEU:HD13	2.44	0.48
2:B:412:LYS:HE2	2:B:413:TYR:CE2	2.49	0.48
1:C:504:LEU:CB	1:C:505:PRO:CD	2.76	0.48
2:D:209:ILE:HG22	2:D:210:ALA:N	2.29	0.48
2:D:367:ILE:O	2:D:367:ILE:HG13	2.13	0.48
2:D:434:VAL:HG23	2:D:435:PRO:N	2.27	0.48
1:E:169:LEU:CD2	1:E:313:ILE:HG22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:GLU:HG2	1:E:397:PRO:HG3	1.95	0.48
1:E:439:ALA:HB3	1:E:451:LEU:HB2	1.96	0.48
1:E:78:VAL:CG1	1:E:96:VAL:HG23	2.44	0.48
2:D:472:VAL:HG11	2:J:181:GLN:HB3	1.91	0.48
2:J:191:PHE:HE2	2:J:195:PHE:CZ	2.32	0.48
2:H:303:GLN:NE2	2:J:297:ARG:CG	2.76	0.48
2:L:369:ILE:C	2:L:370:LEU:HD12	2.34	0.48
1:A:231:ALA:O	1:A:244:MET:HE3	2.14	0.48
1:A:340:LEU:CD2	1:A:344:HIS:HB3	2.44	0.48
1:A:491:ARG:HD2	1:A:492:HIS:CE1	2.49	0.48
1:A:549:ARG:O	1:A:567:ARG:HA	2.13	0.48
2:B:330:ASP:OD2	2:B:332:ARG:NH1	2.46	0.48
2:D:241:LEU:HD12	2:J:418:ILE:HG23	1.96	0.48
2:D:317:LEU:CD2	2:D:334:VAL:CG1	2.92	0.48
1:E:616:ARG:HG3	1:E:630:GLU:HB2	1.95	0.48
1:E:63:ARG:NH2	1:E:356:VAL:HG23	2.28	0.48
2:D:345:ASP:CG	2:F:289:ARG:HH21	2.17	0.48
2:F:403:ASN:HA	2:F:443:GLY:H	1.77	0.48
1:G:135:ASN:ND2	1:G:137:ASP:HB2	2.28	0.48
1:G:202:VAL:HG23	1:G:248:LYS:HA	1.96	0.48
1:G:473:ILE:HG13	1:G:473:ILE:O	2.13	0.48
1:G:513:ALA:HB1	1:G:566:LEU:HD11	1.94	0.48
1:G:536:PRO:CB	2:H:363:HIS:HE1	2.26	0.48
1:I:150:LEU:HD21	1:I:359:GLN:C	2.34	0.48
1:I:302:MET:HA	1:I:331:PHE:CZ	2.49	0.48
1:I:491:ARG:HH11	1:I:492:HIS:CE1	2.32	0.48
1:K:335:GLU:HG3	1:K:336:MET:N	2.29	0.48
1:K:269:LEU:CB	1:K:372:GLN:NE2	2.76	0.48
1:K:77:ALA:O	1:K:95:ALA:HA	2.13	0.48
1:A:217:VAL:CG2	1:A:249:TYR:CD1	2.97	0.48
1:A:350:ILE:HA	1:A:440:TRP:HZ3	1.79	0.48
1:C:327:GLU:O	1:C:329:GLY:N	2.47	0.48
1:C:501:GLN:NE2	1:C:504:LEU:CD2	2.73	0.48
1:C:52:LEU:HD12	1:C:53:LEU:N	2.29	0.48
1:E:327:GLU:O	1:E:329:GLY:N	2.47	0.48
1:E:504:LEU:CB	1:E:505:PRO:CD	2.90	0.48
1:E:71:LEU:HA	1:E:71:LEU:HD23	1.70	0.48
2:F:84:ARG:NH1	2:F:84:ARG:CG	2.72	0.48
1:G:360:ILE:O	1:G:364:ARG:HG3	2.13	0.48
1:G:504:LEU:HB3	1:G:505:PRO:HD2	1.95	0.48
1:G:53:LEU:HG	1:G:54:VAL:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:LYS:HG3	1:I:177:LEU:HD13	1.95	0.48
1:I:309:ALA:O	1:I:312:ALA:HB3	2.14	0.48
2:J:299:GLN:CB	2:J:552:PRO:HD3	2.42	0.48
2:J:436:LYS:HD2	2:J:453:CYS:SG	2.54	0.48
2:J:507:ALA:N	2:J:508:PRO:HD2	2.28	0.48
2:L:255:VAL:CG1	2:L:256:SER:N	2.77	0.48
2:L:408:MET:HG3	2:L:413:TYR:CD2	2.48	0.48
2:L:474:GLY:HA3	2:L:477:GLN:NE2	2.28	0.48
1:A:556:ARG:NH1	1:A:556:ARG:HG2	2.29	0.47
1:C:202:VAL:HG21	1:C:246:VAL:HG13	1.96	0.47
1:C:380:HIS:NE2	1:C:444:ARG:HG3	2.29	0.47
1:E:167:LYS:HG3	1:E:177:LEU:CD2	2.44	0.47
1:E:313:ILE:HD11	1:E:315:TYR:HD2	1.79	0.47
1:E:278:ILE:HG23	1:E:488:PHE:HD2	1.79	0.47
2:F:424:LYS:HB3	2:L:563:MET:CE	2.43	0.47
1:G:218:VAL:CG1	1:G:224:LEU:HD13	2.43	0.47
1:G:386:LEU:CD1	1:G:386:LEU:C	2.82	0.47
1:G:421:ARG:NE	1:G:424:ASP:OD2	2.46	0.47
1:G:452:LEU:HD22	1:G:474:LEU:CB	2.42	0.47
1:G:491:ARG:C	1:G:493:GLN:H	2.17	0.47
1:G:522:GLY:O	1:G:523:HIS:HB2	2.14	0.47
1:G:612:LEU:N	1:G:612:LEU:HD12	2.29	0.47
2:H:398:LEU:HD12	2:H:434:VAL:HG21	1.96	0.47
2:H:490:ALA:HA	2:H:493:ALA:HB3	1.95	0.47
2:H:53:VAL:O	2:H:57:ARG:HG2	2.14	0.47
1:I:82:ILE:HD13	1:I:101:ALA:HB1	1.96	0.47
1:I:315:TYR:HE2	1:I:336:MET:HE1	1.78	0.47
2:J:500:GLU:O	2:J:504:LYS:HG3	2.14	0.47
1:K:516:TRP:CZ2	1:K:631:ALA:HB2	2.48	0.47
1:A:135:ASN:O	1:A:135:ASN:CG	2.52	0.47
1:A:557:CYS:O	1:A:558:ARG:C	2.52	0.47
1:A:693:VAL:O	1:A:714:LEU:HD22	2.14	0.47
1:C:262:ALA:O	1:C:316:VAL:O	2.32	0.47
1:C:590:LEU:C	1:C:590:LEU:HD12	2.34	0.47
2:D:155:ARG:HD2	2:D:155:ARG:O	2.13	0.47
2:D:176:ALA:HB1	2:D:184:VAL:HG11	1.95	0.47
2:D:31:LEU:HD12	2:D:336:ALA:HB2	1.97	0.47
2:D:424:LYS:HD2	2:H:563:MET:SD	2.54	0.47
2:D:444:SER:HG	2:D:449:ASN:ND2	2.12	0.47
1:E:269:LEU:HD23	1:E:269:LEU:N	2.29	0.47
1:E:308:ARG:CG	1:E:308:ARG:NH1	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:PHE:N	1:E:429:PHE:CD2	2.81	0.47
1:G:518:GLN:CB	1:G:590:LEU:HD23	2.43	0.47
1:G:613:ARG:HG2	1:G:614:ARG:N	2.29	0.47
1:G:86:ALA:HB3	1:G:89:VAL:HG23	1.96	0.47
2:H:321:ILE:HD13	2:H:329:TYR:CE1	2.49	0.47
2:H:386:HIS:O	2:H:386:HIS:HD2	1.97	0.47
2:H:68:GLY:C	2:H:70:ALA:N	2.66	0.47
2:J:136:ASN:N	2:J:136:ASN:OD1	2.46	0.47
2:J:248:LYS:HA	2:J:252:GLY:O	2.14	0.47
2:J:28:MET:C	2:J:30:ILE:H	2.16	0.47
2:J:499:VAL:O	2:J:499:VAL:CG1	2.63	0.47
2:J:81:LEU:HD11	2:J:89:ARG:HH21	1.80	0.47
1:K:440:TRP:CD1	1:K:441:GLY:N	2.82	0.47
2:L:498:GLY:O	2:L:500:GLU:N	2.47	0.47
2:B:379:GLU:N	2:B:379:GLU:OE2	2.44	0.47
2:B:68:GLY:O	2:B:70:ALA:N	2.46	0.47
1:C:201:PRO:CD	1:C:328:ARG:NH2	2.71	0.47
1:C:392:GLU:O	1:C:394:ASP:N	2.45	0.47
2:D:357:CYS:HB2	2:D:383:LYS:HE2	1.96	0.47
2:F:100:LEU:O	2:F:152:LYS:HE3	2.14	0.47
2:F:212:VAL:HG21	2:F:232:MET:CG	2.44	0.47
1:G:143:GLU:HA	1:G:147:LEU:O	2.15	0.47
1:G:49:ILE:HD11	1:G:148:LEU:CD1	2.44	0.47
1:G:197:ARG:O	1:G:198:ILE:CG1	2.62	0.47
2:H:81:LEU:HD22	2:H:85:GLU:HB3	1.96	0.47
1:I:76:VAL:HG11	1:I:120:SER:OG	2.14	0.47
1:K:62:CYS:O	1:K:66:ARG:HG3	2.14	0.47
2:L:498:GLY:C	2:L:500:GLU:H	2.17	0.47
1:A:186:GLN:NE2	1:A:190:THR:N	2.47	0.47
1:A:396:LEU:CD1	1:A:464:ARG:HH12	2.05	0.47
2:B:220:GLY:O	2:B:224:PRO:HD2	2.15	0.47
2:B:244:PRO:HA	2:B:247:VAL:CG1	2.42	0.47
2:B:268:LYS:CB	2:B:268:LYS:NZ	2.77	0.47
1:C:262:ALA:HB2	1:C:268:CYS:HB2	1.96	0.47
1:C:280:ARG:O	1:C:280:ARG:NE	2.40	0.47
1:C:388:ALA:HB2	1:C:434:LEU:HD11	1.97	0.47
1:C:549:ARG:HG2	1:C:549:ARG:NH1	2.29	0.47
2:D:338:LEU:O	2:D:538:ARG:CD	2.51	0.47
2:D:464:MET:HE2	2:D:519:PRO:CG	2.35	0.47
1:E:324:LEU:HD22	1:E:334:MET:SD	2.54	0.47
1:E:426:VAL:O	1:E:426:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:GLU:HA	1:E:458:THR:HG23	1.96	0.47
1:E:77:ALA:O	1:E:95:ALA:HA	2.14	0.47
2:F:527:TRP:CH2	2:H:186:PRO:HG3	2.49	0.47
1:G:549:ARG:CG	1:G:549:ARG:NH1	2.77	0.47
2:H:497:LEU:HD11	2:H:501:GLU:HB2	1.96	0.47
1:I:620:LEU:HD12	1:I:621:GLU:N	2.28	0.47
2:J:339:VAL:HG23	2:J:342:SER:HA	1.97	0.47
1:K:148:LEU:HD23	1:K:148:LEU:N	2.30	0.47
1:K:414:ARG:HD3	1:K:454:MET:HG2	1.96	0.47
2:L:109:TYR:CZ	2:L:147:PRO:HD2	2.49	0.47
2:B:178:LEU:CD1	2:L:482:LEU:HD13	2.43	0.47
2:L:431:CYS:O	2:L:556:THR:HG23	2.15	0.47
1:A:144:GLU:O	1:A:144:GLU:HG2	2.12	0.47
1:A:163:LYS:O	1:A:167:LYS:HB2	2.13	0.47
1:A:376:PRO:O	1:A:377:LEU:HB2	2.14	0.47
1:A:565:ARG:HG2	1:A:567:ARG:CZ	2.44	0.47
1:A:652:PRO:HD3	1:A:686:ILE:HG12	1.96	0.47
1:C:232:GLN:H	1:C:233:ARG:CZ	2.27	0.47
1:C:421:ARG:O	1:C:422:GLU:C	2.52	0.47
2:D:400:PHE:CB	2:D:438:THR:HG22	2.44	0.47
2:D:435:PRO:HD3	2:D:553:ILE:HG23	1.97	0.47
1:E:346:VAL:O	1:E:349:ALA:HB3	2.13	0.47
1:E:384:VAL:HG23	1:E:451:LEU:HD21	1.97	0.47
1:E:53:LEU:HD13	1:E:117:ALA:CA	2.44	0.47
1:G:60:ILE:HD12	1:G:63:ARG:HB3	1.96	0.47
1:I:440:TRP:CG	1:I:441:GLY:N	2.82	0.47
2:J:146:TYR:HE1	2:J:180:ARG:HH11	1.62	0.47
1:K:437:LEU:HD22	1:K:455:LEU:CD2	2.43	0.47
1:K:470:LEU:HA	1:K:473:ILE:HG21	1.93	0.47
1:K:482:ALA:C	1:K:484:LEU:HD12	2.34	0.47
1:K:505:PRO:HB2	1:K:507:HIS:CB	2.40	0.47
1:K:508:PHE:O	1:K:509:TRP:C	2.53	0.47
2:B:178:LEU:HB2	2:L:482:LEU:HD13	1.97	0.47
2:B:518:HIS:ND1	2:B:519:PRO:CD	2.69	0.47
1:C:188:LEU:CG	1:C:228:LEU:HD22	2.43	0.47
1:C:185:ALA:CB	1:C:243:ARG:HB2	2.43	0.47
2:D:240:PHE:CE1	2:D:243:GLY:HA2	2.50	0.47
2:D:526:LEU:C	2:D:528:ASP:N	2.68	0.47
2:F:119:ILE:CG2	2:F:149:THR:HG22	2.45	0.47
2:F:45:ASN:HB3	2:F:321:ILE:O	2.14	0.47
1:G:520:GLU:OE1	1:G:613:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:248:LYS:CG	2:H:254:VAL:HG22	2.44	0.47
1:I:386:LEU:HD21	1:I:467:LEU:HD13	1.96	0.47
2:J:114:VAL:HG11	2:J:146:TYR:CE2	2.49	0.47
2:J:164:ARG:NH1	2:J:296:TRP:CZ2	2.83	0.47
2:J:417:GLY:C	2:J:419:ALA:H	2.16	0.47
2:D:492:ARG:NH2	2:J:74:ARG:NH2	2.53	0.47
1:K:250:LEU:CD1	1:K:324:LEU:HD23	2.44	0.47
1:K:561:ARG:O	1:K:562:ARG:HG2	2.13	0.47
2:L:386:HIS:HD2	2:L:386:HIS:O	1.97	0.47
1:A:263:ASP:OD2	1:A:368:LEU:N	2.38	0.47
1:C:440:TRP:CD1	1:C:441:GLY:N	2.82	0.47
2:D:145:TYR:CE1	2:D:149:THR:HG22	2.50	0.47
2:D:30:ILE:HG22	2:D:31:LEU:N	2.30	0.47
2:D:36:ASN:HB3	2:D:39:SER:HB2	1.97	0.47
2:D:462:LEU:O	2:D:462:LEU:HD23	2.14	0.47
2:D:472:VAL:HG22	2:D:473:MET:CG	2.40	0.47
2:D:164:ARG:HB2	2:D:551:ALA:HB2	1.97	0.47
2:D:92:ASP:HB2	2:D:95:SER:HB2	1.96	0.47
1:E:207:ALA:HB2	1:E:243:ARG:NH1	2.30	0.47
1:E:333:PHE:CD1	1:E:333:PHE:C	2.88	0.47
1:E:287:GLU:HG2	1:E:343:GLU:HG3	1.96	0.47
1:E:451:LEU:HD23	1:E:474:LEU:HD13	1.97	0.47
1:E:561:ARG:HH11	1:E:561:ARG:CG	2.26	0.47
2:F:53:VAL:HG12	2:F:57:ARG:NH1	2.29	0.47
1:G:398:ALA:CB	1:G:464:ARG:HE	2.18	0.47
2:H:339:VAL:HG11	2:H:360:ALA:HB1	1.95	0.47
2:H:491:GLU:C	2:H:493:ALA:H	2.17	0.47
2:H:551:ALA:HA	2:H:552:PRO:HD2	1.67	0.47
1:I:272:ASN:ND2	1:I:377:LEU:HD22	2.29	0.47
1:I:315:TYR:CD1	1:I:316:VAL:N	2.82	0.47
1:I:439:ALA:HB3	1:I:451:LEU:HB2	1.96	0.47
2:J:375:ILE:CD1	2:J:375:ILE:N	2.69	0.47
1:K:322:GLU:OE2	1:K:337:ASN:ND2	2.48	0.47
2:L:444:SER:HB2	2:L:470:ILE:CG1	2.44	0.47
1:A:251:LEU:O	1:A:252:LYS:C	2.52	0.47
2:B:486:LYS:HG2	2:B:505:ILE:CD1	2.44	0.47
1:C:114:ILE:HD12	1:C:147:LEU:HD12	1.94	0.47
2:D:206:ILE:O	2:D:207:PRO:C	2.53	0.47
2:D:237:ALA:O	2:D:238:THR:CG2	2.62	0.47
2:D:350:LEU:HD23	2:D:350:LEU:N	2.14	0.47
2:D:420:LYS:O	2:D:423:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:THR:CG2	1:E:466:ASN:N	2.77	0.47
2:F:219:GLY:C	2:F:221:ALA:N	2.68	0.47
2:F:421:HIS:CE1	2:F:424:LYS:HZ2	2.33	0.47
1:G:136:ALA:O	1:G:137:ASP:C	2.53	0.47
1:G:536:PRO:CA	2:H:363:HIS:HE1	2.28	0.47
1:I:392:GLU:OE2	1:I:498:PRO:O	2.32	0.47
1:I:622:TRP:CD1	1:I:622:TRP:O	2.68	0.47
2:J:311:LEU:HB2	2:J:342:SER:OG	2.14	0.47
2:L:39:SER:OG	2:L:40:ALA:N	2.47	0.47
1:A:135:ASN:O	1:A:136:ALA:C	2.53	0.47
1:A:263:ASP:C	1:A:265:HIS:H	2.17	0.47
1:A:60:ILE:HA	1:A:60:ILE:HD12	1.74	0.47
1:C:525:ARG:NH1	1:C:531:ASP:OD1	2.48	0.47
1:C:544:ARG:NH2	2:D:88:ASN:ND2	2.61	0.47
1:E:148:LEU:CD2	1:E:148:LEU:N	2.78	0.47
1:E:451:LEU:HD23	1:E:474:LEU:CD1	2.44	0.47
1:E:627:LEU:H	1:E:627:LEU:HD12	1.80	0.47
2:F:108:VAL:HG11	2:F:148:LEU:HD11	1.96	0.47
1:G:299:ARG:C	1:G:301:ALA:H	2.17	0.47
2:H:311:LEU:HD12	2:H:341:GLY:O	2.15	0.47
2:H:497:LEU:CD2	2:H:502:GLU:HB2	2.45	0.47
1:I:531:ASP:OD2	2:J:298:LYS:CB	2.63	0.47
1:K:142:CYS:SG	1:K:149:PHE:HD2	2.38	0.47
1:K:263:ASP:N	1:K:263:ASP:OD1	2.47	0.47
1:K:395:PHE:HZ	1:K:469:PHE:CE1	2.33	0.47
1:K:407:GLU:OE1	1:K:416:VAL:HG11	2.15	0.47
2:L:169:TYR:HE2	2:L:208:GLN:HE22	1.63	0.47
2:L:209:ILE:HD11	2:L:290:CYS:HB2	1.97	0.47
2:L:41:GLU:O	2:L:44:ALA:HB3	2.14	0.47
1:A:340:LEU:HD22	1:A:344:HIS:HB3	1.96	0.47
1:A:402:LEU:HD11	1:A:420:VAL:HG21	1.96	0.47
1:A:471:ARG:NH2	1:A:624:GLY:O	2.47	0.47
2:B:344:PHE:CE2	2:B:346:GLU:HG3	2.50	0.47
2:B:388:ILE:O	2:B:392:CYS:HB2	2.15	0.47
1:C:189:GLU:O	1:C:192:ARG:HB3	2.15	0.47
1:C:489:ILE:CG2	1:C:490:ALA:N	2.78	0.47
2:D:409:VAL:HB	2:J:247:VAL:HG22	1.96	0.47
1:E:361:ARG:HH11	1:E:361:ARG:CG	2.26	0.47
1:E:608:ARG:O	1:E:608:ARG:HG3	2.14	0.47
2:F:227:SER:O	2:F:228:ASP:C	2.53	0.47
2:F:333:GLU:O	2:F:337:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:PRO:HD2	1:G:328:ARG:NH2	2.30	0.47
1:G:516:TRP:CE3	1:G:613:ARG:NH2	2.83	0.47
2:H:30:ILE:CD1	2:H:343:GLU:HG2	2.44	0.47
1:I:300:ARG:NH1	1:I:300:ARG:CB	2.62	0.47
1:I:412:PRO:CB	1:I:450:ARG:HH11	2.28	0.47
1:I:545:SER:O	2:J:536:GLN:NE2	2.35	0.47
2:J:393:GLN:HG2	2:J:393:GLN:O	2.15	0.47
1:K:118:LEU:HD22	1:K:147:LEU:HD11	1.97	0.47
1:K:379:GLY:CA	1:K:440:TRP:CH2	2.98	0.47
2:L:157:GLN:NE2	2:L:197:ASN:OD1	2.48	0.47
2:L:302:LEU:CD2	2:L:366:PRO:HG2	2.44	0.47
2:L:373:ASN:HD22	2:L:373:ASN:HA	1.57	0.47
2:L:59:LEU:HD22	2:L:520:TYR:HE1	1.79	0.47
2:L:54:ASN:HA	2:L:57:ARG:CD	2.41	0.47
2:L:74:ARG:HH21	2:L:78:ARG:CZ	2.27	0.47
1:A:526:ASP:OD2	1:A:526:ASP:N	2.34	0.47
1:A:540:ASN:HA	2:B:94:GLY:O	2.16	0.47
2:B:224:PRO:CG	2:B:239:ILE:HD13	2.46	0.47
2:B:430:ALA:HB1	2:L:196:PHE:HD1	1.80	0.47
1:C:203:LEU:CD2	1:C:205:LYS:HZ2	2.26	0.47
1:C:178:VAL:HG22	1:C:332:PHE:CB	2.44	0.47
2:D:354:THR:CG2	2:D:375:ILE:N	2.78	0.47
2:D:470:ILE:CG2	2:D:470:ILE:O	2.63	0.47
2:D:499:VAL:O	2:D:499:VAL:HG12	2.14	0.47
2:D:338:LEU:HD22	2:D:537:THR:HG22	1.97	0.47
1:E:181:TYR:HD1	1:E:182:HIS:H	1.62	0.47
1:E:404:LEU:HD11	1:E:612:LEU:HD13	1.94	0.47
1:E:400:GLY:N	1:E:463:LEU:HD11	2.17	0.47
1:E:508:PHE:HB2	1:E:622:TRP:CZ2	2.49	0.47
2:F:190:HIS:O	2:F:191:PHE:O	2.33	0.47
2:F:392:CYS:SG	2:F:556:THR:HG21	2.54	0.47
2:F:83:VAL:CG1	2:F:84:ARG:N	2.76	0.47
1:G:167:LYS:HB2	1:G:167:LYS:HE3	1.64	0.47
1:G:201:PRO:HD2	1:G:328:ARG:HH22	1.79	0.47
2:H:409:VAL:HG23	2:H:410:GLY:N	2.30	0.47
2:H:50:LEU:C	2:H:50:LEU:HD23	2.35	0.47
1:I:451:LEU:HD12	1:I:454:MET:HE2	1.96	0.47
1:I:620:LEU:C	1:I:620:LEU:HD12	2.36	0.47
2:D:527:TRP:CZ2	2:J:186:PRO:HG3	2.50	0.47
2:J:378:ALA:H	2:J:418:ILE:HD12	1.80	0.47
1:K:103:PRO:O	1:K:108:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:71:LEU:O	1:K:71:LEU:HD23	2.14	0.47
2:L:33:THR:HB	2:L:312:TYR:HE2	1.72	0.47
2:L:354:THR:HG22	2:L:375:ILE:N	2.30	0.47
1:A:269:LEU:HB2	1:A:372:GLN:HE21	1.80	0.46
1:A:67:SER:O	1:A:68:ALA:C	2.53	0.46
2:B:481:VAL:HG13	2:L:245:PRO:HB2	1.97	0.46
1:C:333:PHE:CD1	1:C:333:PHE:C	2.88	0.46
2:D:145:TYR:HB2	2:D:176:ALA:HA	1.97	0.46
2:D:190:HIS:C	2:D:191:PHE:O	2.53	0.46
2:D:330:ASP:OD1	2:D:332:ARG:HG3	2.14	0.46
1:E:271:LEU:HD23	1:E:375:VAL:HG21	1.96	0.46
1:E:339:ARG:CG	1:E:339:ARG:HH11	2.17	0.46
1:E:526:ASP:OD2	1:E:526:ASP:N	2.46	0.46
1:G:395:PHE:HZ	1:G:469:PHE:CE1	2.32	0.46
1:G:411:GLY:N	1:G:414:ARG:HG3	2.30	0.46
2:H:119:ILE:CG2	2:H:119:ILE:O	2.63	0.46
2:H:428:ALA:HA	2:H:558:PHE:CE2	2.50	0.46
2:H:446:GLY:O	2:H:448:GLY:N	2.47	0.46
1:I:402:LEU:HD21	1:I:434:LEU:HD21	1.97	0.46
2:J:413:TYR:O	2:J:418:ILE:HB	2.15	0.46
1:K:346:VAL:HG13	1:K:438:ILE:HG23	1.97	0.46
1:K:463:LEU:HD22	1:K:464:ARG:N	2.23	0.46
1:K:549:ARG:HH21	1:K:571:PRO:CA	2.25	0.46
1:K:590:LEU:CD1	1:K:598:LEU:HD12	2.42	0.46
2:L:98:LEU:HD21	2:L:463:TRP:CZ2	2.49	0.46
1:A:354:ASP:OD1	1:A:357:ALA:HB2	2.15	0.46
1:A:420:VAL:HG23	1:A:421:ARG:N	2.29	0.46
1:A:65:MET:HE1	1:A:77:ALA:HB2	1.96	0.46
2:B:386:HIS:C	2:B:386:HIS:CD2	2.89	0.46
2:B:59:LEU:HD22	2:B:520:TYR:CE1	2.50	0.46
1:C:114:ILE:O	1:C:118:LEU:HB2	2.15	0.46
1:C:251:LEU:HB3	1:C:327:GLU:OE2	2.16	0.46
1:C:260:VAL:CG2	1:C:319:GLY:O	2.64	0.46
1:C:405:TYR:HB3	1:C:422:GLU:CB	2.45	0.46
1:C:384:VAL:HG12	1:C:470:LEU:HD13	1.96	0.46
1:C:506:GLU:O	1:C:507:HIS:C	2.53	0.46
1:C:513:ALA:CB	1:C:564:VAL:HG11	2.46	0.46
1:C:565:ARG:CG	1:C:567:ARG:NH2	2.78	0.46
1:C:620:LEU:HD12	1:C:621:GLU:N	2.31	0.46
2:D:230:THR:HG22	2:D:273:ALA:CA	2.41	0.46
2:D:39:SER:HB3	2:D:42:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:LYS:HG3	1:E:177:LEU:HD21	1.97	0.46
1:G:138:PHE:CD1	1:G:142:CYS:HB2	2.50	0.46
1:G:362:VAL:HG23	1:G:363:ALA:N	2.30	0.46
2:H:354:THR:HG21	2:H:375:ILE:C	2.36	0.46
1:I:302:MET:HB3	1:I:323:PHE:CE2	2.50	0.46
2:J:431:CYS:O	2:J:556:THR:HG23	2.15	0.46
2:J:74:ARG:HG2	2:J:74:ARG:O	2.15	0.46
1:K:251:LEU:HD13	1:K:327:GLU:CB	2.31	0.46
1:K:320:THR:HG21	1:K:341:GLN:HB2	1.96	0.46
1:K:258:ILE:HD13	1:K:323:PHE:CD2	2.50	0.46
1:K:504:LEU:HB3	1:K:505:PRO:HD2	1.97	0.46
1:K:51:ARG:HA	1:K:74:GLY:O	2.15	0.46
2:L:127:GLU:O	2:L:129:VAL:HG23	2.15	0.46
2:L:83:VAL:HG22	2:L:84:ARG:N	2.30	0.46
1:A:607:ARG:HB2	1:A:607:ARG:CZ	2.45	0.46
2:B:159:ILE:CD1	2:B:159:ILE:H	2.28	0.46
1:C:152:PRO:HG3	1:C:315:TYR:CZ	2.50	0.46
1:C:69:ARG:CB	1:C:69:ARG:NH1	2.78	0.46
2:D:373:ASN:HA	2:D:373:ASN:HD22	1.52	0.46
1:E:102:LYS:HB2	1:E:105:ASP:OD1	2.15	0.46
1:E:218:VAL:CG2	1:E:218:VAL:O	2.58	0.46
1:E:221:GLU:HG3	1:E:222:ALA:N	2.31	0.46
2:F:218:ALA:HB1	3:I:801:BTI:H5	1.96	0.46
2:F:368:ALA:HB1	2:F:387:PHE:CE2	2.50	0.46
2:F:421:HIS:CE1	2:F:424:LYS:NZ	2.83	0.46
2:H:366:PRO:O	2:H:397:PRO:HD2	2.14	0.46
2:J:195:PHE:CZ	2:J:222:TYR:HB2	2.51	0.46
2:J:427:THR:HB	2:J:561:PHE:HE2	1.81	0.46
1:K:321:VAL:HA	1:K:336:MET:CG	2.44	0.46
1:K:429:PHE:O	1:K:430:TYR:CD2	2.68	0.46
2:L:234:ARG:HE	2:L:234:ARG:HB2	1.32	0.46
2:L:402:GLN:HE21	2:L:444:SER:CB	2.29	0.46
2:L:338:LEU:HD22	2:L:537:THR:CG2	2.46	0.46
1:A:76:VAL:HG13	1:A:94:ILE:HG22	1.97	0.46
2:B:487:ARG:HA	2:B:497:LEU:HD13	1.98	0.46
1:C:111:ASP:O	1:C:114:ILE:HG22	2.15	0.46
1:C:255:HIS:HA	1:C:324:LEU:HD12	1.98	0.46
1:C:272:ASN:OD1	1:C:377:LEU:HB2	2.16	0.46
1:C:566:LEU:C	1:C:567:ARG:HD3	2.35	0.46
1:C:602:VAL:O	1:C:605:VAL:HG22	2.15	0.46
2:D:248:LYS:HG2	2:D:253:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:MET:C	2:D:30:ILE:N	2.69	0.46
2:D:35:ILE:CD1	2:D:320:VAL:HG22	2.46	0.46
2:D:498:GLY:C	2:D:500:GLU:N	2.69	0.46
2:D:520:TYR:H	2:D:520:TYR:HD2	1.61	0.46
1:E:184:GLU:C	1:E:184:GLU:CD	2.74	0.46
1:E:189:GLU:CA	1:E:189:GLU:OE1	2.61	0.46
1:E:437:LEU:HD22	1:E:455:LEU:CD2	2.45	0.46
1:E:596:ASP:CB	1:E:612:LEU:HD23	2.45	0.46
2:F:304:CYS:HB3	2:F:365:TYR:HD1	1.79	0.46
2:F:351:PHE:CZ	2:F:379:GLU:HG3	2.51	0.46
2:F:506:LYS:HZ3	2:F:506:LYS:HB2	1.81	0.46
2:F:433:ARG:CZ	2:F:554:GLU:HG3	2.45	0.46
1:G:339:ARG:NH1	1:G:341:GLN:OE1	2.47	0.46
2:H:251:THR:OG1	2:H:251:THR:O	2.29	0.46
2:H:72:GLN:O	2:H:75:HIS:HB3	2.15	0.46
1:I:450:ARG:O	1:I:453:ALA:HB3	2.15	0.46
1:I:469:PHE:HD2	1:I:470:LEU:N	2.13	0.46
1:K:163:LYS:HE2	1:K:167:LYS:HZ2	1.80	0.46
1:K:630:GLU:HG3	1:K:631:ALA:N	2.30	0.46
2:L:464:MET:O	2:L:531:VAL:HG13	2.15	0.46
1:A:203:LEU:HG	1:A:204:LEU:H	1.74	0.46
2:B:231:VAL:HG21	2:B:286:ILE:HG21	1.96	0.46
2:B:30:ILE:HG22	2:B:31:LEU:N	2.31	0.46
1:C:414:ARG:NH1	1:C:414:ARG:HG2	2.29	0.46
1:C:87:ARG:O	1:C:90:ALA:HB3	2.16	0.46
1:E:252:LYS:HG3	1:E:485:ASP:HB3	1.98	0.46
1:E:602:VAL:O	1:E:605:VAL:HG22	2.16	0.46
2:D:347:PHE:HA	2:F:275:HIS:CE1	2.50	0.46
2:F:53:VAL:CG1	2:F:57:ARG:HH12	2.27	0.46
1:G:185:ALA:O	1:G:186:GLN:O	2.33	0.46
1:G:258:ILE:O	1:G:320:THR:HA	2.15	0.46
1:G:515:ALA:HB2	1:G:598:LEU:CD2	2.45	0.46
2:H:375:ILE:HG21	2:H:408:MET:HB2	1.96	0.46
2:H:83:VAL:HG12	2:H:84:ARG:N	2.29	0.46
1:I:260:VAL:HG23	1:I:319:GLY:O	2.15	0.46
1:I:525:ARG:HH11	1:I:525:ARG:CG	2.29	0.46
1:I:619:PHE:CE2	1:I:628:ALA:HB2	2.51	0.46
2:J:338:LEU:HD21	2:J:537:THR:HB	1.97	0.46
2:J:81:LEU:CD2	2:J:85:GLU:HB3	2.35	0.46
1:K:389:GLU:O	1:K:390:ASP:HB2	2.14	0.46
1:K:512:ALA:HB1	1:K:629:ILE:CD1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:184:VAL:HG12	2:L:184:VAL:O	2.15	0.46
2:L:53:VAL:CG1	2:L:57:ARG:HD2	2.44	0.46
1:A:427:SER:OG	1:A:428:PRO:CD	2.63	0.46
2:B:123:ILE:HA	2:B:131:CYS:O	2.15	0.46
2:B:137:ASP:CB	2:B:140:VAL:HG23	2.31	0.46
1:E:76:VAL:HA	1:E:94:ILE:O	2.15	0.46
1:E:76:VAL:HG22	1:E:94:ILE:HB	1.97	0.46
1:G:299:ARG:O	1:G:301:ALA:N	2.48	0.46
1:G:304:GLU:CA	1:G:307:VAL:HG12	2.46	0.46
1:G:150:LEU:HD21	1:G:363:ALA:HB2	1.94	0.46
2:H:526:LEU:C	2:H:528:ASP:N	2.68	0.46
1:I:469:PHE:C	1:I:469:PHE:CD2	2.88	0.46
2:J:220:GLY:O	2:J:224:PRO:HD2	2.15	0.46
1:K:262:ALA:O	1:K:316:VAL:O	2.33	0.46
1:K:371:THR:O	1:K:374:GLN:HB2	2.16	0.46
2:L:414:GLU:HA	2:L:418:ILE:CG2	2.46	0.46
2:L:398:LEU:HB2	2:L:436:LYS:HG2	1.98	0.46
2:L:516:GLN:HG2	2:L:521:TYR:CZ	2.51	0.46
1:A:83:ASP:C	1:A:85:HIS:N	2.69	0.46
2:B:201:MET:HG2	2:B:206:ILE:HD12	1.97	0.46
2:B:90:LEU:HG	2:B:90:LEU:O	2.16	0.46
1:C:280:ARG:HD3	1:C:283:GLN:NE2	2.31	0.46
1:C:298:LEU:HG	1:C:298:LEU:O	2.16	0.46
1:C:549:ARG:CG	1:C:549:ARG:NH1	2.78	0.46
2:D:105:ALA:HA	2:D:108:VAL:CG2	2.45	0.46
2:D:199:ALA:HB2	2:D:226:MET:HE2	1.97	0.46
2:D:238:THR:HA	2:D:261:GLY:O	2.15	0.46
2:D:317:LEU:O	2:D:318:TYR:C	2.54	0.46
1:E:132:LEU:HD12	1:E:138:PHE:HD2	1.81	0.46
2:F:105:ALA:HA	2:F:108:VAL:HG21	1.96	0.46
1:G:351:THR:OG1	1:G:352:GLY:N	2.47	0.46
1:G:52:LEU:CD2	1:G:360:ILE:HD11	2.46	0.46
1:G:383:GLU:HG3	1:G:438:ILE:HG12	1.97	0.46
2:H:119:ILE:HG23	2:H:119:ILE:O	2.16	0.46
2:F:513:TYR:CZ	2:H:181:GLN:HG2	2.50	0.46
2:J:100:LEU:O	2:J:101:SER:C	2.54	0.46
2:J:181:GLN:NE2	2:J:182:ASP:N	2.64	0.46
2:D:481:VAL:CG1	2:J:245:PRO:HB2	2.44	0.46
2:J:291:VAL:HG12	2:J:291:VAL:O	2.16	0.46
1:K:290:PRO:HD2	1:K:380:HIS:ND1	2.31	0.46
1:K:465:THR:CG2	1:K:467:LEU:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:270:SER:OG	2:L:271:GLY:N	2.46	0.46
2:L:302:LEU:HD22	2:L:366:PRO:CG	2.46	0.46
2:L:501:GLU:OE2	2:L:501:GLU:N	2.47	0.46
2:L:68:GLY:O	2:L:70:ALA:N	2.48	0.46
1:A:159:ALA:C	1:A:161:GLY:H	2.19	0.46
2:B:275:HIS:HE1	2:F:347:PHE:HA	1.80	0.46
2:B:31:LEU:HD12	2:B:336:ALA:CB	2.46	0.46
2:B:389:GLU:HG2	2:B:558:PHE:HE1	1.81	0.46
1:C:63:ARG:NH1	1:C:63:ARG:HG3	2.30	0.46
2:D:291:VAL:HA	2:D:294:LEU:HG	1.96	0.46
2:D:62:ARG:HG2	2:D:62:ARG:NH1	2.31	0.46
1:E:269:LEU:CB	1:E:372:GLN:NE2	2.78	0.46
2:F:103:LEU:O	2:F:524:ALA:HA	2.15	0.46
2:F:39:SER:OG	2:F:40:ALA:N	2.49	0.46
1:G:96:VAL:HG11	1:G:116:ALA:CB	2.46	0.46
1:G:306:ALA:C	1:G:308:ARG:H	2.19	0.46
1:G:371:THR:O	1:G:372:GLN:C	2.54	0.46
2:H:145:TYR:HB2	2:H:176:ALA:HA	1.98	0.46
2:H:433:ARG:H	2:H:556:THR:CG2	2.23	0.46
1:I:112:ARG:HH11	1:I:112:ARG:HG3	1.80	0.46
1:I:251:LEU:HD11	1:I:328:ARG:CZ	2.45	0.46
1:I:274:ARG:HD3	1:I:346:VAL:HG23	1.98	0.46
1:I:294:LEU:CD1	1:I:299:ARG:NH1	2.79	0.46
2:L:207:PRO:HG2	2:L:294:LEU:CD2	2.39	0.46
2:L:216:CYS:HB3	2:L:238:THR:O	2.16	0.46
2:L:400:PHE:O	2:L:401:LEU:HD23	2.15	0.46
2:L:438:THR:CG2	2:L:462:LEU:HG	2.46	0.46
1:A:47:ARG:CZ	1:A:148:LEU:HD22	2.46	0.46
1:A:713:GLU:O	1:A:714:LEU:O	2.32	0.46
2:B:171:VAL:HG11	2:B:216:CYS:SG	2.56	0.46
2:B:184:VAL:O	2:B:184:VAL:HG12	2.15	0.46
2:B:268:LYS:HB2	2:B:268:LYS:NZ	2.31	0.46
2:B:316:GLU:O	2:B:320:VAL:HG23	2.15	0.46
2:B:377:PHE:N	2:B:377:PHE:CD1	2.84	0.46
1:C:398:ALA:HB2	1:C:464:ARG:HE	1.80	0.46
1:C:570:SER:O	1:C:586:SER:N	2.49	0.46
2:D:317:LEU:CD2	2:D:334:VAL:HG12	2.46	0.46
2:D:83:VAL:HG13	2:D:84:ARG:N	2.29	0.46
1:E:396:LEU:HD12	1:E:464:ARG:HH12	1.81	0.46
1:G:226:GLU:N	1:G:226:GLU:OE1	2.49	0.46
1:G:251:LEU:N	1:G:251:LEU:CD1	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:213:MET:HA	2:H:233:VAL:HG23	1.98	0.46
2:H:227:SER:O	2:H:228:ASP:C	2.54	0.46
2:H:232:MET:HE1	2:H:239:ILE:HG13	1.96	0.46
2:J:155:ARG:HD2	2:J:155:ARG:O	2.16	0.46
2:J:338:LEU:O	2:J:538:ARG:NH1	2.48	0.46
1:K:358:TRP:O	1:K:361:ARG:HB2	2.16	0.46
2:L:191:PHE:HE2	2:L:195:PHE:HZ	1.63	0.46
2:J:390:LEU:CD2	2:L:228:ASP:HB3	2.46	0.46
2:L:376:LEU:HD12	2:L:404:ILE:HD13	1.98	0.46
1:A:653:MET:CG	1:A:654:ASN:H	2.17	0.46
2:B:215:SER:HA	2:B:238:THR:OG1	2.16	0.46
1:C:167:LYS:HG3	1:C:177:LEU:CD2	2.46	0.46
1:C:204:LEU:O	1:C:215:MET:HA	2.15	0.46
1:C:273:GLU:H	1:C:273:GLU:CD	2.17	0.46
1:C:416:VAL:HG23	1:C:454:MET:CE	2.46	0.46
1:C:416:VAL:HG23	1:C:454:MET:HE2	1.98	0.46
1:C:567:ARG:NH1	1:C:567:ARG:HG3	2.29	0.46
2:D:476:GLU:CD	2:D:477:GLN:H	2.19	0.46
1:E:202:VAL:HG21	1:E:246:VAL:HG13	1.98	0.46
1:E:249:TYR:CD2	1:E:250:LEU:N	2.84	0.46
1:E:336:MET:CE	1:E:338:THR:HG22	2.46	0.46
1:E:414:ARG:HD3	1:E:454:MET:HG2	1.97	0.46
2:F:190:HIS:C	2:F:191:PHE:O	2.53	0.46
2:F:487:ARG:NH1	2:F:487:ARG:HB3	2.31	0.46
2:H:223:VAL:O	2:H:227:SER:OG	2.34	0.46
2:H:231:VAL:CG1	2:H:283:ALA:HB1	2.44	0.46
2:H:298:LYS:HG2	2:H:550:ASN:HA	1.97	0.46
2:H:317:LEU:HD23	2:H:337:ARG:HD2	1.98	0.46
2:H:36:ASN:HD21	2:H:38:ARG:CD	2.24	0.46
2:H:400:PHE:CE2	2:H:453:CYS:CB	2.96	0.46
1:I:476:HIS:CD2	1:I:496:LEU:HD21	2.51	0.46
1:I:548:ALA:O	1:I:550:GLU:HG3	2.16	0.46
2:J:170:LEU:HD23	2:J:211:VAL:HG23	1.98	0.46
2:J:498:GLY:C	2:J:500:GLU:H	2.19	0.46
1:K:107:TYR:CB	1:K:131:PHE:CE1	2.99	0.46
1:K:141:ALA:HA	1:K:144:GLU:CD	2.37	0.46
1:K:261:PHE:CZ	1:K:358:TRP:HB3	2.51	0.46
1:K:547:LEU:H	1:K:547:LEU:HG	1.33	0.46
2:L:417:GLY:C	2:L:419:ALA:N	2.68	0.46
1:A:185:ALA:O	1:A:186:GLN:O	2.33	0.45
1:A:187:ASP:C	1:A:189:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:O	1:A:193:ARG:HD3	2.17	0.45
1:A:263:ASP:OD1	1:A:265:HIS:HB2	2.16	0.45
1:A:558:ARG:HE	1:A:627:LEU:HD22	1.81	0.45
1:C:136:ALA:O	1:C:137:ASP:C	2.53	0.45
1:C:396:LEU:O	1:C:398:ALA:N	2.48	0.45
1:C:550:GLU:HG2	1:C:567:ARG:HD2	1.97	0.45
1:C:516:TRP:CZ3	1:C:613:ARG:NH1	2.83	0.45
2:D:247:VAL:HG22	2:D:253:GLU:CD	2.36	0.45
1:E:109:ARG:NH1	1:E:111:ASP:OD2	2.49	0.45
1:E:166:ALA:C	1:E:168:ALA:N	2.69	0.45
1:E:299:ARG:C	1:E:301:ALA:N	2.70	0.45
2:F:144:THR:HG21	4:F:591:COA:C5A	2.46	0.45
2:F:408:MET:HG3	2:F:413:TYR:CD2	2.50	0.45
2:F:449:ASN:ND2	2:F:470:ILE:HD11	2.31	0.45
2:F:456:ALA:HA	2:H:188:ARG:HA	1.97	0.45
2:H:486:LYS:HD2	2:H:489:GLN:HE21	1.81	0.45
1:K:384:VAL:CG1	1:K:470:LEU:HD13	2.46	0.45
2:L:240:PHE:CE1	2:L:243:GLY:CA	3.00	0.45
2:B:188:ARG:H	2:L:455:ARG:HG3	1.80	0.45
2:L:483:ALA:HB2	2:L:505:ILE:HG22	1.97	0.45
1:A:258:ILE:HD12	1:A:306:ALA:HB2	1.98	0.45
1:A:87:ARG:O	1:A:90:ALA:HB3	2.15	0.45
2:B:339:VAL:CG2	2:B:342:SER:HA	2.46	0.45
2:B:348:LYS:O	2:B:383:LYS:HE2	2.16	0.45
2:B:487:ARG:HB3	2:B:497:LEU:CD2	2.36	0.45
1:C:201:PRO:CG	1:C:328:ARG:HH21	2.29	0.45
2:D:518:HIS:CD2	2:D:520:TYR:H	2.33	0.45
1:E:298:LEU:HD21	1:E:325:LEU:CD1	2.46	0.45
1:E:289:ALA:CB	1:E:350:ILE:HD13	2.45	0.45
2:F:125:ARG:HD2	2:F:128:GLY:HA2	1.99	0.45
2:F:491:GLU:C	2:F:493:ALA:N	2.70	0.45
2:F:81:LEU:HD21	2:F:89:ARG:HH22	1.81	0.45
1:G:128:GLY:O	1:G:133:SER:HB3	2.16	0.45
1:G:202:VAL:HG23	1:G:247:GLU:O	2.16	0.45
1:G:416:VAL:HG13	1:G:437:LEU:HD12	1.96	0.45
1:G:543:TRP:CH2	2:H:540:VAL:HG22	2.51	0.45
1:A:654:ASN:O	2:H:251:THR:CG2	2.64	0.45
1:I:358:TRP:CZ2	1:I:369:PRO:HG2	2.51	0.45
2:J:218:ALA:O	2:J:221:ALA:CB	2.64	0.45
2:J:457:TYR:CD2	2:J:457:TYR:N	2.83	0.45
1:K:532:ASP:OD2	2:L:365:TYR:OH	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:232:MET:HE1	2:L:266:HIS:HD2	1.81	0.45
2:L:375:ILE:H	2:L:375:ILE:CD1	2.29	0.45
2:L:491:GLU:C	2:L:493:ALA:H	2.18	0.45
1:A:562:ARG:HH11	1:A:562:ARG:CG	2.29	0.45
2:B:335:ILE:O	2:B:339:VAL:HG22	2.17	0.45
1:E:371:THR:O	1:E:372:GLN:C	2.53	0.45
2:F:526:LEU:C	2:F:528:ASP:N	2.70	0.45
1:G:350:ILE:HD12	1:G:377:LEU:CD1	2.41	0.45
1:G:485:ASP:OD2	1:G:491:ARG:NH2	2.48	0.45
2:H:188:ARG:HG2	2:H:188:ARG:NH1	2.31	0.45
2:H:277:ALA:CB	2:H:283:ALA:HB2	2.46	0.45
2:H:488:GLU:O	2:H:492:ARG:HG2	2.15	0.45
1:I:438:ILE:H	1:I:438:ILE:HD12	1.80	0.45
1:I:452:LEU:HD23	1:I:474:LEU:CB	2.45	0.45
1:I:391:PRO:CD	1:I:465:THR:O	2.65	0.45
1:I:601:ARG:NH1	1:I:601:ARG:HB3	2.25	0.45
2:J:161:LEU:HD13	2:J:201:MET:CG	2.46	0.45
2:J:332:ARG:CG	2:J:332:ARG:NH1	2.75	0.45
1:K:305:ALA:O	1:K:308:ARG:HG3	2.16	0.45
1:K:465:THR:CG2	1:K:466:ASN:N	2.78	0.45
1:K:386:LEU:CD2	1:K:467:LEU:HD13	2.41	0.45
2:L:244:PRO:HD3	2:L:260:LEU:HD23	1.98	0.45
2:L:283:ALA:HA	2:L:286:ILE:HD12	1.99	0.45
1:A:217:VAL:HG21	1:A:249:TYR:CE1	2.52	0.45
1:A:231:ALA:HB3	1:A:244:MET:CE	2.45	0.45
1:A:280:ARG:O	1:A:282:HIS:N	2.49	0.45
1:A:365:GLY:O	1:A:366:GLU:C	2.54	0.45
2:B:375:ILE:N	2:B:375:ILE:HD12	2.31	0.45
1:C:222:ALA:O	1:C:224:LEU:N	2.49	0.45
2:D:449:ASN:ND2	2:D:470:ILE:HD11	2.31	0.45
2:D:437:PHE:CE1	2:D:544:ALA:HB1	2.50	0.45
1:E:51:ARG:NH1	1:E:121:GLY:O	2.50	0.45
1:E:123:GLN:H	1:E:123:GLN:CD	2.19	0.45
1:E:132:LEU:HD22	1:E:132:LEU:N	2.32	0.45
1:E:232:GLN:C	1:E:233:ARG:HG2	2.37	0.45
2:F:385:ALA:O	2:F:389:GLU:HG3	2.16	0.45
2:F:432:ALA:HA	2:F:556:THR:CG2	2.40	0.45
1:G:160:MET:HG3	1:G:336:MET:HB3	1.99	0.45
1:G:249:TYR:CE2	1:G:250:LEU:O	2.70	0.45
1:G:65:MET:HG3	1:G:75:SER:HB2	1.98	0.45
2:H:187:ASP:O	2:H:190:HIS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:417:GLY:O	2:H:419:ALA:N	2.50	0.45
2:H:486:LYS:HG2	2:H:505:ILE:HD11	1.97	0.45
1:I:163:LYS:HG2	1:I:167:LYS:NZ	2.32	0.45
1:I:294:LEU:CD1	1:I:299:ARG:HH12	2.29	0.45
1:I:383:GLU:HB2	1:I:438:ILE:HG23	1.98	0.45
1:I:93:ASP:OD2	1:I:93:ASP:N	2.50	0.45
2:J:189:GLU:OE1	2:J:189:GLU:C	2.55	0.45
2:D:423:ALA:HB1	2:J:226:MET:CG	2.45	0.45
2:J:346:GLU:HG2	2:J:349:ALA:HA	1.97	0.45
2:J:164:ARG:HB3	2:J:551:ALA:HB2	1.98	0.45
2:J:98:LEU:C	2:J:98:LEU:HD12	2.36	0.45
1:K:468:ALA:O	1:K:471:ARG:HB3	2.17	0.45
1:K:89:VAL:O	1:K:89:VAL:HG12	2.16	0.45
2:B:562:ARG:HD2	2:L:225:ALA:O	2.17	0.45
2:L:31:LEU:HD12	2:L:336:ALA:HB2	1.98	0.45
2:L:61:GLY:O	2:L:62:ARG:C	2.54	0.45
1:A:231:ALA:HA	1:A:233:ARG:NH2	2.31	0.45
1:A:431:ASP:OD2	1:A:433:MET:N	2.50	0.45
2:B:385:ALA:O	2:B:389:GLU:HG3	2.16	0.45
2:B:75:HIS:O	2:B:77:ALA:N	2.49	0.45
1:C:345:PRO:HB3	1:C:415:ARG:NH1	2.32	0.45
1:C:616:ARG:HD2	1:C:630:GLU:OE1	2.16	0.45
2:D:221:ALA:O	2:D:224:PRO:HD2	2.16	0.45
2:D:465:TRP:HB3	2:D:467:ASN:HD21	1.80	0.45
1:E:135:ASN:CG	1:E:135:ASN:O	2.55	0.45
1:E:125:ILE:HD11	1:E:147:LEU:HD13	1.97	0.45
1:E:623:GLU:H	1:E:623:GLU:CD	2.18	0.45
2:F:308:ARG:NH2	2:F:343:GLU:HG3	2.31	0.45
2:F:445:PHE:HA	2:F:471:GLY:O	2.16	0.45
1:G:277:SER:HB3	1:G:485:ASP:O	2.16	0.45
1:G:156:ALA:HB1	1:G:313:ILE:HD12	1.97	0.45
1:G:354:ASP:HB3	1:G:357:ALA:HB3	1.98	0.45
2:H:179:PRO:HD2	4:H:591:COA:H2A	1.97	0.45
2:H:83:VAL:HG13	2:H:84:ARG:N	2.31	0.45
1:I:343:GLU:H	1:I:343:GLU:CD	2.19	0.45
2:J:109:TYR:HE1	2:J:148:LEU:HD12	1.82	0.45
2:J:317:LEU:O	2:J:318:TYR:C	2.55	0.45
2:J:45:ASN:HB3	2:J:321:ILE:O	2.16	0.45
2:J:368:ALA:HB1	2:J:387:PHE:CZ	2.52	0.45
1:K:408:ALA:H	1:K:458:THR:HG22	1.82	0.45
2:L:412:LYS:HG3	2:L:412:LYS:H	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:498:GLY:C	2:L:500:GLU:N	2.70	0.45
1:A:152:PRO:HA	1:A:316:VAL:HG23	1.98	0.45
1:A:271:LEU:O	1:A:272:ASN:CB	2.65	0.45
1:A:659:ARG:HG3	1:A:676:VAL:CG2	2.47	0.45
2:B:178:LEU:HG	4:B:591:COA:H61A	1.81	0.45
2:B:469:ARG:NH2	2:B:519:PRO:CD	2.80	0.45
2:B:472:VAL:CG1	2:L:181:GLN:HG2	2.47	0.45
2:B:500:GLU:N	2:B:500:GLU:OE2	2.48	0.45
1:C:102:LYS:O	1:C:106:SER:OG	2.26	0.45
1:C:403:MET:HE3	1:C:462:GLY:HA3	1.99	0.45
2:D:199:ALA:HB2	2:D:226:MET:CE	2.46	0.45
2:D:324:ASP:O	2:D:325:SER:C	2.54	0.45
1:E:229:SER:C	1:E:231:ALA:H	2.20	0.45
1:E:322:GLU:OE2	1:E:337:ASN:ND2	2.50	0.45
2:F:100:LEU:HD13	2:F:159:ILE:CD1	2.45	0.45
2:F:321:ILE:O	2:F:321:ILE:HG22	2.17	0.45
2:F:438:THR:O	2:F:462:LEU:HA	2.16	0.45
1:G:198:ILE:HG23	1:G:248:LYS:HG2	1.98	0.45
1:G:452:LEU:CD2	1:G:474:LEU:CB	2.93	0.45
1:G:516:TRP:CG	1:G:555:LEU:HD21	2.52	0.45
1:G:605:VAL:HG12	1:I:96:VAL:CG1	2.26	0.45
2:H:83:VAL:CG2	2:H:136:ASN:O	2.65	0.45
2:H:154:LEU:HD23	2:H:157:GLN:HE21	1.81	0.45
2:H:402:GLN:HE22	2:H:449:ASN:HA	1.78	0.45
1:I:346:VAL:CG1	1:I:383:GLU:HB2	2.46	0.45
1:I:343:GLU:O	1:I:346:VAL:HG22	2.17	0.45
2:J:378:ALA:H	2:J:418:ILE:CD1	2.30	0.45
1:K:392:GLU:O	1:K:394:ASP:N	2.50	0.45
1:K:516:TRP:HZ3	1:K:630:GLU:HA	1.82	0.45
1:A:50:GLN:NE2	1:A:123:GLN:HE21	2.15	0.45
1:A:677:LEU:CD2	1:A:711:LEU:HD11	2.47	0.45
2:B:497:LEU:HA	2:B:501:GLU:OE2	2.17	0.45
2:B:470:ILE:O	2:B:517:GLY:HA2	2.17	0.45
1:C:110:GLY:O	1:C:114:ILE:HG22	2.17	0.45
1:C:132:LEU:HD22	1:C:132:LEU:N	2.31	0.45
1:C:504:LEU:O	1:C:505:PRO:O	2.34	0.45
1:C:605:VAL:HG12	1:E:96:VAL:HG12	1.98	0.45
2:D:456:ALA:C	2:D:457:TYR:HD2	2.20	0.45
2:D:72:GLN:O	2:D:75:HIS:HB3	2.17	0.45
1:E:126:HIS:NE2	1:E:359:GLN:OE1	2.49	0.45
