Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 10:40 PM EDT

PDB ID	:	3DBR
Title	:	Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190Gln-NEDD8Ala72Arg)
Authors	:	Souphron, J.; Schulman, B.A.
Deposited on	:	2008-06-02
Resolution	:	3.05 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

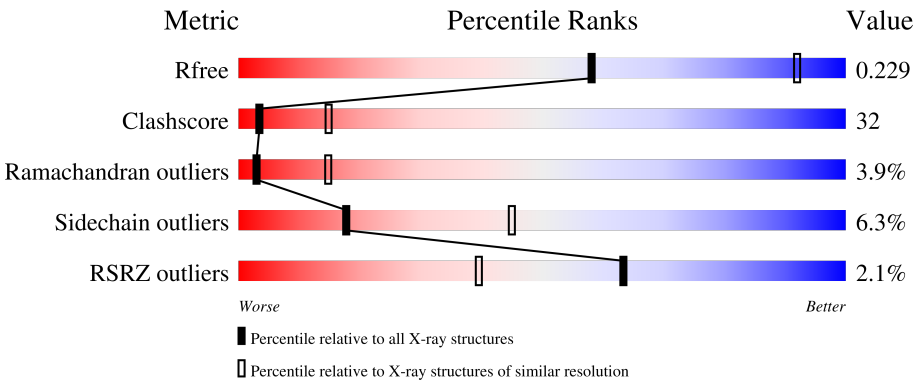
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	531	% 49% 44% 5% •
1	C	531	% 47% 44% 5% • •
1	E	531	2% 55% 36% 5% • •
1	G	531	2% 51% 42% • •
2	B	434	3% 50% 43% 7%

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Mol	Chain	Length	Quality of chain
2	D	434	2% 45% 48% 6%
2	F	434	4% 46% 48% 5%
2	H	434	3% 39% 52% 6%
3	I	88	% 53% 36% 7%
3	J	88	2% 40% 44% 13%
3	K	88	41% 36% 10% 13%
3	L	88	22% 61% 6% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32424 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 NEDD8-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	4104	2600	699	790	15	0	0	0
1	C	516	4096	2596	698	787	15	0	0	0
1	E	515	4093	2597	696	785	15	0	0	0
1	G	508	4038	2563	686	774	15	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q13564
A	0	SER	-	expression tag	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLU	deletion	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLY	deletion	UNP Q13564
A	?	-	ALA	deletion	UNP Q13564
C	-1	GLY	-	expression tag	UNP Q13564
C	0	SER	-	expression tag	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLU	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLY	deletion	UNP Q13564
C	?	-	ALA	deletion	UNP Q13564
E	-1	GLY	-	expression tag	UNP Q13564
E	0	SER	-	expression tag	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLU	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLY	deletion	UNP Q13564
E	?	-	ALA	deletion	UNP Q13564

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q13564
G	0	SER	-	expression tag	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLU	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLY	deletion	UNP Q13564
G	?	-	ALA	deletion	UNP Q13564

- Molecule 2 is a protein called NEDD8-activating enzyme E1 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	432	3402	2174	575	636	17	0	0	0
			Total	C	N	O	S			
2	D	431	3399	2174	575	633	17	0	0	0
			Total	C	N	O	S			
2	F	431	3395	2171	574	633	17	0	0	0
			Total	C	N	O	S			
2	H	431	3387	2164	573	633	17	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	expression tag	UNP Q8TBC4
B	10	LYS	-	expression tag	UNP Q8TBC4
B	11	LEU	-	expression tag	UNP Q8TBC4
B	190	GLN	ARG	engineered mutation	UNP Q8TBC4
B	216	ALA	CYS	engineered mutation	UNP Q8TBC4
D	9	MET	-	expression tag	UNP Q8TBC4
D	10	LYS	-	expression tag	UNP Q8TBC4
D	11	LEU	-	expression tag	UNP Q8TBC4
D	190	GLN	ARG	engineered mutation	UNP Q8TBC4
D	216	ALA	CYS	engineered mutation	UNP Q8TBC4
F	9	MET	-	expression tag	UNP Q8TBC4
F	10	LYS	-	expression tag	UNP Q8TBC4
F	11	LEU	-	expression tag	UNP Q8TBC4
F	190	GLN	ARG	engineered mutation	UNP Q8TBC4
F	216	ALA	CYS	engineered mutation	UNP Q8TBC4
H	9	MET	-	expression tag	UNP Q8TBC4
H	10	LYS	-	expression tag	UNP Q8TBC4
H	11	LEU	-	expression tag	UNP Q8TBC4
H	190	GLN	ARG	engineered mutation	UNP Q8TBC4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	85	666	414	122	128	2	0	0	0
3	J	77	612	384	108	118	2	0	0	0
3	K	77	612	384	108	118	2	0	0	0
3	L	78	616	386	109	119	2	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	89	GLY	-	expression tag	UNP Q15843
I	90	SER	-	expression tag	UNP Q15843
I	91	ARG	-	expression tag	UNP Q15843
I	92	ARG	-	expression tag	UNP Q15843
I	93	ALA	-	expression tag	UNP Q15843
I	94	SER	-	expression tag	UNP Q15843
I	95	VAL	-	expression tag	UNP Q15843
I	96	GLY	-	expression tag	UNP Q15843
I	97	SER	-	expression tag	UNP Q15843
I	98	GLY	-	expression tag	UNP Q15843
I	99	GLY	-	expression tag	UNP Q15843
I	100	SER	-	expression tag	UNP Q15843
I	172	ARG	ALA	engineered mutation	UNP Q15843
J	89	GLY	-	expression tag	UNP Q15843
J	90	SER	-	expression tag	UNP Q15843
J	91	ARG	-	expression tag	UNP Q15843
J	92	ARG	-	expression tag	UNP Q15843
J	93	ALA	-	expression tag	UNP Q15843
J	94	SER	-	expression tag	UNP Q15843
J	95	VAL	-	expression tag	UNP Q15843
J	96	GLY	-	expression tag	UNP Q15843
J	97	SER	-	expression tag	UNP Q15843
J	98	GLY	-	expression tag	UNP Q15843
J	99	GLY	-	expression tag	UNP Q15843
J	100	SER	-	expression tag	UNP Q15843

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Chain	Residue	Modelled	Actual	Comment	Reference
J	172	ARG	ALA	engineered mutation	UNP Q15843
K	89	GLY	-	expression tag	UNP Q15843
K	90	SER	-	expression tag	UNP Q15843
K	91	ARG	-	expression tag	UNP Q15843
K	92	ARG	-	expression tag	UNP Q15843
K	93	ALA	-	expression tag	UNP Q15843
K	94	SER	-	expression tag	UNP Q15843
K	95	VAL	-	expression tag	UNP Q15843
K	96	GLY	-	expression tag	UNP Q15843
K	97	SER	-	expression tag	UNP Q15843
K	98	GLY	-	expression tag	UNP Q15843
K	99	GLY	-	expression tag	UNP Q15843
K	100	SER	-	expression tag	UNP Q15843
K	172	ARG	ALA	engineered mutation	UNP Q15843
L	89	GLY	-	expression tag	UNP Q15843
L	90	SER	-	expression tag	UNP Q15843
L	91	ARG	-	expression tag	UNP Q15843
L	92	ARG	-	expression tag	UNP Q15843
L	93	ALA	-	expression tag	UNP Q15843
L	94	SER	-	expression tag	UNP Q15843
L	95	VAL	-	expression tag	UNP Q15843
L	96	GLY	-	expression tag	UNP Q15843
L	97	SER	-	expression tag	UNP Q15843
L	98	GLY	-	expression tag	UNP Q15843
L	99	GLY	-	expression tag	UNP Q15843
L	100	SER	-	expression tag	UNP Q15843
L	172	ARG	ALA	engineered mutation	UNP Q15843

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

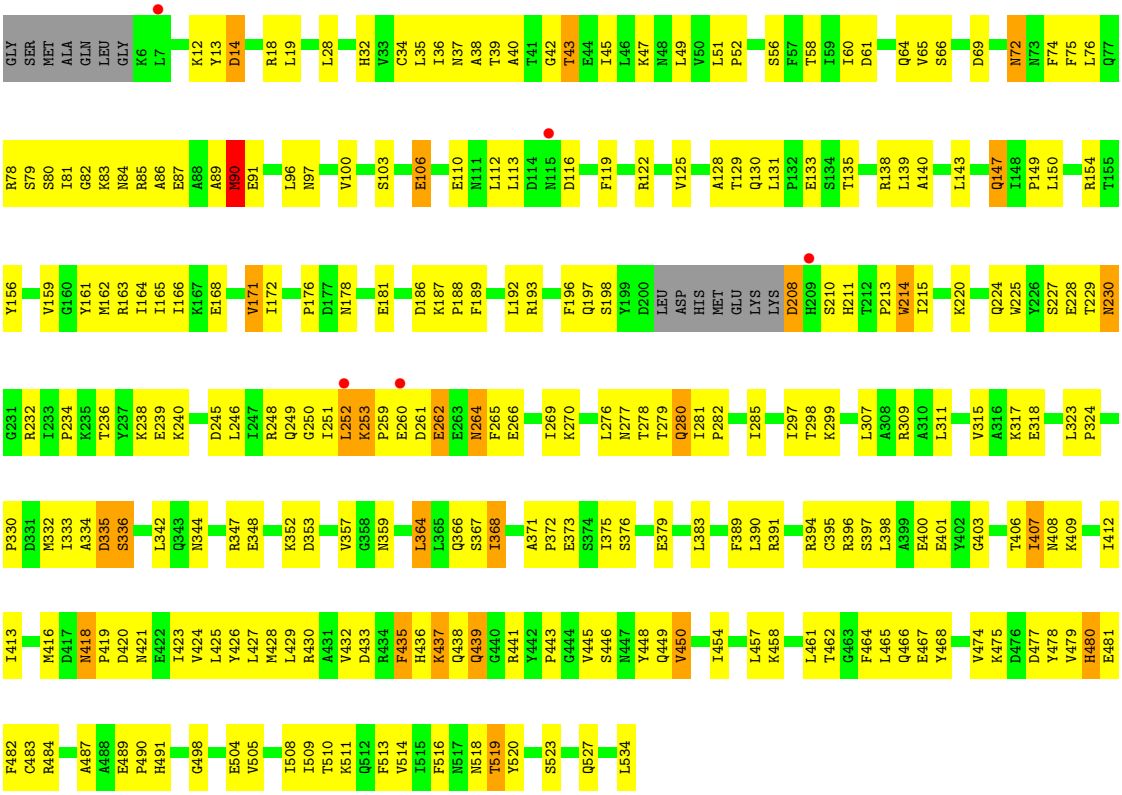
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	1	1	1	0	0
4	D	1	1	1	0	0
4	F	1	1	1	0	0
4	H	1	1	1	0	0

3 Residue-property plots (i)

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

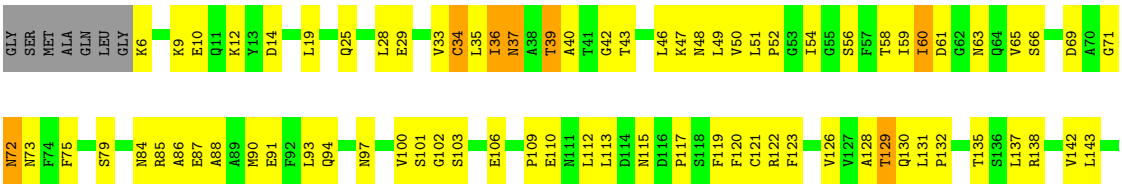
• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

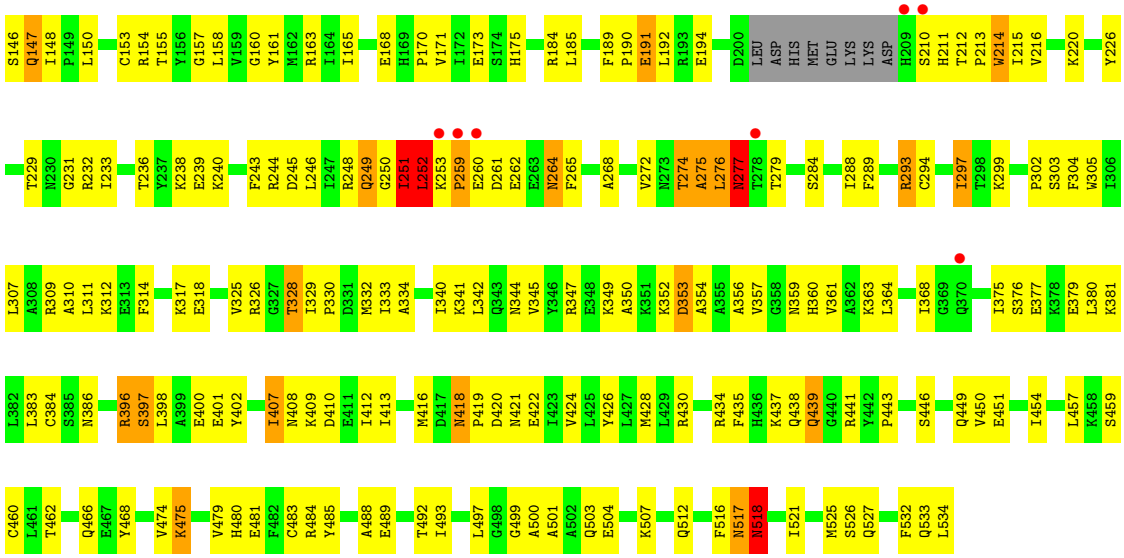
Chain A:



• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

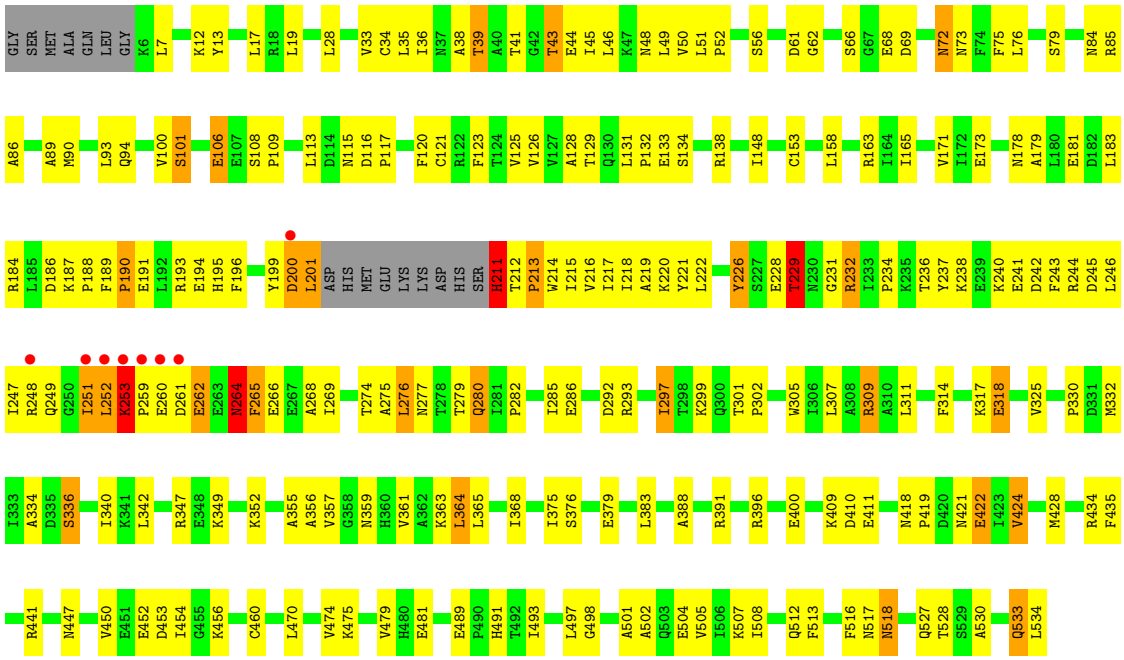
Chain C:





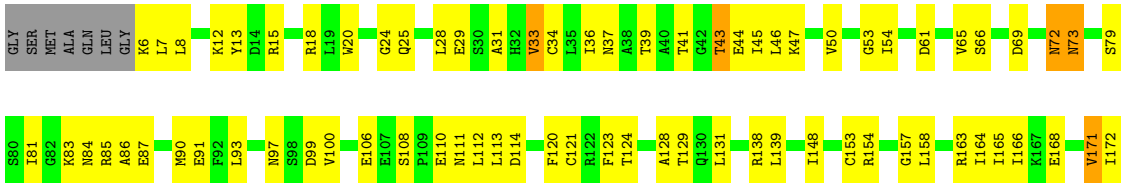
• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain E:



• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain G:



E173 L180 R184 L185 D186 K187 P188 F189 L192 R193 E194 H195 F196 Q197 S198 Y199 ASP LEU ASP HIS MET GLU LYS LYS ASP HIS SER HIS T212 P213 W214 I215 V216 I217 I218 A219 K220 Y221 L222 W225 Y226 T229 N230 G231 R232 I233 P234 K235 T236 Y237 K238 E239 K240 E241 D242

F243 R244 D245 L246 I247 R248 Q249 G250 I251 L252 LYS PRO GLU ASP E262 E263 N264 F265 E266 E267 A268 I269 K270 N271 V272 A275 L276 N277 T278 T279 P282 S283 S284 I285 E286 D287 I288 R293 T298 K299 Q300 W305 I306 L307 L311 F314 E318 G319 Q320 G321 N322 L323

P324 V325 P330 D331 M332 I333 A334 D335 S336 Y339 I340 K341 L342 Q343 N344 V345 Y346 R347 E348 H360 V361 A362 K363 L364 L365 Q366 S367 I368 E377 K381 L382 L383 C384 S385 N386 S387 A388 R391 R394 C395 R396 S397 E400 L404 D405 T406 I407 N408 K409 D410

M416 D417 N418 P419 D420 N421 E422 I423 V424 L425 Y426 L427 M428 V432 D433 R434 F435 H436 K437 Q438 R441 S446 N447 Y448 Q449 Q450 E451 E452 D453 I454 F464 E467 K475 H480 E481 R484 Y485 A488 E489 P490 H491 T492 I493 L497 G498 Q503 E504 K507

I508 I509 T510 K511 Q512 F513 V514 I515 F516 N517 N518 Q527 F532 Q533 L534

- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain B: 3% 50% 43% 7%

MET LYS L11 D12 W13 E14 G15 R16 W17 N18 H19 K22 F23 L24 E25 R26 S27 G28 T31 H32 P33 D34 P37 S38 L46 C49 K50 V51 L52 E62 L63 L64 K65 N66 L67 A68 L69 R73 Q74 I78 D81 T82 I83 D84 V85 S86 N87 F92 L93 F94

R95 P96 K97 D98 I99 P102 K103 A104 E105 L111 R114 V115 P116 N117 C118 N119 H123 K126 I127 Q128 D129 F130 N131 D132 T133 F134 Q137 F138 H139 I149 A150 R151 R152 W153 I154 N155 G156 M157 L158 D166 G167 V168 L177 I178 T182 F185 K186 G187 N188

A189 Q190 V191 G195 M196 T197 A198 C199 I200 T203 Y207 P208 V211 P214 T217 I218 A219 S220 M221 P222 R223 E226 I229 E230 Y231 V232 R233 Q236 W237 P238 K239 E240 Q241 P242 F243 G246 L249 D250 G251 D252 D253 P254 E255 H256 I257 I260 K263

S264 L265 R274 Y278 R279 L280 T281 V284 V285 K286 R287 I288 I289 P290 A291 V292 N296 A300 A301 V302 E306 K309 I310 A311 T312 S313 A314 Y315 I316 P317 L318 N319 N320 Y321 L322 N325 D326 V327 D328 Y331 T334 F335 E336 A337 E338 R339 N342 C343

C346 S347 Q348 L349 P350 Q351 N352 I353 Q354 F355 S356 P357 S358 A359 K360 L361 Q362 E363 V364 Y367 L368 L374 Q375 M376 A380 I381 T382 L385 E386 G387 K388 N389 R390 T391 L392 Y393 L394 S399 I400 E401 E402 R403 T404 R405 P406 N407 L408 T411 L412 K413 E414 L415 G416 L417

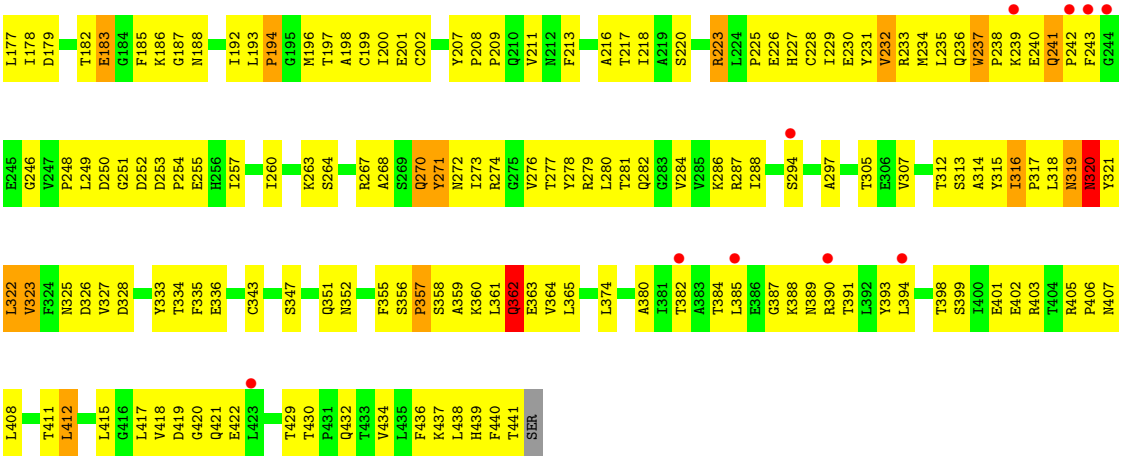
V418 D419 G420 Q421 E422 L423 A424 V425 A426 D427 V428 T429 T430 P431 V434 L435 F436 K437 L438 H439 F440 T441 S442

- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain D: 2% 45% 48% 6%

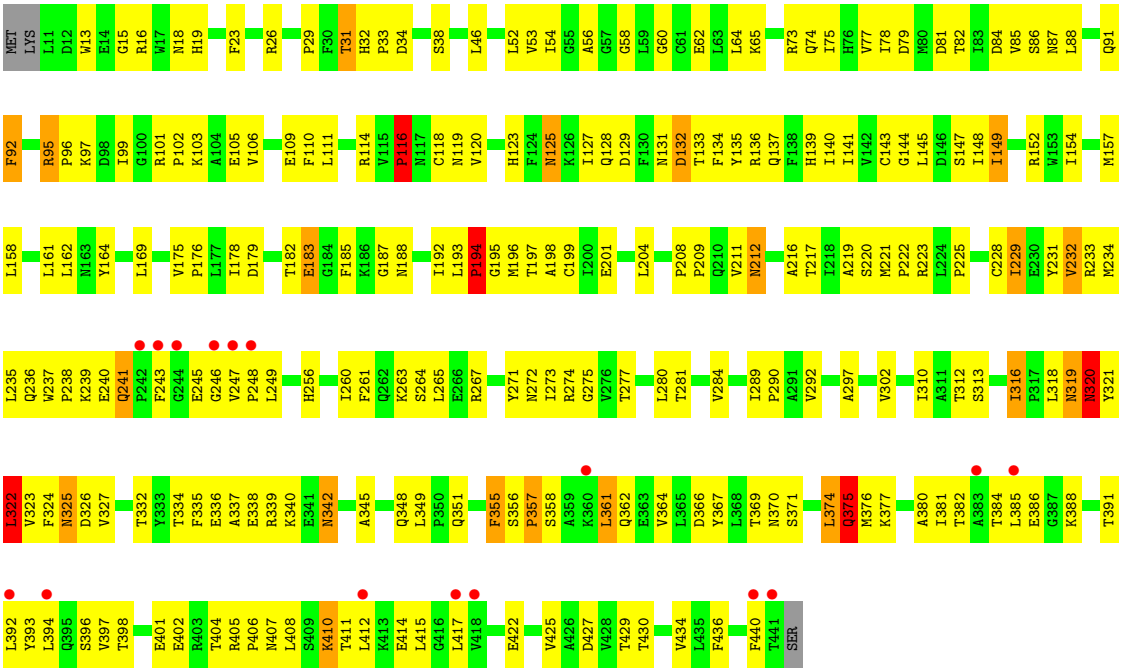
MET LYS L11 D12 W13 E14 G15 R16 W17 N18 H19 V20 K21 K22 F23 L24 E25 R26 S27 G28 P29 F30 T31 H32 P33 D34 P37 S41 L46 I54 G57 G58 E62 L63 L64 K65 N66 L67 F72 R73 Q74 I75 H76 V77 T82 I83 N87 R90 Q91 F92

L93 F94 K97 D98 I99 K103 V106 E109 F110 L111 N112 D113 R114 V115 P116 N119 F124 N125 Q128 N131 D132 R136 Q137 F138 H139 I140 I141 V142 L145 I148 I149 A150 R151 R152 W153 I154 M157 L158 L162 L169 D170 P171 S172 V175 P176



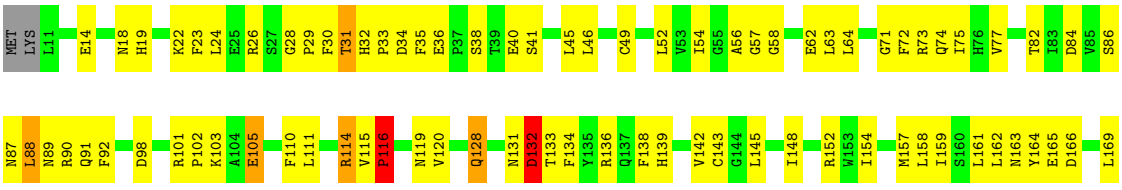
- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

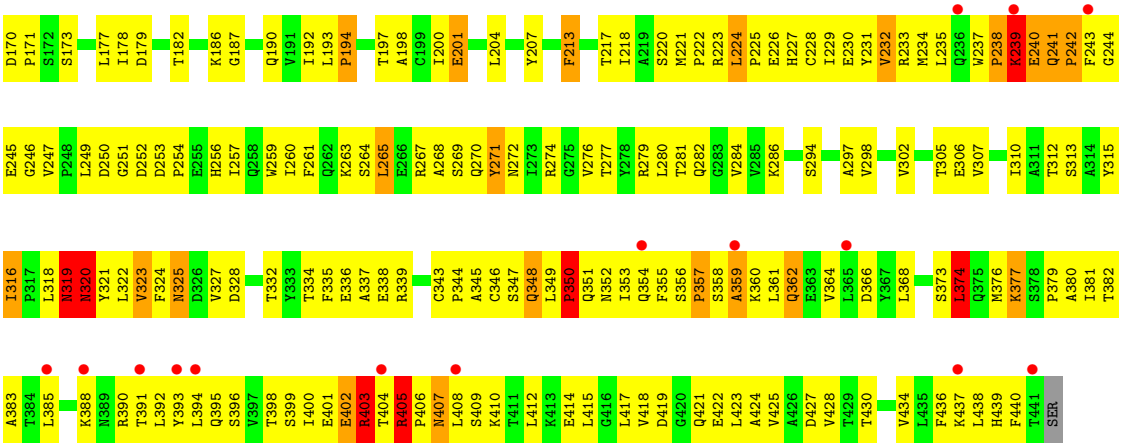
Chain F:



- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

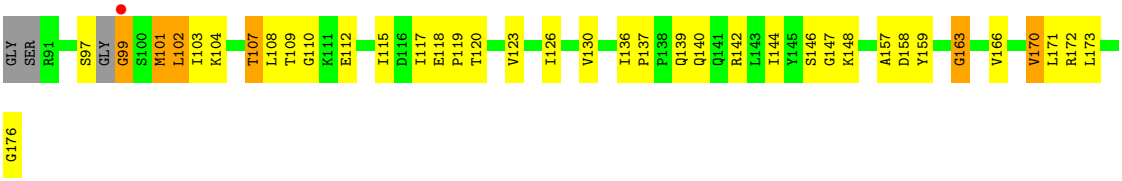
Chain H:





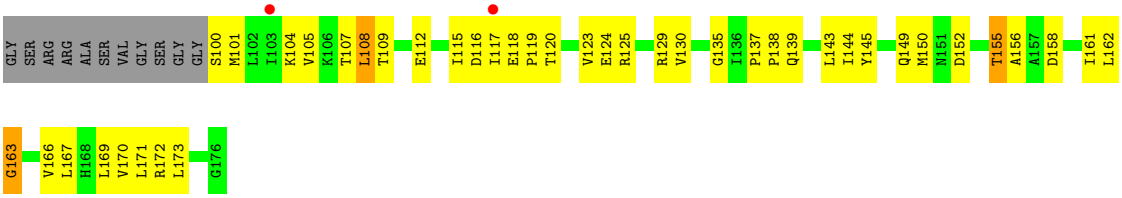
- Molecule 3: NEDD8

Chain I:



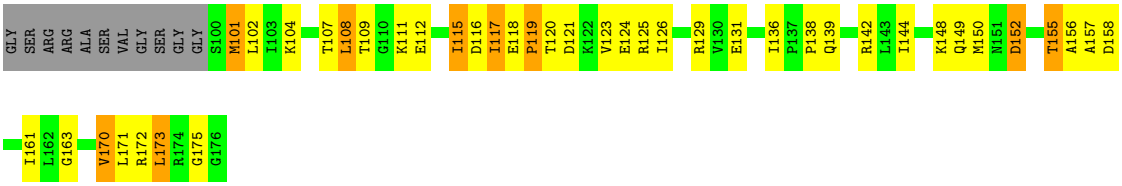
- Molecule 3: NEDD8

Chain J:



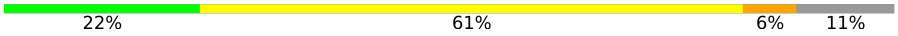
- Molecule 3: NEDD8

Chain K:



- Molecule 3: NEDD8

Chain L:



E153
K154
T155
A156
A157
D158
Y159
K160
I161
L162
G163
G164
S165
V166
L167
H168
L169
V170
L171
R172
L173
R174
G175
G176

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.32Å 198.53Å 208.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.05 48.29 – 3.07	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-3.05) 95.3 (48.29-3.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 3.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.280 0.232 , 0.229	Depositor DCC
R_{free} test set	4982 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32424	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% 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 (i)

5.1 Standard geometry (i)

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

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	0.43	0/4184	0.68	1/5660 (0.0%)
1	C	0.45	0/4176	0.73	9/5649 (0.2%)
1	E	0.48	1/4172 (0.0%)	0.71	2/5643 (0.0%)
1	G	0.41	0/4114	0.67	1/5563 (0.0%)
2	B	0.50	1/3480 (0.0%)	0.75	4/4736 (0.1%)
2	D	0.44	0/3477	0.72	2/4732 (0.0%)
2	F	0.46	0/3473	0.73	3/4728 (0.1%)
2	H	0.50	0/3465	0.85	10/4718 (0.2%)
3	I	0.55	2/670 (0.3%)	0.77	0/891
3	J	0.43	0/617	0.82	1/823 (0.1%)
3	K	0.46	0/617	0.78	0/823
3	L	0.61	1/621 (0.2%)	0.98	5/828 (0.6%)
All	All	0.46	5/33066 (0.0%)	0.74	38/44794 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	442	SER	C-O	8.06	1.38	1.23
1	E	211	HIS	CG-CD2	-6.33	1.25	1.35
3	I	99	GLY	C-O	-5.79	1.14	1.23
3	I	99	GLY	CA-C	5.25	1.60	1.51
3	L	99	GLY	N-CA	5.09	1.53	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	320	ASN	N-CA-C	12.33	144.30	111.00
2	B	442	SER	N-CA-C	-9.77	84.61	111.00
2	D	320	ASN	N-CA-C	9.75	137.32	111.00
3	L	100	SER	N-CA-C	9.41	136.40	111.00
2	H	271	TYR	N-CA-C	-8.89	86.99	111.00
2	H	403	ARG	C-N-CA	-8.72	99.91	121.70
2	B	320	ASN	N-CA-C	8.68	134.43	111.00
1	C	518	ASN	N-CA-C	8.31	133.44	111.00
2	H	240	GLU	N-CA-C	-7.99	89.43	111.00
1	C	277	ASN	N-CA-CB	7.19	123.55	110.60
1	E	252	LEU	CA-CB-CG	-7.04	99.11	115.30
2	F	320	ASN	N-CA-C	7.00	129.91	111.00
3	L	101	MET	N-CA-C	-6.75	92.78	111.00
1	C	276	LEU	N-CA-C	6.74	129.20	111.00
2	H	240	GLU	C-N-CA	-6.69	104.97	121.70
2	F	375	GLN	N-CA-C	6.57	128.75	111.00
3	L	100	SER	CA-C-N	-6.55	102.79	117.20
2	D	319	ASN	N-CA-C	-6.54	93.35	111.00
2	H	239	LYS	N-CA-C	6.17	127.65	111.00
1	C	252	LEU	N-CA-C	6.14	127.58	111.00
2	B	386	GLU	N-CA-C	-5.95	94.94	111.00
1	C	210	SER	N-CA-C	-5.85	95.20	111.00
2	H	359	ALA	N-CA-C	5.79	126.62	111.00
2	B	240	GLU	N-CA-C	-5.74	95.50	111.00
3	J	100	SER	CA-C-N	-5.64	104.80	117.20
1	C	211	HIS	CB-CA-C	5.58	121.57	110.40
1	C	129	THR	CA-CB-CG2	-5.57	104.60	112.40
2	H	241	GLN	C-N-CD	-5.57	108.35	120.60
2	F	322	LEU	CA-CB-CG	5.50	127.96	115.30
2	H	319	ASN	C-N-CA	-5.43	108.12	121.70
1	A	519	THR	N-CA-C	5.40	125.58	111.00
3	L	120	THR	N-CA-C	5.29	125.29	111.00
3	L	100	SER	O-C-N	5.25	131.09	122.70
1	C	260	GLU	N-CA-C	-5.19	96.98	111.00
2	H	321	TYR	N-CA-CB	-5.12	101.38	110.60
1	E	232	ARG	N-CA-C	5.11	124.80	111.00
1	G	252	LEU	CA-CB-CG	-5.08	103.62	115.30
1	C	129	THR	CA-C-N	5.07	128.35	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	319	ASN	Mainchain

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	4104	0	4052	264	0
1	C	4096	0	4048	255	0
1	E	4093	0	4059	220	0
1	G	4038	0	4009	220	0
2	B	3402	0	3380	253	0
2	D	3399	0	3386	241	0
2	F	3395	0	3375	269	0
2	H	3387	0	3354	311	0
3	I	666	0	703	49	0
3	J	612	0	648	46	0
3	K	612	0	648	47	0
3	L	616	0	651	74	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	32424	0	32313	2093	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 32.