1:E:387:TYR:HB3	1:E:389:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:303:GLN:HA	2:F:303:GLN:OE1	2.16	0.45
2:F:507:ALA:HB3	2:F:508:PRO:CD	2.46	0.45
1:G:270:TYR:H	1:G:372:GLN:NE2	2.12	0.45
1:G:356:VAL:HA	1:G:359:GLN:OE1	2.17	0.45
1:G:67:SER:O	1:G:71:LEU:CD1	2.65	0.45
2:H:145:TYR:CE1	2:H:149:THR:HG22	2.52	0.45
2:H:446:GLY:C	2:H:448:GLY:N	2.70	0.45
2:D:389:GLU:CD	2:H:561:PHE:H	2.20	0.45
1:I:343:GLU:C	1:I:345:PRO:CD	2.85	0.45
1:I:376:PRO:O	1:I:377:LEU:HB2	2.17	0.45
1:I:589:ARG:HG2	1:I:590:LEU:N	2.32	0.45
2:L:74:ARG:HE	2:L:78:ARG:HH12	1.64	0.45
1:A:534:HIS:O	2:B:363:HIS:CE1	2.69	0.45
1:A:656:SER:O	1:A:678:GLU:HG3	2.17	0.45
1:A:659:ARG:HG3	1:A:659:ARG:O	2.16	0.45
2:B:248:LYS:HG3	2:B:254:VAL:HG22	1.97	0.45
2:B:277:ALA:HB2	2:B:286:ILE:CD1	2.44	0.45
1:C:375:VAL:HA	1:C:376:PRO:HD2	1.76	0.45
1:C:441:GLY:HA3	1:C:446:GLU:HB3	1.99	0.45
1:C:561:ARG:NH1	1:C:632:VAL:CG2	2.79	0.45
2:D:255:VAL:HG22	2:D:256:SER:N	2.32	0.45
2:D:320:VAL:O	2:D:322:PRO:HD3	2.17	0.45
2:D:507:ALA:N	2:D:508:PRO:CD	2.76	0.45
2:D:507:ALA:HB3	2:D:508:PRO:CD	2.47	0.45
1:E:134:GLU:O	1:E:135:ASN:HB3	2.16	0.45
1:E:164:SER:OG	1:E:165:ALA:N	2.50	0.45
1:E:360:ILE:O	1:E:364:ARG:HG3	2.17	0.45
2:F:252:GLY:O	2:F:253:GLU:O	2.34	0.45
2:F:242:ALA:O	2:F:260:LEU:HD21	2.17	0.45
2:F:528:ASP:C	2:F:530:GLY:H	2.21	0.45
1:G:307:VAL:O	1:G:310:ALA:HB3	2.17	0.45
1:G:306:ALA:O	1:G:308:ARG:N	2.49	0.45
1:G:170:MET:CE	1:G:309:ALA:HB1	2.47	0.45
2:H:161:LEU:HD13	2:H:206:ILE:CD1	2.47	0.45
2:H:331:VAL:O	2:H:331:VAL:HG22	2.16	0.45
2:H:29:ALA:O	2:H:343:GLU:HA	2.17	0.45
4:H:591:COA:H122	4:H:591:COA:O1A	2.17	0.45
1:I:108:LEU:HA	1:I:132:LEU:CD1	2.47	0.45
1:I:135:ASN:CG	1:I:135:ASN:O	2.55	0.45
1:I:153:PRO:O	1:I:154:ALA:C	2.55	0.45
1:I:280:ARG:NH1	1:I:283:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:299:ARG:HH11	1:I:299:ARG:HG3	1.81	0.45
2:J:144:THR:HG22	2:J:175:GLY:H	1.82	0.45
2:J:231:VAL:HG21	2:J:286:ILE:HG22	1.99	0.45
2:J:472:VAL:O	2:J:472:VAL:HG22	2.17	0.45
2:J:433:ARG:HB3	2:J:554:GLU:HB2	1.99	0.45
1:K:497:LEU:N	1:K:498:PRO:CD	2.80	0.45
1:K:549:ARG:NH2	1:K:571:PRO:HB3	2.32	0.45
1:A:123:GLN:OE1	1:A:123:GLN:N	2.49	0.45
1:C:298:LEU:HD21	1:C:325:LEU:CD1	2.47	0.45
1:C:416:VAL:HG22	1:C:437:LEU:HA	1.98	0.45
1:C:452:LEU:CD2	1:C:474:LEU:CB	2.95	0.45
1:E:252:LYS:HB3	1:E:327:GLU:HG3	1.98	0.45
2:F:100:LEU:HD13	2:F:159:ILE:HD12	1.99	0.45
2:F:527:TRP:CZ3	2:H:186:PRO:HG3	2.52	0.45
2:F:533:ASP:O	2:F:534:PRO:C	2.54	0.45
2:F:89:ARG:HG3	2:F:89:ARG:NH2	2.31	0.45
1:G:275:ASP:OD1	1:G:484:LEU:HD22	2.17	0.45
1:G:306:ALA:C	1:G:308:ARG:N	2.69	0.45
1:G:558:ARG:HB3	1:G:559:ASP:H	1.42	0.45
1:G:612:LEU:O	1:G:612:LEU:CD1	2.64	0.45
1:I:412:PRO:HB3	1:I:450:ARG:NH1	2.32	0.45
1:I:455:LEU:HD23	1:I:467:LEU:HD11	1.99	0.45
1:I:519:SER:HB2	1:I:613:ARG:NE	2.20	0.45
1:K:344:HIS:N	1:K:345:PRO:CD	2.80	0.45
1:K:384:VAL:CG2	1:K:451:LEU:HD21	2.43	0.45
2:L:223:VAL:N	2:L:224:PRO:HD2	2.32	0.45
2:L:424:LYS:NZ	2:L:563:MET:HA	2.31	0.45
2:L:83:VAL:O	2:L:87:ILE:HD13	2.17	0.45
1:A:396:LEU:O	1:A:398:ALA:N	2.50	0.45
1:A:675:VAL:HG21	1:A:699:CYS:SG	2.56	0.45
2:B:562:ARG:NH1	2:B:562:ARG:HG3	2.31	0.45
1:C:473:ILE:CA	1:C:496:LEU:HD21	2.47	0.45
1:C:66:ARG:HH11	1:C:66:ARG:HB2	1.82	0.45
1:C:69:ARG:CZ	1:C:69:ARG:HB2	2.46	0.45
2:D:227:SER:O	2:D:228:ASP:C	2.56	0.45
2:D:331:VAL:C	2:D:333:GLU:N	2.71	0.45
2:D:348:LYS:O	2:D:383:LYS:HE3	2.17	0.45
2:D:409:VAL:O	2:D:413:TYR:HD2	2.00	0.45
1:E:339:ARG:CG	1:E:339:ARG:NH1	2.79	0.45
1:E:601:ARG:HE	1:E:601:ARG:HB3	1.52	0.45
2:F:168:ILE:HG23	2:F:209:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:324:ASP:CG	2:F:327:GLN:HB2	2.38	0.45
1:G:232:GLN:CG	1:G:233:ARG:NH1	2.75	0.45
1:G:274:ARG:HD3	1:G:347:THR:OG1	2.17	0.45
1:G:340:LEU:HD22	1:G:344:HIS:HB3	1.99	0.45
2:H:464:MET:O	2:H:531:VAL:HA	2.17	0.45
2:H:562:ARG:HH11	2:H:562:ARG:HG3	1.81	0.45
1:I:500:PRO:O	1:I:501:GLN:HB3	2.17	0.45
2:J:121:ALA:HB1	2:J:134:VAL:HG12	1.98	0.45
2:D:456:ALA:HA	2:J:188:ARG:HA	1.99	0.45
2:J:371:ALA:CB	2:J:401:LEU:HB2	2.47	0.45
1:K:382:ILE:HD12	1:K:448:ARG:N	2.32	0.45
1:K:548:ALA:HB1	1:K:568:HIS:O	2.17	0.45
2:L:312:TYR:O	2:L:313:PRO:C	2.55	0.45
2:L:549:LEU:CD2	2:L:553:ILE:HD11	2.47	0.45
2:L:549:LEU:HD23	2:L:553:ILE:HD11	1.99	0.45
1:A:607:ARG:NH1	1:A:607:ARG:HB3	2.32	0.44
2:B:465:TRP:CB	2:B:467:ASN:HD21	2.28	0.44
1:A:537:TRP:CZ2	2:B:543:LEU:HD22	2.52	0.44
2:B:367:ILE:HG21	2:B:545:LEU:HD11	1.98	0.44
1:C:612:LEU:HD12	1:C:612:LEU:O	2.17	0.44
2:D:345:ASP:OD2	2:D:345:ASP:N	2.49	0.44
2:D:487:ARG:HB2	2:D:497:LEU:HD22	1.99	0.44
2:F:35:ILE:O	2:F:37:PRO:HD3	2.17	0.44
2:F:414:GLU:OE2	2:H:240:PHE:HA	2.17	0.44
1:G:309:ALA:O	1:G:312:ALA:HB3	2.17	0.44
2:H:186:PRO:O	2:H:187:ASP:O	2.36	0.44
2:H:238:THR:HA	2:H:261:GLY:O	2.17	0.44
1:I:342:VAL:HG21	1:I:385:ARG:NH2	2.32	0.44
2:J:167:CYS:HB3	2:J:169:TYR:CE2	2.52	0.44
2:J:220:GLY:HA2	2:J:223:VAL:HG23	1.99	0.44
1:K:516:TRP:CH2	1:K:631:ALA:HB2	2.52	0.44
2:L:347:PHE:CE2	2:L:348:LYS:CG	3.00	0.44
2:L:75:HIS:NE2	2:L:80:LYS:HE2	2.32	0.44
1:A:649:LEU:HD11	1:A:689:PRO:CG	2.45	0.44
1:A:651:ALA:H	1:A:711:LEU:HD12	1.82	0.44
2:B:191:PHE:CD2	2:B:192:GLY:N	2.83	0.44
2:B:320:VAL:HG11	2:B:333:GLU:HB3	1.98	0.44
2:B:464:MET:HE2	2:B:519:PRO:HG3	2.00	0.44
2:B:534:PRO:O	2:B:537:THR:OG1	2.35	0.44
2:D:470:ILE:O	2:D:470:ILE:HG23	2.17	0.44
2:D:476:GLU:CD	2:D:476:GLU:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:HIS:O	2:F:108:VAL:HG23	2.17	0.44
2:F:130:GLU:N	2:F:130:GLU:OE2	2.42	0.44
1:G:450:ARG:O	1:G:453:ALA:HB3	2.17	0.44
1:G:497:LEU:N	1:G:498:PRO:CD	2.78	0.44
1:G:533:PRO:HD2	1:G:534:HIS:CD2	2.52	0.44
1:G:566:LEU:C	1:G:567:ARG:HD3	2.38	0.44
1:G:76:VAL:HA	1:G:94:ILE:O	2.17	0.44
1:I:416:VAL:HG22	1:I:437:LEU:HA	1.99	0.44
1:I:448:ARG:HG2	1:I:474:LEU:HD22	1.99	0.44
2:J:219:GLY:C	2:J:221:ALA:H	2.21	0.44
2:D:188:ARG:HG3	2:J:455:ARG:O	2.17	0.44
2:J:481:VAL:HA	2:J:484:GLN:HB3	1.98	0.44
2:J:497:LEU:HG	2:J:501:GLU:HB2	1.99	0.44
2:J:464:MET:HE1	2:J:519:PRO:HA	1.99	0.44
1:K:175:VAL:O	1:K:177:LEU:HD23	2.17	0.44
1:K:348:GLU:HG2	1:K:353:LEU:O	2.17	0.44
2:L:56:LEU:HD11	2:L:60:LEU:HD11	1.98	0.44
1:A:346:VAL:HG23	1:A:347:THR:N	2.32	0.44
1:A:263:ASP:OD2	1:A:368:LEU:HG	2.17	0.44
1:A:470:LEU:CA	1:A:473:ILE:HG22	2.42	0.44
1:A:650:SER:HB2	1:A:711:LEU:H	1.82	0.44
2:B:403:ASN:CG	2:B:442:GLY:HA3	2.38	0.44
1:C:281:ARG:NH2	1:C:395:PHE:HD2	2.16	0.44
2:D:386:HIS:CD2	2:D:386:HIS:O	2.71	0.44
2:D:433:ARG:HH11	2:D:433:ARG:CG	2.27	0.44
2:D:89:ARG:CG	2:D:89:ARG:HH21	2.26	0.44
1:E:371:THR:HG23	1:E:374:GLN:HG3	1.98	0.44
2:F:332:ARG:HG3	2:F:332:ARG:HH11	1.81	0.44
2:F:417:GLY:O	2:F:419:ALA:N	2.50	0.44
1:G:104:ALA:HA	1:G:108:LEU:CD1	2.47	0.44
1:G:139:ALA:HA	1:G:142:CYS:HB3	1.99	0.44
1:G:71:LEU:HB3	1:G:73:ILE:HD12	2.00	0.44
2:H:513:TYR:CD1	2:H:513:TYR:N	2.85	0.44
1:I:440:TRP:CD1	1:I:441:GLY:N	2.85	0.44
1:K:294:LEU:HB2	1:K:298:LEU:HD22	1.98	0.44
1:K:437:LEU:N	1:K:437:LEU:HD12	2.33	0.44
1:K:47:ARG:HG2	1:K:148:LEU:HD11	1.99	0.44
2:L:402:GLN:NE2	2:L:449:ASN:HD22	2.15	0.44
1:A:299:ARG:C	1:A:301:ALA:H	2.21	0.44
1:A:306:ALA:HB1	1:A:321:VAL:CG2	2.46	0.44
2:B:180:ARG:HG3	2:B:180:ARG:HH11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:ALA:O	2:B:289:ARG:HG2	2.16	0.44
2:B:324:ASP:O	2:B:325:SER:C	2.56	0.44
2:D:161:LEU:HB2	2:D:201:MET:CE	2.46	0.44
1:E:107:TYR:CB	1:E:131:PHE:CD2	3.00	0.44
1:E:201:PRO:CD	1:E:328:ARG:HH21	2.30	0.44
2:F:446:GLY:O	2:F:447:ALA:C	2.53	0.44
2:F:365:TYR:CB	2:F:545:LEU:HD13	2.47	0.44
1:G:114:ILE:HD12	1:G:147:LEU:HD13	1.98	0.44
1:G:466:ASN:O	1:G:469:PHE:HB3	2.16	0.44
1:G:547:LEU:HD11	2:H:64:HIS:CE1	2.51	0.44
1:G:60:ILE:HD12	1:G:60:ILE:O	2.16	0.44
2:H:81:LEU:HD23	2:H:82:LEU:N	2.31	0.44
1:I:287:GLU:HG2	1:I:343:GLU:HG3	2.00	0.44
1:I:445:GLU:HB3	1:I:448:ARG:HH21	1.83	0.44
1:I:605:VAL:CG2	1:I:605:VAL:O	2.63	0.44
2:J:362:LEU:HD21	2:J:538:ARG:HG2	1.99	0.44
1:K:412:PRO:HB3	1:K:450:ARG:HH11	1.83	0.44
2:L:125:ARG:HD2	2:L:128:GLY:HA2	1.99	0.44
1:A:188:LEU:HD23	1:A:228:LEU:CD2	2.39	0.44
1:A:358:TRP:HH2	1:A:370:LEU:HD12	1.81	0.44
1:A:413:GLY:N	1:A:450:ARG:HH11	2.15	0.44
1:A:388:ALA:HB2	1:A:434:LEU:HD11	2.00	0.44
1:A:705:VAL:HG12	1:A:709:THR:HG21	2.00	0.44
2:B:186:PRO:HG3	2:L:527:TRP:CH2	2.52	0.44
2:B:246:LEU:HD12	2:B:246:LEU:H	1.82	0.44
2:B:507:ALA:HB3	2:B:508:PRO:CD	2.47	0.44
2:D:303:GLN:NE2	2:F:297:ARG:HD2	2.33	0.44
2:D:378:ALA:HB3	2:D:379:GLU:OE1	2.18	0.44
2:D:396:ILE:O	2:D:434:VAL:HG21	2.18	0.44
1:E:105:ASP:O	1:E:109:ARG:HD2	2.17	0.44
1:E:170:MET:SD	1:E:309:ALA:CB	3.03	0.44
1:E:289:ALA:O	1:E:350:ILE:HG21	2.16	0.44
1:E:389:GLU:O	1:E:390:ASP:HB2	2.17	0.44
1:E:470:LEU:HA	1:E:473:ILE:HG23	1.98	0.44
2:F:234:ARG:HD2	2:F:276:TYR:OH	2.17	0.44
1:G:201:PRO:CB	1:G:251:LEU:HD11	2.47	0.44
1:G:261:PHE:O	1:G:368:LEU:HD21	2.16	0.44
1:G:607:ARG:HB2	1:G:607:ARG:CZ	2.47	0.44
2:H:307:PRO:HB3	2:H:363:HIS:CD2	2.38	0.44
2:H:348:LYS:O	2:H:383:LYS:HE3	2.17	0.44
1:I:112:ARG:HG3	1:I:112:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:TYR:H	1:I:372:GLN:NE2	2.12	0.44
1:I:294:LEU:O	1:I:294:LEU:HD12	2.17	0.44
1:I:320:THR:O	1:I:336:MET:HG2	2.18	0.44
1:I:371:THR:O	1:I:374:GLN:HB2	2.17	0.44
1:I:446:GLU:HG2	1:I:450:ARG:HH21	1.82	0.44
1:I:278:ILE:CG2	1:I:473:ILE:HD11	2.42	0.44
1:I:546:ALA:HB3	2:J:60:LEU:CD1	2.48	0.44
1:I:596:ASP:HB3	1:I:612:LEU:HG	2.00	0.44
1:I:516:TRP:CD2	1:I:613:ARG:NH2	2.85	0.44
2:J:157:GLN:OE1	2:J:194:ILE:HG23	2.17	0.44
2:J:220:GLY:O	2:J:223:VAL:HG23	2.17	0.44
2:J:351:PHE:O	2:J:352:GLY:C	2.54	0.44
2:J:484:GLN:CA	2:J:484:GLN:NE2	2.75	0.44
2:J:486:LYS:CG	2:J:497:LEU:HD22	2.48	0.44
1:K:135:ASN:HB2	1:K:137:ASP:OD1	2.17	0.44
1:K:85:HIS:NE2	1:K:424:ASP:OD1	2.50	0.44
1:K:588:TYR:N	1:K:588:TYR:HD1	2.14	0.44
2:L:316:GLU:CB	2:L:337:ARG:HE	2.31	0.44
2:L:518:HIS:O	2:L:521:TYR:N	2.51	0.44
2:L:525:ARG:CG	2:L:525:ARG:NH1	2.75	0.44
1:A:500:PRO:O	1:A:501:GLN:HB3	2.17	0.44
1:A:81:ASP:HB3	1:A:100:GLY:C	2.37	0.44
2:B:489:GLN:HA	2:B:492:ARG:HE	1.82	0.44
2:B:498:GLY:C	2:B:500:GLU:N	2.71	0.44
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.69	0.44
2:B:28:MET:HG2	1:C:633:ASP:OD2	2.17	0.44
2:D:176:ALA:H	4:D:591:COA:H21	1.81	0.44
2:D:289:ARG:O	2:D:293:ASN:ND2	2.51	0.44
2:D:300:GLY:O	2:D:301:GLN:CB	2.66	0.44
1:E:396:LEU:HD12	1:E:464:ARG:NH1	2.33	0.44
1:E:421:ARG:O	1:E:422:GLU:C	2.55	0.44
1:E:598:LEU:C	1:E:598:LEU:HD12	2.38	0.44
2:F:373:ASN:HD22	2:F:373:ASN:HA	1.43	0.44
1:G:191:PHE:CE2	1:G:228:LEU:HD13	2.53	0.44
1:G:217:VAL:HG21	1:G:249:TYR:CD1	2.53	0.44
1:G:200:TYR:OH	1:G:224:LEU:CD2	2.65	0.44
1:G:518:GLN:HB2	1:G:590:LEU:HD23	2.00	0.44
1:G:59:GLU:HB3	1:G:419:GLY:N	2.32	0.44
2:H:499:VAL:O	2:H:499:VAL:HG12	2.18	0.44
1:I:536:PRO:HD3	2:J:363:HIS:CD2	2.53	0.44
1:K:289:ALA:HB1	1:K:350:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:270:SER:OG	2:L:272:VAL:HG23	2.18	0.44
2:L:286:ILE:O	2:L:289:ARG:HB2	2.17	0.44
2:L:365:TYR:HB2	2:L:545:LEU:CD1	2.42	0.44
2:L:455:ARG:HD3	2:L:455:ARG:HA	1.77	0.44
2:L:516:GLN:HA	2:L:521:TYR:CD2	2.53	0.44
1:A:202:VAL:HA	1:A:249:TYR:H	1.83	0.44
1:A:261:PHE:CE1	1:A:358:TRP:HB3	2.53	0.44
1:A:470:LEU:O	1:A:471:ARG:C	2.55	0.44
2:B:102:ALA:C	2:B:104:ALA:H	2.20	0.44
2:B:311:LEU:HB2	2:B:312:TYR:CE1	2.53	0.44
2:B:546:SER:HA	2:B:549:LEU:HD12	2.00	0.44
1:C:202:VAL:HA	1:C:249:TYR:H	1.82	0.44
1:C:345:PRO:HB3	1:C:438:ILE:HD13	1.99	0.44
1:C:342:VAL:HG11	1:C:385:ARG:NH2	2.33	0.44
1:C:60:ILE:O	1:C:63:ARG:HB3	2.17	0.44
2:D:108:VAL:HG11	2:D:148:LEU:HD11	1.98	0.44
2:D:170:LEU:HD23	2:D:211:VAL:CG2	2.47	0.44
2:D:234:ARG:HA	2:D:263:ALA:HB3	1.98	0.44
4:D:591:COA:H62A	4:D:591:COA:H62	1.83	0.44
1:E:205:LYS:HB3	1:E:206:ALA:H	1.61	0.44
1:E:47:ARG:CG	1:E:48:SER:N	2.77	0.44
1:E:500:PRO:O	1:E:501:GLN:CB	2.65	0.44
1:E:54:VAL:HG13	1:E:64:VAL:HG11	2.00	0.44
1:E:603:ASP:O	1:E:605:VAL:HG13	2.17	0.44
1:G:451:LEU:HD23	1:G:474:LEU:HD21	2.00	0.44
2:H:161:LEU:HD12	2:H:161:LEU:C	2.38	0.44
2:H:435:PRO:HG3	2:H:460:ARG:NH2	2.33	0.44
2:H:401:LEU:HD23	2:H:439:VAL:HB	2.00	0.44
1:I:47:ARG:NH2	1:I:148:LEU:HD22	2.33	0.44
1:I:473:ILE:O	1:I:473:ILE:HG12	2.17	0.44
2:J:140:VAL:O	2:J:141:LYS:C	2.55	0.44
2:J:53:VAL:HG12	2:J:57:ARG:NH1	2.33	0.44
1:K:114:ILE:HD13	1:K:138:PHE:CE2	2.52	0.44
1:K:296:ALA:O	1:K:299:ARG:HB3	2.18	0.44
1:K:396:LEU:HB2	1:K:464:ARG:NH2	2.33	0.44
1:K:78:VAL:HG12	1:K:96:VAL:HG23	1.99	0.44
2:L:169:TYR:N	2:L:169:TYR:CD2	2.85	0.44
2:L:169:TYR:N	2:L:169:TYR:HD2	2.15	0.44
2:L:209:ILE:HG22	2:L:209:ILE:O	2.18	0.44
2:L:338:LEU:O	2:L:538:ARG:NH1	2.51	0.44
1:A:127:PRO:HB2	1:A:133:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLY:O	1:A:523:HIS:HB2	2.18	0.44
1:A:586:SER:HB2	1:A:587:GLN:H	1.52	0.44
1:C:152:PRO:HD2	1:C:157:ILE:HD11	1.99	0.44
1:C:306:ALA:HB1	1:C:321:VAL:HG21	2.00	0.44
1:C:415:ARG:HD3	1:C:438:ILE:HD12	2.00	0.44
1:C:416:VAL:HG22	1:C:437:LEU:CD1	2.47	0.44
1:C:497:LEU:N	1:C:498:PRO:CD	2.81	0.44
1:C:49:ILE:CD1	1:C:49:ILE:N	2.72	0.44
2:D:101:SER:CB	2:D:526:LEU:HD23	2.47	0.44
2:D:100:LEU:O	2:D:101:SER:C	2.55	0.44
2:D:521:TYR:CE1	2:D:525:ARG:NH1	2.86	0.44
2:D:536:GLN:O	2:D:537:THR:C	2.55	0.44
2:D:549:LEU:HD23	2:D:549:LEU:HA	1.73	0.44
1:E:186:GLN:NE2	1:E:189:GLU:HB2	2.33	0.44
1:E:320:THR:OG1	1:E:341:GLN:HG3	2.16	0.44
2:F:301:GLN:HA	2:F:301:GLN:NE2	2.32	0.44
2:F:311:LEU:HG	2:F:342:SER:CB	2.45	0.44
2:F:402:GLN:OE1	2:F:452:MET:HB2	2.18	0.44
2:F:491:GLU:HA	2:F:495:GLN:O	2.17	0.44
2:F:106:HIS:HB3	2:F:524:ALA:HB2	1.99	0.44
1:G:232:GLN:HB2	1:G:233:ARG:H	1.66	0.44
1:G:525:ARG:HB3	1:G:531:ASP:OD1	2.18	0.44
1:G:550:GLU:HG2	1:G:567:ARG:CZ	2.48	0.44
1:I:135:ASN:O	1:I:136:ALA:C	2.56	0.44
1:I:166:ALA:C	1:I:168:ALA:N	2.69	0.44
1:I:171:GLU:HB2	1:I:177:LEU:HD11	2.00	0.44
1:I:320:THR:HG21	1:I:341:GLN:HB2	1.99	0.44
2:J:220:GLY:HA2	2:J:223:VAL:CG2	2.48	0.44
2:J:42:PHE:CE1	2:J:319:GLY:HA3	2.51	0.44
2:J:329:TYR:OH	2:J:441:ILE:CD1	2.66	0.44
2:J:469:ARG:CG	2:J:469:ARG:HH21	2.12	0.44
1:K:333:PHE:CD1	1:K:333:PHE:C	2.91	0.44
1:K:340:LEU:CD1	1:K:359:GLN:HE22	2.31	0.44
2:L:344:PHE:CZ	2:L:358:GLY:HA3	2.52	0.44
1:A:451:LEU:CD2	1:A:474:LEU:HD11	2.48	0.44
1:A:700:SER:O	1:A:701:GLU:C	2.56	0.44
2:B:191:PHE:HA	2:B:194:ILE:HD13	2.00	0.44
2:B:242:ALA:O	2:B:260:LEU:HD21	2.18	0.44
2:B:294:LEU:HA	2:B:294:LEU:HD23	1.55	0.44
2:B:393:GLN:HB3	2:B:393:GLN:HE21	1.59	0.44
1:C:253:PRO:HG2	1:C:486:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:PRO:HD2	1:E:248:LYS:CB	2.48	0.44
1:G:127:PRO:HB2	1:G:133:SER:HA	2.00	0.44
1:G:217:VAL:CG2	1:G:249:TYR:CD1	3.01	0.44
1:G:251:LEU:N	1:G:251:LEU:HD12	2.33	0.44
1:G:273:GLU:N	1:G:273:GLU:OE1	2.51	0.44
1:G:440:TRP:CD1	1:G:441:GLY:N	2.86	0.44
1:G:414:ARG:CB	1:G:454:MET:SD	3.06	0.44
1:G:612:LEU:HD12	1:G:612:LEU:H	1.83	0.44
1:I:126:HIS:HE2	1:I:356:VAL:HG22	1.83	0.44
1:I:336:MET:CE	1:I:338:THR:HG23	2.47	0.44
2:J:239:ILE:O	2:J:266:HIS:NE2	2.51	0.44
2:J:321:ILE:HA	2:J:321:ILE:HD13	1.83	0.44
1:K:114:ILE:O	1:K:118:LEU:HD23	2.18	0.44
2:L:140:VAL:O	2:L:141:LYS:C	2.56	0.44
2:L:250:ALA:O	2:L:252:GLY:N	2.51	0.44
2:L:74:ARG:NH2	2:L:78:ARG:NH1	2.54	0.44
1:A:203:LEU:CG	1:A:204:LEU:N	2.73	0.43
1:A:442:GLU:N	1:A:442:GLU:OE2	2.45	0.43
2:B:155:ARG:CZ	2:B:159:ILE:HD11	2.48	0.43
2:B:507:ALA:N	2:B:508:PRO:HD2	2.33	0.43
2:B:59:LEU:O	2:B:63:ILE:HG13	2.18	0.43
1:C:60:ILE:HD13	1:C:129:TYR:CZ	2.53	0.43
1:C:596:ASP:CG	1:C:612:LEU:HD23	2.38	0.43
1:E:132:LEU:CB	1:E:138:PHE:CD2	3.00	0.43
1:E:304:GLU:C	1:E:307:VAL:HG12	2.36	0.43
2:F:287:ALA:O	2:F:288:ARG:C	2.56	0.43
2:F:400:PHE:CE2	2:F:453:CYS:HB2	2.52	0.43
1:G:278:ILE:HD13	1:G:286:VAL:O	2.18	0.43
1:G:295:GLY:O	1:G:297:GLU:N	2.51	0.43
1:G:350:ILE:HG13	1:G:351:THR:N	2.32	0.43
2:H:218:ALA:HB2	2:H:241:LEU:O	2.18	0.43
2:H:243:GLY:C	2:H:245:PRO:CD	2.87	0.43
2:H:83:VAL:HG12	2:H:84:ARG:H	1.82	0.43
1:I:263:ASP:C	1:I:265:HIS:H	2.21	0.43
1:I:51:ARG:O	1:I:122:ALA:HB1	2.18	0.43
2:J:302:LEU:CD1	2:J:549:LEU:HD11	2.47	0.43
2:J:426:VAL:HG13	2:J:451:GLY:HA2	2.00	0.43
2:J:423:ALA:O	2:J:426:VAL:HG23	2.18	0.43
2:L:100:LEU:O	2:L:101:SER:C	2.57	0.43
2:L:237:ALA:C	2:L:238:THR:HG23	2.37	0.43
2:L:71:ALA:HA	2:L:74:ARG:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HG23	1:A:488:PHE:CD2	2.53	0.43
1:A:251:LEU:HD11	1:A:328:ARG:NH2	2.33	0.43
1:A:344:HIS:CG	1:A:345:PRO:HD3	2.53	0.43
1:A:497:LEU:O	1:A:498:PRO:O	2.36	0.43
2:B:72:GLN:O	2:B:75:HIS:HB3	2.18	0.43
1:C:138:PHE:HD1	1:C:142:CYS:HB2	1.78	0.43
1:C:274:ARG:HH11	1:C:347:THR:HG1	1.59	0.43
1:C:300:ARG:NH1	1:C:300:ARG:CB	2.76	0.43
1:C:350:ILE:HD12	1:C:351:THR:N	2.34	0.43
1:C:587:GLN:HA	1:C:587:GLN:OE1	2.18	0.43
1:E:60:ILE:HA	1:E:60:ILE:HD12	1.70	0.43
2:F:123:ILE:HA	2:F:131:CYS:O	2.18	0.43
2:F:223:VAL:N	2:F:224:PRO:HD2	2.33	0.43
2:F:509:ILE:N	2:F:509:ILE:HD13	2.32	0.43
1:G:291:ALA:HA	1:G:292:PRO:HD3	1.82	0.43
1:G:325:LEU:C	1:G:325:LEU:HD23	2.38	0.43
1:G:64:VAL:HG21	1:G:126:HIS:CD2	2.53	0.43
2:H:489:GLN:O	2:H:493:ALA:HB2	2.18	0.43
1:I:170:MET:SD	1:I:309:ALA:CB	3.06	0.43
1:I:170:MET:SD	1:I:309:ALA:HB1	2.57	0.43
1:I:328:ARG:HH11	1:I:328:ARG:CB	2.31	0.43
1:I:416:VAL:HG22	1:I:437:LEU:HG	2.00	0.43
1:I:486:THR:HG22	1:I:486:THR:O	2.17	0.43
2:J:255:VAL:HG22	2:J:256:SER:N	2.33	0.43
2:J:288:ARG:HH21	2:J:288:ARG:HG2	1.83	0.43
2:J:486:LYS:HE2	2:J:497:LEU:HD13	2.01	0.43
1:K:439:ALA:CB	1:K:451:LEU:HB2	2.45	0.43
2:L:195:PHE:HB3	2:L:226:MET:CE	2.48	0.43
2:L:49:MET:HE3	2:L:321:ILE:HG21	2.00	0.43
2:B:125:ARG:HD2	2:B:128:GLY:HA2	2.00	0.43
2:B:194:ILE:H	2:B:194:ILE:CD1	2.31	0.43
2:D:102:ALA:C	2:D:104:ALA:H	2.21	0.43
2:D:316:GLU:HB2	2:D:337:ARG:HE	1.83	0.43
2:D:60:LEU:O	2:D:64:HIS:ND1	2.46	0.43
2:D:87:ILE:HG22	2:D:88:ASN:N	2.33	0.43
1:E:278:ILE:HD12	1:E:278:ILE:N	2.03	0.43
1:E:340:LEU:HD23	1:E:340:LEU:HA	1.49	0.43
1:E:437:LEU:N	1:E:437:LEU:HD12	2.32	0.43
1:E:489:ILE:HG23	1:E:490:ALA:H	1.83	0.43
2:F:212:VAL:CG2	2:F:232:MET:HG2	2.48	0.43
1:G:444:ARG:HG2	1:G:444:ARG:NH1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:144:THR:HG21	4:H:591:COA:C5A	2.48	0.43
2:H:338:LEU:HD23	2:H:538:ARG:HB2	2.00	0.43
2:H:533:ASP:HB3	2:H:536:GLN:NE2	2.29	0.43
1:I:476:HIS:ND1	1:I:477:PRO:CD	2.77	0.43
2:J:317:LEU:O	2:J:320:VAL:N	2.47	0.43
1:K:440:TRP:CG	1:K:441:GLY:N	2.86	0.43
1:K:58:GLY:O	1:K:60:ILE:N	2.52	0.43
2:L:242:ALA:HA	2:L:246:LEU:HD12	2.01	0.43
2:L:300:GLY:O	2:L:301:GLN:HG3	2.17	0.43
2:L:45:ASN:HB3	2:L:321:ILE:O	2.18	0.43
1:A:300:ARG:NH2	1:A:304:GLU:OE1	2.51	0.43
1:A:311:GLN:HA	1:A:311:GLN:OE1	2.18	0.43
2:B:51:GLU:HA	2:B:54:ASN:ND2	2.32	0.43
1:C:136:ALA:HB1	1:C:154:ALA:HB1	2.00	0.43
1:C:350:ILE:HD12	1:C:351:THR:HG22	1.99	0.43
1:E:413:GLY:HA3	1:E:450:ARG:NH1	2.33	0.43
2:F:31:LEU:HD12	2:F:336:ALA:HB2	2.00	0.43
2:F:321:ILE:HD13	2:F:329:TYR:CE2	2.53	0.43
2:F:338:LEU:HD21	2:F:537:THR:CB	2.47	0.43
2:F:435:PRO:HD2	2:F:553:ILE:HD12	2.00	0.43
1:G:198:ILE:HG23	1:G:248:LYS:CG	2.49	0.43
1:G:404:LEU:HD21	1:G:612:LEU:HD11	2.01	0.43
1:G:384:VAL:HB	1:G:470:LEU:CD1	2.49	0.43
2:H:244:PRO:HA	2:H:247:VAL:HG12	2.01	0.43
1:I:512:ALA:HB2	1:I:620:LEU:HD23	2.00	0.43
1:I:540:ASN:HA	2:J:94:GLY:O	2.19	0.43
2:J:403:ASN:HA	2:J:443:GLY:H	1.84	0.43
1:K:500:PRO:O	1:K:501:GLN:CB	2.64	0.43
1:K:549:ARG:NH2	1:K:571:PRO:CB	2.82	0.43
1:K:59:GLU:OE2	1:K:436:LYS:NZ	2.51	0.43
2:L:277:ALA:HB2	2:L:286:ILE:HD12	2.00	0.43
2:L:311:LEU:C	2:L:312:TYR:CD1	2.92	0.43
2:L:412:LYS:HB2	2:L:412:LYS:HE3	1.78	0.43
1:A:149:PHE:O	1:A:151:GLY:N	2.51	0.43
1:A:169:LEU:HD12	1:A:169:LEU:N	2.33	0.43
1:A:225:ALA:O	1:A:228:LEU:HB3	2.18	0.43
1:A:392:GLU:O	1:A:394:ASP:N	2.51	0.43
1:A:463:LEU:HD22	1:A:464:ARG:H	1.84	0.43
1:A:549:ARG:CG	1:A:549:ARG:HH11	2.32	0.43
2:B:255:VAL:HG22	2:B:256:SER:N	2.33	0.43
2:B:272:VAL:O	2:B:272:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LYS:CG	2:B:413:TYR:N	2.82	0.43
2:B:49:MET:O	2:B:52:GLN:HB2	2.18	0.43
1:C:445:GLU:OE1	1:C:445:GLU:HA	2.17	0.43
1:C:384:VAL:HG13	1:C:470:LEU:HD22	2.00	0.43
1:C:77:ALA:HB1	1:C:88:HIS:HD2	1.84	0.43
2:D:371:ALA:CB	2:D:401:LEU:HB2	2.49	0.43
1:E:203:LEU:HG	1:E:204:LEU:N	2.34	0.43
1:E:251:LEU:HD11	1:E:328:ARG:NH1	2.33	0.43
1:E:288:GLU:HB3	1:E:382:ILE:HG12	1.99	0.43
1:E:452:LEU:CD1	1:E:452:LEU:O	2.66	0.43
1:E:549:ARG:CG	1:E:549:ARG:HH11	2.05	0.43
2:F:157:GLN:HE21	2:F:197:ASN:CB	2.32	0.43
2:F:238:THR:HA	2:F:261:GLY:O	2.18	0.43
2:F:282:HIS:O	2:F:285:ALA:HB3	2.18	0.43
2:F:315:GLU:C	2:F:317:LEU:N	2.69	0.43
2:F:375:ILE:N	2:F:375:ILE:CD1	2.73	0.43
2:F:382:GLN:OE1	2:F:421:HIS:CE1	2.71	0.43
2:F:507:ALA:HB3	2:F:508:PRO:HD3	2.00	0.43
1:G:169:LEU:HD12	1:G:169:LEU:N	2.33	0.43
2:H:212:VAL:HG12	2:H:237:ALA:HB1	2.00	0.43
2:H:347:PHE:O	2:H:348:LYS:C	2.56	0.43
2:H:407:PHE:CD1	2:H:407:PHE:N	2.86	0.43
2:H:68:GLY:C	2:H:70:ALA:H	2.21	0.43
1:I:108:LEU:HA	1:I:132:LEU:HD11	1.99	0.43
1:I:294:LEU:HD11	1:I:299:ARG:NH1	2.31	0.43
1:I:375:VAL:HA	1:I:376:PRO:HD2	1.70	0.43
1:I:508:PHE:O	1:I:511:ALA:N	2.51	0.43
2:J:216:CYS:O	2:J:216:CYS:SG	2.76	0.43
2:J:370:LEU:HD11	2:J:387:PHE:HD2	1.83	0.43
1:K:276:CYS:HB2	1:K:284:LYS:HE2	2.01	0.43
1:K:384:VAL:HG11	1:K:470:LEU:HD13	2.00	0.43
1:K:516:TRP:CZ3	1:K:630:GLU:HA	2.53	0.43
2:L:223:VAL:O	2:L:227:SER:OG	2.36	0.43
2:L:536:GLN:O	2:L:537:THR:C	2.57	0.43
1:A:190:THR:HA	1:A:193:ARG:HD3	1.99	0.43
1:A:224:LEU:HD23	1:A:224:LEU:O	2.19	0.43
1:A:304:GLU:HB3	1:A:308:ARG:NH2	2.34	0.43
1:A:69:ARG:NH2	1:A:91:GLU:O	2.47	0.43
2:B:180:ARG:HG3	2:B:180:ARG:NH1	2.33	0.43
2:B:469:ARG:HD3	2:B:518:HIS:HA	2.00	0.43
2:D:121:ALA:HB1	2:D:134:VAL:HG22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:414:GLU:C	2:D:416:GLY:H	2.21	0.43
2:D:90:LEU:O	2:D:288:ARG:NH2	2.51	0.43
1:E:135:ASN:O	1:E:136:ALA:C	2.57	0.43
1:E:169:LEU:O	1:E:173:ALA:HB2	2.18	0.43
1:E:437:LEU:CD2	1:E:455:LEU:CD2	2.97	0.43
1:E:516:TRP:CE2	1:E:613:ARG:NH2	2.86	0.43
2:F:170:LEU:HD23	2:F:211:VAL:HB	2.01	0.43
2:F:381:ALA:HA	2:F:425:LEU:HD13	1.99	0.43
2:F:476:GLU:H	2:F:476:GLU:CD	2.22	0.43
1:G:232:GLN:H	1:G:233:ARG:CZ	2.32	0.43
1:G:470:LEU:O	1:G:471:ARG:C	2.56	0.43
1:G:516:TRP:CD1	1:G:555:LEU:HD21	2.53	0.43
1:I:384:VAL:HG11	1:I:470:LEU:HD22	1.99	0.43
1:I:553:LEU:HD12	1:I:566:LEU:CD1	2.48	0.43
2:J:100:LEU:HG	2:J:122:GLY:HA2	2.00	0.43
2:J:150:VAL:HG21	2:J:184:VAL:HG13	2.01	0.43
2:J:341:GLY:O	2:J:343:GLU:HG2	2.19	0.43
1:K:488:PHE:CE1	1:K:492:HIS:ND1	2.81	0.43
2:L:313:PRO:HD2	2:L:316:GLU:OE1	2.19	0.43
2:L:478:ALA:O	2:L:482:LEU:HB2	2.19	0.43
2:L:68:GLY:C	2:L:70:ALA:N	2.72	0.43
1:A:673:THR:HA	1:A:687:ARG:HA	1.99	0.43
2:B:351:PHE:O	2:B:383:LYS:HD2	2.18	0.43
2:B:74:ARG:O	2:B:77:ALA:HB3	2.19	0.43
1:C:443:THR:OG1	1:C:444:ARG:N	2.51	0.43
1:C:536:PRO:HD3	2:D:363:HIS:HD2	1.83	0.43
2:D:375:ILE:CG2	2:D:376:LEU:H	2.20	0.43
2:D:476:GLU:CA	2:D:510:LEU:HD21	2.49	0.43
1:E:289:ALA:HB1	1:E:350:ILE:CD1	2.44	0.43
1:E:351:THR:HA	1:E:376:PRO:HG2	2.01	0.43
1:E:392:GLU:OE2	1:E:500:PRO:HD3	2.18	0.43
1:A:361:ARG:NH2	1:E:442:GLU:OE2	2.51	0.43
1:E:412:PRO:HB3	1:E:450:ARG:CZ	2.48	0.43
1:E:613:ARG:HG2	1:E:614:ARG:H	1.83	0.43
2:F:167:CYS:HB3	2:F:169:TYR:CE2	2.54	0.43
2:F:536:GLN:HA	2:F:539:GLU:HG3	2.00	0.43
1:G:150:LEU:HD21	1:G:363:ALA:HB3	2.01	0.43
2:H:127:GLU:OE2	2:H:292:ALA:HB2	2.19	0.43
2:H:184:VAL:HG12	2:H:184:VAL:O	2.18	0.43
2:H:270:SER:OG	2:H:271:GLY:N	2.51	0.43
1:I:339:ARG:HG3	1:I:339:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:428:PRO:HG2	1:I:429:PHE:N	2.34	0.43
1:I:534:HIS:HB3	2:J:307:PRO:CG	2.48	0.43
2:J:68:GLY:C	2:J:70:ALA:N	2.72	0.43
2:J:98:LEU:C	2:J:98:LEU:CD1	2.87	0.43
1:A:663:GLU:CG	1:A:666:GLN:HB2	2.49	0.43
1:A:669:GLU:HB3	1:A:670:ALA:H	1.69	0.43
1:A:673:THR:HG21	1:A:685:SER:OG	2.18	0.43
2:B:224:PRO:HB2	2:B:230:THR:HG21	2.01	0.43
2:B:375:ILE:H	2:B:375:ILE:CD1	2.29	0.43
1:C:138:PHE:O	1:C:139:ALA:C	2.57	0.43
1:C:254:ARG:HH22	1:C:292:PRO:HD2	1.83	0.43
1:C:619:PHE:HB3	1:C:626:LEU:HD11	2.00	0.43
1:C:69:ARG:HB3	1:C:69:ARG:NH1	2.34	0.43
2:D:377:PHE:CD1	2:D:377:PHE:N	2.82	0.43
2:D:355:LEU:HB2	2:D:380:ALA:HB1	2.01	0.43
2:H:476:GLU:CB	2:H:510:LEU:HD21	2.49	0.43
1:I:160:MET:SD	1:I:160:MET:N	2.92	0.43
1:I:517:LEU:HD22	1:I:566:LEU:CD1	2.49	0.43
1:I:81:ASP:HB2	1:I:100:GLY:CA	2.47	0.43
2:J:83:VAL:CG1	2:J:84:ARG:H	2.23	0.43
1:K:114:ILE:CD1	1:K:138:PHE:CZ	3.02	0.43
1:K:140:ARG:O	1:K:144:GLU:HB3	2.19	0.43
1:K:541:ASP:O	1:K:549:ARG:HG2	2.18	0.43
2:L:197:ASN:HA	2:L:197:ASN:HD22	1.65	0.43
1:A:598:LEU:HD12	1:A:598:LEU:HA	1.79	0.43
2:B:402:GLN:HB3	2:B:402:GLN:HE21	1.57	0.43
2:B:441:ILE:HB	2:B:465:TRP:CE3	2.54	0.43
1:C:274:ARG:HH22	1:C:320:THR:CG2	2.30	0.43
1:C:513:ALA:CB	1:C:566:LEU:HD21	2.49	0.43
2:D:476:GLU:O	2:D:480:GLY:N	2.52	0.43
1:E:204:LEU:O	1:E:215:MET:HA	2.19	0.43
1:E:553:LEU:HB2	1:E:564:VAL:HG22	2.01	0.43
1:E:567:ARG:CG	1:E:567:ARG:HH11	2.26	0.43
2:F:191:PHE:HD2	2:F:192:GLY:N	2.16	0.43
2:F:299:GLN:CB	2:F:552:PRO:HD3	2.49	0.43
2:F:331:VAL:C	2:F:333:GLU:N	2.73	0.43
2:F:375:ILE:HD13	2:F:377:PHE:HE1	1.84	0.43
1:G:202:VAL:HG22	1:G:247:GLU:O	2.19	0.43
1:G:251:LEU:HD11	1:G:328:ARG:HH21	1.84	0.43
2:H:155:ARG:NH2	2:H:460:ARG:O	2.52	0.43
2:H:65:GLU:O	2:H:72:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:PHE:O	1:I:139:ALA:C	2.57	0.43
1:I:324:LEU:HB2	1:I:334:MET:HG3	2.00	0.43
1:I:98:LEU:HA	1:I:98:LEU:HD23	1.64	0.43
2:J:248:LYS:C	2:J:248:LYS:HD2	2.40	0.43
2:L:148:LEU:HD23	2:L:148:LEU:HA	1.80	0.43
1:A:331:PHE:O	1:A:332:PHE:CD2	2.71	0.43
1:A:658:VAL:HG12	1:A:658:VAL:O	2.19	0.43
1:A:704:LEU:HG	1:A:704:LEU:H	1.69	0.43
2:B:194:ILE:O	2:B:198:GLN:HB2	2.18	0.43
2:B:370:LEU:HD11	2:B:387:PHE:HD2	1.83	0.43
1:C:251:LEU:O	1:C:327:GLU:HG3	2.19	0.43
2:D:309:ALA:HB1	2:D:310:PRO:CD	2.49	0.43
1:E:248:LYS:HD3	1:E:248:LYS:C	2.39	0.43
1:E:505:PRO:CB	1:E:507:HIS:CB	2.92	0.43
1:E:63:ARG:HH11	1:E:63:ARG:HG3	1.84	0.43
2:F:114:VAL:HG11	2:F:146:TYR:CE2	2.53	0.43
2:F:206:ILE:O	2:F:207:PRO:C	2.57	0.43
2:F:325:SER:HB3	2:F:326:LYS:HZ2	1.83	0.43
2:F:332:ARG:HG3	2:F:332:ARG:NH1	2.34	0.43
1:G:404:LEU:HD22	1:G:612:LEU:HD11	1.99	0.43
1:I:261:PHE:CE1	1:I:318:ALA:CB	2.99	0.43
1:I:320:THR:OG1	1:I:341:GLN:HG3	2.19	0.43
2:J:192:GLY:HA2	2:J:195:PHE:CD2	2.54	0.43
2:J:377:PHE:N	2:J:377:PHE:HD1	2.14	0.43
2:J:440:LEU:HB2	2:J:464:MET:HG3	2.01	0.43
1:K:255:HIS:CE1	1:K:322:GLU:CG	2.99	0.43
2:B:260:LEU:HD12	2:L:411:GLN:HA	2.00	0.43
2:L:57:ARG:HH11	2:L:57:ARG:HG2	1.84	0.43
2:L:91:LEU:HD23	2:L:125:ARG:O	2.19	0.43
1:A:223:GLU:O	1:A:227:ALA:HB2	2.19	0.42
1:A:283:GLN:O	1:A:285:VAL:HG23	2.19	0.42
1:A:714:LEU:HB3	1:A:715:ASP:H	1.61	0.42
2:B:331:VAL:O	2:B:333:GLU:N	2.52	0.42
2:B:498:GLY:C	2:B:500:GLU:H	2.21	0.42
1:C:126:HIS:HB2	1:C:150:LEU:HD12	2.00	0.42
1:C:175:VAL:O	1:C:175:VAL:HG12	2.18	0.42
1:C:251:LEU:O	1:C:252:LYS:C	2.58	0.42
1:C:279:GLN:HE21	1:C:279:GLN:HB3	1.62	0.42
1:C:263:ASP:HB2	1:C:362:VAL:HG12	1.97	0.42
1:C:491:ARG:C	1:C:493:GLN:H	2.22	0.42
2:D:433:ARG:HG3	2:D:433:ARG:NH1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:HIS:NE2	2:D:80:LYS:HE2	2.34	0.42
1:E:590:LEU:HD12	1:E:597:ASP:O	2.19	0.42
2:F:223:VAL:O	2:F:227:SER:OG	2.34	0.42
2:F:350:LEU:N	2:F:350:LEU:HD23	2.34	0.42
2:F:370:LEU:HD12	2:F:398:LEU:HD23	2.00	0.42
1:G:136:ALA:HB1	1:G:154:ALA:HB1	2.00	0.42
1:G:189:GLU:O	1:G:192:ARG:N	2.51	0.42
1:G:509:TRP:HB3	1:G:564:VAL:HG11	2.01	0.42
1:G:64:VAL:HG13	1:G:65:MET:N	2.34	0.42
1:G:71:LEU:HD22	1:G:360:ILE:HG21	2.01	0.42
2:H:30:ILE:CG2	2:H:31:LEU:N	2.82	0.42
2:H:393:GLN:HB3	2:H:393:GLN:HE21	1.55	0.42
1:I:306:ALA:CB	1:I:321:VAL:HG21	2.31	0.42
1:I:356:VAL:O	1:I:359:GLN:HB2	2.18	0.42
1:I:396:LEU:O	1:I:398:ALA:N	2.52	0.42
1:I:534:HIS:HB3	2:J:307:PRO:HG3	2.00	0.42
2:J:373:ASN:HA	2:J:373:ASN:HD22	1.49	0.42
1:K:261:PHE:O	1:K:268:CYS:HA	2.19	0.42
2:L:205:GLY:O	2:L:207:PRO:HD3	2.19	0.42
2:L:240:PHE:CE1	2:L:243:GLY:HA2	2.54	0.42
2:L:335:ILE:O	2:L:339:VAL:HG13	2.19	0.42
1:A:307:VAL:HG22	1:A:307:VAL:O	2.20	0.42
1:A:680:MET:O	1:A:681:LYS:C	2.57	0.42
1:A:65:MET:CE	1:A:92:ALA:HB2	2.49	0.42
2:B:487:ARG:O	2:B:491:GLU:HB2	2.19	0.42
2:B:479:ALA:HB2	2:B:509:ILE:HG21	2.01	0.42
1:C:103:PRO:O	1:C:108:LEU:HD12	2.19	0.42
1:C:297:GLU:O	1:C:300:ARG:HG3	2.18	0.42
2:D:512:GLN:HB3	2:D:512:GLN:HE21	1.61	0.42
2:D:560:VAL:HG13	2:H:389:GLU:CB	2.43	0.42
1:E:179:PRO:HD2	1:E:248:LYS:HB3	2.01	0.42
2:F:137:ASP:C	2:F:139:THR:N	2.73	0.42
2:F:291:VAL:O	2:F:291:VAL:HG12	2.18	0.42
1:G:440:TRP:CG	1:G:441:GLY:N	2.86	0.42
1:G:476:HIS:ND1	1:G:477:PRO:HD2	2.34	0.42
1:G:501:GLN:NE2	1:G:504:LEU:HG	2.34	0.42
2:H:513:TYR:N	2:H:513:TYR:HD1	2.17	0.42
2:H:520:TYR:HD2	2:H:520:TYR:N	2.16	0.42
1:I:607:ARG:CZ	1:I:607:ARG:HB2	2.49	0.42
2:J:327:GLN:HA	2:J:328:PRO:HD3	1.80	0.42
1:K:133:SER:OG	1:K:339:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:463:LEU:CD2	1:K:464:ARG:N	2.74	0.42
1:K:463:LEU:HD23	1:K:464:ARG:H	1.78	0.42
2:L:440:LEU:HG	2:L:463:TRP:O	2.20	0.42
2:L:526:LEU:C	2:L:528:ASP:H	2.23	0.42
1:A:154:ALA:O	1:A:155:ALA:C	2.57	0.42
1:A:218:VAL:O	1:A:218:VAL:CG2	2.65	0.42
1:A:229:SER:C	1:A:231:ALA:H	2.22	0.42
1:A:440:TRP:CD1	1:A:441:GLY:N	2.87	0.42
1:A:493:GLN:HE21	1:A:497:LEU:HG	1.85	0.42
1:A:517:LEU:HB2	1:A:553:LEU:HD11	2.00	0.42
3:A:801:BTI:O3	2:F:407:PHE:N	2.51	0.42
2:B:172:ASP:OD1	2:B:214:GLY:HA3	2.20	0.42
2:B:412:LYS:HG3	2:B:413:TYR:N	2.34	0.42
2:B:487:ARG:CA	2:B:497:LEU:HD13	2.49	0.42
2:B:144:THR:HG21	4:B:591:COA:C5A	2.50	0.42
2:D:240:PHE:CD1	2:D:243:GLY:HA2	2.54	0.42
2:D:418:ILE:CG2	2:D:419:ALA:N	2.82	0.42
2:D:436:LYS:HB2	2:D:436:LYS:HE3	1.88	0.42
1:E:134:GLU:HG2	1:E:338:THR:OG1	2.19	0.42
2:F:197:ASN:O	2:F:201:MET:HG3	2.19	0.42
1:G:602:VAL:O	1:G:603:ASP:HB2	2.18	0.42
2:H:278:GLU:O	2:H:279:ASP:HB3	2.18	0.42
2:H:236:GLN:OE1	2:H:280:ASP:OD1	2.37	0.42
1:I:256:VAL:HG13	1:I:274:ARG:O	2.18	0.42
1:I:472:ARG:H	1:I:472:ARG:HG2	1.59	0.42
1:I:501:GLN:C	1:I:504:LEU:H	2.22	0.42
1:I:587:GLN:HB3	1:I:588:TYR:CD1	2.50	0.42
2:J:164:ARG:O	2:J:164:ARG:HG2	2.18	0.42
2:J:305:ARG:HH21	2:J:361:HIS:CE1	2.38	0.42
2:J:489:GLN:O	2:J:493:ALA:HB2	2.19	0.42
2:J:85:GLU:HA	2:J:85:GLU:OE1	2.19	0.42
1:K:280:ARG:O	1:K:282:HIS:N	2.52	0.42
1:K:298:LEU:HD11	1:K:325:LEU:HD11	2.01	0.42
1:K:361:ARG:HG2	1:K:361:ARG:NH1	2.32	0.42
1:K:46:TYR:C	1:K:46:TYR:CD2	2.92	0.42
1:K:470:LEU:CA	1:K:473:ILE:CG2	2.95	0.42
2:L:324:ASP:O	2:L:325:SER:C	2.58	0.42
1:A:200:TYR:OH	1:A:224:LEU:HD13	2.19	0.42
1:A:129:TYR:CD2	1:A:342:VAL:HA	2.53	0.42
1:A:531:ASP:OD1	1:A:531:ASP:N	2.52	0.42
2:B:119:ILE:O	2:B:119:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:HIS:O	2:B:191:PHE:O	2.37	0.42
2:B:36:ASN:HD21	2:B:38:ARG:HB2	1.84	0.42
2:B:533:ASP:HB3	2:B:536:GLN:HB2	2.01	0.42
1:C:270:TYR:N	1:C:372:GLN:HE22	2.02	0.42
1:C:523:HIS:ND1	1:C:523:HIS:C	2.72	0.42
2:D:100:LEU:HA	2:D:100:LEU:HD22	1.74	0.42
2:D:31:LEU:HD12	2:D:336:ALA:CA	2.49	0.42
2:D:507:ALA:HB3	2:D:508:PRO:HD3	2.02	0.42
2:D:521:TYR:CE1	2:D:525:ARG:CZ	3.02	0.42
1:E:188:LEU:HD23	1:E:228:LEU:CD2	2.46	0.42
1:E:79:HIS:CD2	1:E:84:ARG:HA	2.55	0.42
2:F:140:VAL:O	2:F:143:GLY:N	2.41	0.42
2:F:219:GLY:O	2:F:221:ALA:N	2.52	0.42
2:F:467:ASN:ND2	2:F:467:ASN:H	2.17	0.42
2:F:464:MET:O	2:F:531:VAL:HA	2.19	0.42
1:G:136:ALA:O	1:G:140:ARG:HB2	2.19	0.42
1:G:414:ARG:HB2	1:G:454:MET:SD	2.59	0.42
1:G:67:SER:O	1:G:71:LEU:HD12	2.18	0.42
2:H:150:VAL:HG21	2:H:184:VAL:HG13	2.00	0.42
2:H:188:ARG:HG2	2:H:188:ARG:HH11	1.84	0.42
2:H:509:ILE:HD13	2:H:509:ILE:HA	1.69	0.42
4:H:591:COA:H62A	4:H:591:COA:H62	1.84	0.42
1:I:114:ILE:CD1	1:I:142:CYS:HA	2.49	0.42
1:I:444:ARG:CG	1:I:444:ARG:NH1	2.82	0.42
1:K:307:VAL:HG22	1:K:311:GLN:HE22	1.84	0.42
1:K:402:LEU:CD2	1:K:460:VAL:HG12	2.50	0.42
1:K:47:ARG:HE	1:K:148:LEU:HD22	1.80	0.42
1:K:55:ALA:HA	1:K:78:VAL:HG21	2.02	0.42
1:A:232:GLN:H	1:A:233:ARG:NH2	2.14	0.42
1:A:284:LYS:HZ2	1:A:341:GLN:NE2	2.16	0.42
1:A:463:LEU:HD23	1:A:464:ARG:H	1.84	0.42
2:B:305:ARG:O	2:B:364:GLY:HA2	2.18	0.42
1:C:269:LEU:HD13	1:C:375:VAL:HG11	2.01	0.42
1:C:160:MET:SD	1:C:313:ILE:HD13	2.60	0.42
1:C:565:ARG:CG	1:C:567:ARG:CZ	2.98	0.42
1:C:537:TRP:CH2	2:D:123:ILE:HG22	2.54	0.42
2:D:295:ASN:O	2:D:295:ASN:ND2	2.53	0.42
2:D:306:ALA:HA	2:D:307:PRO:HD3	1.84	0.42
2:D:438:THR:HG21	2:D:453:CYS:O	2.20	0.42
1:E:56:ASN:HD22	1:E:128:GLY:HA3	1.85	0.42
1:E:191:PHE:HZ	1:E:244:MET:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:PHE:O	1:E:509:TRP:C	2.57	0.42
1:E:567:ARG:CG	1:E:567:ARG:NH1	2.80	0.42
1:E:512:ALA:CB	1:E:629:ILE:HD13	2.46	0.42
2:F:401:LEU:HA	2:F:401:LEU:HD23	1.71	0.42
2:F:81:LEU:HD21	2:F:89:ARG:NH2	2.34	0.42
1:G:172:GLU:OE1	1:G:172:GLU:HA	2.20	0.42
1:G:549:ARG:NH1	1:G:549:ARG:HG2	2.33	0.42
2:H:525:ARG:O	2:H:526:LEU:HB2	2.19	0.42
1:I:251:LEU:HD12	1:I:327:GLU:HB2	2.00	0.42
1:I:465:THR:HG22	1:I:466:ASN:N	2.35	0.42
1:I:531:ASP:OD2	2:J:298:LYS:HG3	2.19	0.42
1:I:554:MET:HB3	1:I:554:MET:HE2	1.87	0.42
2:J:441:ILE:CD1	2:J:441:ILE:O	2.64	0.42
2:J:533:ASP:HB3	2:J:536:GLN:HG3	2.00	0.42
2:J:164:ARG:HB2	2:J:551:ALA:HB2	2.00	0.42
1:K:284:LYS:O	1:K:385:ARG:NH1	2.53	0.42
1:K:387:TYR:HE2	1:K:433:MET:HB2	1.81	0.42
2:L:130:GLU:O	2:L:165:LEU:HD22	2.20	0.42
2:L:331:VAL:HG21	2:L:371:ALA:HB1	2.01	0.42
2:L:49:MET:CE	2:L:321:ILE:HG21	2.49	0.42
1:A:126:HIS:HA	1:A:127:PRO:HD2	1.83	0.42
1:A:268:CYS:SG	1:A:307:VAL:CG2	2.99	0.42
2:B:31:LEU:HD13	2:B:336:ALA:HB2	2.01	0.42
1:C:477:PRO:O	1:C:480:ALA:HB3	2.19	0.42
2:D:331:VAL:O	2:D:333:GLU:N	2.53	0.42
1:E:114:ILE:CG2	1:E:114:ILE:O	2.67	0.42
1:E:508:PHE:O	1:E:511:ALA:N	2.53	0.42
1:E:78:VAL:HG13	1:E:96:VAL:HG23	2.02	0.42
2:F:164:ARG:CB	2:F:551:ALA:HB2	2.49	0.42
2:F:412:LYS:CG	2:F:413:TYR:N	2.82	0.42
1:G:47:ARG:CG	1:G:148:LEU:HD11	2.47	0.42
1:G:501:GLN:HG3	1:G:501:GLN:O	2.20	0.42
2:H:213:MET:HA	2:H:233:VAL:HG21	2.01	0.42
2:H:470:ILE:O	2:H:517:GLY:HA2	2.19	0.42
2:J:401:LEU:HD23	2:J:401:LEU:HA	1.83	0.42
2:J:518:HIS:NE2	2:J:520:TYR:CG	2.87	0.42
1:K:47:ARG:HG3	1:K:48:SER:N	2.34	0.42
1:K:536:PRO:HG2	2:L:543:LEU:HD23	2.00	0.42
2:L:285:ALA:O	2:L:289:ARG:HG2	2.20	0.42
2:L:367:ILE:O	2:L:367:ILE:HG13	2.19	0.42
1:A:299:ARG:HB2	1:A:299:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:HG23	1:A:363:ALA:N	2.35	0.42
1:A:444:ARG:HG2	1:A:444:ARG:HH11	1.85	0.42
1:A:693:VAL:O	1:A:714:LEU:CD2	2.68	0.42
2:B:235:GLU:OE2	2:B:235:GLU:HA	2.20	0.42
2:B:247:VAL:HG23	2:L:409:VAL:CG2	2.50	0.42
2:B:491:GLU:C	2:B:493:ALA:H	2.21	0.42
1:C:166:ALA:O	1:C:167:LYS:C	2.58	0.42
1:C:194:GLU:C	1:C:196:GLY:N	2.71	0.42
1:C:525:ARG:NH1	1:C:531:ASP:CG	2.73	0.42
2:D:145:TYR:CD1	2:D:149:THR:HG22	2.55	0.42
2:D:317:LEU:HD21	2:D:334:VAL:HA	2.02	0.42
2:D:411:GLN:HA	2:J:260:LEU:HD12	2.02	0.42
1:E:178:VAL:HA	1:E:179:PRO:HD3	1.79	0.42
1:E:269:LEU:HD12	1:E:375:VAL:HG23	2.02	0.42
1:E:436:LYS:C	1:E:437:LEU:HD12	2.40	0.42
1:E:549:ARG:O	1:E:567:ARG:HA	2.20	0.42
2:F:201:MET:CE	2:F:208:GLN:HE22	2.32	0.42
2:F:487:ARG:HB3	2:F:487:ARG:HH11	1.85	0.42
1:G:57:ARG:HG3	1:G:57:ARG:HH11	1.85	0.42
1:G:596:ASP:OD1	1:G:596:ASP:N	2.52	0.42
2:H:185:PHE:H	2:H:186:PRO:HD2	1.84	0.42
2:H:351:PHE:O	2:H:383:LYS:HD2	2.20	0.42
1:I:302:MET:HG2	1:I:331:PHE:CD2	2.53	0.42
1:I:365:GLY:O	1:I:366:GLU:C	2.57	0.42
2:J:234:ARG:HB3	2:J:276:TYR:CZ	2.55	0.42
2:J:462:LEU:CD2	2:J:462:LEU:C	2.88	0.42
2:J:89:ARG:HG3	2:J:89:ARG:NH2	2.35	0.42
1:K:250:LEU:HD13	1:K:324:LEU:HD23	2.01	0.42
1:K:331:PHE:CD2	1:K:331:PHE:N	2.88	0.42
1:K:395:PHE:CZ	1:K:469:PHE:CE1	3.07	0.42
2:L:403:ASN:ND2	2:L:442:GLY:CA	2.66	0.42
2:L:476:GLU:O	2:L:480:GLY:N	2.45	0.42
1:A:476:HIS:CE1	1:A:478:ALA:HB2	2.54	0.42
2:B:331:VAL:C	2:B:333:GLU:N	2.72	0.42
1:C:132:LEU:HD22	1:C:132:LEU:H	1.85	0.42
1:C:205:LYS:HB3	1:C:206:ALA:H	1.74	0.42
1:C:392:GLU:C	1:C:394:ASP:H	2.22	0.42
1:C:426:VAL:HG21	1:C:463:LEU:CD1	2.50	0.42
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.78	0.42
1:C:47:ARG:NH1	1:C:47:ARG:HB2	2.15	0.42
2:D:270:SER:OG	2:D:272:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:ALA:C	1:E:168:ALA:H	2.22	0.42
1:E:533:PRO:C	1:E:535:SER:N	2.72	0.42
2:F:121:ALA:HA	2:F:133:ILE:O	2.20	0.42
2:F:362:LEU:CD2	2:F:538:ARG:HG3	2.50	0.42
1:G:110:GLY:O	1:G:114:ILE:CG2	2.58	0.42
1:G:218:VAL:CB	1:G:224:LEU:HD13	2.49	0.42
1:G:50:GLN:HE21	1:G:123:GLN:HE22	1.66	0.42
2:H:321:ILE:HG22	2:H:321:ILE:O	2.18	0.42
2:H:375:ILE:CG2	2:H:408:MET:HB2	2.50	0.42
2:H:457:TYR:N	2:H:457:TYR:HD2	2.16	0.42
1:I:170:MET:HB3	1:I:177:LEU:HD21	2.01	0.42
1:I:289:ALA:HB1	1:I:350:ILE:CD1	2.49	0.42
1:I:452:LEU:HD22	1:I:452:LEU:HA	1.71	0.42
2:J:379:GLU:N	2:J:379:GLU:OE1	2.52	0.42
1:K:305:ALA:C	1:K:308:ARG:HG3	2.39	0.42
2:L:155:ARG:NE	2:L:159:ILE:CD1	2.83	0.42
2:L:186:PRO:O	2:L:187:ASP:O	2.38	0.42
2:B:455:ARG:HG3	2:L:188:ARG:N	2.34	0.42
2:L:305:ARG:CB	2:L:305:ARG:NH1	2.82	0.42
2:L:311:LEU:HB2	2:L:312:TYR:CD1	2.55	0.42
2:L:377:PHE:O	2:L:378:ALA:C	2.58	0.42
2:L:404:ILE:CG2	2:L:404:ILE:O	2.68	0.42
1:A:371:THR:O	1:A:374:GLN:HB2	2.20	0.42
1:A:446:GLU:OE2	1:C:361:ARG:NH1	2.48	0.42
1:A:650:SER:HA	1:A:711:LEU:HB2	2.01	0.42
1:A:654:ASN:HD22	1:A:707:GLU:HG2	1.84	0.42
1:A:79:HIS:CD2	1:A:80:SER:O	2.73	0.42
2:B:341:GLY:O	2:B:343:GLU:HG2	2.19	0.42
1:C:135:ASN:O	1:C:136:ALA:C	2.58	0.42
1:C:254:ARG:HH21	1:C:275:ASP:CG	2.23	0.42
1:C:298:LEU:HD21	1:C:325:LEU:HD11	2.01	0.42
1:C:413:GLY:N	1:C:450:ARG:HH11	2.17	0.42
1:C:460:VAL:O	1:C:626:LEU:HD23	2.20	0.42
1:C:494:ASP:O	1:C:498:PRO:HD3	2.20	0.42
1:C:565:ARG:HG2	1:C:567:ARG:CZ	2.50	0.42
2:D:400:PHE:CD2	2:D:453:CYS:HB2	2.55	0.42
2:D:481:VAL:HG23	2:D:482:LEU:H	1.85	0.42
2:D:85:GLU:O	2:D:86:ARG:C	2.58	0.42
1:E:460:VAL:O	1:E:626:LEU:HD23	2.19	0.42
2:F:244:PRO:N	2:F:245:PRO:CD	2.83	0.42
2:F:35:ILE:HD12	2:F:337:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:68:GLY:O	2:F:70:ALA:N	2.53	0.42
2:F:74:ARG:HH22	2:F:78:ARG:HH11	1.67	0.42
1:G:251:LEU:HD22	1:G:328:ARG:CD	2.50	0.42
1:G:274:ARG:HG2	1:G:289:ALA:HB2	2.01	0.42
1:G:601:ARG:HB3	1:G:601:ARG:HE	1.35	0.42
1:G:67:SER:O	1:G:68:ALA:C	2.58	0.42
2:H:171:VAL:O	2:H:171:VAL:HG23	2.19	0.42
1:I:463:LEU:CD2	1:I:464:ARG:H	2.33	0.42
2:J:242:ALA:HA	2:J:246:LEU:HD22	2.02	0.42
2:J:331:VAL:H	2:J:373:ASN:HD21	1.68	0.42
1:K:534:HIS:O	2:L:363:HIS:NE2	2.53	0.42
1:K:537:TRP:O	2:L:125:ARG:HG3	2.20	0.42
2:L:42:PHE:CE1	2:L:319:GLY:HA3	2.55	0.42
2:L:63:ILE:O	2:L:63:ILE:HG22	2.20	0.42
1:A:267:HIS:O	1:A:268:CYS:HB2	2.19	0.42
1:A:695:LYS:HD3	1:A:715:ASP:CB	2.50	0.42
2:B:186:PRO:O	2:B:187:ASP:O	2.38	0.42
2:B:157:GLN:HE22	2:B:194:ILE:HA	1.85	0.42
2:B:161:LEU:HD13	2:B:206:ILE:HD12	2.00	0.42
2:B:35:ILE:HD11	2:B:337:ARG:HH12	1.83	0.42
2:B:481:VAL:O	2:B:484:GLN:N	2.53	0.42
2:B:532:ILE:HD11	2:B:537:THR:HG23	2.02	0.42
1:C:524:ARG:HD2	1:C:533:PRO:O	2.20	0.42
1:C:58:GLY:O	1:C:60:ILE:N	2.53	0.42
2:D:169:TYR:CD2	2:D:169:TYR:N	2.88	0.42
1:C:536:PRO:HD3	2:D:363:HIS:CD2	2.55	0.42
1:A:71:LEU:HD21	1:E:446:GLU:HG2	2.02	0.42
1:E:503:ALA:CB	1:E:560:GLU:OE1	2.66	0.42
1:E:568:HIS:H	1:E:568:HIS:HD2	1.61	0.42
2:F:490:ALA:HA	2:F:493:ALA:HB3	2.02	0.42
1:G:104:ALA:CA	1:G:108:LEU:HD12	2.48	0.42
1:G:343:GLU:O	1:G:346:VAL:HG22	2.19	0.42
1:G:386:LEU:C	1:G:386:LEU:HD13	2.41	0.42
1:G:421:ARG:N	1:G:421:ARG:HD3	2.35	0.42
1:G:520:GLU:C	1:G:522:GLY:H	2.22	0.42
2:H:109:TYR:CE2	2:H:147:PRO:HD2	2.55	0.42
2:H:339:VAL:CG1	2:H:360:ALA:CB	2.98	0.42
2:F:245:PRO:HB2	2:H:481:VAL:HG13	2.02	0.42
2:H:487:ARG:HB3	2:H:497:LEU:CB	2.50	0.42
1:I:132:LEU:HD23	1:I:138:PHE:CE2	2.51	0.42
1:I:328:ARG:HH11	1:I:328:ARG:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:350:ILE:HA	1:I:440:TRP:HZ3	1.85	0.42
1:I:360:ILE:O	1:I:364:ARG:HG3	2.19	0.42
1:I:513:ALA:HB2	1:I:564:VAL:HG11	2.02	0.42
2:J:250:ALA:O	2:J:252:GLY:N	2.53	0.42
2:J:258:GLU:O	2:J:258:GLU:HG3	2.20	0.42
2:D:192:GLY:HA3	2:J:450:TYR:CE1	2.55	0.42
2:J:400:PHE:CD2	2:J:453:CYS:HB2	2.54	0.42
2:J:526:LEU:C	2:J:528:ASP:H	2.22	0.42
1:K:114:ILE:O	1:K:118:LEU:HB2	2.19	0.42
1:K:294:LEU:CD1	1:K:299:ARG:NH2	2.83	0.42
1:K:63:ARG:CZ	1:K:356:VAL:HG21	2.50	0.42
2:B:242:ALA:HB2	2:L:409:VAL:HG11	2.02	0.42
1:A:313:ILE:HD11	1:A:315:TYR:CD2	2.52	0.41
1:A:342:VAL:HB	1:A:385:ARG:NH2	2.35	0.41
1:A:520:GLU:OE1	1:A:613:ARG:NH2	2.53	0.41
1:A:709:THR:CG2	1:A:710:PRO:HD2	2.48	0.41
2:B:163:ASN:OD1	2:B:460:ARG:NH1	2.50	0.41
2:B:264:ASP:OD1	2:B:276:TYR:CE1	2.71	0.41
2:B:486:LYS:HG2	2:B:505:ILE:HD11	2.00	0.41
1:C:415:ARG:HD3	1:C:438:ILE:HD13	2.00	0.41
1:C:619:PHE:CD2	1:C:628:ALA:HB2	2.55	0.41
1:E:506:GLU:O	1:E:507:HIS:C	2.58	0.41
1:E:619:PHE:HB3	1:E:626:LEU:HD11	2.02	0.41
2:F:144:THR:HG22	2:F:175:GLY:H	1.85	0.41
2:F:433:ARG:H	2:F:556:THR:CG2	2.32	0.41
2:F:466:PRO:HD3	2:F:532:ILE:O	2.20	0.41
1:G:270:TYR:CE1	1:G:372:GLN:CD	2.94	0.41
2:H:89:ARG:HD3	2:H:281:ASP:OD1	2.20	0.41
1:I:251:LEU:HB2	1:I:327:GLU:CG	2.47	0.41
1:I:336:MET:HE1	1:I:338:THR:HG23	2.01	0.41
2:J:191:PHE:CD2	2:J:192:GLY:N	2.86	0.41
2:J:191:PHE:C	2:J:193:ARG:H	2.24	0.41
2:J:256:SER:OG	2:J:259:GLU:HB2	2.20	0.41
2:H:347:PHE:HA	2:J:275:HIS:HE1	1.85	0.41
1:K:135:ASN:O	1:K:136:ALA:C	2.58	0.41
1:K:135:ASN:ND2	1:K:138:PHE:HB2	2.34	0.41
1:K:71:LEU:HD21	1:K:364:ARG:HH12	1.85	0.41
2:L:437:PHE:CD2	2:L:437:PHE:N	2.88	0.41
2:L:82:LEU:H	2:L:82:LEU:CD1	2.27	0.41
2:L:83:VAL:CG2	2:L:120:VAL:HG11	2.50	0.41
1:A:139:ALA:HB2	1:A:149:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG22	1:A:247:GLU:O	2.20	0.41
1:A:46:TYR:CD2	1:A:46:TYR:O	2.73	0.41
2:B:497:LEU:HD23	2:B:502:GLU:HB2	2.02	0.41
1:C:218:VAL:CG2	1:C:218:VAL:O	2.68	0.41
1:C:346:VAL:HG23	1:C:347:THR:N	2.36	0.41
1:C:270:TYR:CE1	1:C:372:GLN:NE2	2.88	0.41
1:C:351:THR:HB	1:C:376:PRO:HG2	2.02	0.41
1:C:66:ARG:HA	1:C:69:ARG:NH1	2.35	0.41
2:D:164:ARG:O	2:D:164:ARG:CG	2.68	0.41
1:E:186:GLN:HB3	1:E:187:ASP:H	1.56	0.41
1:E:321:VAL:HG11	1:E:323:PHE:CE2	2.55	0.41
1:E:365:GLY:O	1:E:366:GLU:C	2.58	0.41
1:E:51:ARG:HA	1:E:74:GLY:O	2.20	0.41
2:H:100:LEU:O	2:H:101:SER:C	2.57	0.41
2:H:349:ALA:HB3	2:H:350:LEU:HD23	2.02	0.41
2:H:442:GLY:O	2:H:468:ALA:HA	2.20	0.41
1:I:414:ARG:HH22	1:I:453:ALA:HB1	1.85	0.41
1:I:613:ARG:O	1:I:614:ARG:CD	2.66	0.41
2:J:82:LEU:H	2:J:82:LEU:HD12	1.83	0.41
1:K:282:HIS:ND1	1:K:282:HIS:N	2.67	0.41
2:L:176:ALA:O	2:L:178:LEU:N	2.52	0.41
2:L:520:TYR:N	2:L:520:TYR:CD2	2.88	0.41
2:L:433:ARG:NH2	2:L:554:GLU:HG3	2.33	0.41
1:A:411:GLY:O	1:A:412:PRO:C	2.58	0.41
2:B:198:GLN:HG3	2:B:208:GLN:OE1	2.20	0.41
2:B:268:LYS:HZ2	2:B:268:LYS:HB2	1.85	0.41
2:B:462:LEU:HD12	2:B:463:TRP:N	2.35	0.41
1:C:448:ARG:HD3	1:C:474:LEU:O	2.21	0.41
1:C:513:ALA:HB1	1:C:566:LEU:HD21	2.02	0.41
1:E:109:ARG:HG2	1:E:109:ARG:NH1	2.34	0.41
1:E:395:PHE:C	1:E:397:PRO:HD3	2.39	0.41
2:F:311:LEU:CD1	2:F:342:SER:HB2	2.50	0.41
1:G:138:PHE:C	1:G:138:PHE:HD1	2.22	0.41
1:G:506:GLU:O	1:G:507:HIS:C	2.59	0.41
2:H:250:ALA:O	2:H:252:GLY:N	2.52	0.41
1:I:140:ARG:HD3	1:I:141:ALA:N	2.35	0.41
1:I:315:TYR:HE2	1:I:336:MET:HE3	1.85	0.41
1:I:342:VAL:HB	1:I:343:GLU:OE1	2.20	0.41
1:I:446:GLU:O	1:I:450:ARG:HB2	2.20	0.41
1:K:270:TYR:CE2	1:K:303:GLY:HA3	2.55	0.41
1:K:349:ALA:CB	1:K:381:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:360:ILE:HG13	1:K:360:ILE:H	1.35	0.41
1:K:269:LEU:CD1	1:K:375:VAL:CG2	2.98	0.41
2:L:219:GLY:C	2:L:221:ALA:H	2.23	0.41
2:L:396:ILE:HA	2:L:397:PRO:HD3	1.89	0.41
1:A:249:TYR:O	1:A:250:LEU:HD23	2.20	0.41
1:A:308:ARG:HG3	1:A:308:ARG:NH1	2.31	0.41
1:A:550:GLU:OE2	1:A:567:ARG:HB3	2.20	0.41
1:A:73:ILE:HG22	1:A:74:GLY:N	2.34	0.41
2:B:376:LEU:HD23	2:B:380:ALA:HB3	2.01	0.41
1:C:321:VAL:HG22	1:C:336:MET:HG3	2.02	0.41
2:D:224:PRO:HG2	2:D:225:ALA:N	2.35	0.41
2:D:129:VAL:HG13	2:D:296:TRP:CD1	2.54	0.41
2:D:354:THR:CG2	2:D:375:ILE:H	2.34	0.41
2:D:354:THR:HG22	2:D:375:ILE:N	2.35	0.41
2:D:492:ARG:HH22	2:J:74:ARG:CZ	2.31	0.41
2:D:537:THR:HG22	2:D:538:ARG:N	2.34	0.41
1:E:186:GLN:CB	1:E:190:THR:HB	2.50	0.41
1:E:196:GLY:O	1:E:198:ILE:N	2.53	0.41
1:E:269:LEU:HB2	1:E:372:GLN:HE22	1.85	0.41
1:E:336:MET:HE1	1:E:338:THR:HG22	2.01	0.41
1:E:497:LEU:N	1:E:498:PRO:HD3	2.36	0.41
1:E:618:LEU:HD23	1:E:629:ILE:HB	2.02	0.41
2:F:134:VAL:HG11	2:F:153:HIS:HD2	1.85	0.41
2:F:212:VAL:HG21	2:F:232:MET:HG3	2.03	0.41
2:F:489:GLN:O	2:F:493:ALA:HB2	2.20	0.41
1:G:132:LEU:HD23	1:G:138:PHE:HD2	1.84	0.41
1:G:144:GLU:O	1:G:144:GLU:HG2	2.20	0.41
1:G:166:ALA:C	1:G:168:ALA:N	2.73	0.41
1:G:205:LYS:HD3	1:G:247:GLU:OE2	2.20	0.41
1:G:516:TRP:CH2	1:G:631:ALA:HB2	2.55	0.41
1:G:622:TRP:O	1:G:622:TRP:CD1	2.73	0.41
2:H:134:VAL:HG11	2:H:153:HIS:CD2	2.56	0.41
2:H:373:ASN:HD22	2:H:373:ASN:HA	1.58	0.41
2:H:518:HIS:CD2	2:H:520:TYR:H	2.38	0.41
1:I:598:LEU:C	1:I:598:LEU:HD12	2.41	0.41
2:J:102:ALA:C	2:J:104:ALA:N	2.73	0.41
2:J:154:LEU:HD23	2:J:157:GLN:NE2	2.36	0.41
2:J:483:ALA:HB3	2:J:506:LYS:CE	2.49	0.41
2:J:68:GLY:O	2:J:69:SER:C	2.58	0.41
1:K:112:ARG:HH11	1:K:112:ARG:HG3	1.85	0.41
1:K:298:LEU:HD23	1:K:298:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:349:ALA:HB3	1:K:381:ALA:CB	2.51	0.41
2:L:126:VAL:HG12	2:L:291:VAL:HG11	2.01	0.41
2:L:247:VAL:O	2:L:247:VAL:HG12	2.19	0.41
2:J:348:LYS:HE2	2:L:274:ASP:OD1	2.19	0.41
1:A:415:ARG:HB3	1:A:438:ILE:HG13	2.02	0.41
1:A:440:TRP:CG	1:A:441:GLY:N	2.86	0.41
1:A:589:ARG:HG2	1:A:590:LEU:N	2.35	0.41
1:A:653:MET:CG	1:A:654:ASN:N	2.80	0.41
2:B:525:ARG:HH11	2:B:525:ARG:HG3	1.86	0.41
2:B:536:GLN:O	2:B:539:GLU:HG2	2.20	0.41
2:B:75:HIS:C	2:B:77:ALA:H	2.23	0.41
2:B:77:ALA:C	2:B:79:GLY:H	2.24	0.41
1:C:153:PRO:O	1:C:154:ALA:C	2.58	0.41
1:C:201:PRO:HB2	1:C:251:LEU:HD11	2.02	0.41
1:C:222:ALA:C	1:C:224:LEU:N	2.72	0.41
1:C:401:ARG:HH11	1:C:401:ARG:HG2	1.86	0.41
1:C:79:HIS:CD2	1:C:80:SER:O	2.74	0.41
2:D:309:ALA:O	2:D:310:PRO:O	2.38	0.41
2:D:472:VAL:CG2	2:D:473:MET:HG2	2.43	0.41
2:D:464:MET:O	2:D:531:VAL:HA	2.20	0.41
1:E:298:LEU:HD21	1:E:325:LEU:HD11	2.01	0.41
1:E:514:GLU:OE1	1:E:568:HIS:CE1	2.74	0.41
1:E:63:ARG:HH22	1:E:356:VAL:HG23	1.85	0.41
2:F:533:ASP:C	2:F:533:ASP:OD2	2.59	0.41
1:G:351:THR:HA	1:G:376:PRO:HG2	2.02	0.41
1:G:445:GLU:OE2	1:G:448:ARG:NH2	2.53	0.41
1:G:553:LEU:HD12	1:G:566:LEU:HD12	2.02	0.41
2:H:95:SER:HB2	2:H:125:ARG:HB2	2.01	0.41
1:I:277:SER:O	1:I:279:GLN:N	2.54	0.41
1:I:412:PRO:HB2	1:I:450:ARG:HH11	1.85	0.41
2:D:188:ARG:HA	2:J:456:ALA:HA	2.03	0.41
1:K:340:LEU:HD12	1:K:359:GLN:OE1	2.20	0.41
2:L:231:VAL:HG21	2:L:286:ILE:CG2	2.51	0.41
2:L:324:ASP:C	2:L:324:ASP:OD2	2.59	0.41
2:L:45:ASN:HA	2:L:323:ALA:HB2	2.02	0.41
1:A:140:ARG:HD3	1:A:141:ALA:N	2.35	0.41
1:A:232:GLN:HE21	1:A:232:GLN:HB3	1.66	0.41
1:A:198:ILE:O	1:A:248:LYS:HE2	2.20	0.41
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.64	0.41
1:A:393:GLY:O	1:A:396:LEU:CG	2.58	0.41
1:A:562:ARG:CG	1:A:562:ARG:NH1	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:O	1:A:567:ARG:HD3	2.20	0.41
1:A:678:GLU:CG	1:A:678:GLU:O	2.68	0.41
2:B:35:ILE:HD12	2:B:337:ARG:CZ	2.50	0.41
1:C:129:TYR:HE2	1:C:342:VAL:HA	1.80	0.41
1:C:482:ALA:C	1:C:484:LEU:H	2.23	0.41
1:C:602:VAL:O	1:C:603:ASP:HB2	2.21	0.41
2:D:175:GLY:HA3	4:D:591:COA:HN4	1.84	0.41
1:E:107:TYR:HB3	1:E:131:PHE:CD2	2.56	0.41
1:E:608:ARG:O	1:E:608:ARG:CG	2.68	0.41
2:F:265:VAL:O	2:F:269:VAL:HG23	2.20	0.41
2:F:479:ALA:HB1	2:F:506:LYS:HG3	2.01	0.41
1:G:520:GLU:O	1:G:522:GLY:N	2.54	0.41
2:H:31:LEU:HD12	2:H:336:ALA:HB2	2.03	0.41
1:I:334:MET:O	1:I:335:GLU:HB3	2.20	0.41
1:I:359:GLN:O	1:I:362:VAL:HG23	2.20	0.41
1:K:325:LEU:HD23	1:K:326:ASP:N	2.36	0.41
1:K:386:LEU:HB3	1:K:435:ALA:H	1.85	0.41
1:K:558:ARG:NH2	1:K:625:GLU:OE1	2.54	0.41
1:K:85:HIS:HD1	1:K:86:ALA:N	2.18	0.41
1:A:138:PHE:CD1	1:A:142:CYS:HB2	2.55	0.41
1:A:229:SER:O	1:A:231:ALA:N	2.53	0.41
1:A:385:ARG:HB3	1:A:387:TYR:CE1	2.56	0.41
1:A:53:LEU:HD11	1:A:78:VAL:HG13	2.03	0.41
1:A:65:MET:HG3	1:A:75:SER:HB2	2.01	0.41
2:B:306:ALA:HA	2:B:307:PRO:HD3	1.86	0.41
2:B:338:LEU:O	2:B:538:ARG:NH1	2.47	0.41
1:C:109:ARG:NH1	1:C:111:ASP:OD2	2.54	0.41
1:C:152:PRO:HG3	1:C:315:TYR:CE1	2.56	0.41
1:C:384:VAL:HG11	1:C:470:LEU:HD22	2.02	0.41
2:D:351:PHE:CE1	2:F:271:GLY:HA3	2.56	0.41
2:D:442:GLY:O	2:D:468:ALA:HA	2.20	0.41
1:E:311:GLN:O	1:E:312:ALA:C	2.59	0.41
2:F:137:ASP:CB	2:F:140:VAL:HG23	2.32	0.41
2:F:277:ALA:HB2	2:F:286:ILE:HD12	2.02	0.41
2:F:365:TYR:HB2	2:F:545:LEU:HD13	2.02	0.41
2:F:400:PHE:CD2	2:F:453:CYS:HB3	2.56	0.41
2:F:543:LEU:HA	2:F:543:LEU:HD23	1.75	0.41
4:F:591:COA:H62	4:F:591:COA:H62A	1.86	0.41
1:G:284:LYS:NZ	1:G:322:GLU:OE2	2.52	0.41
1:G:539:ARG:HB2	1:G:541:ASP:OD2	2.21	0.41
2:H:49:MET:HG2	2:H:318:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:351:PHE:O	2:H:352:GLY:C	2.59	0.41
1:I:370:LEU:HD22	1:I:374:GLN:HB3	2.03	0.41
1:I:404:LEU:O	1:I:460:VAL:HA	2.20	0.41
2:J:223:VAL:HG23	2:J:223:VAL:H	1.45	0.41
2:J:476:GLU:O	2:J:480:GLY:N	2.49	0.41
2:J:498:GLY:C	2:J:500:GLU:N	2.74	0.41
1:K:170:MET:HG3	1:K:333:PHE:CE2	2.56	0.41
1:K:358:TRP:HZ2	1:K:369:PRO:HG2	1.85	0.41
1:K:555:LEU:HA	1:K:555:LEU:HD23	1.91	0.41
1:K:53:LEU:HD11	1:K:78:VAL:CG1	2.51	0.41
2:L:393:GLN:O	2:L:393:GLN:HG2	2.20	0.41
2:L:375:ILE:HG21	2:L:408:MET:CE	2.51	0.41
1:A:170:MET:HG3	1:A:333:PHE:CE1	2.56	0.41
1:A:708:GLY:O	1:A:709:THR:O	2.39	0.41
2:B:244:PRO:N	2:B:245:PRO:CD	2.84	0.41
1:C:160:MET:HE2	1:C:160:MET:HB3	1.84	0.41
1:C:228:LEU:HD23	1:C:229:SER:H	1.81	0.41
1:C:389:GLU:HB3	1:C:390:ASP:H	1.50	0.41
1:C:47:ARG:HE	1:C:148:LEU:CD2	2.33	0.41
1:C:47:ARG:NE	1:C:148:LEU:CD2	2.83	0.41
1:C:90:ALA:O	1:C:92:ALA:N	2.54	0.41
2:D:81:LEU:HD12	2:D:280:ASP:HB3	2.02	0.41
2:D:36:ASN:OD1	2:D:39:SER:N	2.54	0.41
2:D:508:PRO:O	2:D:511:GLU:HG3	2.21	0.41
1:E:107:TYR:HB2	1:E:131:PHE:CD2	2.55	0.41
1:E:348:GLU:HG2	1:E:355:LEU:HG	2.02	0.41
1:E:411:GLY:O	1:E:412:PRO:C	2.59	0.41
1:E:448:ARG:HD3	1:E:474:LEU:O	2.20	0.41
1:E:56:ASN:OD1	1:E:57:ARG:N	2.44	0.41
2:F:49:MET:HG2	2:F:318:TYR:HA	2.02	0.41
2:F:362:LEU:HB2	2:F:367:ILE:HD13	2.03	0.41
2:F:424:LYS:HE2	2:F:562:ARG:O	2.20	0.41
1:G:251:LEU:N	1:G:326:ASP:OD2	2.50	0.41
2:H:247:VAL:HG11	2:H:255:VAL:HG12	2.03	0.41
1:I:308:ARG:NH1	1:I:308:ARG:CG	2.84	0.41
1:I:262:ALA:O	1:I:316:VAL:O	2.38	0.41
1:K:136:ALA:O	1:K:140:ARG:HB2	2.21	0.41
1:K:47:ARG:NE	1:K:148:LEU:HD21	2.35	0.41
1:K:302:MET:HA	1:K:305:ALA:HB3	2.01	0.41
1:K:485:ASP:CG	1:K:491:ARG:NH2	2.74	0.41
2:J:351:PHE:CE1	2:L:271:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:376:LEU:HB2	2:L:404:ILE:HD11	2.02	0.41
2:B:193:ARG:NH1	2:L:458:ASP:OD1	2.43	0.41
2:L:507:ALA:HA	2:L:510:LEU:HD12	2.02	0.41
1:A:150:LEU:HA	1:A:150:LEU:HD23	1.67	0.41
1:A:354:ASP:O	1:A:357:ALA:HB3	2.21	0.41
1:A:508:PHE:O	1:A:511:ALA:N	2.53	0.41
2:B:227:SER:O	2:B:228:ASP:C	2.59	0.41
2:B:240:PHE:CD1	2:B:243:GLY:HA2	2.55	0.41
2:B:367:ILE:CG2	2:B:545:LEU:HD11	2.50	0.41
2:B:420:LYS:O	2:B:423:ALA:HB3	2.21	0.41
1:C:299:ARG:C	1:C:301:ALA:N	2.75	0.41
1:C:337:ASN:HD22	1:C:341:GLN:HE21	1.68	0.41
1:C:469:PHE:O	1:C:472:ARG:HG3	2.21	0.41
1:C:525:ARG:CB	1:C:525:ARG:HH11	2.34	0.41
2:D:347:PHE:O	2:D:348:LYS:C	2.58	0.41
2:D:41:GLU:O	2:D:44:ALA:CB	2.60	0.41
2:D:434:VAL:HG23	2:D:435:PRO:CD	2.51	0.41
1:E:343:GLU:C	1:E:345:PRO:HD2	2.41	0.41
1:E:601:ARG:HA	1:E:606:THR:HG23	2.02	0.41
2:F:216:CYS:CB	2:F:238:THR:O	2.68	0.41
2:F:247:VAL:HG12	2:F:247:VAL:O	2.20	0.41
1:G:344:HIS:N	1:G:345:PRO:HD3	2.35	0.41
1:G:534:HIS:H	1:G:534:HIS:CD2	2.36	0.41
2:H:234:ARG:HD2	2:H:276:TYR:OH	2.21	0.41
2:H:455:ARG:HH22	2:H:529:ASP:CG	2.24	0.41
1:I:455:LEU:HB3	1:I:471:ARG:HD3	2.02	0.41
1:I:414:ARG:NH1	1:I:457:GLU:OE1	2.54	0.41
2:H:326:LYS:HE3	1:I:681:LYS:HD3	2.02	0.41
2:J:186:PRO:O	2:J:187:ASP:O	2.38	0.41
2:J:206:ILE:O	2:J:207:PRO:C	2.58	0.41
1:K:144:GLU:CG	1:K:144:GLU:O	2.66	0.41
1:K:380:HIS:CE1	1:K:444:ARG:HG3	2.56	0.41
1:K:504:LEU:CD2	1:K:505:PRO:HD2	2.45	0.41
1:K:537:TRP:CH2	2:L:123:ILE:HG22	2.56	0.41
1:A:408:ALA:HB2	1:A:457:GLU:HB2	2.02	0.41
2:B:169:TYR:N	2:B:169:TYR:CD2	2.89	0.41
2:B:417:GLY:O	2:B:419:ALA:N	2.54	0.41
1:C:263:ASP:HA	1:C:362:VAL:CG1	2.51	0.41
2:D:483:ALA:O	2:D:486:LYS:HB3	2.21	0.41
1:E:557:CYS:SG	1:E:627:LEU:HD23	2.61	0.41
2:F:189:GLU:H	2:F:189:GLU:CD	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:350:LEU:H	2:F:350:LEU:HD23	1.86	0.41
2:F:400:PHE:CD2	2:F:453:CYS:CB	3.04	0.41
2:F:106:HIS:H	2:F:524:ALA:HB1	1.86	0.41
1:G:109:ARG:NH1	1:G:111:ASP:OD2	2.54	0.41
1:G:275:ASP:OD2	1:G:277:SER:OG	2.23	0.41
1:G:280:ARG:HD3	1:G:283:GLN:NE2	2.36	0.41
2:H:114:VAL:HG11	2:H:146:TYR:CE2	2.55	0.41
2:H:400:PHE:HB2	2:H:438:THR:OG1	2.20	0.41
2:H:500:GLU:O	2:H:504:LYS:HG2	2.21	0.41
2:H:66:GLY:C	2:H:68:GLY:H	2.24	0.41
1:I:128:GLY:O	1:I:133:SER:HB3	2.21	0.41
1:I:136:ALA:O	1:I:137:ASP:C	2.58	0.41
1:I:258:ILE:HD12	1:I:302:MET:O	2.21	0.41
1:I:522:GLY:O	1:I:523:HIS:CB	2.64	0.41
2:J:537:THR:HG22	2:J:541:LEU:CD1	2.50	0.41
2:J:73:ALA:C	2:J:75:HIS:N	2.74	0.41
2:L:49:MET:HG2	2:L:318:TYR:HA	2.03	0.41
2:L:324:ASP:HB3	2:L:327:GLN:HB2	2.03	0.41
1:A:182:HIS:HA	1:A:245:LEU:CD2	2.51	0.41
1:A:71:LEU:HD21	1:A:364:ARG:HH22	1.85	0.41
1:A:663:GLU:HG2	1:A:663:GLU:H	1.50	0.41
2:B:234:ARG:O	2:B:235:GLU:HB2	2.20	0.41
2:B:26:SER:C	2:B:28:MET:H	2.23	0.41
2:B:61:GLY:O	2:B:64:HIS:HB2	2.20	0.41
1:C:269:LEU:HD12	1:C:271:LEU:HD21	2.03	0.41
1:C:320:THR:CG2	1:C:341:GLN:HB2	2.50	0.41
1:C:327:GLU:C	1:C:329:GLY:N	2.74	0.41
1:C:473:ILE:HD13	1:C:473:ILE:HG21	1.86	0.41
1:C:516:TRP:CD2	1:C:613:ARG:NH2	2.87	0.41
2:D:198:GLN:HG2	2:D:208:GLN:OE1	2.20	0.41
2:D:394:ARG:HB2	2:D:396:ILE:CD1	2.51	0.41
2:D:418:ILE:HG23	2:J:241:LEU:HD12	2.02	0.41
2:D:433:ARG:NH1	2:D:433:ARG:CG	2.82	0.41
1:E:57:ARG:HD2	1:E:107:TYR:CE2	2.56	0.41
1:E:132:LEU:HA	1:E:132:LEU:HD13	1.87	0.41
1:E:207:ALA:CB	1:E:243:ARG:NH1	2.83	0.41
1:E:622:TRP:HB3	1:E:627:LEU:HD13	2.03	0.41
2:F:212:VAL:CG2	2:F:232:MET:CG	2.99	0.41
2:F:479:ALA:HB1	2:F:506:LYS:HG2	2.02	0.41
1:G:165:ALA:O	1:G:169:LEU:CD1	2.67	0.41
1:G:178:VAL:HG23	1:G:332:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:213:MET:HE3	2:H:284:LEU:HG	2.03	0.41
2:H:309:ALA:HB1	2:H:310:PRO:CD	2.50	0.41
2:H:322:PRO:CD	2:H:329:TYR:CD1	3.04	0.41
1:G:536:PRO:CB	2:H:363:HIS:CE1	2.94	0.41
2:H:378:ALA:HB2	2:H:418:ILE:HD12	2.02	0.41
1:I:275:ASP:OD2	1:I:275:ASP:C	2.60	0.41
1:I:60:ILE:HD12	1:I:60:ILE:HA	1.77	0.41
2:J:334:VAL:HG12	2:J:338:LEU:HD11	2.02	0.41
2:J:516:GLN:HB3	2:J:521:TYR:CE2	2.56	0.41
1:K:569:ALA:O	1:K:571:PRO:HD3	2.21	0.41
1:K:555:LEU:HD22	1:K:629:ILE:HG22	2.02	0.41
2:L:204:ARG:HB2	2:L:204:ARG:HE	1.17	0.41
4:L:591:COA:H62	4:L:591:COA:H62A	1.85	0.41
1:K:544:ARG:HH21	2:L:88:ASN:ND2	2.19	0.41
1:A:382:ILE:HG22	1:A:383:GLU:N	2.35	0.40
1:A:518:GLN:HB3	1:A:590:LEU:HD23	2.03	0.40
1:A:667:THR:O	1:A:668:VAL:O	2.39	0.40
1:A:695:LYS:HD3	1:A:715:ASP:HB2	2.03	0.40
2:B:321:ILE:O	2:B:321:ILE:HG22	2.21	0.40
2:D:212:VAL:HG23	2:D:231:VAL:O	2.22	0.40
2:D:331:VAL:C	2:D:333:GLU:H	2.24	0.40
2:F:163:ASN:OD1	2:F:460:ARG:HD2	2.21	0.40
2:F:545:LEU:HA	2:F:545:LEU:HD23	1.65	0.40
1:G:389:GLU:HG2	1:G:397:PRO:HG3	2.03	0.40
1:G:57:ARG:HG3	1:G:58:GLY:N	2.36	0.40
1:G:84:ARG:H	1:G:84:ARG:HG2	1.66	0.40
1:I:127:PRO:HG3	1:I:149:PHE:CE2	2.56	0.40
1:I:385:ARG:HD3	1:I:387:TYR:HE1	1.86	0.40
1:I:452:LEU:O	1:I:452:LEU:CD1	2.65	0.40
1:I:469:PHE:CD2	1:I:470:LEU:N	2.90	0.40
3:I:801:BTI:HN2	3:I:801:BTI:H72	1.60	0.40
2:J:222:TYR:HA	2:J:225:ALA:HB3	2.03	0.40
2:L:112:GLU:HG2	2:L:112:GLU:H	1.55	0.40
2:L:157:GLN:NE2	2:L:197:ASN:HB2	2.36	0.40
2:L:192:GLY:HA2	2:L:195:PHE:HD2	1.83	0.40
2:L:215:SER:HA	2:L:238:THR:HG1	1.85	0.40
2:L:420:LYS:HE3	2:L:563:MET:O	2.21	0.40
1:A:323:PHE:CD1	1:A:333:PHE:HA	2.56	0.40
1:A:398:ALA:HB3	1:A:464:ARG:HB2	2.03	0.40
1:A:489:ILE:HD12	1:A:489:ILE:HA	1.70	0.40
1:A:489:ILE:CG2	1:A:490:ALA:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HD11	1:A:148:LEU:CD1	2.51	0.40
1:A:57:ARG:HG3	1:A:57:ARG:HH11	1.86	0.40
2:B:158:ALA:O	2:B:159:ILE:C	2.60	0.40
2:B:331:VAL:HG12	2:B:373:ASN:ND2	2.36	0.40
1:C:613:ARG:HG2	1:C:614:ARG:H	1.85	0.40
2:D:191:PHE:HD2	2:D:192:GLY:H	1.69	0.40
2:D:221:ALA:C	2:D:224:PRO:HD2	2.41	0.40
2:D:240:PHE:CE1	2:D:243:GLY:CA	3.04	0.40
2:D:476:GLU:OE2	2:D:477:GLN:HB2	2.21	0.40
2:F:408:MET:CG	2:F:413:TYR:CE2	3.04	0.40
1:G:327:GLU:O	1:G:329:GLY:N	2.55	0.40
2:H:102:ALA:C	2:H:104:ALA:N	2.75	0.40
2:F:482:LEU:HD21	2:H:179:PRO:HG3	2.02	0.40
2:F:481:VAL:HG13	2:H:245:PRO:HB3	2.02	0.40
2:H:486:LYS:HD2	2:H:489:GLN:NE2	2.35	0.40
1:I:169:LEU:HD22	1:I:313:ILE:CG2	2.48	0.40
1:I:251:LEU:O	1:I:252:LYS:C	2.59	0.40
1:I:537:TRP:HB3	2:J:125:ARG:HG2	2.01	0.40
2:D:423:ALA:HB1	2:J:226:MET:HG3	2.02	0.40
2:J:465:TRP:HB3	2:J:467:ASN:HD21	1.87	0.40
1:K:112:ARG:HG3	1:K:112:ARG:NH1	2.36	0.40
1:K:170:MET:SD	1:K:309:ALA:CB	3.04	0.40
1:K:508:PHE:O	1:K:510:GLN:N	2.54	0.40
2:L:164:ARG:CG	2:L:164:ARG:O	2.67	0.40
2:B:186:PRO:HG3	2:L:527:TRP:CZ2	2.57	0.40
1:A:109:ARG:CZ	1:A:112:ARG:HH22	2.34	0.40
1:A:271:LEU:CD1	1:A:355:LEU:HD21	2.51	0.40
1:A:384:VAL:HG13	1:A:470:LEU:HD22	2.03	0.40
2:B:42:PHE:C	2:B:42:PHE:CD2	2.94	0.40
1:C:190:THR:HG23	1:C:193:ARG:NH1	2.36	0.40
1:C:229:SER:C	1:C:231:ALA:H	2.25	0.40
1:C:320:THR:HG21	1:C:341:GLN:CG	2.51	0.40
1:C:333:PHE:CZ	1:C:335:GLU:HA	2.55	0.40
2:D:170:LEU:HD23	2:D:211:VAL:HG23	2.02	0.40
1:E:150:LEU:HD21	1:E:359:GLN:O	2.21	0.40
1:E:186:GLN:HB3	1:E:190:THR:HB	2.02	0.40
1:E:607:ARG:CG	1:E:607:ARG:HH11	2.35	0.40
2:F:190:HIS:O	2:F:191:PHE:C	2.59	0.40
1:G:359:GLN:O	1:G:362:VAL:HG22	2.21	0.40
1:G:83:ASP:O	1:G:89:VAL:HG21	2.22	0.40
2:F:450:TYR:CE1	2:H:192:GLY:HA3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:270:SER:HG	2:H:272:VAL:HG23	1.85	0.40
2:H:479:ALA:O	2:H:506:LYS:HG2	2.21	0.40
1:I:256:VAL:O	1:I:323:PHE:HB2	2.21	0.40
1:I:421:ARG:O	1:I:422:GLU:C	2.60	0.40
2:H:405:THR:HG23	1:I:681:LYS:HG2	2.03	0.40
2:J:27:HIS:CB	1:K:616:ARG:NH2	2.85	0.40
1:K:274:ARG:NH2	1:K:320:THR:HG21	2.37	0.40
1:K:532:ASP:O	1:K:535:SER:HB2	2.21	0.40
2:L:106:HIS:O	2:L:107:GLU:HB2	2.22	0.40
2:L:222:TYR:HE2	2:L:241:LEU:HD21	1.86	0.40
1:A:112:ARG:NH1	1:A:112:ARG:HG3	2.36	0.40
1:A:414:ARG:CB	1:A:454:MET:SD	3.09	0.40
1:A:506:GLU:O	1:A:507:HIS:C	2.60	0.40
1:A:531:ASP:HB3	2:B:298:LYS:HB2	2.02	0.40
1:A:65:MET:HE3	1:A:92:ALA:HB2	2.02	0.40
1:A:682:MET:SD	2:F:405:THR:HG21	2.62	0.40
2:B:241:LEU:HA	2:B:241:LEU:HD23	1.67	0.40
2:B:457:TYR:N	2:B:457:TYR:HD2	2.19	0.40
1:C:179:PRO:HB2	1:C:198:ILE:HG12	2.03	0.40
1:C:340:LEU:HD21	1:C:344:HIS:CG	2.57	0.40
2:D:165:LEU:HD21	2:D:547:ALA:O	2.21	0.40
2:D:394:ARG:HB2	2:D:396:ILE:HD12	2.04	0.40
1:E:309:ALA:O	1:E:312:ALA:HB3	2.20	0.40
1:E:340:LEU:HG	1:E:359:GLN:HE22	1.84	0.40
2:F:161:LEU:CD2	2:F:201:MET:HG2	2.43	0.40
1:G:518:GLN:HB3	1:G:590:LEU:HD23	2.03	0.40
1:G:52:LEU:HD12	1:G:124:ALA:C	2.42	0.40
2:H:101:SER:O	2:H:152:LYS:HE3	2.22	0.40
2:H:164:ARG:NH1	2:H:296:TRP:CZ2	2.90	0.40
2:H:331:VAL:HG21	2:H:371:ALA:HB1	2.03	0.40
2:H:491:GLU:HA	2:H:495:GLN:O	2.21	0.40
1:I:374:GLN:O	1:I:376:PRO:CD	2.68	0.40
2:L:222:TYR:O	2:L:223:VAL:C	2.60	0.40
2:L:305:ARG:HB3	2:L:305:ARG:HH11	1.85	0.40
2:L:308:ARG:NH2	2:L:343:GLU:CD	2.75	0.40
2:L:376:LEU:HD12	2:L:404:ILE:CD1	2.52	0.40
2:B:242:ALA:CB	2:L:409:VAL:HG11	2.52	0.40
4:B:591:COA:OAP	2:L:485:VAL:HG11	2.21	0.40
2:L:507:ALA:N	2:L:508:PRO:HD2	2.36	0.40
1:A:187:ASP:O	1:A:189:GLU:N	2.55	0.40
1:A:248:LYS:NZ	1:A:328:ARG:HH12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ARG:CB	1:A:562:ARG:NH1	2.74	0.40
1:A:672:ALA:O	1:A:674:LEU:N	2.54	0.40
1:A:713:GLU:C	1:A:714:LEU:O	2.60	0.40
2:B:247:VAL:O	2:B:250:ALA:HB3	2.21	0.40
2:B:320:VAL:O	2:B:322:PRO:HD3	2.22	0.40
2:B:541:LEU:HA	2:B:541:LEU:HD23	1.80	0.40
1:C:470:LEU:O	1:C:471:ARG:C	2.57	0.40
1:C:519:SER:HB2	1:C:613:ARG:HE	1.86	0.40
2:D:56:LEU:O	2:D:57:ARG:C	2.59	0.40
2:D:89:ARG:NH2	2:D:89:ARG:CG	2.82	0.40
1:E:154:ALA:O	1:E:155:ALA:C	2.60	0.40
1:E:279:GLN:HB2	1:E:283:GLN:O	2.21	0.40
1:E:384:VAL:CG1	1:E:470:LEU:CD2	2.91	0.40
1:E:544:ARG:HG3	1:E:550:GLU:OE1	2.21	0.40
1:E:516:TRP:CE3	1:E:555:LEU:HD21	2.57	0.40
2:F:119:ILE:HG22	2:F:149:THR:CG2	2.51	0.40
2:F:484:GLN:NE2	2:F:487:ARG:HH12	2.19	0.40
2:F:508:PRO:HG2	2:F:509:ILE:H	1.85	0.40
1:G:114:ILE:HD11	1:G:147:LEU:CD1	2.51	0.40
1:G:199:GLY:O	1:G:201:PRO:CD	2.69	0.40
1:G:182:HIS:CB	1:G:245:LEU:CD2	2.93	0.40
1:G:386:LEU:HD11	1:G:465:THR:CG2	2.52	0.40
1:G:387:TYR:N	1:G:466:ASN:OD1	2.54	0.40
2:H:338:LEU:HD21	2:H:537:THR:HB	2.04	0.40
1:I:273:GLU:H	1:I:273:GLU:CD	2.23	0.40
1:I:543:TRP:O	1:I:544:ARG:NH1	2.55	0.40
2:J:424:LYS:H	2:J:424:LYS:HG3	1.64	0.40
1:K:282:HIS:O	1:K:283:GLN:HB2	2.22	0.40
1:K:298:LEU:O	1:K:301:ALA:HB3	2.22	0.40
1:K:332:PHE:O	1:K:334:MET:HE3	2.21	0.40
1:K:340:LEU:HD12	1:K:359:GLN:HE22	1.86	0.40
1:K:405:TYR:HB3	1:K:422:GLU:CB	2.42	0.40
1:K:47:ARG:CZ	1:K:47:ARG:HB2	2.47	0.40
1:K:85:HIS:ND1	1:K:86:ALA:N	2.70	0.40
2:L:247:VAL:O	2:L:247:VAL:CG1	2.69	0.40
2:L:382:GLN:HE21	2:L:382:GLN:HB2	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	613/655 (94%)	427 (70%)	114 (19%)	72 (12%)	0 5
1	C	546/655 (83%)	382 (70%)	113 (21%)	51 (9%)	0 8
1	E	546/655 (83%)	384 (70%)	109 (20%)	53 (10%)	0 7
1	G	546/655 (83%)	381 (70%)	113 (21%)	52 (10%)	0 8
1	I	493/655 (75%)	353 (72%)	101 (20%)	39 (8%)	1 10
1	K	493/655 (75%)	364 (74%)	88 (18%)	41 (8%)	1 9
2	B	535/555 (96%)	448 (84%)	63 (12%)	24 (4%)	2 21
2	D	535/555 (96%)	456 (85%)	62 (12%)	17 (3%)	4 29
2	F	535/555 (96%)	439 (82%)	73 (14%)	23 (4%)	2 22
2	H	535/555 (96%)	450 (84%)	60 (11%)	25 (5%)	2 20
2	J	535/555 (96%)	452 (84%)	65 (12%)	18 (3%)	3 28
2	L	535/555 (96%)	438 (82%)	76 (14%)	21 (4%)	3 25
All	All	6447/7260 (89%)	4974 (77%)	1037 (16%)	436 (7%)	1 13