All (2093) 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:252:LEU:O	1:C:259:PRO:HD2	1.17	1.33
1:A:252:LEU:O	1:A:259:PRO:HD2	1.25	1.30
1:C:517:ASN:ND2	1:C:518:ASN:H	1.31	1.28
2:F:371:SER:CB	2:F:374:LEU:HD11	1.64	1.26
1:C:517:ASN:HD22	1:C:518:ASN:N	1.35	1.24
2:F:371:SER:HB3	2:F:374:LEU:HD11	1.20	1.12
1:A:259:PRO:HB2	1:A:262:GLU:OE1	1.51	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:123:VAL:HB	3:K:152:ASP:HA	1.29	1.11
2:F:149:ILE:HD12	2:F:149:ILE:H	1.06	1.10
1:G:333:ILE:HG22	2:H:223:ARG:NH2	1.66	1.10
1:A:36:ILE:HD12	1:A:60:ILE:HB	1.25	1.10
3:J:123:VAL:HB	3:J:152:ASP:HA	1.33	1.09
2:D:149:ILE:H	2:D:149:ILE:HD12	1.11	1.09
2:B:338:GLU:HG3	3:I:148:LYS:HG2	1.30	1.09
2:F:325:ASN:HD21	2:F:327:VAL:HG23	0.98	1.08
2:D:207:TYR:CE1	3:J:172:ARG:HD3	1.89	1.07
1:E:226:TYR:CD1	1:E:231:GLY:HA2	1.89	1.07
1:A:208:ASP:N	1:A:211:HIS:HB2	1.69	1.07
2:B:357:PRO:HD2	2:B:442:SER:O	1.56	1.05
1:C:35:LEU:HD11	1:C:129:THR:CG2	1.87	1.05
1:G:333:ILE:HG22	2:H:223:ARG:HH22	1.13	1.04
1:A:518:ASN:HD22	1:A:534:LEU:N	1.56	1.03
2:H:362:GLN:HG2	2:H:408:LEU:HB3	1.36	1.03
1:C:35:LEU:HD11	1:C:129:THR:HG21	1.42	1.01
2:H:403:ARG:HG2	2:H:403:ARG:O	1.54	1.01
2:H:232:VAL:HG21	2:H:264:SER:HA	1.39	1.00
1:C:252:LEU:O	1:C:259:PRO:CD	2.10	1.00
1:E:226:TYR:HD1	1:E:231:GLY:HA2	1.23	1.00
1:A:236:THR:HB	1:A:239:GLU:HG3	1.43	0.99
2:F:325:ASN:ND2	2:F:327:VAL:HG23	1.77	0.98
1:G:489:GLU:H	2:H:19:HIS:HD2	1.00	0.98
2:F:380:ALA:CB	2:F:394:LEU:HD12	1.93	0.98
2:H:380:ALA:CB	2:H:394:LEU:HD12	1.93	0.98
1:A:518:ASN:ND2	1:A:534:LEU:N	2.12	0.97
1:C:130:GLN:OE1	1:C:155:THR:HB	1.63	0.97
2:D:402:GLU:HA	2:D:405:ARG:HH12	1.26	0.97
3:K:155:THR:HG22	3:K:158:ASP:OD1	1.63	0.97
1:E:184:ARG:HH12	1:E:325:VAL:HG22	1.27	0.97
2:F:362:GLN:HG2	2:F:408:LEU:HD22	1.45	0.96
1:C:259:PRO:HB2	1:C:262:GLU:OE1	1.66	0.96
2:H:128:GLN:HE21	2:H:128:GLN:H	1.12	0.96
2:F:361:LEU:HB3	2:F:408:LEU:HD23	1.48	0.96
2:B:386:GLU:O	2:B:388:LYS:N	1.99	0.95
1:A:518:ASN:ND2	1:A:534:LEU:H	1.64	0.95
1:A:252:LEU:C	1:A:259:PRO:HD2	1.87	0.95
2:B:207:TYR:CE2	3:I:172:ARG:HG2	2.02	0.95
1:E:211:HIS:CE1	2:F:221:MET:SD	2.60	0.94
1:E:347:ARG:HH22	2:F:274:ARG:HD2	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:376:MET:HB3	2:F:427:ASP:OD1	1.67	0.94
2:F:374:LEU:H	2:F:374:LEU:HD12	1.33	0.94
1:G:489:GLU:H	2:H:19:HIS:CD2	1.85	0.94
1:G:293:ARG:HG2	1:G:293:ARG:HH11	1.29	0.94
2:F:371:SER:HB3	2:F:374:LEU:CD1	1.98	0.93
3:I:99:GLY:O	3:I:118:GLU:CB	2.16	0.93
1:A:252:LEU:O	1:A:259:PRO:CD	2.16	0.93
2:D:257:ILE:HD13	2:D:282:GLN:HG2	1.50	0.93
3:I:107:THR:HG22	3:I:109:THR:H	1.31	0.92
2:D:149:ILE:H	2:D:149:ILE:CD1	1.81	0.92
2:B:214:PRO:HG2	2:B:217:THR:HG23	1.52	0.92
1:C:35:LEU:CD1	1:C:129:THR:CG2	2.48	0.92
1:E:201:LEU:N	1:E:201:LEU:HD23	1.85	0.91
2:F:64:LEU:HD11	2:F:77:VAL:HG21	1.51	0.91
2:F:362:GLN:HE21	2:F:408:LEU:HD13	1.35	0.90
2:B:236:GLN:HE22	2:B:263:LYS:HD2	1.35	0.90
3:L:107:THR:HG23	3:L:109:THR:H	1.35	0.90
2:F:342:ASN:HD22	2:F:342:ASN:H	1.18	0.90
2:F:149:ILE:H	2:F:149:ILE:CD1	1.82	0.90
2:F:380:ALA:HB1	2:F:394:LEU:HA	1.54	0.90
2:B:342:ASN:H	2:B:342:ASN:HD22	1.18	0.89
2:F:74:GLN:HE22	2:F:119:ASN:HD22	1.15	0.89
2:H:223:ARG:HB2	2:H:227:HIS:CE1	2.08	0.89
1:G:121:CYS:HA	1:G:148:ILE:HD11	1.53	0.89
2:D:380:ALA:HB2	2:D:394:LEU:HD12	1.53	0.89
3:K:118:GLU:HG2	3:K:121:ASP:OD1	1.73	0.88
1:G:180:LEU:H	1:G:180:LEU:HD12	1.39	0.88
2:B:380:ALA:HB2	2:B:394:LEU:HD12	1.56	0.88
2:H:128:GLN:H	2:H:128:GLN:NE2	1.72	0.87
3:L:120:THR:HA	3:L:155:THR:OG1	1.73	0.87
2:F:131:ASN:HB3	2:H:131:ASN:HD22	1.35	0.87
2:B:380:ALA:CB	2:B:394:LEU:HD12	2.04	0.87
2:F:340:LYS:HB3	2:F:342:ASN:HD21	1.38	0.87
2:B:327:VAL:HG23	2:B:328:ASP:H	1.39	0.87
2:D:232:VAL:HG11	2:D:263:LYS:HB2	1.56	0.86
2:F:380:ALA:HB1	2:F:394:LEU:HD12	1.56	0.86
3:J:161:ILE:HD11	3:J:167:LEU:HD21	1.56	0.86
1:E:211:HIS:N	1:E:211:HIS:CD2	2.39	0.86
2:H:58:GLY:H	2:H:91:GLN:HG2	1.40	0.86
1:E:184:ARG:NH1	1:E:325:VAL:HG22	1.89	0.86
2:H:318:LEU:HD11	2:H:334:THR:CG2	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:ASN:HD21	2:F:327:VAL:CG2	1.87	0.85
2:B:343:CYS:O	2:B:347:SER:HB3	1.76	0.85
1:C:36:ILE:HB	1:C:128:ALA:HA	1.58	0.85
1:E:297:ILE:H	1:E:297:ILE:HD12	1.41	0.85
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.57	0.85
1:E:212:THR:OG1	1:E:217:ILE:HD11	1.76	0.85
3:L:170:VAL:HG12	3:L:171:LEU:H	1.40	0.85
1:E:307:LEU:HD13	1:E:383:LEU:HD22	1.58	0.85
2:H:380:ALA:HB2	2:H:394:LEU:HD12	1.59	0.85
1:G:421:ASN:O	1:G:424:VAL:HG23	1.76	0.85
2:B:218:ILE:HD11	2:B:230:GLU:HG2	1.59	0.85
1:C:37:ASN:O	1:C:129:THR:OG1	1.94	0.84
2:F:134:PHE:O	2:F:137:GLN:HG2	1.77	0.84
1:E:51:LEU:HD11	2:F:92:PHE:HB3	1.58	0.84
2:H:271:TYR:N	2:H:271:TYR:CD2	2.42	0.84
2:B:355:PHE:O	2:B:440:PHE:HA	1.76	0.84
2:F:411:THR:H	2:F:414:GLU:HB3	1.40	0.84
3:K:125:ARG:HD3	3:K:129:ARG:HH21	1.41	0.83
2:B:361:LEU:HD23	2:B:408:LEU:HD23	1.60	0.83
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.58	0.83
2:F:149:ILE:HD12	2:F:149:ILE:N	1.90	0.83
2:F:411:THR:H	2:F:414:GLU:CB	1.91	0.83
1:A:229:THR:CG2	1:A:232:ARG:HB3	2.08	0.83
2:F:371:SER:OG	2:F:374:LEU:HD11	1.79	0.83
2:H:318:LEU:HG	2:H:319:ASN:O	1.79	0.83
1:E:248:ARG:O	1:E:251:ILE:CG1	2.27	0.83
1:G:518:ASN:HB3	1:G:533:GLN:HA	1.61	0.83
2:B:316:ILE:H	2:B:316:ILE:HD12	1.42	0.82
3:L:123:VAL:HG11	3:L:150:MET:HB3	1.60	0.82
2:D:380:ALA:CB	2:D:394:LEU:HD12	2.08	0.82
2:B:342:ASN:H	2:B:342:ASN:ND2	1.75	0.82
1:G:518:ASN:CB	1:G:533:GLN:HA	2.10	0.81
2:H:318:LEU:HD11	2:H:334:THR:HG23	1.61	0.81
1:A:418:ASN:ND2	1:A:420:ASP:H	1.79	0.81
1:C:35:LEU:CD1	1:C:129:THR:HG21	2.08	0.81
1:C:299:LYS:HA	1:C:368:ILE:HG23	1.63	0.81
2:D:149:ILE:HD12	2:D:149:ILE:N	1.94	0.81
1:A:224:GLN:NE2	1:A:246:LEU:HD11	1.96	0.81
1:C:35:LEU:CD1	1:C:129:THR:HG23	2.10	0.80
3:J:101:MET:SD	3:J:162:LEU:HA	2.21	0.80
2:B:13:TRP:CZ3	2:B:116:PRO:HG2	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:GLN:HB2	2:D:318:LEU:HD13	1.64	0.80
2:B:240:GLU:O	2:B:242:PRO:CD	2.30	0.80
1:E:252:LEU:C	1:E:259:PRO:HD2	2.01	0.80
1:E:211:HIS:N	1:E:211:HIS:HD2	1.76	0.79
2:D:318:LEU:HG	2:D:319:ASN:O	1.82	0.79
2:F:74:GLN:NE2	2:F:119:ASN:HD22	1.79	0.79
3:J:118:GLU:HG3	3:J:120:THR:HG22	1.62	0.79
2:H:277:THR:HG23	2:H:280:LEU:H	1.47	0.79
3:I:99:GLY:O	3:I:118:GLU:HB2	1.81	0.79
1:C:229:THR:CG2	1:C:232:ARG:HB2	2.12	0.79
3:J:170:VAL:HG22	3:J:171:LEU:H	1.48	0.79
3:I:99:GLY:O	3:I:118:GLU:HB3	1.81	0.79
1:E:201:LEU:N	1:E:201:LEU:CD2	2.45	0.79
2:F:412:LEU:HD13	2:F:440:PHE:HE2	1.49	0.78
1:G:6:LYS:N	1:G:6:LYS:HD2	1.97	0.78
2:H:231:TYR:HA	2:H:235:LEU:HD23	1.64	0.78
1:A:462:THR:O	1:A:466:GLN:HG3	1.83	0.78
2:H:380:ALA:HB1	2:H:394:LEU:HD12	1.64	0.78
1:C:518:ASN:HB2	1:C:533:GLN:HA	1.63	0.78
1:G:360:HIS:O	1:G:364:LEU:HD13	1.83	0.78
1:C:297:ILE:H	1:C:297:ILE:HD13	1.48	0.78
1:E:262:GLU:OE2	1:E:262:GLU:HA	1.83	0.78
1:A:125:VAL:HG12	1:A:149:PRO:HB2	1.65	0.78
1:A:259:PRO:CB	1:A:262:GLU:OE1	2.31	0.78
2:F:87:ASN:ND2	2:F:103:LYS:HE2	1.99	0.78
1:E:186:ASP:OD2	1:E:279:THR:HB	1.84	0.78
2:H:241:GLN:OE1	2:H:245:GLU:HA	1.83	0.77
1:A:418:ASN:HD22	1:A:420:ASP:H	1.29	0.77
2:D:402:GLU:HA	2:D:405:ARG:NH1	1.98	0.77
2:B:240:GLU:O	2:B:242:PRO:HD3	1.84	0.77
2:H:351:GLN:H	2:H:436:PHE:HA	1.47	0.77
2:F:277:THR:HG23	2:F:280:LEU:H	1.47	0.77
1:G:333:ILE:HA	2:H:223:ARG:CZ	2.15	0.77
1:A:317:LYS:HB3	1:A:318:GLU:OE1	1.85	0.77
1:C:35:LEU:HD11	1:C:129:THR:HG23	1.65	0.77
2:B:356:SER:HB3	2:B:441:THR:OG1	1.84	0.77
2:F:340:LYS:HB3	2:F:342:ASN:ND2	2.00	0.77
1:G:489:GLU:N	2:H:19:HIS:HD2	1.81	0.77
2:H:162:LEU:HA	2:H:173:SER:OG	1.83	0.77
2:H:403:ARG:O	2:H:403:ARG:CG	2.33	0.77
1:G:447:ASN:HD22	2:H:26:ARG:HH21	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:316:ILE:H	2:H:316:ILE:HD12	1.48	0.77
1:A:28:LEU:HD12	1:A:509:ILE:HG21	1.67	0.76
1:G:226:TYR:OH	1:G:233:ILE:HG22	1.85	0.76
3:L:105:VAL:HG23	3:L:167:LEU:HB2	1.67	0.76
1:C:163:ARG:CZ	1:C:518:ASN:OD1	2.34	0.76
1:C:418:ASN:ND2	1:C:420:ASP:H	1.81	0.76
1:C:51:LEU:HD11	2:D:92:PHE:HB3	1.68	0.76
1:E:248:ARG:O	1:E:251:ILE:HG13	1.84	0.76
2:H:164:TYR:CE2	2:H:169:LEU:HB2	2.21	0.76
1:G:267:GLU:OE2	1:G:333:ILE:HG12	1.85	0.76
3:L:120:THR:CA	3:L:155:THR:OG1	2.34	0.76
1:A:75:PHE:O	1:A:76:LEU:HD23	1.85	0.75
2:B:357:PRO:CD	2:B:442:SER:O	2.34	0.75
1:G:41:THR:O	1:G:45:ILE:HG13	1.85	0.75
2:H:217:THR:HG21	2:H:223:ARG:HH21	1.50	0.75
1:C:129:THR:O	1:C:153:CYS:O	2.03	0.75
1:E:253:LYS:HA	1:E:253:LYS:HE3	1.69	0.75