All (436) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	225	ALA
1	A	230	SER
1	A	294	LEU
1	A	366	GLU
1	A	377	LEU
1	A	397	PRO
1	A	412	PRO
1	A	498	PRO
1	A	504	LEU
1	A	505	PRO
1	A	586	SER

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Mol	Chain	Res	Type
1	A	587	GLN
1	A	661	LEU
1	A	666	GLN
1	A	668	VAL
1	A	696	ALA
1	A	701	GLU
1	A	703	GLU
1	A	705	VAL
1	A	714	LEU
2	B	70	ALA
2	B	186	PRO
2	B	187	ASP
2	B	375	ILE
2	B	376	LEU
2	B	474	GLY
1	C	186	GLN
1	C	225	ALA
1	C	292	PRO
1	C	294	LEU
1	C	366	GLU
1	C	377	LEU
1	C	397	PRO
1	C	412	PRO
1	C	501	GLN
1	C	504	LEU
1	C	505	PRO
1	C	523	HIS
2	D	70	ALA
2	D	186	PRO
2	D	187	ASP
2	D	310	PRO
1	E	86	ALA
1	E	186	GLN
1	E	225	ALA
1	E	278	ILE
1	E	294	LEU
1	E	366	GLU
1	E	397	PRO
1	E	412	PRO
1	E	501	GLN
1	E	504	LEU
1	E	505	PRO