2:D:380:ALA:CB	2:D:394:LEU:CD1	2.64	0.75
1:E:489:GLU:H	2:F:19:HIS:CD2	2.04	0.75
2:F:62:GLU:HG2	2:F:297:ALA:HA	1.68	0.74
1:A:112:LEU:H	1:A:112:LEU:HD22	1.50	0.74
1:A:229:THR:HG21	1:A:232:ARG:HB3	1.68	0.74
1:E:409:LYS:HG2	1:E:470:LEU:HD21	1.68	0.74
2:B:342:ASN:HD22	2:B:342:ASN:N	1.79	0.74
1:C:259:PRO:HB2	1:C:262:GLU:CD	2.07	0.74
1:E:61:ASP:HB3	1:E:86:ALA:HB2	1.70	0.74
1:G:341:LYS:O	1:G:345:VAL:HG23	1.87	0.74
2:H:62:GLU:HG2	2:H:297:ALA:HA	1.69	0.74
2:B:81:ASP:HB2	2:B:103:LYS:HD2	1.68	0.74
1:C:115:ASN:O	1:C:117:PRO:HD3	1.88	0.74
1:A:34:CYS:SG	1:A:36:ILE:HD11	2.28	0.74
2:B:214:PRO:HG2	2:B:217:THR:CG2	2.18	0.74
1:C:252:LEU:C	1:C:259:PRO:HD2	2.06	0.74
1:C:396:ARG:HD2	1:C:534:LEU:O	1.88	0.74
2:B:419:ASP:OD1	2:B:440:PHE:HD1	1.71	0.74
2:B:229:ILE:HD13	2:B:281:THR:HA	1.69	0.73
1:G:293:ARG:HG2	1:G:293:ARG:NH1	2.00	0.73
2:B:95:ARG:HH11	2:B:95:ARG:HG3	1.52	0.73
1:C:229:THR:HG21	1:C:232:ARG:HB2	1.69	0.73
2:H:240:GLU:O	2:H:242:PRO:HD3	1.88	0.73
2:H:339:ARG:HH21	2:H:346:CYS:HB3	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:TRP:HZ3	2:B:116:PRO:HG2	1.53	0.73
1:C:84:ASN:HB3	1:C:87:GLU:HB3	1.71	0.73
1:C:397:SER:OG	1:C:400:GLU:HG3	1.89	0.73
2:F:316:ILE:HD12	2:F:316:ILE:H	1.52	0.73
1:A:36:ILE:CD1	1:A:60:ILE:HB	2.11	0.73
1:C:143:LEU:HD22	1:C:148:ILE:HB	1.70	0.73
2:H:252:ASP:O	2:H:254:PRO:HD3	1.88	0.73
2:H:356:SER:O	2:H:358:SER:N	2.21	0.73
1:A:236:THR:CB	1:A:239:GLU:HG3	2.19	0.73
1:E:307:LEU:HB3	1:E:383:LEU:HD22	1.71	0.73
2:F:217:THR:HG21	2:F:223:ARG:NH2	2.03	0.73
2:F:382:THR:HG22	2:F:391:THR:HA	1.70	0.73
2:H:223:ARG:HB2	2:H:227:HIS:HE1	1.52	0.73
2:F:348:GLN:O	2:F:349:LEU:HD12	1.89	0.73
2:F:199:CYS:SG	2:F:201:GLU:HB2	2.29	0.73
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.69	0.73
2:B:200:ILE:HD13	3:I:172:ARG:HH22	1.54	0.73
1:C:130:GLN:HG2	1:C:154:ARG:HA	1.71	0.72
2:D:223:ARG:HB2	2:D:223:ARG:HH11	1.52	0.72
2:B:318:LEU:HD11	2:B:334:THR:CG2	2.19	0.72
2:F:371:SER:O	2:F:374:LEU:HD12	1.90	0.72
2:H:404:THR:HG22	2:H:407:ASN:HD22	1.54	0.72
1:A:236:THR:HG22	1:A:238:LYS:H	1.55	0.72
2:B:353:ILE:HG23	2:B:355:PHE:HD1	1.54	0.72
2:H:38:SER:HB3	2:H:41:SER:OG	1.90	0.72
2:F:58:GLY:H	2:F:91:GLN:HG2	1.54	0.72
2:F:351:GLN:HB2	2:F:436:PHE:CD2	2.24	0.72
1:G:45:ILE:HG12	1:G:498:GLY:HA2	1.72	0.72
2:D:162:LEU:HD22	2:D:169:LEU:HD11	1.71	0.72
1:A:489:GLU:H	2:B:19:HIS:CD2	2.08	0.71
1:E:347:ARG:NH2	2:F:274:ARG:HD2	2.04	0.71
2:D:16:ARG:HD3	2:D:17:TRP:NE1	2.05	0.71
1:A:259:PRO:C	1:A:261:ASP:H	1.94	0.71
1:C:259:PRO:C	1:C:261:ASP:H	1.93	0.71
1:E:211:HIS:HE1	2:F:221:MET:SD	2.13	0.71
2:B:217:THR:HA	2:B:221:MET:HG3	1.70	0.71
2:B:253:ASP:HB3	2:B:256:HIS:HB2	1.70	0.71
1:C:409:LYS:HE2	1:C:468:TYR:O	1.91	0.71
2:H:224:LEU:HG	2:H:227:HIS:CE1	2.26	0.71
2:H:207:TYR:CE1	3:L:172:ARG:HD3	2.25	0.71
3:L:170:VAL:HG12	3:L:171:LEU:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:O	1:A:270:LYS:HG3	1.91	0.71
1:G:446:SER:HB2	1:G:449:GLN:HG3	1.73	0.71
2:H:325:ASN:ND2	2:H:327:VAL:HG23	2.06	0.71
1:A:397:SER:OG	1:A:400:GLU:HG3	1.90	0.70
1:C:251:ILE:HG22	1:C:262:GLU:OE1	1.90	0.70
2:H:235:LEU:O	2:H:238:PRO:HD2	1.91	0.70
2:B:217:THR:HB	2:B:223:ARG:NH2	2.06	0.70
2:D:232:VAL:CG1	2:D:263:LYS:HB2	2.20	0.70
1:G:196:PHE:O	1:G:220:LYS:HE3	1.91	0.70
1:E:184:ARG:HG3	1:E:184:ARG:HH11	1.55	0.70
2:F:374:LEU:HD12	2:F:374:LEU:N	1.98	0.70
1:A:264:ASN:HD22	1:A:264:ASN:N	1.89	0.70
2:B:240:GLU:O	2:B:240:GLU:HG3	1.91	0.70
2:B:325:ASN:HD21	2:B:327:VAL:HG22	1.56	0.70
2:F:411:THR:OG1	2:F:414:GLU:HB2	1.91	0.70
2:H:239:LYS:HG3	2:H:239:LYS:O	1.91	0.70
2:H:74:GLN:HE22	2:H:119:ASN:HD22	1.39	0.70
2:H:318:LEU:C	2:H:319:ASN:O	2.24	0.70
1:A:299:LYS:HG2	1:A:368:ILE:O	1.90	0.70
2:B:74:GLN:HE22	2:B:119:ASN:HD22	1.40	0.70
2:F:241:GLN:HG2	2:F:245:GLU:HA	1.72	0.70
3:K:116:ASP:O	3:K:117:ILE:HD12	1.92	0.70
1:A:297:ILE:HD12	1:A:297:ILE:N	2.06	0.70
1:C:248:ARG:O	1:C:251:ILE:HG13	1.92	0.70
2:H:234:MET:O	2:H:235:LEU:HD13	1.92	0.70
2:D:325:ASN:HD21	2:D:327:VAL:HG22	1.56	0.70
2:F:32:HIS:CD2	2:F:34:ASP:H	2.10	0.70
1:A:84:ASN:OD1	1:A:106:GLU:HG2	1.92	0.69
2:B:64:LEU:HB3	2:B:111:LEU:CD1	2.22	0.69
2:H:148:ILE:HG12	3:L:174:ARG:HG2	1.73	0.69
2:H:157:MET:HE3	2:H:157:MET:O	1.92	0.69
2:H:164:TYR:CD2	2:H:169:LEU:HB2	2.27	0.69
2:H:187:GLY:HA2	3:L:173:LEU:HD13	1.74	0.69
2:H:294:SER:O	2:H:298:VAL:HG23	1.92	0.69
2:H:398:THR:O	2:H:402:GLU:HG3	1.92	0.69
1:A:518:ASN:CG	1:A:519:THR:H	1.94	0.69
2:D:318:LEU:HD11	2:D:334:THR:CG2	2.22	0.69
1:A:36:ILE:O	1:A:60:ILE:O	2.08	0.69
1:C:317:LYS:HB3	1:C:318:GLU:OE1	1.93	0.69
2:D:141:ILE:CD1	2:D:158:LEU:HD21	2.22	0.69
2:D:380:ALA:HB1	2:D:394:LEU:CD1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:TRP:HB3	2:F:238:PRO:HD3	1.75	0.69
1:G:507:LYS:HG2	1:G:513:PHE:HB2	1.73	0.69
2:B:356:SER:HB3	2:B:442:SER:H	1.55	0.69
2:B:380:ALA:CB	2:B:394:LEU:CD1	2.71	0.69
1:C:146:SER:O	1:C:147:GLN:HB2	1.90	0.69
1:G:185:LEU:HD12	1:G:275:ALA:HB1	1.73	0.69
2:B:361:LEU:HB3	2:B:408:LEU:HA	1.74	0.69
1:A:527:GLN:HB2	2:B:318:LEU:HD13	1.75	0.69
1:E:297:ILE:H	1:E:297:ILE:CD1	2.03	0.69
2:F:125:ASN:HD22	2:F:125:ASN:N	1.91	0.69
1:A:154:ARG:HB3	1:A:161:TYR:HB3	1.76	0.68
2:B:64:LEU:HB3	2:B:111:LEU:HD11	1.74	0.68
2:B:203:THR:OG1	3:I:172:ARG:NH1	2.25	0.68
1:C:274:THR:O	1:C:276:LEU:N	2.26	0.68
2:F:131:ASN:HD22	2:H:131:ASN:HB3	1.58	0.68
1:G:33:VAL:CG2	1:G:54:ILE:HG12	2.22	0.68
1:C:163:ARG:NH1	1:C:165:ILE:HG12	2.07	0.68
2:D:17:TRP:O	2:D:21:LYS:HB2	1.92	0.68
3:K:104:LYS:HD2	3:K:112:GLU:OE2	1.91	0.68
2:H:355:PHE:O	2:H:440:PHE:HA	1.93	0.68
2:D:125:ASN:HD22	2:D:125:ASN:N	1.92	0.68
2:F:217:THR:HG21	2:F:223:ARG:HH22	1.56	0.68
2:F:355:PHE:CE1	2:F:364:VAL:HG22	2.28	0.68
1:A:61:ASP:OD2	1:A:85:ARG:HB3	1.92	0.68
2:D:74:GLN:NE2	2:D:119:ASN:HD22	1.92	0.68
2:F:54:ILE:HG22	2:F:145:LEU:HD21	1.75	0.68
2:H:271:TYR:N	2:H:271:TYR:HD2	1.90	0.68
1:C:46:LEU:O	1:C:50:VAL:HG23	1.94	0.68
1:G:248:ARG:O	1:G:251:ILE:HG13	1.93	0.68
2:H:232:VAL:HG21	2:H:264:SER:CA	2.21	0.68
2:B:182:THR:HG21	2:B:296:ASN:OD1	1.94	0.68
2:D:322:LEU:HD12	2:D:323:VAL:N	2.08	0.68
1:E:309:ARG:HH11	1:E:309:ARG:HG3	1.59	0.68
2:F:362:GLN:NE2	2:F:408:LEU:HD13	2.08	0.68
1:A:87:GLU:O	1:A:91:GLU:HG3	1.94	0.68
2:H:192:ILE:HG22	2:H:194:PRO:HD3	1.76	0.68
1:C:163:ARG:HD2	1:C:518:ASN:O	1.93	0.68
1:E:259:PRO:C	1:E:261:ASP:H	1.96	0.67
1:C:42:GLY:HA2	1:C:129:THR:HG21	1.77	0.67
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.77	0.67
2:F:229:ILE:HD13	2:F:281:THR:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:PRO:HA	2:F:412:LEU:HB2	1.76	0.67
2:H:228:CYS:O	2:H:232:VAL:HG23	1.94	0.67
2:H:357:PRO:HA	2:H:440:PHE:CE2	2.29	0.67
1:C:248:ARG:C	1:C:250:GLY:H	1.98	0.67
2:D:322:LEU:HD12	2:D:322:LEU:C	2.14	0.67
2:H:362:GLN:OE1	2:H:408:LEU:HD13	1.93	0.67
2:H:361:LEU:O	2:H:364:VAL:HG22	1.95	0.67
1:A:446:SER:HB2	1:A:449:GLN:NE2	2.10	0.67
1:C:226:TYR:CE1	1:C:231:GLY:HA2	2.29	0.67
2:H:64:LEU:HD21	2:H:77:VAL:CG2	2.25	0.67
2:F:132:ASP:HB3	2:F:157:MET:HE1	1.74	0.67
1:C:421:ASN:O	1:C:424:VAL:HG22	1.95	0.67
2:H:325:ASN:HD21	2:H:327:VAL:HG23	1.58	0.67
1:E:297:ILE:HB	1:E:368:ILE:HD11	1.75	0.67
2:F:380:ALA:CB	2:F:394:LEU:HA	2.25	0.67
1:G:518:ASN:HD22	1:G:534:LEU:H	1.43	0.67
2:B:400:ILE:H	2:B:400:ILE:HD12	1.58	0.67
1:A:461:LEU:O	1:A:465:LEU:HG	1.95	0.66
2:H:253:ASP:HB3	2:H:256:HIS:HB2	1.77	0.66
2:B:361:LEU:HB2	2:B:407:ASN:O	1.95	0.66
1:C:264:ASN:HD22	1:C:264:ASN:H	1.44	0.66
2:F:220:SER:C	2:F:222:PRO:HD3	2.15	0.66
1:G:333:ILE:HG22	2:H:223:ARG:CZ	2.25	0.66
2:H:128:GLN:HE21	2:H:128:GLN:N	1.91	0.66
2:D:380:ALA:HB1	2:D:394:LEU:HD13	1.78	0.66
2:F:398:THR:O	2:F:401:GLU:HG2	1.96	0.66
1:A:446:SER:HB2	1:A:449:GLN:HE21	1.59	0.66
1:E:307:LEU:HB3	1:E:383:LEU:CD2	2.25	0.66
1:E:422:GLU:HG3	1:E:530:ALA:HB3	1.78	0.66
2:F:362:GLN:HE21	2:F:408:LEU:CD1	2.06	0.66
3:L:117:ILE:HD13	3:L:126:ILE:HG12	1.76	0.66
2:D:411:THR:O	2:D:415:LEU:HG	1.96	0.66
2:D:412:LEU:HD22	2:D:417:LEU:HD12	1.77	0.66
2:H:348:GLN:HB3	2:H:349:LEU:HD12	1.77	0.66
2:D:192:ILE:CD1	2:D:200:ILE:HG13	2.26	0.66
2:D:418:VAL:HG22	2:D:421:GLN:NE2	2.10	0.66
1:G:112:LEU:C	1:G:114:ASP:H	1.96	0.66
1:A:125:VAL:HG21	1:A:505:VAL:HG13	1.77	0.66
1:A:430:ARG:HB3	1:A:430:ARG:NH1	2.10	0.66
2:D:231:TYR:C	2:D:233:ARG:H	1.98	0.66
2:F:241:GLN:HE21	2:F:246:GLY:H	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:ASP:OD2	1:G:85:ARG:HD2	1.95	0.66
1:G:307:LEU:HB3	1:G:383:LEU:CD2	2.25	0.66