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Mol	Chain	Res	Type
2	F	70	ALA
2	F	186	PRO
2	F	187	ASP
2	F	375	ILE
1	G	186	GLN
1	G	188	LEU
1	G	200	TYR
1	G	225	ALA
1	G	294	LEU
1	G	366	GLU
1	G	397	PRO
1	G	412	PRO
1	G	504	LEU
1	G	505	PRO
1	G	586	SER
1	G	587	GLN
2	H	177	ASN
2	H	186	PRO
2	H	187	ASP
2	H	218	ALA
2	H	310	PRO
2	H	375	ILE
2	H	499	VAL
1	I	278	ILE
1	I	292	PRO
1	I	366	GLU
1	I	397	PRO
1	I	412	PRO
1	I	504	LEU
1	I	505	PRO
1	I	523	HIS
1	I	586	SER
2	J	70	ALA
2	J	177	ASN
2	J	186	PRO
2	J	187	ASP
2	J	253	GLU
2	J	499	VAL
1	K	59	GLU
1	K	366	GLU
1	K	412	PRO
1	K	501	GLN

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Mol	Chain	Res	Type
1	K	504	LEU
1	K	505	PRO
1	K	586	SER
2	L	70	ALA
2	L	177	ASN
2	L	186	PRO
2	L	187	ASP
2	L	375	ILE
1	A	82	ILE
1	A	86	ALA
1	A	150	LEU
1	A	188	LEU
1	A	198	ILE
1	A	268	CYS
1	A	281	ARG
1	A	283	GLN
1	A	293	GLY
1	A	317	GLY
1	A	482	ALA
1	A	509	TRP
1	A	650	SER
1	A	680	MET
1	A	687	ARG
2	B	69	SER
2	B	174	GLY
2	B	177	ASN
2	B	191	PHE
2	B	253	GLU
2	B	499	VAL
1	C	59	GLU
1	C	105	ASP
1	C	135	ASN
1	C	188	LEU
1	C	198	ILE
1	C	230	SER
1	C	278	ILE
1	C	281	ARG
1	C	283	GLN
1	C	293	GLY
1	C	317	GLY
1	C	328	ARG
1	C	393	GLY