2:H:412:LEU:HD22	2:H:440:PHE:CE2	2.31	0.66
2:B:407:ASN:ND2	2:B:415:LEU:HD22	2.10	0.65
3:K:156:ALA:HA	3:K:161:ILE:HD12	1.78	0.65
1:A:58:THR:HA	1:A:103:SER:O	1.96	0.65
1:A:61:ASP:OD2	1:A:85:ARG:HD2	1.95	0.65
2:B:385:LEU:HD12	2:B:390:ARG:HD3	1.78	0.65
2:D:360:LYS:HA	2:D:411:THR:HA	1.77	0.65
3:L:123:VAL:HA	3:L:126:ILE:HD12	1.78	0.65
2:B:400:ILE:HD12	2:B:400:ILE:N	2.12	0.65
2:B:427:ASP:HB3	2:B:429:THR:HG22	1.77	0.65
1:C:43:THR:HG21	1:C:73:ASN:OD1	1.97	0.65
1:C:407:ILE:HG13	1:C:408:ASN:N	2.12	0.65
2:D:200:ILE:HG12	3:J:172:ARG:HH22	1.61	0.65
2:F:125:ASN:N	2:F:125:ASN:ND2	2.41	0.65
2:H:128:GLN:NE2	2:H:128:GLN:N	2.42	0.65
3:L:107:THR:CG2	3:L:111:LYS:HB3	2.26	0.65
3:I:104:LYS:HD3	3:I:112:GLU:OE2	1.96	0.65
3:K:124:GLU:HB2	3:K:152:ASP:O	1.96	0.65
3:K:125:ARG:HD3	3:K:129:ARG:NH2	2.09	0.65
1:G:226:TYR:HB3	1:G:231:GLY:HA2	1.79	0.65
1:A:220:LYS:HE2	1:A:220:LYS:HA	1.78	0.65
2:B:200:ILE:CD1	3:I:172:ARG:HH22	2.09	0.65
2:F:342:ASN:H	2:F:342:ASN:ND2	1.92	0.65
3:I:101:MET:N	3:I:117:ILE:O	2.23	0.65
2:F:154:ILE:O	2:F:158:LEU:HD23	1.97	0.65
3:K:117:ILE:HG12	3:K:126:ILE:HG12	1.77	0.65
1:A:311:LEU:O	1:A:315:VAL:HG23	1.97	0.65
2:H:354:GLN:HE22	2:H:439:HIS:HB3	1.61	0.65
3:K:172:ARG:C	3:K:173:LEU:HG	2.17	0.65
2:H:405:ARG:HB3	2:H:406:PRO:HD3	1.77	0.65
1:A:518:ASN:HD21	1:A:534:LEU:HB2	1.60	0.64
2:B:380:ALA:HB1	2:B:394:LEU:CD1	2.28	0.64
2:D:343:CYS:O	2:D:347:SER:HB3	1.98	0.64
1:A:150:LEU:HD23	1:A:165:ILE:HD12	1.79	0.64
1:A:248:ARG:HA	1:A:251:ILE:HD11	1.79	0.64
2:B:318:LEU:HG	2:B:319:ASN:O	1.96	0.64
1:C:357:VAL:O	1:C:361:VAL:HG23	1.97	0.64
1:E:45:ILE:HG12	1:E:498:GLY:HA2	1.79	0.64
1:A:229:THR:O	1:A:230:ASN:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:HD22	1:A:253:LYS:N	2.12	0.64
2:B:102:PRO:HG2	2:B:105:GLU:HB3	1.78	0.64
2:B:425:VAL:HB	2:B:434:VAL:HG13	1.77	0.64
1:A:430:ARG:HB3	1:A:430:ARG:HH11	1.62	0.64
2:H:32:HIS:HD2	2:H:34:ASP:H	1.43	0.64
3:L:99:GLY:O	3:L:116:ASP:HB3	1.97	0.64
3:L:125:ARG:HD3	3:L:129:ARG:NH2	2.12	0.64
2:B:302:VAL:HG11	2:B:322:LEU:HD23	1.79	0.64
1:C:163:ARG:NH2	1:C:518:ASN:OD1	2.31	0.64
2:D:29:PRO:HG2	2:D:30:PHE:H	1.63	0.64
2:D:357:PRO:HG3	2:D:440:PHE:CG	2.33	0.64
1:G:527:GLN:HB2	2:H:318:LEU:HD13	1.79	0.64
2:D:132:ASP:HB3	2:D:157:MET:HE1	1.80	0.64
1:E:211:HIS:HB2	1:E:334:ALA:HA	1.79	0.64
2:F:201:GLU:HG3	2:F:345:ALA:HB2	1.80	0.64
2:B:233:ARG:HB3	2:B:233:ARG:HH11	1.63	0.64
2:F:16:ARG:HH22	2:F:116:PRO:HB2	1.63	0.64
2:F:412:LEU:HD23	2:F:417:LEU:HD22	1.78	0.64
2:B:188:ASN:OD1	3:I:173:LEU:HD12	1.98	0.64
3:J:161:ILE:CD1	3:J:167:LEU:HD21	2.26	0.64
2:B:200:ILE:CD1	3:I:172:ARG:NH2	2.61	0.63
1:C:84:ASN:HB3	1:C:87:GLU:CB	2.27	0.63
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.79	0.63
2:F:371:SER:CB	2:F:374:LEU:CD1	2.58	0.63
1:C:396:ARG:HG3	1:C:518:ASN:HD21	1.62	0.63
2:H:35:PHE:HD1	2:H:313:SER:O	1.80	0.63
2:H:344:PRO:HG3	2:H:374:LEU:HD13	1.80	0.63
1:C:51:LEU:HB2	1:C:52:PRO:HD3	1.81	0.63
3:L:107:THR:HG21	3:L:111:LYS:HB3	1.79	0.63
1:G:215:ILE:H	1:G:332:MET:HE1	1.64	0.63
2:H:132:ASP:OD1	2:H:132:ASP:N	2.30	0.63
3:L:120:THR:HA	3:L:155:THR:HG1	1.63	0.63
2:H:270:GLN:O	2:H:272:ASN:OD1	2.16	0.63
2:B:430:THR:HG22	2:B:431:PRO:HD2	1.79	0.63
2:D:268:ALA:HB2	2:D:276:VAL:HG21	1.80	0.63
2:H:318:LEU:HD11	2:H:334:THR:HG21	1.80	0.63
1:C:259:PRO:C	1:C:261:ASP:N	2.49	0.63
1:C:274:THR:C	1:C:276:LEU:H	2.01	0.63
2:H:238:PRO:O	2:H:241:GLN:HG3	1.98	0.63
1:C:517:ASN:ND2	1:C:518:ASN:N	2.10	0.63
3:J:155:THR:HG23	3:J:158:ASP:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:384:THR:O	2:F:385:LEU:HD23	1.99	0.63
2:H:178:ILE:HD11	2:H:310:ILE:CD1	2.29	0.63
2:H:187:GLY:CA	3:L:173:LEU:HD13	2.29	0.63
1:A:409:LYS:HE2	1:A:468:TYR:O	1.99	0.62
1:A:458:LYS:O	1:A:458:LYS:HD3	1.99	0.62
2:B:96:PRO:O	2:B:99:ILE:HG13	1.99	0.62
3:I:170:VAL:HG13	3:I:171:LEU:N	2.13	0.62
1:C:33:VAL:HG22	1:C:34:CYS:N	2.12	0.62
2:D:380:ALA:HB2	2:D:394:LEU:CD1	2.26	0.62
2:D:207:TYR:CE1	3:J:172:ARG:CD	2.76	0.62
1:A:178:ASN:ND2	3:I:136:ILE:HG12	2.14	0.62
1:C:503:GLN:O	1:C:507:LYS:HG3	1.99	0.62
2:D:250:ASP:OD2	2:D:253:ASP:HB2	1.99	0.62
2:H:404:THR:HG22	2:H:407:ASN:ND2	2.14	0.62
1:E:113:LEU:O	1:E:117:PRO:HG3	1.99	0.62
1:E:309:ARG:HB3	1:E:364:LEU:HD21	1.81	0.62
1:C:434:ARG:HD3	1:C:460:CYS:HB3	1.80	0.62
2:D:232:VAL:O	2:D:232:VAL:HG12	1.99	0.62
2:F:46:LEU:HD22	2:F:73:ARG:CZ	2.30	0.62
2:F:267:ARG:HG2	2:F:267:ARG:HH11	1.64	0.62
1:G:158:LEU:HD12	1:G:493:ILE:HD11	1.80	0.62
1:G:311:LEU:O	1:G:314:PHE:HB3	2.00	0.62
1:G:397:SER:OG	1:G:400:GLU:HG3	1.98	0.62
2:B:356:SER:CB	2:B:441:THR:OG1	2.47	0.62
3:I:107:THR:HG22	3:I:109:THR:N	2.09	0.62
1:C:61:ASP:OD1	1:C:63:ASN:HB2	1.99	0.62
1:E:36:ILE:HG21	1:E:131:LEU:HD21	1.82	0.62
1:E:243:PHE:O	1:E:247:ILE:HG13	1.99	0.62
1:G:264:ASN:HB3	1:G:333:ILE:HG13	1.80	0.62
2:B:442:SER:O	2:B:442:SER:OG	2.12	0.62
1:G:332:MET:HG2	1:G:339:TYR:HE1	1.65	0.62
1:G:333:ILE:N	2:H:223:ARG:NH1	2.46	0.62
2:F:183:GLU:HG3	2:F:289:ILE:HG21	1.80	0.62
1:E:253:LYS:N	1:E:259:PRO:HD2	2.14	0.62
2:F:342:ASN:HD22	2:F:342:ASN:N	1.85	0.62
2:H:58:GLY:N	2:H:91:GLN:HG2	2.14	0.62
2:H:237:TRP:HB3	2:H:238:PRO:HD3	1.81	0.62
1:A:112:LEU:H	1:A:112:LEU:CD2	2.13	0.61
1:C:294:CYS:O	1:C:309:ARG:HD3	2.00	0.61
3:K:155:THR:HG23	3:K:157:ALA:H	1.65	0.61
2:H:391:THR:O	2:H:404:THR:HG21	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:123:VAL:HA	3:L:126:ILE:CD1	2.29	0.61
2:B:74:GLN:NE2	2:B:119:ASN:HD22	1.97	0.61
1:E:214:TRP:O	1:E:218:ILE:HG13	1.99	0.61
2:F:31:THR:HG23	2:F:32:HIS:O	2.00	0.61
2:F:232:VAL:O	2:F:232:VAL:HG12	1.99	0.61
2:H:233:ARG:NH1	2:H:234:MET:HB2	2.15	0.61
2:F:192:ILE:HG22	2:F:194:PRO:HD3	1.82	0.61
1:G:185:LEU:CD1	1:G:275:ALA:HB1	2.30	0.61
1:G:199:TYR:CD2	1:G:216:VAL:HG11	2.35	0.61
2:H:237:TRP:CE3	2:H:242:PRO:HG2	2.35	0.61
1:A:234:PRO:HB2	1:A:276:LEU:CD1	2.30	0.61
2:D:157:MET:O	2:D:157:MET:HE3	2.00	0.61
2:D:390:ARG:HG2	2:D:391:THR:N	2.14	0.61
1:E:447:ASN:ND2	2:F:26:ARG:HH21	1.97	0.61
1:G:50:VAL:HG13	1:G:100:VAL:HG21	1.82	0.61
1:G:241:GLU:O	1:G:244:ARG:HB2	1.99	0.61
2:H:234:MET:C	2:H:235:LEU:HD22	2.20	0.61
1:A:450:VAL:O	1:A:454:ILE:HG13	1.99	0.61
2:B:415:LEU:HB2	2:B:417:LEU:CD2	2.30	0.61
3:J:104:LYS:HB2	3:J:166:VAL:HG12	1.81	0.61
2:F:139:HIS:C	2:F:140:ILE:HD12	2.20	0.61
2:F:316:ILE:H	2:F:316:ILE:CD1	2.09	0.61
1:A:366:GLN:C	1:A:368:ILE:H	2.04	0.61
2:B:316:ILE:H	2:B:316:ILE:CD1	2.08	0.61
1:C:58:THR:HA	1:C:103:SER:O	2.01	0.61
1:C:492:THR:HB	2:D:305:THR:OG1	2.01	0.61
1:G:61:ASP:HB3	1:G:86:ALA:HB2	1.83	0.61
1:G:72:ASN:HD22	1:G:72:ASN:H	1.48	0.61
2:H:320:ASN:HD22	2:H:337:ALA:HB3	1.66	0.61
2:B:368:LEU:HD21	2:B:436:PHE:CE2	2.35	0.61
2:D:15:GLY:HA2	2:D:18:ASN:ND2	2.16	0.61
2:F:362:GLN:CG	2:F:408:LEU:HD22	2.27	0.61
2:H:92:PHE:H	2:H:92:PHE:HD2	1.48	0.61
2:H:405:ARG:CB	2:H:405:ARG:HH11	2.13	0.61
1:A:423:ILE:O	1:A:426:TYR:HB3	2.01	0.61
1:E:252:LEU:C	1:E:259:PRO:CD	2.69	0.61
2:H:58:GLY:H	2:H:91:GLN:CG	2.14	0.61
1:A:281:ILE:HD11	1:A:315:VAL:HG11	1.82	0.61
2:B:131:ASN:HB3	2:D:131:ASN:HD22	1.64	0.61
2:D:185:PHE:HB3	2:D:326:ASP:HB2	1.83	0.61
2:D:192:ILE:HD11	2:D:200:ILE:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:MET:CE	3:L:167:LEU:HD13	2.31	0.61
1:A:36:ILE:HD12	1:A:60:ILE:CB	2.16	0.61
1:G:192:LEU:O	1:G:195:HIS:HB3	2.01	0.61
2:H:32:HIS:CG	2:H:33:PRO:HD2	2.36	0.61
2:H:405:ARG:HB3	2:H:405:ARG:HH11	1.65	0.61
2:H:419:ASP:OD2	2:H:440:PHE:HB2	2.01	0.61
1:A:168:GLU:HG3	1:A:394:ARG:HE	1.66	0.60
1:C:376:SER:OG	1:C:379:GLU:HG3	2.01	0.60
1:C:501:ALA:O	1:C:504:GLU:N	2.34	0.60
1:G:214:TRP:HB2	1:G:268:ALA:HB2	1.82	0.60
1:G:336:SER:HB2	2:H:221:MET:HA	1.83	0.60
2:B:49:CYS:HA	2:B:139:HIS:HD2	1.65	0.60
2:B:233:ARG:HD2	2:B:285:VAL:HG13	1.82	0.60
2:B:353:ILE:HG23	2:B:355:PHE:CD1	2.35	0.60
2:B:374:LEU:O	2:B:376:MET:HG3	2.01	0.60
1:C:430:ARG:NH1	1:C:430:ARG:HB3	2.16	0.60
3:J:101:MET:HB2	3:J:117:ILE:O	1.99	0.60
1:G:229:THR:HG21	1:G:232:ARG:HH21	1.65	0.60
2:H:217:THR:HG21	2:H:223:ARG:HE	1.65	0.60
2:B:218:ILE:CD1	2:B:230:GLU:HG2	2.29	0.60
1:C:6:LYS:O	1:C:9:LYS:HG2	2.01	0.60
1:C:438:GLN:O	1:C:438:GLN:HG2	2.01	0.60
2:F:178:ILE:HD11	2:F:310:ILE:HD12	1.82	0.60
1:G:306:ILE:HD13	1:G:365:LEU:CD2	2.31	0.60
2:H:178:ILE:N	2:H:178:ILE:HD12	2.16	0.60
2:H:349:LEU:HB3	2:H:350:PRO:HD2	1.83	0.60
1:A:407:ILE:HD13	1:A:408:ASN:N	2.16	0.60
2:B:412:LEU:O	2:B:417:LEU:HB2	2.02	0.60
1:E:240:LYS:HE2	1:E:276:LEU:HD12	1.84	0.60
1:E:489:GLU:H	2:F:19:HIS:HD2	1.46	0.60
2:F:223:ARG:HH11	2:F:223:ARG:HG3	1.67	0.60
1:G:306:ILE:HD13	1:G:365:LEU:HD23	1.83	0.60
2:H:390:ARG:NH2	2:H:407:ASN:HD21	1.99	0.60
3:L:124:GLU:HB2	3:L:152:ASP:O	2.00	0.60
1:A:147:GLN:N	1:A:147:GLN:HE21	1.99	0.60
1:C:284:SER:O	1:C:288:ILE:HG13	2.01	0.60
2:D:236:GLN:HE22	2:D:263:LYS:HD2	1.67	0.60
1:G:307:LEU:HB3	1:G:383:LEU:HD22	1.84	0.60
1:A:437:LYS:HA	1:A:437:LYS:HZ3	1.65	0.60
2:D:199:CYS:O	2:D:202:CYS:HB2	2.02	0.60
1:E:365:LEU:HD11	1:E:375:ILE:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:376:MET:HE1	2:F:427:ASP:HB2	1.82	0.60
2:F:384:THR:C	2:F:385:LEU:HD23	2.22	0.60
2:H:400:ILE:O	2:H:404:THR:N	2.35	0.60
2:D:325:ASN:ND2	2:D:327:VAL:HG22	2.17	0.60
3:J:144:ILE:HD13	3:J:149:GLN:HA	1.84	0.60
2:H:158:LEU:CD1	2:H:177:LEU:HD22	2.32	0.60
2:F:425:VAL:HB	2:F:434:VAL:HG13	1.82	0.60
1:G:265:PHE:O	1:G:269:ILE:HG13	2.02	0.60
2:H:237:TRP:CD2	2:H:242:PRO:HG2	2.37	0.60
2:F:131:ASN:HB3	2:H:131:ASN:ND2	2.14	0.60
2:F:361:LEU:HD12	2:F:407:ASN:O	2.02	0.60
2:D:158:LEU:HD22	2:D:175:VAL:HB	1.84	0.59
1:E:219:ALA:O	1:E:222:LEU:HB3	2.02	0.59
3:K:144:ILE:HD11	3:K:170:VAL:HG11	1.83	0.59
1:C:126:VAL:O	1:C:150:LEU:HD12	2.02	0.59
1:C:360:HIS:O	1:C:364:LEU:HD23	2.02	0.59
1:G:184:ARG:HD3	1:G:279:THR:OG1	2.02	0.59
1:C:407:ILE:HG13	1:C:408:ASN:H	1.66	0.59
1:G:36:ILE:HB	1:G:128:ALA:HA	1.85	0.59
2:H:90:ARG:HH11	2:H:90:ARG:HG2	1.68	0.59
2:H:131:ASN:O	2:H:133:THR:N	2.35	0.59
1:C:113:LEU:HD13	1:C:138:ARG:HG2	1.84	0.59
1:E:39:THR:O	1:E:43:THR:HB	2.01	0.59
1:E:447:ASN:ND2	2:F:26:ARG:HE	2.00	0.59
2:F:410:LYS:HB3	2:F:414:GLU:HG2	1.84	0.59
2:B:158:LEU:HD12	2:B:177:LEU:HB2	1.85	0.59
1:C:61:ASP:CB	1:C:86:ALA:HB2	2.33	0.59
1:C:277:ASN:O	1:C:277:ASN:ND2	2.36	0.59
2:F:241:GLN:CG	2:F:245:GLU:HA	2.32	0.59
3:L:117:ILE:CD1	3:L:126:ILE:HG23	2.32	0.59
1:A:47:LYS:HG3	1:A:75:PHE:HZ	1.67	0.59
3:I:103:ILE:CD1	3:I:117:ILE:HD12	2.33	0.59
1:C:113:LEU:O	1:C:117:PRO:HG3	2.03	0.59
1:G:422:GLU:OE1	1:G:422:GLU:N	2.33	0.59
1:G:492:THR:HB	2:H:305:THR:OG1	2.02	0.59
2:B:385:LEU:CD1	2:B:390:ARG:HD3	2.32	0.59
1:C:158:LEU:HA	1:C:493:ILE:HG13	1.82	0.59
2:D:200:ILE:HG12	3:J:172:ARG:NH2	2.17	0.59
3:L:117:ILE:HG23	3:L:121:ASP:HB2	1.82	0.59
2:F:15:GLY:HA2	2:F:18:ASN:HD21	1.67	0.59
2:H:335:PHE:HE2	3:L:170:VAL:HG11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LYS:HB2	2:B:288:ILE:HG13	1.85	0.59
1:C:42:GLY:CA	1:C:129:THR:HG21	2.32	0.59
1:E:13:TYR:O	1:E:17:LEU:HG	2.03	0.59
1:E:226:TYR:CD1	1:E:231:GLY:CA	2.78	0.59
2:F:219:ALA:HA	2:F:267:ARG:HH22	1.67	0.59
2:F:411:THR:O	2:F:414:GLU:HB3	2.02	0.59
3:K:149:GLN:HG3	3:K:149:GLN:O	2.03	0.59
3:I:117:ILE:HG22	3:I:118:GLU:N	2.17	0.59
2:D:237:TRP:CE3	2:D:242:PRO:HG2	2.38	0.59
2:F:249:LEU:CD1	2:F:260:ILE:HD11	2.33	0.59
1:G:264:ASN:HA	1:G:333:ILE:HD11	1.85	0.58
1:C:173:GLU:HA	1:C:386:ASN:ND2	2.18	0.58
1:C:441:ARG:HB3	2:H:270:GLN:OE1	2.03	0.58
1:E:248:ARG:O	1:E:251:ILE:HG12	2.00	0.58
1:E:340:ILE:HG21	2:F:272:ASN:ND2	2.18	0.58
2:H:224:LEU:H	2:H:227:HIS:CE1	2.20	0.58
2:H:368:LEU:HD13	2:H:425:VAL:HG11	1.84	0.58
1:C:262:GLU:HG2	1:C:265:PHE:CD1	2.38	0.58
2:D:124:PHE:C	2:D:125:ASN:HD22	2.05	0.58
2:D:128:GLN:NE2	2:D:128:GLN:H	2.01	0.58
1:E:282:PRO:HB2	1:E:285:ILE:HD13	1.84	0.58
2:H:356:SER:C	2:H:358:SER:N	2.57	0.58
2:B:393:TYR:CE2	2:B:408:LEU:HD21	2.39	0.58
2:D:384:THR:HA	2:D:389:ASN:HB3	1.83	0.58
1:E:236:THR:HG22	1:E:238:LYS:H	1.67	0.58
1:E:507:LYS:HG2	1:E:513:PHE:HB2	1.84	0.58
2:F:222:PRO:O	2:F:273:ILE:HD11	2.01	0.58
1:A:307:LEU:HB3	1:A:383:LEU:CD2	2.32	0.58
2:B:380:ALA:HB1	2:B:394:LEU:HD12	1.84	0.58
2:D:430:THR:OG1	2:D:432:GLN:HG2	2.02	0.58
1:E:200:ASP:C	1:E:201:LEU:HD23	2.24	0.58
2:F:225:PRO:O	2:F:229:ILE:HG13	2.03	0.58
2:H:35:PHE:CD1	2:H:313:SER:O	2.57	0.58
3:L:106:LYS:HG2	3:L:112:GLU:HG2	1.84	0.58
1:A:518:ASN:OD1	1:A:519:THR:N	2.35	0.58
1:C:229:THR:HG22	1:C:232:ARG:HD2	1.85	0.58
3:J:105:VAL:CG1	3:J:115:ILE:HD11	2.34	0.58
2:F:366:ASP:HB3	2:F:370:ASN:HD22	1.68	0.58
2:H:177:LEU:HG	2:H:177:LEU:O	2.03	0.58
2:H:249:LEU:CD1	2:H:260:ILE:HD11	2.34	0.58
3:L:126:ILE:O	3:L:130:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:HD21	2:B:290:PRO:HB2	1.86	0.58
1:A:49:LEU:O	1:A:52:PRO:HG2	2.03	0.58
2:B:15:GLY:HA2	2:B:18:ASN:OD1	2.03	0.58
2:B:196:MET:O	2:B:339:ARG:HD2	2.03	0.58
2:D:320:ASN:HB2	2:D:336:GLU:HA	1.86	0.58
1:E:41:THR:O	1:E:45:ILE:HG13	2.04	0.58
2:F:221:MET:N	2:F:222:PRO:HD3	2.19	0.58
3:L:103:ILE:HD12	3:L:103:ILE:O	2.04	0.58
1:C:236:THR:HB	1:C:239:GLU:HG3	1.86	0.58
2:F:325:ASN:HD22	2:F:326:ASP:N	2.01	0.58
2:H:238:PRO:O	2:H:241:GLN:CG	2.51	0.58
1:C:130:GLN:OE1	1:C:155:THR:CB	2.48	0.58
1:C:418:ASN:C	1:C:418:ASN:HD22	2.07	0.58
2:D:13:TRP:HZ3	2:D:116:PRO:HG2	1.67	0.58
1:A:436:HIS:HA	1:A:441:ARG:O	2.04	0.58
1:A:518:ASN:HD22	1:A:534:LEU:H	1.29	0.58
2:B:153:TRP:CE2	2:B:431:PRO:HG3	2.39	0.58
1:E:184:ARG:HD3	1:E:279:THR:OG1	2.04	0.58
3:K:107:THR:HG22	3:K:109:THR:H	1.69	0.58
1:G:226:TYR:HE2	1:G:233:ILE:HA	1.67	0.58
2:H:84:ASP:H	2:H:87:ASN:ND2	2.02	0.58
2:D:193:LEU:H	2:D:197:THR:HB	1.68	0.57
2:F:239:LYS:O	2:F:240:GLU:HG2	2.04	0.57
2:B:325:ASN:ND2	2:B:327:VAL:HG22	2.19	0.57
2:F:410:LYS:CB	2:F:414:GLU:HG2	2.33	0.57
3:K:115:ILE:HG23	3:K:117:ILE:HD13	1.85	0.57
1:G:84:ASN:OD1	1:G:106:GLU:HG3	2.04	0.57
1:G:488:ALA:C	1:G:490:PRO:HD3	2.25	0.57
2:H:32:HIS:CD2	2:H:34:ASP:H	2.22	0.57
1:A:418:ASN:HD22	1:A:418:ASN:C	2.08	0.57
1:C:72:ASN:OD1	1:C:489:GLU:HG2	2.04	0.57
1:C:88:ALA:O	1:C:91:GLU:HB2	2.05	0.57
1:G:65:VAL:HB	1:G:81:ILE:HA	1.86	0.57
3:L:102:LEU:HD11	3:L:114:GLU:HB3	1.85	0.57
2:H:270:GLN:C	2:H:272:ASN:OD1	2.43	0.57
2:H:318:LEU:O	2:H:319:ASN:O	2.22	0.57
2:B:327:VAL:HG23	2:B:328:ASP:N	2.17	0.57
2:F:152:ARG:CZ	2:F:429:THR:HG21	2.35	0.57
2:F:187:GLY:CA	3:K:173:LEU:HD13	2.35	0.57
2:F:236:GLN:HE22	2:F:263:LYS:HB3	1.70	0.57
2:F:371:SER:O	2:F:374:LEU:CD1	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLN:HE21	1:A:246:LEU:HD11	1.70	0.57
2:F:187:GLY:HA2	3:K:173:LEU:HD13	1.87	0.57
1:G:20:TRP:O	1:G:24:GLY:HA3	2.04	0.57
1:A:484:ARG:HH12	2:B:31:THR:HG22	1.68	0.57
1:C:438:GLN:O	1:C:439:GLN:HG2	2.04	0.57
2:F:178:ILE:HD11	2:F:310:ILE:CD1	2.34	0.57
2:F:381:ILE:HD12	2:F:381:ILE:H	1.70	0.57
2:B:353:ILE:HD11	2:B:367:TYR:CE2	2.40	0.57
1:C:97:ASN:HB3	1:C:100:VAL:HG23	1.87	0.57
2:D:316:ILE:H	2:D:316:ILE:HD12	1.70	0.57
2:D:335:PHE:HE2	3:J:170:VAL:HG21	1.70	0.57
3:K:118:GLU:HG3	3:K:120:THR:HG22	1.86	0.57
1:G:33:VAL:HG22	1:G:54:ILE:HG12	1.86	0.57
2:H:201:GLU:HB3	2:H:343:CYS:SG	2.44	0.57
2:H:359:ALA:O	2:H:412:LEU:HD12	2.05	0.57
3:L:102:LEU:HD12	3:L:115:ILE:O	2.04	0.57
2:B:318:LEU:HD11	2:B:334:THR:HG21	1.87	0.57
1:C:163:ARG:CD	1:C:518:ASN:O	2.52	0.57
1:C:189:PHE:CE1	1:C:192:LEU:HB2	2.39	0.57
1:C:418:ASN:HD22	1:C:419:PRO:N	2.02	0.57
2:F:411:THR:N	2:F:414:GLU:HB3	2.16	0.57
1:G:6:LYS:C	1:G:8:LEU:H	2.08	0.57
1:G:275:ALA:O	1:G:278:THR:HG23	2.05	0.57
1:A:156:TYR:CE1	1:A:487:ALA:HA	2.40	0.56
2:B:385:LEU:HD12	2:B:390:ARG:CD	2.34	0.56
2:F:385:LEU:HD11	2:F:392:LEU:HD21	1.86	0.56
1:G:518:ASN:ND2	1:G:534:LEU:H	2.03	0.56
1:A:259:PRO:C	1:A:261:ASP:N	2.59	0.56
2:D:252:ASP:O	2:D:254:PRO:HD3	2.05	0.56
2:H:376:MET:HB3	2:H:427:ASP:OD1	2.04	0.56
1:A:441:ARG:HG2	1:A:441:ARG:HH11	1.71	0.56
1:A:527:GLN:HG3	2:B:306:GLU:OE1	2.05	0.56
2:F:222:PRO:HG2	2:F:267:ARG:NH2	2.19	0.56
2:F:236:GLN:O	2:F:240:GLU:HG3	2.05	0.56
1:G:215:ILE:O	1:G:218:ILE:HG22	2.05	0.56
1:G:434:ARG:NH1	1:G:464:PHE:HA	2.19	0.56
1:A:484:ARG:NH1	2:B:31:THR:HG22	2.21	0.56
2:B:427:ASP:OD2	2:B:428:VAL:N	2.38	0.56
2:D:216:ALA:O	2:D:220:SER:HB2	2.06	0.56
2:D:352:ASN:HB3	2:D:439:HIS:CD2	2.39	0.56
2:F:96:PRO:O	2:F:99:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:422:GLU:C	2:H:423:LEU:HD12	2.25	0.56
1:A:371:ALA:C	1:A:373:GLU:H	2.08	0.56
1:C:59:ILE:HG22	1:C:60:ILE:H	1.69	0.56
1:C:307:LEU:HD22	1:C:383:LEU:HD22	1.88	0.56
1:E:215:ILE:HG13	1:E:332:MET:SD	2.46	0.56
2:H:383:ALA:HB3	2:H:392:LEU:HD21	1.87	0.56
1:C:430:ARG:HB3	1:C:430:ARG:HH11	1.70	0.56
2:F:164:TYR:CZ	2:F:348:GLN:HG3	2.41	0.56
1:G:331:ASP:OD1	2:H:223:ARG:HB3	2.04	0.56
2:H:46:LEU:HD23	2:H:71:GLY:O	2.05	0.56
1:E:193:ARG:HG3	1:E:193:ARG:HH11	1.70	0.56
1:G:299:LYS:HA	1:G:368:ILE:CG2	2.36	0.56
2:H:229:ILE:HD13	2:H:281:THR:HA	1.88	0.56
2:D:148:ILE:HG12	2:D:207:TYR:CE2	2.40	0.56
1:E:218:ILE:O	1:E:222:LEU:HB2	2.06	0.56
1:E:264:ASN:HD22	1:E:265:PHE:N	2.04	0.56
3:L:155:THR:HG23	3:L:158:ASP:H	1.70	0.56