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Mol	Chain	Res	Type
1	C	402	LEU
1	C	509	TRP
1	C	571	PRO
1	C	586	SER
1	C	587	GLN
2	D	69	SER
2	D	101	SER
2	D	177	ASN
2	D	301	GLN
2	D	375	ILE
2	D	499	VAL
1	E	59	GLU
1	E	131	PHE
1	E	135	ASN
1	E	188	LEU
1	E	198	ILE
1	E	230	SER
1	E	293	GLY
1	E	299	ARG
1	E	300	ARG
1	E	328	ARG
1	E	391	PRO
1	E	521	PRO
1	E	523	HIS
1	E	539	ARG
1	E	586	SER
1	E	587	GLN
1	E	602	VAL
2	F	253	GLU
2	F	301	GLN
2	F	499	VAL
1	G	82	ILE
1	G	99	GLY
1	G	135	ASN
1	G	150	LEU
1	G	282	HIS
1	G	283	GLN
1	G	293	GLY
1	G	317	GLY
1	G	328	ARG
1	G	501	GLN
1	G	571	PRO

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Mol	Chain	Res	Type
2	H	47	ALA
2	H	69	SER
2	H	70	ALA
2	H	101	SER
2	H	236	GLN
2	H	253	GLU
2	H	301	GLN
2	H	376	LEU
2	H	474	GLY
1	I	59	GLU
1	I	107	TYR
1	I	282	HIS
1	I	283	GLN
1	I	293	GLY
1	I	294	LEU
1	I	501	GLN
1	I	587	GLN
2	J	69	SER
2	J	101	SER
2	J	375	ILE
2	J	376	LEU
1	K	135	ASN
1	K	278	ILE
1	K	281	ARG
1	K	283	GLN
1	K	293	GLY
1	K	294	LEU
1	K	317	GLY
1	K	397	PRO
1	K	491	ARG
1	K	523	HIS
1	K	587	GLN
1	K	602	VAL
2	L	101	SER
2	L	474	GLY
2	L	499	VAL
1	A	59	GLU
1	A	135	ASN
1	A	292	PRO
1	A	300	ARG
1	A	398	ALA
1	A	402	LEU

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Mol	Chain	Res	Type
1	A	483	GLU
1	A	491	ARG
1	A	501	GLN
1	A	503	ALA
1	A	623	GLU
1	A	673	THR
1	A	681	LYS
2	B	236	GLN
1	C	91	GLU
1	C	155	ALA
1	C	282	HIS
1	C	300	ARG
1	C	391	PRO
1	C	498	PRO
1	C	508	PHE
1	C	521	PRO
1	C	602	VAL
2	D	207	PRO
2	D	253	GLU
1	E	281	ARG
1	E	283	GLN
1	E	292	PRO
1	E	377	LEU
1	E	393	GLY
1	E	422	GLU
1	E	500	PRO
1	E	503	ALA
1	E	534	HIS
1	E	603	ASP
2	F	69	SER
2	F	177	ASN
2	F	191	PHE
2	F	218	ALA
2	F	236	GLN
1	G	59	GLU
1	G	131	PHE
1	G	268	CYS
1	G	292	PRO
1	G	296	ALA
1	G	377	LEU
1	G	391	PRO
1	G	398	ALA

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Mol	Chain	Res	Type
1	G	521	PRO
2	H	115	ALA
1	I	82	ILE
1	I	86	ALA
1	I	135	ASN
1	I	300	ARG
1	I	377	LEU
1	I	393	GLY
1	I	482	ALA
1	I	491	ARG
1	I	498	PRO
1	I	571	PRO
2	J	301	GLN
1	K	292	PRO
1	K	498	PRO
1	K	521	PRO
1	K	603	ASP
2	L	69	SER
2	L	141	LYS
2	L	174	GLY
2	L	236	GLN
2	L	253	GLU
1	A	98	LEU
1	A	131	PHE
1	A	389	GLU
1	A	508	PHE
1	A	523	HIS
1	A	571	PRO
2	B	76	SER
2	B	141	LYS
2	B	251	THR
2	B	403	ASN
1	C	104	ALA
1	C	131	PHE
1	C	389	GLU
1	C	500	PRO
2	D	47	ALA
1	E	99	GLY
1	E	268	CYS
1	E	282	HIS
1	E	571	PRO
1	E	623	GLU

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Mol	Chain	Res	Type
2	F	101	SER
2	F	141	LYS
1	G	86	ALA
1	G	160	MET
1	G	171	GLU
1	G	198	ILE
1	G	389	GLU
1	G	463	LEU
1	G	482	ALA
1	G	491	ARG
2	H	39	SER
2	H	207	PRO
2	H	537	THR
1	I	255	HIS
1	I	391	PRO
1	I	503	ALA
1	I	509	TRP
2	J	207	PRO
2	J	236	GLN
1	K	150	LEU
1	K	155	ALA
1	K	282	HIS
1	K	301	ALA
1	K	482	ALA
1	K	500	PRO
1	K	509	TRP
1	K	571	PRO
1	A	272	ASN
1	A	282	HIS
1	A	299	ARG
1	A	328	ARG
1	A	391	PRO
1	A	393	GLY
2	B	83	VAL
2	B	93	PRO
2	B	185	PHE
2	B	325	SER
1	C	137	ASP
1	C	223	GLU
1	C	268	CYS
1	C	422	GLU
1	C	491	ARG

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Mol	Chain	Res	Type
2	D	27	HIS
2	D	39	SER
2	D	174	GLY
2	D	236	GLN
1	E	150	LEU
1	E	349	ALA
1	E	389	GLU
1	E	498	PRO
1	E	509	TRP
2	F	93	PRO
2	F	228	ASP
1	G	248	LYS
1	G	281	ARG
1	G	432	PRO
1	G	483	GLU
1	G	498	PRO
1	G	523	HIS
2	H	174	GLY
2	H	185	PHE
2	H	245	PRO
1	I	105	ASP
1	I	154	ALA
1	I	296	ALA
2	J	103	LEU
1	K	131	PHE
1	K	391	PRO
1	K	503	ALA
2	L	185	PHE
2	L	218	ALA
2	L	376	LEU
1	A	492	HIS
1	A	521	PRO
1	A	625	GLU
2	B	101	SER
2	B	115	ALA
1	C	58	GLY
1	C	99	GLY
1	C	109	ARG
1	E	482	ALA
2	F	112	GLU
2	F	245	PRO
2	F	300	GLY

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Mol	Chain	Res	Type
1	G	58	GLY
1	I	428	PRO
1	I	500	PRO
1	I	521	PRO
2	J	174	GLY
2	J	310	PRO
1	K	105	ASP
1	K	377	LEU
1	A	278	ILE
1	A	428	PRO
1	A	500	PRO
1	A	709	THR
1	E	82	ILE
1	E	317	GLY
1	E	432	PRO
2	F	220	GLY
2	J	474	GLY
2	L	93	PRO
2	L	207	PRO
1	A	200	TYR
2	B	310	PRO
2	F	174	GLY
1	G	393	GLY
1	I	390	ASP
1	K	82	ILE
1	K	428	PRO
1	A	376	PRO
1	A	432	PRO
1	E	379	GLY
2	F	185	PHE
2	F	219	GLY
1	G	278	ILE
1	G	307	VAL
1	G	500	PRO
1	I	432	PRO
2	J	185	PHE
1	K	58	GLY
1	K	390	ASP
1	K	393	GLY
2	L	245	PRO
1	G	352	GLY
2	H	534	PRO

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Mol	Chain	Res	Type
2	H	552	PRO
2	L	178	LEU
1	A	352	GLY
2	L	310	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	477/496 (96%)	384 (80%)	93 (20%)	1 7
1	C	423/496 (85%)	336 (79%)	87 (21%)	1 6
1	E	423/496 (85%)	330 (78%)	93 (22%)	1 5
1	G	423/496 (85%)	329 (78%)	94 (22%)	1 5
1	I	382/496 (77%)	305 (80%)	77 (20%)	1 6
1	K	381/496 (77%)	300 (79%)	81 (21%)	1 5
2	B	401/418 (96%)	341 (85%)	60 (15%)	3 17
2	D	401/418 (96%)	340 (85%)	61 (15%)	3 17
2	F	401/418 (96%)	339 (84%)	62 (16%)	2 16
2	H	401/418 (96%)	338 (84%)	63 (16%)	2 15
2	J	401/418 (96%)	354 (88%)	47 (12%)	5 26
2	L	401/418 (96%)	341 (85%)	60 (15%)	3 17
All	All	4915/5484 (90%)	4037 (82%)	878 (18%)	2 9

All (878) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	50	GLN
1	A	59	GLU
1	A	65	MET
1	A	75	SER
1	A	80	SER

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Mol	Chain	Res	Type
1	A	87	ARG
1	A	96	VAL
1	A	105	ASP
1	A	118	LEU
1	A	123	GLN
1	A	129	TYR
1	A	132	LEU
1	A	137	ASP
1	A	144	GLU
1	A	148	LEU
1	A	171	GLU
1	A	186	GLN
1	A	192	ARG
1	A	197	ARG
1	A	198	ILE
1	A	200	TYR
1	A	202	VAL
1	A	215	MET
1	A	216	LYS
1	A	217	VAL
1	A	221	GLU
1	A	226	GLU
1	A	232	GLN
1	A	233	ARG
1	A	244	MET
1	A	249	TYR
1	A	261	PHE
1	A	269	LEU
1	A	276	CYS
1	A	278	ILE
1	A	292	PRO
1	A	316	VAL
1	A	327	GLU
1	A	328	ARG
1	A	336	MET
1	A	340	LEU
1	A	341	GLN
1	A	361	ARG
1	A	371	THR
1	A	386	LEU
1	A	412	PRO
1	A	420	VAL

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Mol	Chain	Res	Type
1	A	421	ARG
1	A	431	ASP
1	A	438	ILE
1	A	440	TRP
1	A	443	THR
1	A	446	GLU
1	A	449	GLN
1	A	452	LEU
1	A	460	VAL
1	A	463	LEU
1	A	465	THR
1	A	469	PHE
1	A	471	ARG
1	A	492	HIS
1	A	495	ASP
1	A	505	PRO
1	A	518	GLN
1	A	519	SER
1	A	525	ARG
1	A	526	ASP
1	A	540	ASN
1	A	544	ARG
1	A	550	GLU
1	A	559	ASP
1	A	562	ARG
1	A	565	ARG
1	A	567	ARG
1	A	586	SER
1	A	597	ASP
1	A	602	VAL
1	A	606	THR
1	A	612	LEU
1	A	614	ARG
1	A	621	GLU
1	A	654	ASN
1	A	667	THR
1	A	668	VAL
1	A	677	LEU
1	A	678	GLU
1	A	682	MET
1	A	686	ILE
1	A	687	ARG

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Mol	Chain	Res	Type
1	A	697	LEU
1	A	698	TYR
1	A	704	LEU
2	B	33	THR
2	B	35	ILE
2	B	36	ASN
2	B	57	ARG
2	B	62	ARG
2	B	64	HIS
2	B	69	SER
2	B	81	LEU
2	B	85	GLU
2	B	89	ARG
2	B	93	PRO
2	B	99	GLU
2	B	112	GLU
2	B	114	VAL
2	B	120	VAL
2	B	139	THR
2	B	147	PRO
2	B	149	THR
2	B	161	LEU
2	B	162	GLU
2	B	187	ASP
2	B	189	GLU
2	B	191	PHE
2	B	227	SER
2	B	230	THR
2	B	240	PHE
2	B	247	VAL
2	B	256	SER
2	B	264	ASP
2	B	281	ASP
2	B	308	ARG
2	B	312	TYR
2	B	327	GLN
2	B	331	VAL
2	B	350	LEU
2	B	353	THR
2	B	354	THR
2	B	362	LEU
2	B	370	LEU

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Mol	Chain	Res	Type
2	B	373	ASN
2	B	392	CYS
2	B	393	GLN
2	B	403	ASN
2	B	408	MET
2	B	455	ARG
2	B	466	PRO
2	B	467	ASN
2	B	473	MET
2	B	476	GLU
2	B	481	VAL
2	B	484	GLN
2	B	487	ARG
2	B	491	GLU
2	B	499	VAL
2	B	502	GLU
2	B	510	LEU
2	B	511	GLU
2	B	537	THR
2	B	545	LEU
2	B	553	ILE
1	C	47	ARG
1	C	50	GLN
1	C	66	ARG
1	C	71	LEU
1	C	84	ARG
1	C	85	HIS
1	C	105	ASP
1	C	111	ASP
1	C	118	LEU
1	C	123	GLN
1	C	129	TYR
1	C	132	LEU
1	C	135	ASN
1	C	138	PHE
1	C	148	LEU
1	C	171	GLU
1	C	192	ARG
1	C	197	ARG
1	C	198	ILE
1	C	200	TYR
1	C	217	VAL

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Mol	Chain	Res	Type
1	C	220	ARG
1	C	221	GLU
1	C	226	GLU
1	C	232	GLN
1	C	233	ARG
1	C	243	ARG
1	C	251	LEU
1	C	261	PHE
1	C	268	CYS
1	C	269	LEU
1	C	278	ILE
1	C	280	ARG
1	C	292	PRO
1	C	300	ARG
1	C	311	GLN
1	C	313	ILE
1	C	328	ARG
1	C	336	MET
1	C	341	GLN
1	C	353	LEU
1	C	362	VAL
1	C	370	LEU
1	C	397	PRO
1	C	412	PRO
1	C	414	ARG
1	C	420	VAL
1	C	421	ARG
1	C	424	ASP
1	C	438	ILE
1	C	440	TRP
1	C	443	THR
1	C	445	GLU
1	C	446	GLU
1	C	449	GLN
1	C	452	LEU
1	C	455	LEU
1	C	469	PHE
1	C	471	ARG
1	C	472	ARG
1	C	486	THR
1	C	493	GLN
1	C	495	ASP

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Mol	Chain	Res	Type
1	C	498	PRO
1	C	505	PRO
1	C	525	ARG
1	C	526	ASP
1	C	531	ASP
1	C	540	ASN
1	C	547	LEU
1	C	549	ARG
1	C	554	MET
1	C	562	ARG
1	C	564	VAL
1	C	571	PRO
1	C	586	SER
1	C	590	LEU
1	C	597	ASP
1	C	598	LEU
1	C	600	SER
1	C	606	THR
1	C	608	ARG
1	C	612	LEU
1	C	616	ARG
1	C	618	LEU
1	C	620	LEU
1	C	621	GLU
2	D	41	GLU
2	D	65	GLU
2	D	74	ARG
2	D	78	ARG
2	D	81	LEU
2	D	85	GLU
2	D	89	ARG
2	D	98	LEU
2	D	100	LEU
2	D	136	ASN
2	D	147	PRO
2	D	157	GLN
2	D	178	LEU
2	D	187	ASP
2	D	188	ARG
2	D	189	GLU
2	D	191	PHE
2	D	197	ASN

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Mol	Chain	Res	Type
2	D	211	VAL
2	D	212	VAL
2	D	230	THR
2	D	235	GLU
2	D	236	GLN
2	D	240	PHE
2	D	245	PRO
2	D	247	VAL
2	D	248	LYS
2	D	260	LEU
2	D	270	SER
2	D	281	ASP
2	D	293	ASN
2	D	327	GLN
2	D	334	VAL
2	D	345	ASP
2	D	350	LEU
2	D	351	PHE
2	D	353	THR
2	D	354	THR
2	D	357	CYS
2	D	370	LEU
2	D	373	ASN
2	D	379	GLU
2	D	402	GLN
2	D	434	VAL
2	D	438	THR
2	D	441	ILE
2	D	453	CYS
2	D	472	VAL
2	D	473	MET
2	D	476	GLU
2	D	481	VAL
2	D	484	GLN
2	D	486	LYS
2	D	489	GLN
2	D	505	ILE
2	D	511	GLU
2	D	512	GLN
2	D	519	PRO
2	D	520	TYR
2	D	525	ARG