1:A:147:GLN:HE21	1:A:147:GLN:CA	2.18	0.56
1:C:435:PHE:O	1:C:439:GLN:HB2	2.05	0.56
2:F:147:SER:HB2	2:F:149:ILE:HD13	1.87	0.56
3:K:107:THR:HG22	3:K:109:THR:N	2.20	0.56
1:G:407:ILE:HG13	1:G:408:ASN:N	2.21	0.56
2:H:324:PHE:HD1	2:H:332:THR:HG22	1.70	0.56
2:H:356:SER:C	2:H:358:SER:H	2.08	0.56
2:B:425:VAL:HB	2:B:434:VAL:CG1	2.35	0.56
1:C:297:ILE:H	1:C:297:ILE:CD1	2.16	0.56
2:D:158:LEU:HD13	2:D:177:LEU:HB2	1.86	0.56
3:J:116:ASP:O	3:J:117:ILE:HD13	2.06	0.56
1:E:518:ASN:HB2	1:E:533:GLN:HA	1.87	0.56
2:F:16:ARG:NH2	2:F:116:PRO:HB2	2.21	0.56
2:F:312:THR:O	2:F:313:SER:HB2	2.05	0.56
2:B:198:ALA:H	2:B:320:ASN:HD21	1.54	0.55
2:B:252:ASP:O	2:B:254:PRO:HD3	2.06	0.55
1:C:233:ILE:N	1:C:233:ILE:HD12	2.21	0.55
2:D:57:GLY:C	2:D:91:GLN:HG2	2.26	0.55
1:E:299:LYS:HE2	1:E:368:ILE:O	2.06	0.55
2:F:256:HIS:O	2:F:260:ILE:HG13	2.06	0.55
1:A:66:SER:O	1:A:81:ILE:HG23	2.06	0.55
1:A:264:ASN:HD22	1:A:264:ASN:H	1.53	0.55
1:C:426:TYR:O	1:C:430:ARG:HG2	2.06	0.55
1:E:158:LEU:HD12	1:E:158:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:ASN:HD22	2:F:26:ARG:NH2	2.04	0.55
2:F:381:ILE:HG22	2:F:382:THR:N	2.20	0.55
1:G:7:LEU:O	1:G:7:LEU:HD23	2.06	0.55
2:H:52:LEU:HD22	2:H:138:PHE:CE1	2.42	0.55
2:B:197:THR:CG2	2:B:198:ALA:N	2.70	0.55
2:B:356:SER:N	2:B:441:THR:OG1	2.38	0.55
1:C:61:ASP:HB2	1:C:86:ALA:HB2	1.88	0.55
1:C:481:GLU:OE2	2:D:29:PRO:HD2	2.05	0.55
2:F:348:GLN:O	2:F:348:GLN:HG2	2.06	0.55
2:F:351:GLN:H	2:F:436:PHE:HA	1.70	0.55
2:F:412:LEU:HD13	2:F:440:PHE:CE2	2.35	0.55
1:A:19:LEU:HD21	2:B:290:PRO:CB	2.36	0.55
1:C:119:PHE:O	1:C:122:ARG:HG2	2.07	0.55
1:C:259:PRO:CB	1:C:262:GLU:OE1	2.47	0.55
1:E:84:ASN:OD1	1:E:106:GLU:HG2	2.06	0.55
1:E:212:THR:O	1:E:213:PRO:C	2.44	0.55
1:E:234:PRO:HG2	1:E:243:PHE:CD1	2.42	0.55
2:F:15:GLY:HA2	2:F:18:ASN:ND2	2.21	0.55
2:F:234:MET:O	2:F:235:LEU:HD23	2.06	0.55
2:F:320:ASN:ND2	2:F:337:ALA:O	2.40	0.55
1:G:18:ARG:HH12	2:H:279:ARG:HG3	1.71	0.55
1:A:74:PHE:CD1	2:B:65:LYS:HG3	2.42	0.55
2:D:230:GLU:HG3	2:D:230:GLU:O	2.07	0.55
1:E:357:VAL:O	1:E:361:VAL:HG23	2.06	0.55
1:G:180:LEU:H	1:G:180:LEU:CD1	2.17	0.55
1:G:267:GLU:O	1:G:270:LYS:HG2	2.06	0.55
3:L:113:ILE:HG13	3:L:113:ILE:O	2.06	0.55
1:A:14:ASP:O	1:A:18:ARG:HG3	2.07	0.55
1:A:112:LEU:HD22	1:A:112:LEU:N	2.19	0.55
1:G:164:ILE:HD11	1:G:166:ILE:HD11	1.89	0.55
1:G:299:LYS:HG2	1:G:368:ILE:HG22	1.89	0.55
1:A:193:ARG:O	1:A:197:GLN:HG3	2.07	0.55
3:J:170:VAL:HG22	3:J:171:LEU:N	2.18	0.55
1:E:396:ARG:NH2	1:E:400:GLU:HB3	2.22	0.55
2:F:425:VAL:HB	2:F:434:VAL:CG1	2.37	0.55
2:B:435:LEU:C	2:B:436:PHE:HD1	2.10	0.55
2:D:240:GLU:HG3	2:D:240:GLU:O	2.07	0.55
1:A:47:LYS:HG3	1:A:75:PHE:CZ	2.42	0.55
2:B:353:ILE:HD11	2:B:367:TYR:HE2	1.71	0.55
3:J:123:VAL:CB	3:J:152:ASP:HA	2.22	0.55
1:E:173:GLU:O	1:E:512:GLN:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:THR:HG22	1:G:322:ASN:ND2	2.22	0.55
2:H:217:THR:HG21	2:H:223:ARG:NH2	2.19	0.55
2:D:74:GLN:HE22	2:D:119:ASN:HD22	1.52	0.54
2:H:228:CYS:SG	2:H:268:ALA:HB2	2.47	0.54
1:A:418:ASN:HD22	1:A:419:PRO:N	2.05	0.54
1:C:412:ILE:O	1:C:416:MET:HB2	2.07	0.54
2:F:236:GLN:HE22	2:F:263:LYS:HD2	1.72	0.54
1:G:87:GLU:O	1:G:91:GLU:HG3	2.07	0.54
1:G:248:ARG:O	1:G:251:ILE:CG1	2.55	0.54
1:G:516:PHE:H	1:G:516:PHE:HD2	1.54	0.54
1:C:243:PHE:O	1:C:246:LEU:HB3	2.08	0.54
2:D:229:ILE:HD13	2:D:281:THR:HA	1.89	0.54
1:E:215:ILE:HD12	1:E:332:MET:HE1	1.89	0.54
1:E:252:LEU:O	1:E:259:PRO:N	2.40	0.54
2:F:87:ASN:HD21	2:F:103:LYS:HE2	1.70	0.54
2:H:200:ILE:HD13	3:L:172:ARG:HH22	1.72	0.54
2:H:412:LEU:HD23	2:H:438:LEU:HD21	1.88	0.54
2:B:182:THR:HG22	3:I:176:GLY:HA2	1.90	0.54
1:C:154:ARG:HB3	1:C:161:TYR:HB3	1.88	0.54
1:C:232:ARG:C	1:C:233:ILE:HD12	2.28	0.54
2:F:318:LEU:HD11	2:F:334:THR:CG2	2.37	0.54
3:K:123:VAL:CB	3:K:152:ASP:HA	2.21	0.54
1:G:37:ASN:HB3	1:G:39:THR:HG23	1.89	0.54
1:G:518:ASN:HB3	1:G:532:PHE:O	2.07	0.54
1:E:171:VAL:CG1	1:E:391:ARG:HB2	2.37	0.54
1:E:332:MET:O	2:F:223:ARG:NE	2.40	0.54
1:A:45:ILE:HG12	1:A:498:GLY:HA2	1.90	0.54
1:A:178:ASN:CG	3:I:136:ILE:HG12	2.28	0.54
1:A:461:LEU:HD21	1:A:474:VAL:HG11	1.89	0.54
1:C:34:CYS:HB2	1:C:123:PHE:CD2	2.42	0.54
1:G:215:ILE:H	1:G:332:MET:CE	2.20	0.54
1:A:78:ARG:HA	1:A:81:ILE:HG13	1.90	0.54
1:C:248:ARG:O	1:C:250:GLY:N	2.41	0.54
2:D:32:HIS:ND1	2:D:33:PRO:HD2	2.23	0.54
1:E:302:PRO:HG2	1:E:305:TRP:HD1	1.72	0.54
1:G:434:ARG:O	1:G:438:GLN:HG2	2.08	0.54
2:H:229:ILE:HD12	2:H:284:VAL:HG21	1.88	0.54
3:L:143:LEU:C	3:L:144:ILE:HD12	2.28	0.54
1:A:96:LEU:HD23	2:B:95:ARG:HH21	1.73	0.54
1:E:220:LYS:C	1:E:222:LEU:H	2.11	0.54
1:E:260:GLU:O	1:E:261:ASP:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:ILE:CG2	2:F:145:LEU:HD21	2.37	0.54
2:F:415:LEU:HB2	2:F:417:LEU:CD1	2.38	0.54
1:G:307:LEU:HB3	1:G:383:LEU:HD21	1.89	0.54
2:H:38:SER:C	2:H:40:GLU:H	2.10	0.54
2:H:132:ASP:HB3	2:H:157:MET:HE1	1.90	0.54
2:H:259:TRP:CE2	2:H:263:LYS:HG3	2.42	0.54
1:A:396:ARG:HD3	1:A:534:LEU:O	2.08	0.54
2:B:226:GLU:HG3	2:B:280:LEU:HD11	1.90	0.54
1:C:274:THR:C	1:C:276:LEU:N	2.61	0.54
2:D:357:PRO:HG3	2:D:440:PHE:CD2	2.43	0.54
2:H:231:TYR:O	2:H:233:ARG:N	2.41	0.54
1:A:12:LYS:HG3	1:A:13:TYR:CD2	2.43	0.54
1:A:214:TRP:CZ3	1:A:332:MET:HB3	2.43	0.54
2:B:359:ALA:O	2:B:412:LEU:HD23	2.08	0.54
1:E:163:ARG:NH1	1:E:518:ASN:HD21	2.05	0.54
1:G:269:ILE:HG22	1:G:269:ILE:O	2.08	0.54
1:A:78:ARG:O	1:A:81:ILE:HG13	2.08	0.53
2:B:62:GLU:HG2	2:B:300:ALA:HB3	1.89	0.53
2:D:362:GLN:NE2	2:D:365:LEU:HD23	2.23	0.53
3:L:117:ILE:CG2	3:L:121:ASP:HB2	2.38	0.53
2:B:46:LEU:HD22	2:B:73:ARG:CZ	2.38	0.53
2:B:241:GLN:OE1	2:B:246:GLY:N	2.40	0.53
2:B:351:GLN:HB3	2:B:436:PHE:CG	2.43	0.53
2:B:419:ASP:HA	2:B:440:PHE:HE1	1.72	0.53
1:C:130:GLN:CD	1:C:155:THR:H	2.12	0.53
2:D:183:GLU:HB3	3:J:173:LEU:HD22	1.89	0.53
2:D:415:LEU:HD11	2:D:417:LEU:HG	1.90	0.53
2:D:415:LEU:CD1	2:D:417:LEU:HG	2.38	0.53
3:K:119:PRO:O	3:K:157:ALA:HB2	2.08	0.53
1:A:162:MET:HB3	1:A:520:TYR:HB3	1.90	0.53
1:A:214:TRP:C	1:A:214:TRP:CD1	2.82	0.53
3:J:118:GLU:HG3	3:J:120:THR:CG2	2.37	0.53
1:E:158:LEU:HD11	2:F:23:PHE:CE2	2.43	0.53
2:F:125:ASN:HB2	2:F:129:ASP:OD2	2.07	0.53
2:H:207:TYR:OH	3:L:172:ARG:NE	2.40	0.53
2:H:224:LEU:N	2:H:227:HIS:ND1	2.55	0.53
2:H:344:PRO:HG3	2:H:374:LEU:HD22	1.90	0.53
1:A:282:PRO:HB2	1:A:285:ILE:HD13	1.91	0.53
2:B:74:GLN:HE22	2:B:119:ASN:ND2	2.06	0.53
2:F:322:LEU:HD13	2:F:323:VAL:N	2.23	0.53
1:E:246:LEU:O	1:E:246:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:356:SER:C	2:F:358:SER:H	2.12	0.53
2:H:402:GLU:HA	2:H:405:ARG:HH12	1.73	0.53
1:A:437:LYS:HA	1:A:437:LYS:NZ	2.24	0.53
2:B:49:CYS:HA	2:B:139:HIS:CD2	2.43	0.53
2:B:195:GLY:O	2:B:339:ARG:NH1	2.41	0.53
1:C:59:ILE:O	1:C:60:ILE:HG13	2.08	0.53
1:C:297:ILE:HD13	1:C:297:ILE:N	2.19	0.53
1:E:171:VAL:HG12	1:E:391:ARG:HB2	1.89	0.53
2:F:391:THR:HG21	2:F:394:LEU:HB2	1.90	0.53
1:G:333:ILE:CA	2:H:223:ARG:NH1	2.71	0.53
2:B:251:GLY:O	2:B:257:ILE:HD11	2.09	0.53
2:B:361:LEU:O	2:B:364:VAL:HG23	2.09	0.53
1:C:341:LYS:O	1:C:345:VAL:HG23	2.08	0.53
1:E:68:GLU:HG2	2:F:18:ASN:HD22	1.73	0.53
1:A:72:ASN:ND2	1:A:72:ASN:C	2.62	0.53
1:A:172:ILE:HA	1:A:390:LEU:HD23	1.91	0.53
2:B:190:GLN:HG3	2:B:191:VAL:N	2.23	0.53
1:C:120:PHE:C	1:C:122:ARG:H	2.12	0.53
1:E:447:ASN:HD22	2:F:26:ARG:HH21	1.55	0.53
1:E:527:GLN:HB2	2:F:318:LEU:HD13	1.89	0.53
1:A:130:GLN:OE1	1:A:154:ARG:HA	2.09	0.53
2:B:241:GLN:O	2:B:242:PRO:C	2.47	0.53
1:C:36:ILE:CB	1:C:128:ALA:HA	2.36	0.53
1:A:72:ASN:C	1:A:72:ASN:HD22	2.11	0.53
2:B:178:ILE:HD11	2:B:310:ILE:CD1	2.39	0.53
2:B:207:TYR:O	3:I:142:ARG:NH1	2.42	0.53
1:C:59:ILE:HG22	1:C:60:ILE:N	2.23	0.53
1:C:132:PRO:HD2	1:C:135:THR:HB	1.90	0.53
2:D:398:THR:O	2:D:402:GLU:HG3	2.09	0.53
1:E:113:LEU:HB3	1:E:138:ARG:NH2	2.23	0.53
1:G:404:LEU:HD21	1:G:467:GLU:HG2	1.89	0.53
3:L:126:ILE:HD11	3:L:156:ALA:HB2	1.91	0.53
1:A:518:ASN:ND2	1:A:534:LEU:CA	2.72	0.52
2:D:405:ARG:HB3	2:D:405:ARG:HH11	1.73	0.52
2:H:234:MET:O	2:H:234:MET:HG2	2.08	0.52
2:H:243:PHE:O	2:H:247:VAL:HB	2.09	0.52
2:H:380:ALA:HB1	2:H:394:LEU:CD1	2.35	0.52
2:H:382:THR:OG1	2:H:424:ALA:HB3	2.08	0.52
2:B:51:VAL:HG11	2:B:67:LEU:HD13	1.89	0.52
2:B:360:LYS:O	2:B:363:GLU:HB2	2.09	0.52
2:B:407:ASN:HB3	2:B:415:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:GLU:HG3	2:B:436:PHE:O	2.10	0.52
3:I:102:LEU:O	3:I:102:LEU:HD23	2.09	0.52
1:G:226:TYR:CZ	1:G:233:ILE:HG22	2.44	0.52
2:H:338:GLU:CD	3:L:148:LYS:HE3	2.29	0.52
2:H:348:GLN:CA	2:H:348:GLN:HE21	2.21	0.52
1:E:194:GLU:O	1:E:196:PHE:N	2.42	0.52