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Mol	Chain	Res	Type
2	D	534	PRO
1	E	47	ARG
1	E	51	ARG
1	E	59	GLU
1	E	60	ILE
1	E	66	ARG
1	E	78	VAL
1	E	84	ARG
1	E	85	HIS
1	E	87	ARG
1	E	93	ASP
1	E	96	VAL
1	E	105	ASP
1	E	111	ASP
1	E	112	ARG
1	E	123	GLN
1	E	129	TYR
1	E	148	LEU
1	E	169	LEU
1	E	177	LEU
1	E	178	VAL
1	E	182	HIS
1	E	184	GLU
1	E	186	GLN
1	E	189	GLU
1	E	193	ARG
1	E	197	ARG
1	E	198	ILE
1	E	200	TYR
1	E	205	LYS
1	E	216	LYS
1	E	217	VAL
1	E	232	GLN
1	E	233	ARG
1	E	243	ARG
1	E	251	LEU
1	E	261	PHE
1	E	267	HIS
1	E	269	LEU
1	E	278	ILE
1	E	280	ARG
1	E	292	PRO

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Mol	Chain	Res	Type
1	E	300	ARG
1	E	326	ASP
1	E	328	ARG
1	E	335	GLU
1	E	340	LEU
1	E	341	GLN
1	E	345	PRO
1	E	347	THR
1	E	362	VAL
1	E	371	THR
1	E	376	PRO
1	E	378	ASN
1	E	386	LEU
1	E	392	GLU
1	E	406	ARG
1	E	412	PRO
1	E	418	SER
1	E	421	ARG
1	E	440	TRP
1	E	443	THR
1	E	452	LEU
1	E	459	SER
1	E	463	LEU
1	E	467	LEU
1	E	473	ILE
1	E	505	PRO
1	E	510	GLN
1	E	519	SER
1	E	520	GLU
1	E	525	ARG
1	E	526	ASP
1	E	541	ASP
1	E	547	LEU
1	E	549	ARG
1	E	550	GLU
1	E	556	ARG
1	E	560	GLU
1	E	561	ARG
1	E	562	ARG
1	E	568	HIS
1	E	571	PRO
1	E	589	ARG

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Mol	Chain	Res	Type
1	E	591	ASP
1	E	597	ASP
1	E	601	ARG
1	E	606	THR
1	E	612	LEU
1	E	616	ARG
1	E	617	GLN
1	E	618	LEU
1	E	621	GLU
1	E	623	GLU
2	F	28	MET
2	F	33	THR
2	F	34	GLN
2	F	57	ARG
2	F	60	LEU
2	F	65	GLU
2	F	78	ARG
2	F	82	LEU
2	F	84	ARG
2	F	85	GLU
2	F	95	SER
2	F	98	LEU
2	F	112	GLU
2	F	114	VAL
2	F	119	ILE
2	F	120	VAL
2	F	134	VAL
2	F	136	ASN
2	F	139	THR
2	F	149	THR
2	F	161	LEU
2	F	169	TYR
2	F	179	PRO
2	F	180	ARG
2	F	187	ASP
2	F	189	GLU
2	F	191	PHE
2	F	209	ILE
2	F	211	VAL
2	F	212	VAL
2	F	223	VAL
2	F	240	PHE

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Mol	Chain	Res	Type
2	F	255	VAL
2	F	269	VAL
2	F	280	ASP
2	F	281	ASP
2	F	301	GLN
2	F	304	CYS
2	F	305	ARG
2	F	329	TYR
2	F	350	LEU
2	F	353	THR
2	F	354	THR
2	F	362	LEU
2	F	373	ASN
2	F	375	ILE
2	F	377	PHE
2	F	392	CYS
2	F	405	THR
2	F	426	VAL
2	F	427	THR
2	F	435	PRO
2	F	472	VAL
2	F	476	GLU
2	F	491	GLU
2	F	499	VAL
2	F	501	GLU
2	F	519	PRO
2	F	536	GLN
2	F	539	GLU
2	F	545	LEU
2	F	556	THR
1	G	47	ARG
1	G	50	GLN
1	G	59	GLU
1	G	65	MET
1	G	66	ARG
1	G	81	ASP
1	G	83	ASP
1	G	85	HIS
1	G	102	LYS
1	G	105	ASP
1	G	109	ARG
1	G	112	ARG

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Mol	Chain	Res	Type
1	G	118	LEU
1	G	123	GLN
1	G	126	HIS
1	G	132	LEU
1	G	135	ASN
1	G	138	PHE
1	G	140	ARG
1	G	143	GLU
1	G	172	GLU
1	G	182	HIS
1	G	186	GLN
1	G	192	ARG
1	G	197	ARG
1	G	200	TYR
1	G	203	LEU
1	G	216	LYS
1	G	217	VAL
1	G	220	ARG
1	G	226	GLU
1	G	232	GLN
1	G	233	ARG
1	G	247	GLU
1	G	249	TYR
1	G	250	LEU
1	G	251	LEU
1	G	261	PHE
1	G	269	LEU
1	G	276	CYS
1	G	278	ILE
1	G	311	GLN
1	G	328	ARG
1	G	330	GLN
1	G	335	GLU
1	G	336	MET
1	G	338	THR
1	G	339	ARG
1	G	340	LEU
1	G	341	GLN
1	G	346	VAL
1	G	355	LEU
1	G	356	VAL
1	G	378	ASN

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Mol	Chain	Res	Type
1	G	386	LEU
1	G	421	ARG
1	G	424	ASP
1	G	437	LEU
1	G	438	ILE
1	G	440	TRP
1	G	444	ARG
1	G	446	GLU
1	G	452	LEU
1	G	454	MET
1	G	459	SER
1	G	460	VAL
1	G	463	LEU
1	G	471	ARG
1	G	473	ILE
1	G	484	LEU
1	G	485	ASP
1	G	492	HIS
1	G	495	ASP
1	G	505	PRO
1	G	518	GLN
1	G	526	ASP
1	G	539	ARG
1	G	540	ASN
1	G	541	ASP
1	G	547	LEU
1	G	549	ARG
1	G	552	ASP
1	G	554	MET
1	G	556	ARG
1	G	558	ARG
1	G	559	ASP
1	G	562	ARG
1	G	565	ARG
1	G	571	PRO
1	G	596	ASP
1	G	601	ARG
1	G	602	VAL
1	G	612	LEU
1	G	621	GLU
2	H	35	ILE
2	H	38	ARG

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Mol	Chain	Res	Type
2	H	59	LEU
2	H	78	ARG
2	H	81	LEU
2	H	83	VAL
2	H	85	GLU
2	H	89	ARG
2	H	95	SER
2	H	98	LEU
2	H	112	GLU
2	H	136	ASN
2	H	139	THR
2	H	147	PRO
2	H	161	LEU
2	H	183	GLU
2	H	189	GLU
2	H	191	PHE
2	H	207	PRO
2	H	240	PHE
2	H	247	VAL
2	H	248	LYS
2	H	251	THR
2	H	256	SER
2	H	264	ASP
2	H	270	SER
2	H	280	ASP
2	H	281	ASP
2	H	294	LEU
2	H	297	ARG
2	H	299	GLN
2	H	315	GLU
2	H	327	GLN
2	H	339	VAL
2	H	345	ASP
2	H	350	LEU
2	H	353	THR
2	H	354	THR
2	H	370	LEU
2	H	373	ASN
2	H	376	LEU
2	H	393	GLN
2	H	398	LEU
2	H	403	ASN

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Mol	Chain	Res	Type
2	H	405	THR
2	H	418	ILE
2	H	438	THR
2	H	453	CYS
2	H	472	VAL
2	H	476	GLU
2	H	487	ARG
2	H	491	GLU
2	H	500	GLU
2	H	502	GLU
2	H	505	ILE
2	H	509	ILE
2	H	510	LEU
2	H	519	PRO
2	H	526	LEU
2	H	545	LEU
2	H	554	GLU
2	H	556	THR
2	H	561	PHE
1	I	50	GLN
1	I	59	GLU
1	I	65	MET
1	I	71	LEU
1	I	83	ASP
1	I	85	HIS
1	I	93	ASP
1	I	96	VAL
1	I	105	ASP
1	I	111	ASP
1	I	123	GLN
1	I	129	TYR
1	I	135	ASN
1	I	147	LEU
1	I	148	LEU
1	I	167	LYS
1	I	169	LEU
1	I	178	VAL
1	I	179	PRO
1	I	251	LEU
1	I	255	HIS
1	I	260	VAL
1	I	261	PHE

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Mol	Chain	Res	Type
1	I	269	LEU
1	I	280	ARG
1	I	286	VAL
1	I	300	ARG
1	I	311	GLN
1	I	315	TYR
1	I	325	LEU
1	I	335	GLU
1	I	338	THR
1	I	340	LEU
1	I	341	GLN
1	I	353	LEU
1	I	356	VAL
1	I	362	VAL
1	I	386	LEU
1	I	421	ARG
1	I	427	SER
1	I	438	ILE
1	I	440	TRP
1	I	443	THR
1	I	444	ARG
1	I	449	GLN
1	I	452	LEU
1	I	459	SER
1	I	463	LEU
1	I	465	THR
1	I	469	PHE
1	I	471	ARG
1	I	473	ILE
1	I	474	LEU
1	I	483	GLU
1	I	504	LEU
1	I	505	PRO
1	I	519	SER
1	I	525	ARG
1	I	526	ASP
1	I	538	SER
1	I	539	ARG
1	I	540	ASN
1	I	541	ASP
1	I	554	MET
1	I	561	ARG

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Mol	Chain	Res	Type
1	I	565	ARG
1	I	571	PRO
1	I	589	ARG
1	I	597	ASP
1	I	598	LEU
1	I	601	ARG
1	I	608	ARG
1	I	612	LEU
1	I	616	ARG
1	I	618	LEU
1	I	620	LEU
1	I	623	GLU
2	J	35	ILE
2	J	59	LEU
2	J	62	ARG
2	J	64	HIS
2	J	81	LEU
2	J	85	GLU
2	J	98	LEU
2	J	136	ASN
2	J	149	THR
2	J	161	LEU
2	J	183	GLU
2	J	187	ASP
2	J	189	GLU
2	J	209	ILE
2	J	211	VAL
2	J	217	THR
2	J	223	VAL
2	J	235	GLU
2	J	236	GLN
2	J	240	PHE
2	J	281	ASP
2	J	289	ARG
2	J	297	ARG
2	J	304	CYS
2	J	311	LEU
2	J	327	GLN
2	J	329	TYR
2	J	331	VAL
2	J	337	ARG
2	J	339	VAL

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Mol	Chain	Res	Type
2	J	350	LEU
2	J	353	THR
2	J	354	THR
2	J	370	LEU
2	J	373	ASN
2	J	377	PHE
2	J	379	GLU
2	J	405	THR
2	J	414	GLU
2	J	418	ILE
2	J	426	VAL
2	J	453	CYS
2	J	464	MET
2	J	469	ARG
2	J	476	GLU
2	J	487	ARG
2	J	538	ARG
1	K	47	ARG
1	K	52	LEU
1	K	59	GLU
1	K	66	ARG
1	K	71	LEU
1	K	85	HIS
1	K	96	VAL
1	K	109	ARG
1	K	118	LEU
1	K	123	GLN
1	K	129	TYR
1	K	137	ASP
1	K	140	ARG
1	K	144	GLU
1	K	148	LEU
1	K	150	LEU
1	K	251	LEU
1	K	261	PHE
1	K	263	ASP
1	K	264	ARG
1	K	269	LEU
1	K	273	GLU
1	K	278	ILE
1	K	280	ARG
1	K	282	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	K	286	VAL
1	K	288	GLU
1	K	292	PRO
1	K	294	LEU
1	K	308	ARG
1	K	311	GLN
1	K	322	GLU
1	K	336	MET
1	K	339	ARG
1	K	347	THR
1	K	356	VAL
1	K	358	TRP
1	K	359	GLN
1	K	360	ILE
1	K	386	LEU
1	K	392	GLU
1	K	401	ARG
1	K	412	PRO
1	K	414	ARG
1	K	421	ARG
1	K	424	ASP
1	K	429	PHE
1	K	438	ILE
1	K	443	THR
1	K	445	GLU
1	K	446	GLU
1	K	452	LEU
1	K	460	VAL
1	K	463	LEU
1	K	469	PHE
1	K	471	ARG
1	K	473	ILE
1	K	479	PHE
1	K	504	LEU
1	K	505	PRO
1	K	507	HIS
1	K	510	GLN
1	K	518	GLN
1	K	526	ASP
1	K	540	ASN
1	K	547	LEU
1	K	552	ASP

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Mol	Chain	Res	Type
1	K	565	ARG
1	K	566	LEU
1	K	588	TYR
1	K	591	ASP
1	K	597	ASP
1	K	600	SER
1	K	605	VAL
1	K	606	THR
1	K	612	LEU
1	K	618	LEU
1	K	620	LEU
1	K	625	GLU
1	K	627	LEU
1	K	630	GLU
2	L	28	MET
2	L	31	LEU
2	L	38	ARG
2	L	60	LEU
2	L	62	ARG
2	L	65	GLU
2	L	78	ARG
2	L	82	LEU
2	L	84	ARG
2	L	85	GLU
2	L	95	SER
2	L	98	LEU
2	L	99	GLU
2	L	100	LEU
2	L	114	VAL
2	L	119	ILE
2	L	136	ASN
2	L	161	LEU
2	L	169	TYR
2	L	187	ASP
2	L	188	ARG
2	L	189	GLU
2	L	191	PHE
2	L	202	SER
2	L	206	ILE
2	L	208	GLN
2	L	212	VAL
2	L	217	THR

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Mol	Chain	Res	Type
2	L	234	ARG
2	L	240	PHE
2	L	269	VAL
2	L	279	ASP
2	L	280	ASP
2	L	297	ARG
2	L	302	LEU
2	L	304	CYS
2	L	305	ARG
2	L	315	GLU
2	L	327	GLN
2	L	329	TYR
2	L	350	LEU
2	L	353	THR
2	L	354	THR
2	L	373	ASN
2	L	377	PHE
2	L	392	CYS
2	L	403	ASN
2	L	405	THR
2	L	412	LYS
2	L	426	VAL
2	L	455	ARG
2	L	470	ILE
2	L	472	VAL
2	L	476	GLU
2	L	499	VAL
2	L	520	TYR
2	L	532	ILE
2	L	538	ARG
2	L	541	LEU
2	L	560	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	79	HIS
1	A	186	GLN
1	A	232	GLN
1	A	272	ASN
1	A	279	GLN

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Mol	Chain	Res	Type
1	A	372	GLN
1	A	493	GLN
1	A	501	GLN
1	A	540	ASN
1	A	666	GLN
2	B	36	ASN
2	B	54	ASN
2	B	64	HIS
2	B	72	GLN
2	B	75	HIS
2	B	106	HIS
2	B	157	GLN
2	B	197	ASN
2	B	198	GLN
2	B	208	GLN
2	B	236	GLN
2	B	266	HIS
2	B	303	GLN
2	B	363	HIS
2	B	373	ASN
2	B	382	GLN
2	B	386	HIS
2	B	393	GLN
2	B	402	GLN
2	B	403	ASN
2	B	411	GLN
2	B	449	ASN
2	B	467	ASN
2	B	496	GLN
2	B	512	GLN
1	C	79	HIS
1	C	123	GLN
1	C	186	GLN
1	C	232	GLN
1	C	279	GLN
1	C	311	GLN
1	C	337	ASN
1	C	372	GLN
1	C	378	ASN
1	C	492	HIS
1	C	501	GLN
1	C	617	GLN

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Mol	Chain	Res	Type
2	D	54	ASN
2	D	88	ASN
2	D	236	GLN
2	D	293	ASN
2	D	303	GLN
2	D	373	ASN
2	D	386	HIS
2	D	393	GLN
2	D	402	GLN
2	D	403	ASN
2	D	467	ASN
2	D	484	GLN
2	D	512	GLN
2	D	536	GLN
1	E	88	HIS
1	E	186	GLN
1	E	265	HIS
1	E	279	GLN
1	E	283	GLN
1	E	372	GLN
1	E	380	HIS
1	E	501	GLN
1	E	568	HIS
1	E	617	GLN
2	F	36	ASN
2	F	72	GLN
2	F	75	HIS
2	F	88	ASN
2	F	177	ASN
2	F	200	ASN
2	F	208	GLN
2	F	236	GLN
2	F	275	HIS
2	F	293	ASN
2	F	301	GLN
2	F	361	HIS
2	F	363	HIS
2	F	373	ASN
2	F	386	HIS
2	F	402	GLN
2	F	421	HIS
2	F	467	ASN

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Mol	Chain	Res	Type
2	F	484	GLN
2	F	489	GLN
2	F	536	GLN
1	G	50	GLN
1	G	186	GLN
1	G	232	GLN
1	G	279	GLN
1	G	283	GLN
1	G	372	GLN
1	G	501	GLN
1	G	510	GLN
1	G	534	HIS
1	G	540	ASN
2	H	36	ASN
2	H	72	GLN
2	H	75	HIS
2	H	157	GLN
2	H	197	ASN
2	H	200	ASN
2	H	236	GLN
2	H	275	HIS
2	H	303	GLN
2	H	363	HIS
2	H	373	ASN
2	H	382	GLN
2	H	386	HIS
2	H	393	GLN
2	H	402	GLN
2	H	403	ASN
2	H	449	ASN
2	H	467	ASN
2	H	489	GLN
2	H	512	GLN
2	H	516	GLN
2	H	536	GLN
1	I	79	HIS
1	I	88	HIS
1	I	279	GLN
1	I	311	GLN
1	I	372	GLN
1	I	492	HIS
1	I	501	GLN

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Mol	Chain	Res	Type
1	I	540	ASN
2	J	36	ASN
2	J	72	GLN
2	J	75	HIS
2	J	157	GLN
2	J	177	ASN
2	J	198	GLN
2	J	208	GLN
2	J	303	GLN
2	J	363	HIS
2	J	373	ASN
2	J	382	GLN
2	J	386	HIS
2	J	393	GLN
2	J	402	GLN
2	J	403	ASN
2	J	449	ASN
2	J	467	ASN
2	J	484	GLN
2	J	489	GLN
1	K	79	HIS
1	K	255	HIS
1	K	267	HIS
1	K	279	GLN
1	K	311	GLN
1	K	372	GLN
1	K	501	GLN
2	L	45	ASN
2	L	88	ASN
2	L	106	HIS
2	L	157	GLN
2	L	197	ASN
2	L	198	GLN
2	L	208	GLN
2	L	275	HIS
2	L	303	GLN
2	L	373	ASN
2	L	382	GLN
2	L	386	HIS
2	L	393	GLN
2	L	402	GLN
2	L	403	ASN

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Mol	Chain	Res	Type
2	L	449	ASN
2	L	467	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	$\#\|Z\| > 2$
3	BTI	A	801	1	16,16,16	1.66	1 (6%)	21,21,21	2.73	8 (38%)
4	COA	H	591	-	41,50,50	0.83	1 (2%)	52,75,75	1.07	2 (3%)
4	COA	J	591	-	41,50,50	0.83	1 (2%)	52,75,75	1.14	3 (5%)
4	COA	L	591	-	41,50,50	0.82	0	52,75,75	1.22	4 (7%)
4	COA	B	591	-	41,50,50	0.83	0	52,75,75	1.09	3 (5%)
4	COA	D	591	-	41,50,50	0.83	0	52,75,75	1.12	4 (7%)
4	COA	F	591	-	41,50,50	0.83	1 (2%)	52,75,75	1.21	3 (5%)
3	BTI	I	801	1	16,16,16	1.67	1 (6%)	21,21,21	2.67	8 (38%)

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
3	BTI	A	801	1	-	5/5/27/27	0/2/2/2
4	COA	H	591	-	-	13/44/64/64	0/3/3/3
4	COA	J	591	-	-	14/44/64/64	0/3/3/3
4	COA	L	591	-	-	15/44/64/64	0/3/3/3
4	COA	B	591	-	-	12/44/64/64	0/3/3/3
4	COA	D	591	-	-	12/44/64/64	0/3/3/3
4	COA	F	591	-	-	13/44/64/64	0/3/3/3
3	BTI	I	801	1	-	5/5/27/27	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	801	BTI	O3-C3	6.23	1.36	1.23
3	A	801	BTI	O3-C3	6.19	1.36	1.23
4	F	591	COA	O4B-C1B	2.06	1.43	1.41
4	J	591	COA	O4B-C1B	2.05	1.43	1.41
4	H	591	COA	O4B-C1B	2.02	1.43	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	BTI	C4-N2-C3	-6.72	106.36	112.62
3	I	801	BTI	C4-N2-C3	-5.80	107.22	112.62
3	I	801	BTI	N2-C3-N3	4.87	113.33	108.76
4	D	591	COA	N3A-C2A-N1A	-4.68	121.36	128.68
4	L	591	COA	P2A-O3A-P1A	-4.55	117.23	132.83
4	J	591	COA	N3A-C2A-N1A	-4.54	121.58	128.68
4	L	591	COA	N3A-C2A-N1A	-4.51	121.62	128.68
4	B	591	COA	N3A-C2A-N1A	-4.47	121.69	128.68
3	A	801	BTI	C6-S1-C2	4.44	99.01	89.89
4	F	591	COA	N3A-C2A-N1A	-4.42	121.77	128.68
3	A	801	BTI	N2-C3-N3	4.40	112.89	108.76
3	I	801	BTI	C6-S1-C2	4.35	98.82	89.89
4	F	591	COA	P2A-O3A-P1A	-4.30	118.07	132.83
4	H	591	COA	N3A-C2A-N1A	-4.28	121.99	128.68
3	A	801	BTI	C6-C5-N3	-4.21	107.68	113.03
3	I	801	BTI	C6-C5-N3	-4.17	107.73	113.03
3	A	801	BTI	C5-C6-S1	-3.91	102.96	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	801	BTI	C5-C6-S1	-3.65	103.18	106.31
4	J	591	COA	P2A-O3A-P1A	-3.52	120.73	132.83
4	H	591	COA	P2A-O3A-P1A	-3.32	121.42	132.83
3	I	801	BTI	C5-N3-C3	-3.28	108.18	112.46
3	A	801	BTI	C5-N3-C3	-3.18	108.31	112.46
4	D	591	COA	P2A-O3A-P1A	-3.01	122.50	132.83
3	I	801	BTI	C6-C5-C4	2.85	111.14	108.66
4	B	591	COA	P2A-O3A-P1A	-2.65	123.73	132.83
3	A	801	BTI	C2-C4-C5	2.48	111.82	108.94
4	B	591	COA	O4B-C1B-C2B	-2.40	103.41	106.93
3	I	801	BTI	C2-C4-C5	2.30	111.61	108.94
4	D	591	COA	O4B-C1B-C2B	-2.29	103.58	106.93
3	A	801	BTI	C6-C5-C4	2.21	110.58	108.66
4	L	591	COA	C4A-C5A-N7A	-2.11	107.20	109.40
4	D	591	COA	C4A-C5A-N7A	-2.07	107.24	109.40
4	L	591	COA	O4B-C1B-C2B	-2.06	103.91	106.93
4	J	591	COA	O4B-C1B-C2B	-2.05	103.94	106.93
4	F	591	COA	O4B-C1B-C2B	-2.04	103.95	106.93

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	BTI	C11-C10-C9-C8
3	A	801	BTI	S1-C2-C7-C8
3	A	801	BTI	C4-C2-C7-C8
4	H	591	COA	O4B-C4B-C5B-O5B
4	H	591	COA	C5B-O5B-P1A-O2A
4	H	591	COA	CCP-O6A-P2A-O3A
4	H	591	COA	CCP-O6A-P2A-O4A
4	H	591	COA	CCP-O6A-P2A-O5A
4	H	591	COA	CDP-CBP-CCP-O6A
4	H	591	COA	CEP-CBP-CCP-O6A
4	H	591	COA	CAP-CBP-CCP-O6A
4	H	591	COA	S1P-C2P-C3P-N4P
4	J	591	COA	O4B-C4B-C5B-O5B
4	J	591	COA	C5B-O5B-P1A-O2A
4	J	591	COA	CCP-O6A-P2A-O3A
4	J	591	COA	CCP-O6A-P2A-O4A
4	J	591	COA	CCP-O6A-P2A-O5A
4	J	591	COA	CDP-CBP-CCP-O6A
4	J	591	COA	CEP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
4	J	591	COA	CAP-CBP-CCP-O6A
4	J	591	COA	S1P-C2P-C3P-N4P
4	L	591	COA	O4B-C4B-C5B-O5B
4	L	591	COA	C5B-O5B-P1A-O2A
4	L	591	COA	CCP-O6A-P2A-O3A
4	L	591	COA	CCP-O6A-P2A-O4A
4	L	591	COA	CCP-O6A-P2A-O5A
4	L	591	COA	CDP-CBP-CCP-O6A
4	L	591	COA	CAP-CBP-CCP-O6A
4	L	591	COA	S1P-C2P-C3P-N4P
4	B	591	COA	O4B-C4B-C5B-O5B
4	B	591	COA	C5B-O5B-P1A-O2A
4	B	591	COA	CCP-O6A-P2A-O3A
4	B	591	COA	CCP-O6A-P2A-O4A
4	B	591	COA	CCP-O6A-P2A-O5A
4	B	591	COA	CDP-CBP-CCP-O6A
4	B	591	COA	CEP-CBP-CCP-O6A
4	B	591	COA	CAP-CBP-CCP-O6A
4	B	591	COA	S1P-C2P-C3P-N4P
4	D	591	COA	O4B-C4B-C5B-O5B
4	D	591	COA	C5B-O5B-P1A-O1A
4	D	591	COA	C5B-O5B-P1A-O2A
4	D	591	COA	CCP-O6A-P2A-O3A
4	D	591	COA	CCP-O6A-P2A-O4A
4	D	591	COA	CCP-O6A-P2A-O5A
4	D	591	COA	CDP-CBP-CCP-O6A
4	D	591	COA	CEP-CBP-CCP-O6A
4	D	591	COA	CAP-CBP-CCP-O6A
4	D	591	COA	S1P-C2P-C3P-N4P
4	F	591	COA	O4B-C4B-C5B-O5B
4	F	591	COA	C5B-O5B-P1A-O2A
4	F	591	COA	CCP-O6A-P2A-O3A
4	F	591	COA	CCP-O6A-P2A-O4A
4	F	591	COA	CCP-O6A-P2A-O5A
4	F	591	COA	CDP-CBP-CCP-O6A
4	F	591	COA	CEP-CBP-CCP-O6A
4	F	591	COA	CAP-CBP-CCP-O6A
4	F	591	COA	S1P-C2P-C3P-N4P
3	I	801	BTI	C11-C10-C9-C8
3	I	801	BTI	S1-C2-C7-C8
3	I	801	BTI	C4-C2-C7-C8
4	H	591	COA	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	J	591	COA	C3B-C4B-C5B-O5B
4	L	591	COA	C3B-C4B-C5B-O5B
4	B	591	COA	C3B-C4B-C5B-O5B
4	D	591	COA	C3B-C4B-C5B-O5B
4	F	591	COA	C3B-C4B-C5B-O5B
4	L	591	COA	CEP-CBP-CCP-O6A
3	A	801	BTI	C2-C7-C8-C9
3	I	801	BTI	C2-C7-C8-C9
3	I	801	BTI	C7-C8-C9-C10
4	L	591	COA	O5P-C5P-N4P-C3P
4	H	591	COA	C5B-O5B-P1A-O3A
4	J	591	COA	C5B-O5B-P1A-O3A
4	L	591	COA	C5B-O5B-P1A-O3A
4	B	591	COA	C5B-O5B-P1A-O3A
4	D	591	COA	C5B-O5B-P1A-O3A
4	F	591	COA	C5B-O5B-P1A-O3A
4	H	591	COA	C5B-O5B-P1A-O1A
4	J	591	COA	C5B-O5B-P1A-O1A
4	L	591	COA	C5B-O5B-P1A-O1A
4	B	591	COA	C5B-O5B-P1A-O1A
4	F	591	COA	C5B-O5B-P1A-O1A
3	A	801	BTI	C7-C8-C9-C10
4	J	591	COA	C2P-C3P-N4P-C5P
4	L	591	COA	C6P-C5P-N4P-C3P
4	J	591	COA	C5P-C6P-C7P-N8P
4	L	591	COA	C5P-C6P-C7P-N8P
4	F	591	COA	C5P-C6P-C7P-N8P
4	H	591	COA	O9P-C9P-CAP-OAP

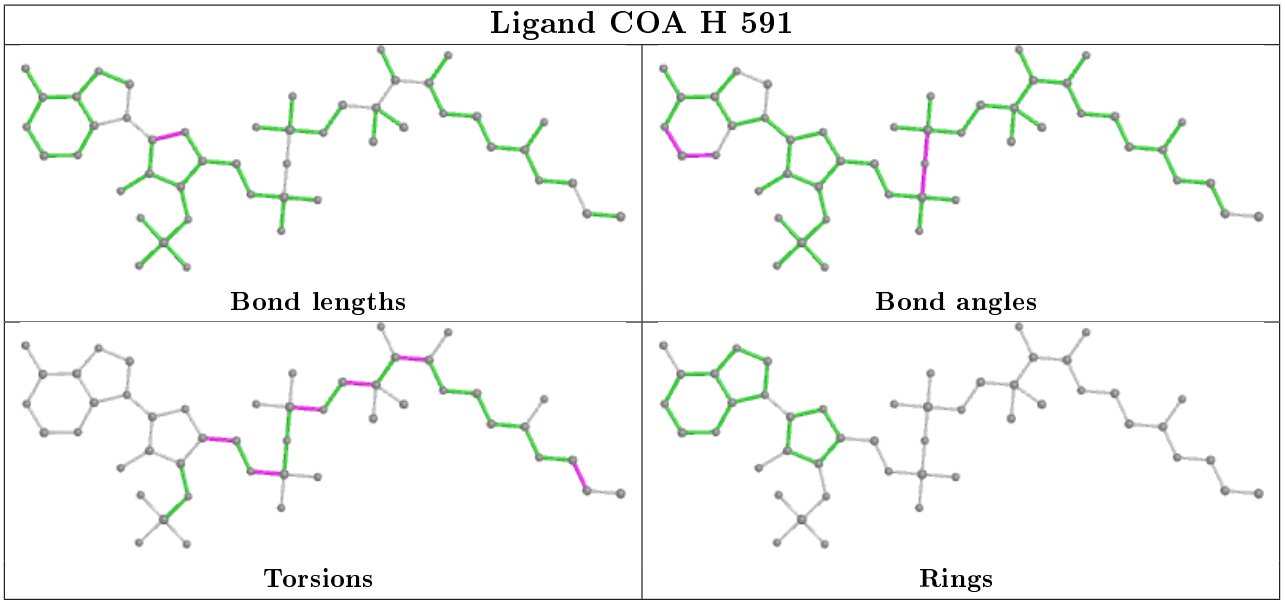
There are no ring outliers.

8 monomers are involved in 29 short contacts:

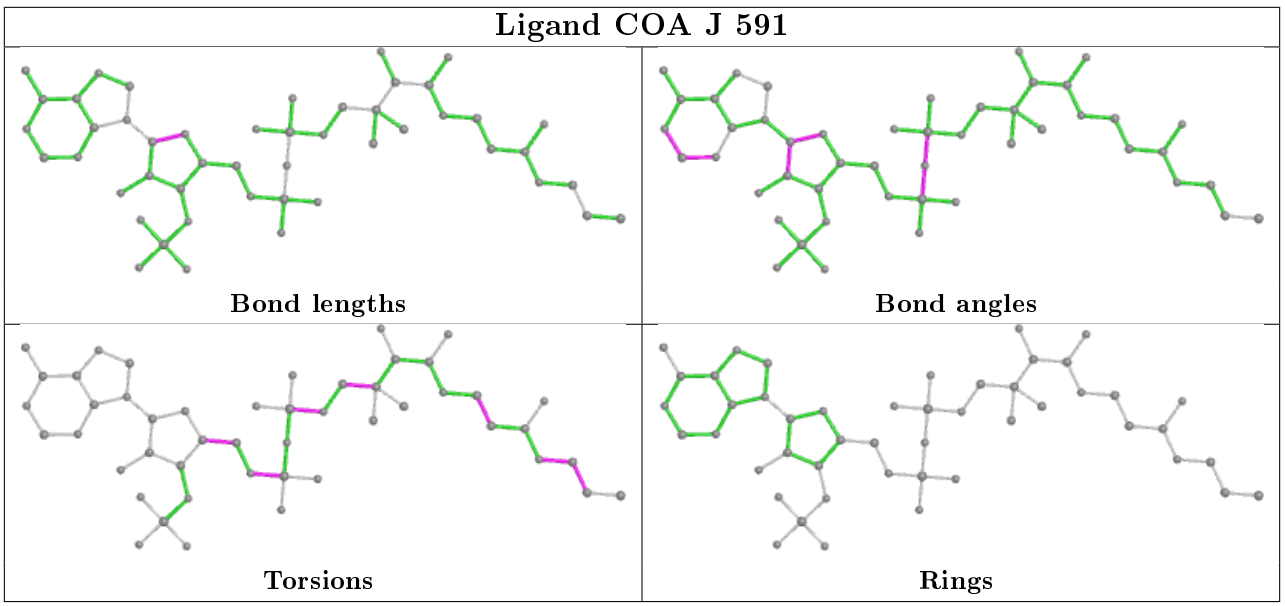
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	BTI	3	0
4	H	591	COA	6	0
4	J	591	COA	4	0
4	L	591	COA	2	0
4	B	591	COA	4	0
4	D	591	COA	3	0
4	F	591	COA	3	0
3	I	801	BTI	4	0

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

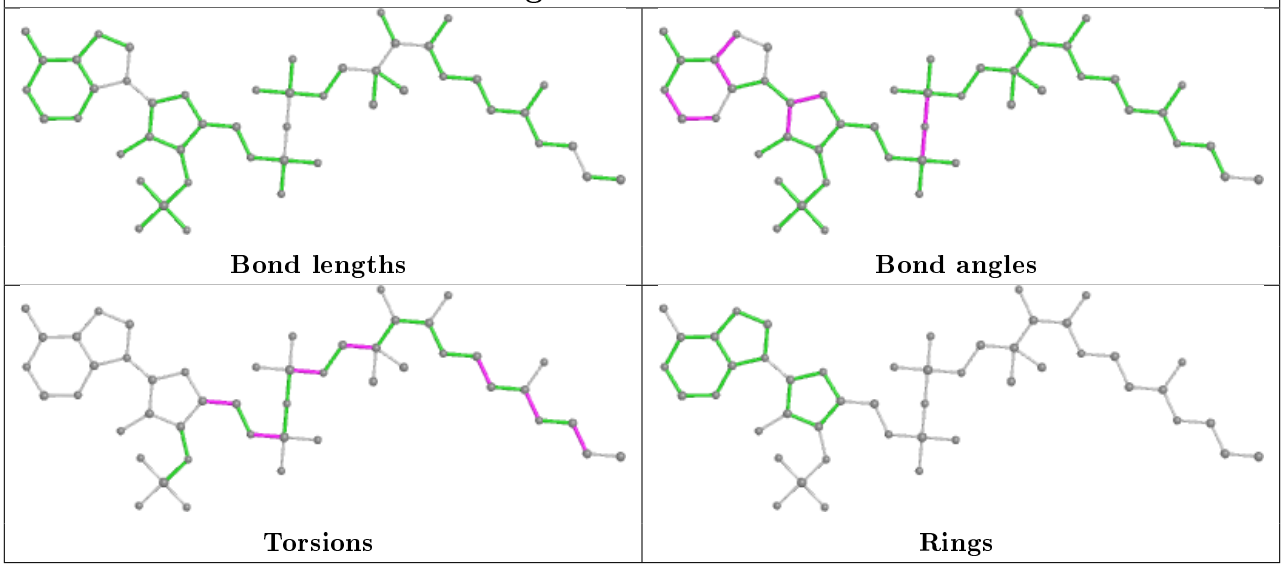
Ligand COA H 591



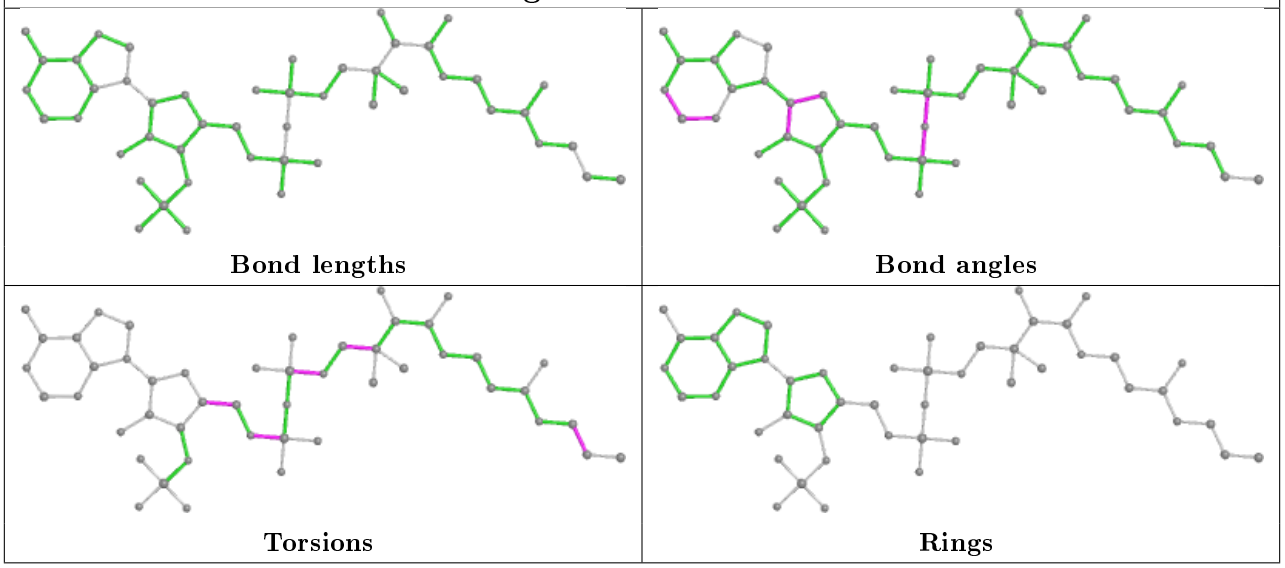
Ligand COA J 591

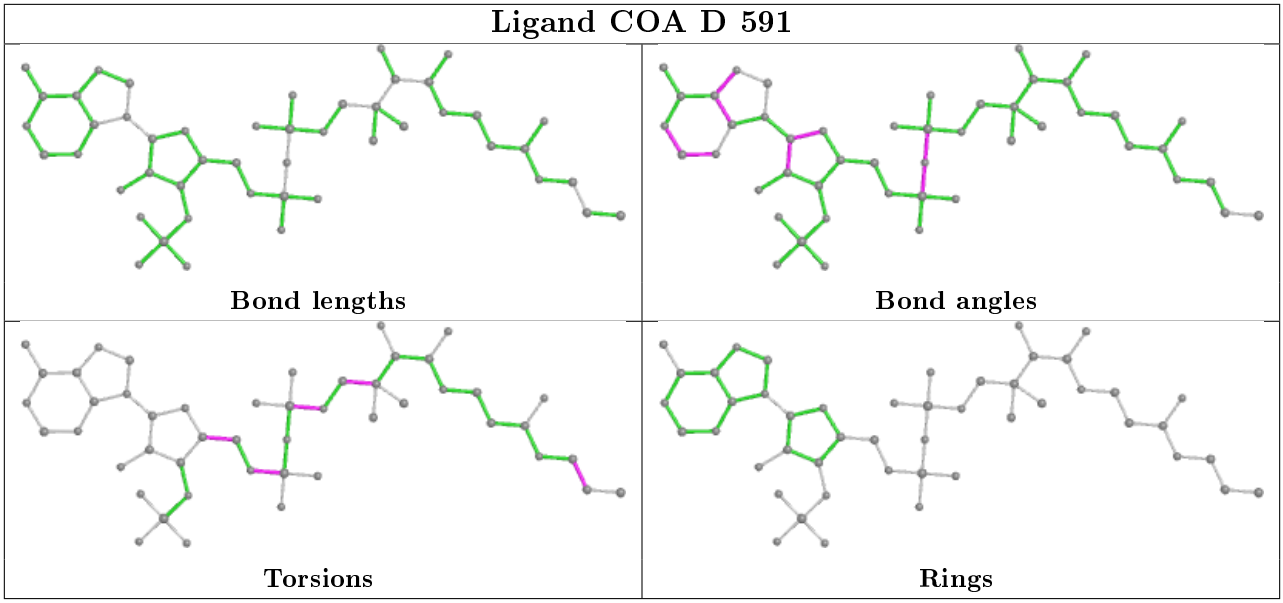


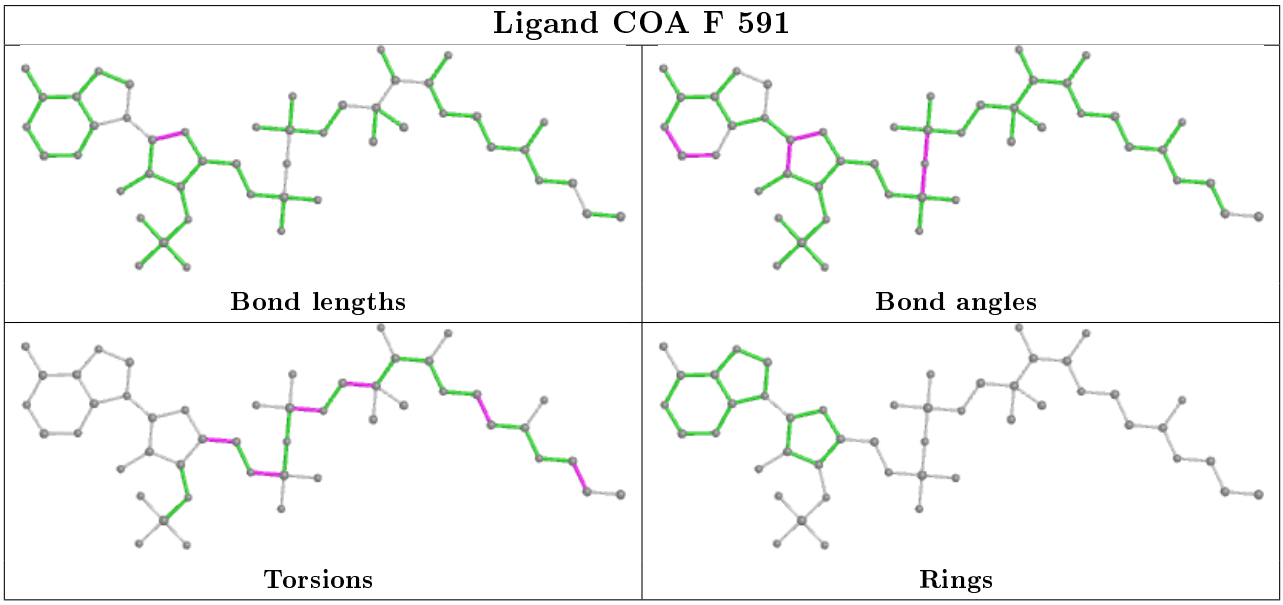
Ligand COA L 591



Ligand COA B 591







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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	621/655 (94%)	0.12	34 (5%) 25 22	71, 115, 170, 200	0
1	C	552/655 (84%)	-0.03	8 (1%) 75 69	69, 113, 154, 187	0
1	E	552/655 (84%)	-0.05	3 (0%) 91 88	71, 113, 154, 189	0
1	G	552/655 (84%)	-0.04	4 (0%) 87 83	76, 112, 155, 187	0
1	I	498/655 (76%)	-0.02	5 (1%) 82 77	73, 113, 146, 193	0
1	K	497/655 (75%)	0.05	8 (1%) 72 66	65, 115, 146, 187	0
2	B	537/555 (96%)	-0.39	0 100 100	60, 87, 140, 169	0
2	D	537/555 (96%)	-0.33	2 (0%) 92 90	58, 89, 143, 171	0
2	F	537/555 (96%)	-0.36	1 (0%) 95 93	58, 88, 142, 167	0
2	H	537/555 (96%)	-0.35	0 100 100	59, 88, 138, 169	0
2	J	537/555 (96%)	-0.21	7 (1%) 77 71	55, 88, 142, 168	0
2	L	537/555 (96%)	-0.29	6 (1%) 80 75	57, 88, 139, 167	0
All	All	6494/7260 (89%)	-0.16	78 (1%) 79 73	55, 103, 153, 200	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	647	GLY	6.4
1	A	648	GLY	5.0
1	C	391	PRO	4.5
1	A	715	ASP	4.4
2	L	497	LEU	4.2
1	A	694	VAL	4.0
1	A	712	VAL	3.8
2	J	497	LEU	3.5
1	K	180	GLY	3.3
1	A	699	CYS	3.2
2	D	497	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	244	MET	3.0
1	A	697	LEU	3.0
1	A	392	GLU	3.0
1	A	677	LEU	3.0
2	L	495	GLN	3.0
1	A	711	LEU	2.9
1	A	703	GLU	2.8
2	J	496	GLN	2.8
1	I	394	ASP	2.8
2	J	486	LYS	2.8
1	A	705	VAL	2.8
1	A	714	LEU	2.8
1	A	696	ALA	2.8
1	G	183	GLY	2.7
1	A	669	GLU	2.7
1	K	521	PRO	2.7
1	A	188	LEU	2.6
1	A	670	ALA	2.6
2	F	497	LEU	2.6
1	G	561	ARG	2.6
1	E	394	ASP	2.5
1	K	484	LEU	2.5
1	A	668	VAL	2.5
1	A	693	VAL	2.5
1	A	649	LEU	2.5
1	A	674	LEU	2.5
2	J	505	ILE	2.5
1	C	633	ASP	2.5
1	K	555	LEU	2.4
1	A	657	ILE	2.4
1	K	488	PHE	2.4
1	A	691	ALA	2.4
1	A	690	HIS	2.4
1	A	692	GLY	2.4
1	G	391	PRO	2.3
2	L	483	ALA	2.3
1	A	651	ALA	2.3
1	I	391	PRO	2.3
1	A	557	CYS	2.3
1	A	650	SER	2.3
1	C	205	LYS	2.3
1	I	250	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	204	LEU	2.2
1	K	434	LEU	2.2
1	A	228	LEU	2.2
1	E	183	GLY	2.2
1	G	188	LEU	2.2
2	J	503	ALA	2.2
1	A	667	THR	2.2
1	A	675	VAL	2.2
2	J	482	LEU	2.2
1	A	244	MET	2.2
2	L	499	VAL	2.2
1	A	689	PRO	2.2
1	A	706	GLU	2.2
1	I	630	GLU	2.1
1	K	250	LEU	2.1
1	K	47	ARG	2.1
1	C	246	VAL	2.1
2	L	486	LYS	2.1
1	I	555	LEU	2.0
1	C	397	PRO	2.0
2	D	496	GLN	2.0
1	E	553	LEU	2.0
1	C	392	GLU	2.0
2	J	501	GLU	2.0
2	L	500	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

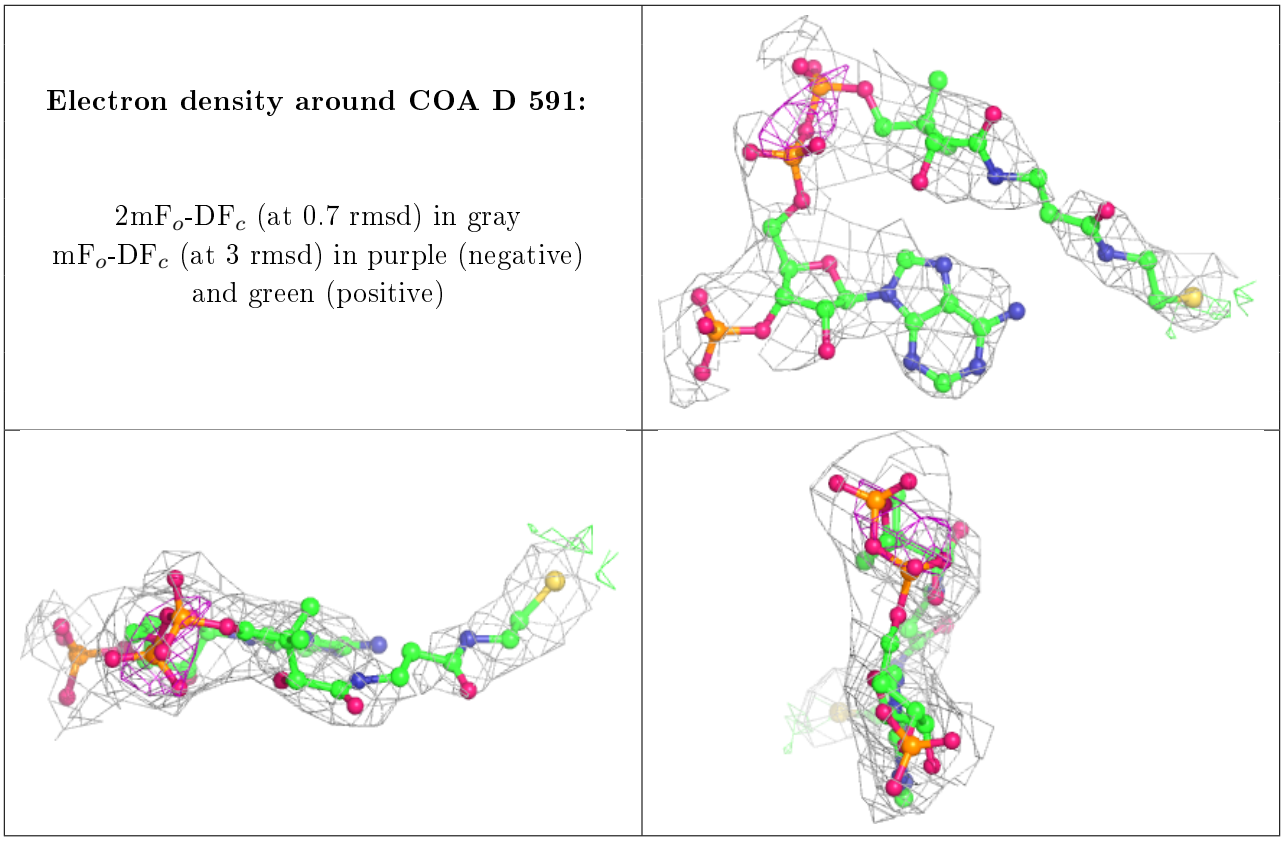
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BTI	A	801	15/15	0.84	0.50	140,152,154,155	0
3	BTI	I	801	15/15	0.84	0.43	142,152,155,158	0
4	COA	D	591	48/48	0.88	0.28	102,129,142,145	0
4	COA	F	591	48/48	0.89	0.28	97,124,134,135	0
4	COA	B	591	48/48	0.89	0.24	103,129,139,142	0
4	COA	J	591	48/48	0.91	0.21	101,127,136,137	0
4	COA	L	591	48/48	0.91	0.29	98,125,132,135	0
4	COA	H	591	48/48	0.93	0.22	102,128,137,139	0

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

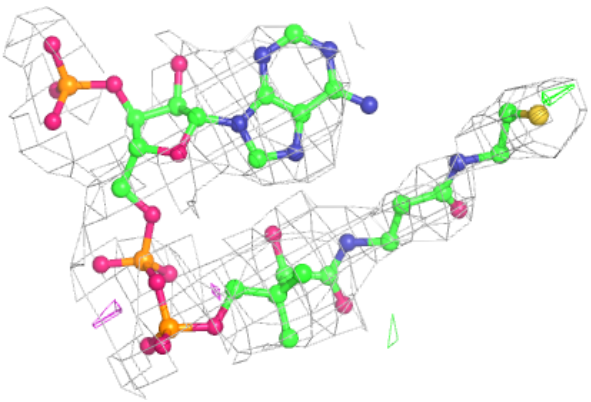
Electron density around COA D 591:

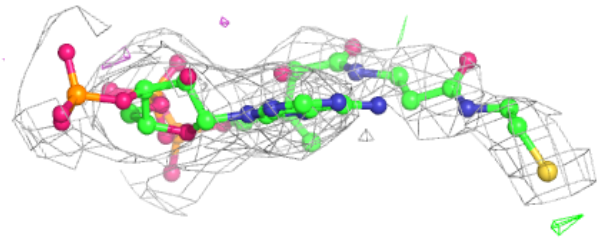
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

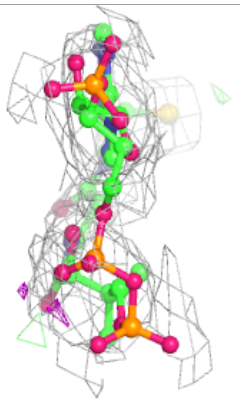


Electron density around COA F 591:

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

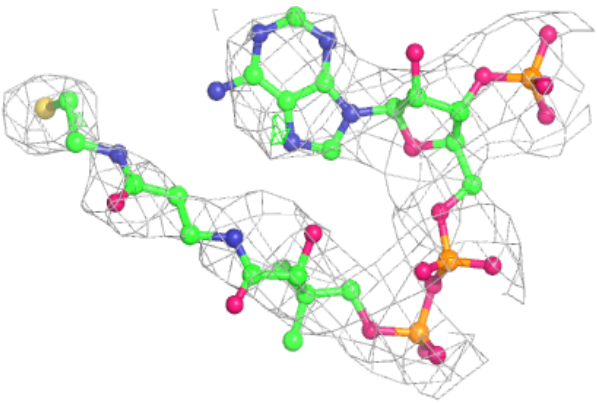


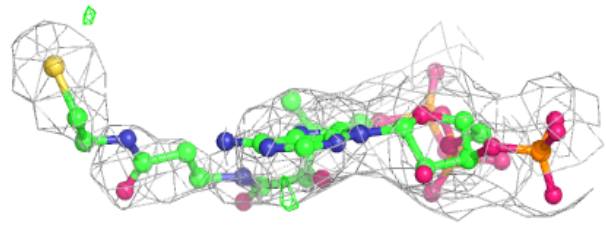


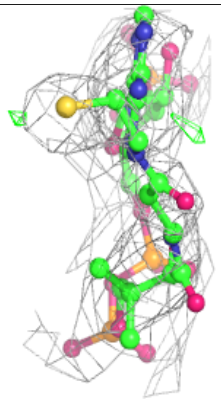


Electron density around COA B 591:

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

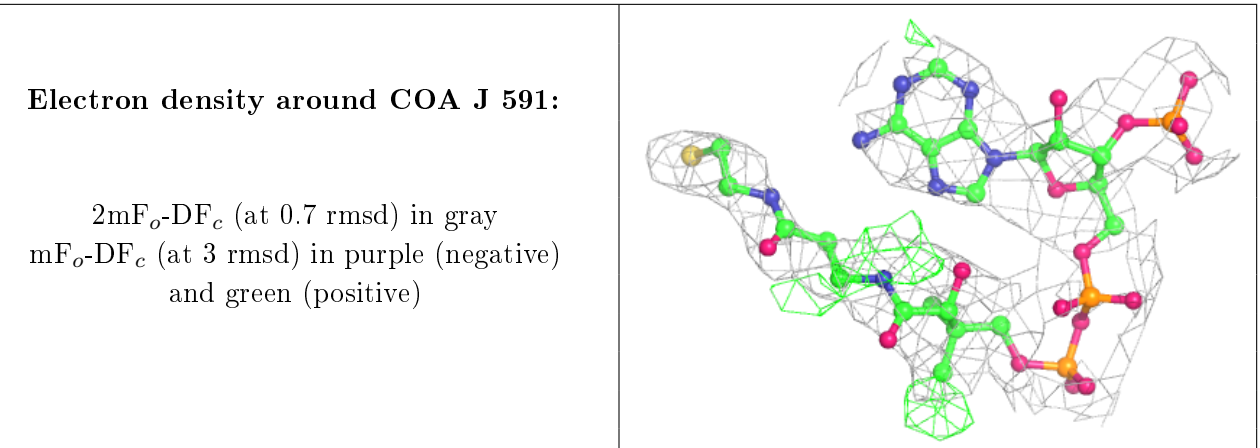


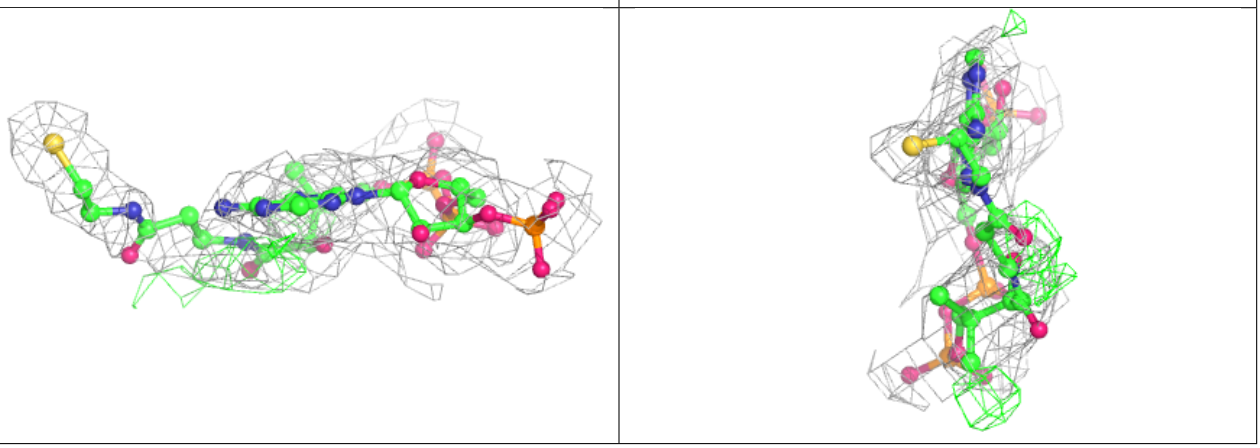




Electron density around COA J 591:

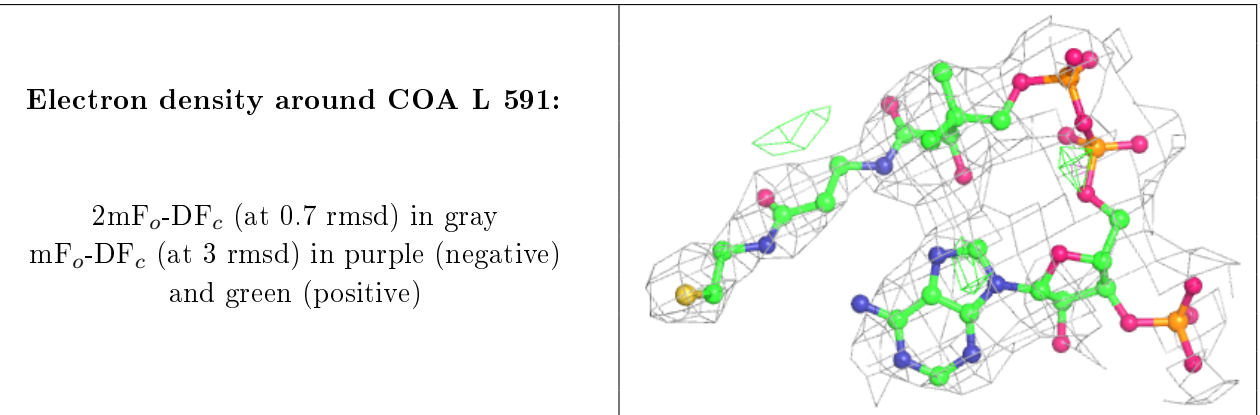
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

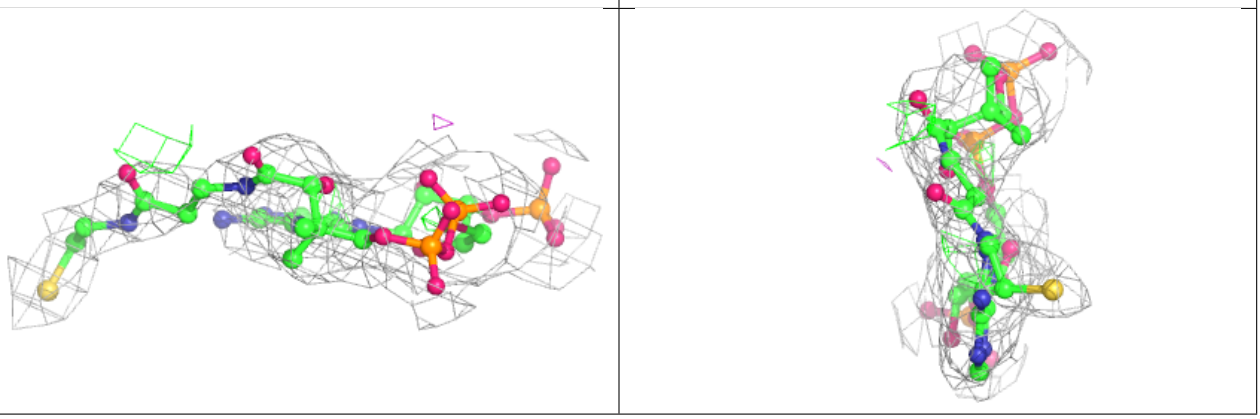




Electron density around COA L 591:

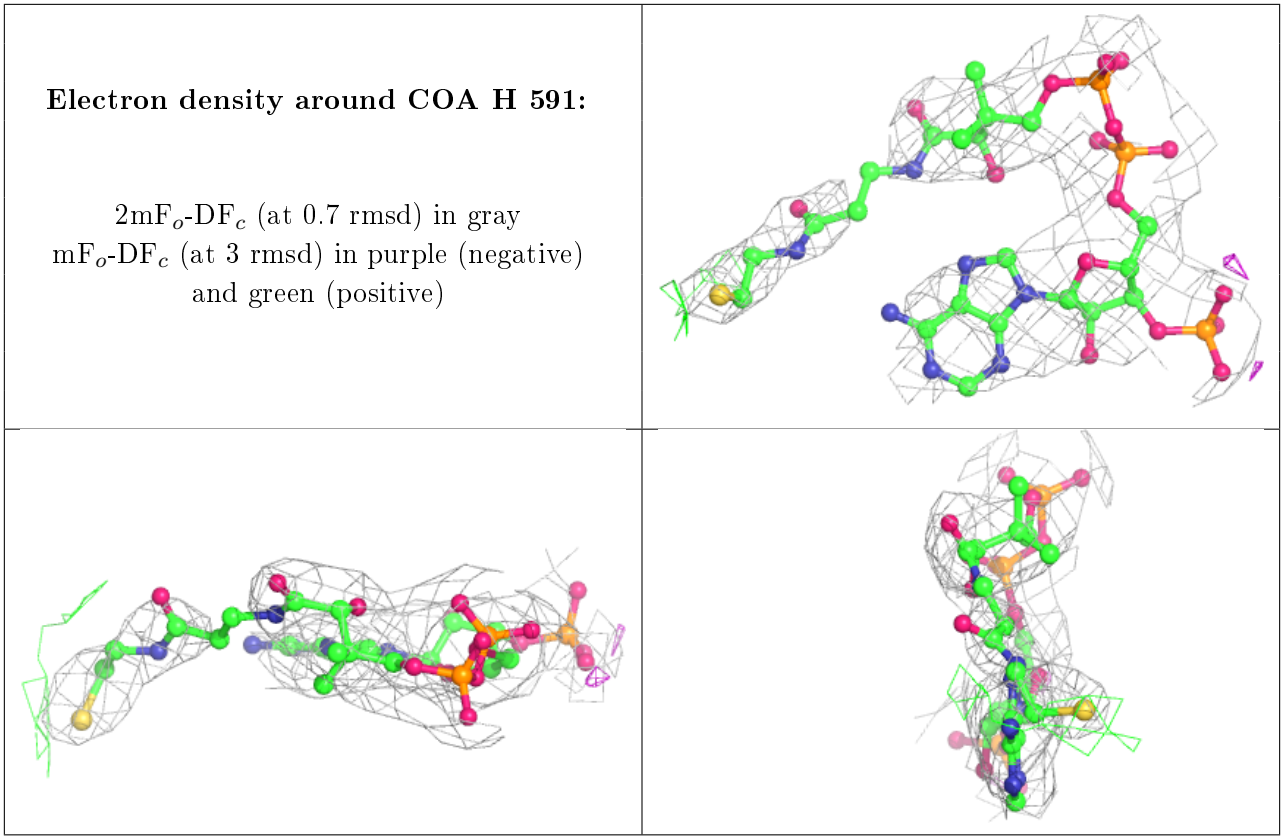
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around COA H 591:

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



6.5 Other polymers (i)

There are no such residues in this entry.