3:K:123:VAL:HB	3:K:152:ASP:CA	2.21	0.52
1:G:299:LYS:HE2	1:G:368:ILE:O	2.09	0.52
1:G:518:ASN:HB2	1:G:533:GLN:HA	1.89	0.52
2:H:412:LEU:HD22	2:H:440:PHE:HE2	1.73	0.52
2:D:246:GLY:O	2:D:248:PRO:HD3	2.09	0.52
2:F:195:GLY:O	2:F:196:MET:HG2	2.10	0.52
1:A:248:ARG:C	1:A:250:GLY:H	2.12	0.52
3:K:102:LEU:O	3:K:163:GLY:O	2.28	0.52
1:G:244:ARG:HH11	1:G:244:ARG:HG3	1.74	0.52
2:H:343:CYS:O	2:H:347:SER:HB3	2.10	0.52
1:A:119:PHE:O	1:A:122:ARG:HG2	2.10	0.52
3:J:105:VAL:HG11	3:J:115:ILE:HD11	1.90	0.52
2:H:102:PRO:HG2	2:H:105:GLU:HB2	1.91	0.52
2:B:83:ILE:HD13	2:B:94:PHE:HB3	1.91	0.52
2:B:434:VAL:HG22	2:B:436:PHE:HE1	1.75	0.52
1:E:307:LEU:HD21	1:E:375:ILE:HG21	1.91	0.52
1:E:376:SER:OG	1:E:379:GLU:HG3	2.09	0.52
2:F:183:GLU:HG3	2:F:289:ILE:CG2	2.39	0.52
2:F:324:PHE:HD1	2:F:332:THR:HG22	1.74	0.52
1:G:25:GLN:O	1:G:29:GLU:HG3	2.10	0.52
1:G:377:GLU:OE2	1:G:381:LYS:HE2	2.09	0.52
2:H:231:TYR:C	2:H:233:ARG:H	2.14	0.52
2:H:381:ILE:HD12	2:H:381:ILE:N	2.25	0.52
2:B:419:ASP:CA	2:B:440:PHE:HE1	2.23	0.52
3:I:115:ILE:HD11	3:I:126:ILE:HG23	1.90	0.52
2:H:385:LEU:HD12	2:H:390:ARG:HD3	1.92	0.52
1:A:309:ARG:HG3	1:A:364:LEU:HD21	1.92	0.52
1:A:516:PHE:CD1	1:A:518:ASN:O	2.63	0.52
2:B:232:VAL:CG1	2:B:260:ILE:HG23	2.40	0.52
1:C:66:SER:H	1:C:69:ASP:HB2	1.74	0.52
2:D:152:ARG:CZ	2:D:429:THR:HG21	2.40	0.52
2:D:152:ARG:HB3	2:D:429:THR:CG2	2.39	0.52
2:D:231:TYR:CD1	2:D:235:LEU:HD12	2.45	0.52
2:D:318:LEU:HD11	2:D:334:THR:HG21	1.89	0.52
1:G:333:ILE:HA	2:H:223:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ALA:HB1	1:A:131:LEU:CD1	2.40	0.52
1:C:521:ILE:HD12	1:C:532:PHE:HE1	1.75	0.52
2:D:327:VAL:HG23	2:D:328:ASP:H	1.75	0.52
2:D:362:GLN:HG2	2:D:408:LEU:HB3	1.92	0.52
1:E:309:ARG:HG3	1:E:309:ARG:NH1	2.24	0.52
1:E:450:VAL:O	1:E:454:ILE:HG13	2.10	0.52
3:K:142:ARG:HB2	3:K:170:VAL:HG12	1.92	0.52
1:C:226:TYR:CZ	1:C:231:GLY:HA2	2.45	0.51
1:C:462:THR:O	1:C:466:GLN:HB2	2.09	0.51
3:K:107:THR:C	3:K:109:THR:H	2.13	0.51
2:H:148:ILE:HD11	3:L:174:ARG:HD3	1.91	0.51
2:B:13:TRP:CH2	2:B:116:PRO:HG2	2.44	0.51
1:C:33:VAL:CG2	1:C:34:CYS:N	2.74	0.51
1:C:49:LEU:C	1:C:52:PRO:HD2	2.30	0.51
1:E:121:CYS:HA	1:E:148:ILE:HD11	1.92	0.51
1:E:317:LYS:HD3	1:E:318:GLU:OE1	2.10	0.51
1:G:298:THR:OG1	1:G:300:GLN:HG2	2.09	0.51
1:G:331:ASP:OD1	2:H:224:LEU:HD21	2.10	0.51
1:A:516:PHE:CE1	1:A:518:ASN:O	2.64	0.51
2:B:132:ASP:O	2:B:133:THR:C	2.49	0.51
2:F:228:CYS:SG	2:F:273:ILE:HD12	2.50	0.51
2:H:350:PRO:HB2	2:H:437:LYS:HG3	1.91	0.51
1:A:35:LEU:O	1:A:36:ILE:HD13	2.11	0.51
1:A:432:VAL:HG21	1:A:482:PHE:HD2	1.75	0.51
1:A:448:TYR:CE1	1:A:449:GLN:HG3	2.45	0.51
2:B:64:LEU:CB	2:B:111:LEU:HD11	2.41	0.51
2:B:309:LYS:HG2	2:B:315:TYR:HB2	1.92	0.51
2:B:318:LEU:HD11	2:B:334:THR:HG23	1.93	0.51
1:C:397:SER:HG	1:C:400:GLU:HG3	1.74	0.51
1:E:43:THR:HG21	1:E:73:ASN:OD1	2.10	0.51
1:E:72:ASN:HD22	1:E:73:ASN:N	2.08	0.51
2:F:64:LEU:HD21	2:F:77:VAL:CG2	2.41	0.51
1:A:12:LYS:HE3	1:A:13:TYR:CE2	2.46	0.51
2:B:32:HIS:ND1	2:B:33:PRO:HD2	2.26	0.51
2:D:223:ARG:HB2	2:D:223:ARG:NH1	2.24	0.51
1:E:317:LYS:HB3	1:E:318:GLU:OE1	2.10	0.51
2:H:355:PHE:O	2:H:440:PHE:HD2	1.94	0.51
1:C:426:TYR:CE2	1:C:534:LEU:HD13	2.45	0.51
2:D:152:ARG:HB3	2:D:429:THR:HG23	1.90	0.51
1:G:112:LEU:C	1:G:114:ASP:N	2.64	0.51
1:G:168:GLU:HG3	1:G:394:ARG:HE	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:LEU:HD21	2:H:312:THR:HG21	1.91	0.51
2:H:90:ARG:HG2	2:H:90:ARG:NH1	2.24	0.51
1:C:48:ASN:O	1:C:52:PRO:HG2	2.11	0.51
2:D:270:GLN:C	2:D:272:ASN:H	2.13	0.51
3:J:108:LEU:HD22	3:J:169:LEU:O	2.10	0.51
1:E:265:PHE:O	1:E:269:ILE:HG13	2.10	0.51
2:H:350:PRO:HB3	2:H:436:PHE:C	2.31	0.51
1:A:229:THR:HG22	1:A:232:ARG:HB3	1.88	0.51
1:A:445:VAL:O	2:B:22:LYS:HE2	2.11	0.51
2:B:441:THR:C	2:B:442:SER:OXT	2.44	0.51
1:C:185:LEU:HD12	1:C:275:ALA:HB1	1.92	0.51
1:C:446:SER:HB2	1:C:449:GLN:HB3	1.93	0.51
1:E:184:ARG:NH1	1:E:184:ARG:HG3	2.23	0.51
2:F:366:ASP:HB3	2:F:370:ASN:ND2	2.26	0.51
1:G:199:TYR:CE2	1:G:216:VAL:HG11	2.45	0.51
2:H:136:ARG:HG2	2:H:161:LEU:HD22	1.93	0.51
2:H:316:ILE:H	2:H:316:ILE:CD1	2.14	0.51
1:A:176:PRO:HG2	1:A:389:PHE:CD2	2.45	0.51
2:B:27:SER:HB3	2:B:37:PRO:HG3	1.93	0.51
2:B:84:ASP:OD1	2:B:85:VAL:N	2.44	0.51
2:B:187:GLY:HA2	3:I:173:LEU:HD13	1.93	0.51
1:C:236:THR:HG22	1:C:238:LYS:H	1.76	0.51
2:D:25:GLU:O	2:D:37:PRO:HB2	2.11	0.51
1:E:116:ASP:N	1:E:117:PRO:HD3	2.26	0.51
1:G:408:ASN:OD1	1:G:408:ASN:O	2.29	0.51
2:H:339:ARG:HE	2:H:346:CYS:HB3	1.75	0.51
2:H:339:ARG:NH2	2:H:346:CYS:HB3	2.25	0.51
2:H:380:ALA:CB	2:H:394:LEU:CD1	2.78	0.51
1:A:215:ILE:HD12	1:A:342:LEU:HD21	1.93	0.51
1:A:248:ARG:HA	1:A:251:ILE:CD1	2.39	0.51
1:C:113:LEU:HD22	1:C:142:VAL:HG21	1.91	0.51
1:C:344:ASN:HD22	1:C:347:ARG:HH12	1.58	0.51
1:G:447:ASN:HD22	2:H:26:ARG:NH2	2.05	0.51
2:H:74:GLN:NE2	2:H:119:ASN:HD22	2.07	0.51
2:H:320:ASN:HB2	2:H:337:ALA:N	2.26	0.51
2:H:418:VAL:HG22	2:H:421:GLN:OE1	2.11	0.51
1:A:65:VAL:HB	1:A:82:GLY:H	1.75	0.50
2:B:422:GLU:O	2:B:423:LEU:HG	2.10	0.50
1:G:72:ASN:HD22	1:G:72:ASN:N	2.06	0.50
1:G:330:PRO:O	1:G:339:TYR:OH	2.24	0.50
2:H:350:PRO:HB3	2:H:436:PHE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ARG:HH11	2:B:95:ARG:CG	2.22	0.50
1:C:216:VAL:O	1:C:220:LYS:HG2	2.11	0.50
1:E:61:ASP:CB	1:E:86:ALA:HB2	2.40	0.50
2:F:197:THR:HG23	2:F:320:ASN:OD1	2.12	0.50
1:G:184:ARG:NH1	1:G:325:VAL:HG22	2.26	0.50
1:C:259:PRO:CB	1:C:262:GLU:OE2	2.59	0.50
1:E:108:SER:HB2	1:E:109:PRO:HD2	1.92	0.50
2:F:320:ASN:HD22	2:F:337:ALA:N	2.09	0.50
1:G:214:TRP:CZ3	1:G:332:MET:HB3	2.46	0.50
2:H:64:LEU:HD21	2:H:77:VAL:HG21	1.92	0.50
2:H:320:ASN:HB2	2:H:337:ALA:H	1.77	0.50
1:A:112:LEU:O	1:A:116:ASP:O	2.29	0.50
1:C:268:ALA:O	1:C:272:VAL:HG23	2.12	0.50
1:E:187:LYS:HD2	1:E:279:THR:HG21	1.93	0.50
1:E:441:ARG:NH2	1:E:453:ASP:OD1	2.44	0.50
1:G:396:ARG:NH2	1:G:406:THR:O	2.44	0.50
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.93	0.50
1:C:264:ASN:ND2	1:C:265:PHE:N	2.60	0.50
2:D:16:ARG:HD3	2:D:17:TRP:HE1	1.75	0.50
1:E:66:SER:H	1:E:69:ASP:HB2	1.75	0.50
1:E:264:ASN:ND2	1:E:265:PHE:N	2.60	0.50
2:F:232:VAL:HG21	2:F:264:SER:HA	1.93	0.50
2:F:236:GLN:NE2	2:F:263:LYS:HB3	2.26	0.50
2:F:280:LEU:O	2:F:284:VAL:HG23	2.11	0.50
2:H:250:ASP:HB3	2:H:253:ASP:HB2	1.94	0.50
2:H:270:GLN:C	2:H:271:TYR:HD2	2.14	0.50
2:D:314:ALA:O	2:D:315:TYR:CD1	2.65	0.50
2:F:338:GLU:OE1	3:K:148:LYS:HE3	2.12	0.50
1:G:226:TYR:O	1:G:231:GLY:N	2.44	0.50
1:G:450:VAL:O	1:G:454:ILE:HG13	2.11	0.50
2:H:220:SER:O	2:H:222:PRO:HD3	2.11	0.50
2:H:322:LEU:HD12	2:H:323:VAL:O	2.12	0.50
1:A:227:SER:C	1:A:229:THR:H	2.15	0.50
1:A:491:HIS:CD2	2:B:69:LEU:HD12	2.46	0.50
1:C:215:ILE:HD12	1:C:342:LEU:HD21	1.93	0.50
1:C:325:VAL:HG21	1:C:349:LYS:HG2	1.94	0.50
2:D:24:LEU:CD2	2:D:312:THR:HB	2.41	0.50
2:D:142:VAL:HG12	2:D:178:ILE:HB	1.93	0.50
1:E:375:ILE:N	1:E:375:ILE:HD12	2.27	0.50
2:B:376:MET:HB3	2:B:427:ASP:OD1	2.12	0.50
2:D:83:ILE:HD12	2:D:98:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:THR:HG22	2:D:278:TYR:N	2.27	0.50
1:E:447:ASN:HD21	2:F:26:ARG:HE	1.59	0.50
2:F:376:MET:CE	2:F:427:ASP:HB2	2.42	0.50
2:F:401:GLU:HG3	2:F:402:GLU:N	2.27	0.50
2:H:393:TYR:HA	2:H:404:THR:HB	1.93	0.50
2:B:430:THR:HG22	2:B:431:PRO:CD	2.41	0.49
3:I:103:ILE:HD11	3:I:117:ILE:HD12	1.94	0.49
3:I:104:LYS:O	3:I:166:VAL:HA	2.12	0.49
1:C:34:CYS:SG	1:C:60:ILE:HD12	2.51	0.49
2:H:231:TYR:C	2:H:233:ARG:N	2.66	0.49
3:L:120:THR:CB	3:L:155:THR:OG1	2.60	0.49
2:B:197:THR:HG23	2:B:198:ALA:N	2.27	0.49
2:B:391:THR:HG21	2:B:400:ILE:HG21	1.94	0.49
2:B:415:LEU:HB2	2:B:417:LEU:HD21	1.93	0.49
1:C:454:ILE:HD13	1:C:480:HIS:ND1	2.27	0.49
1:E:19:LEU:HG	2:F:290:PRO:HB2	1.94	0.49
1:E:199:TYR:CD2	1:E:216:VAL:HG11	2.46	0.49
1:E:309:ARG:HB3	1:E:364:LEU:CD2	2.42	0.49
1:G:218:ILE:O	1:G:222:LEU:HB2	2.12	0.49
2:H:407:ASN:C	2:H:409:SER:H	2.15	0.49
2:B:284:VAL:O	2:B:287:ARG:NH1	2.45	0.49
2:B:319:ASN:CG	2:B:336:GLU:HG3	2.32	0.49
2:D:152:ARG:NE	2:D:429:THR:HG21	2.27	0.49
2:D:352:ASN:HB3	2:D:439:HIS:HD2	1.78	0.49
1:G:43:THR:HG21	1:G:73:ASN:OD1	2.11	0.49
2:H:240:GLU:O	2:H:242:PRO:CD	2.59	0.49
2:H:322:LEU:HD12	2:H:323:VAL:N	2.26	0.49
3:L:105:VAL:HG13	3:L:105:VAL:O	2.11	0.49
2:B:197:THR:HG23	2:B:320:ASN:HD21	1.78	0.49
1:C:409:LYS:O	1:C:413:ILE:HG13	2.11	0.49
2:F:342:ASN:ND2	2:F:342:ASN:N	2.57	0.49
1:G:34:CYS:HB2	1:G:123:PHE:CG	2.48	0.49
1:G:288:ILE:HG23	1:G:305:TRP:CZ3	2.47	0.49
2:H:344:PRO:CD	2:H:374:LEU:HD22	2.42	0.49
2:B:37:PRO:O	2:B:38:SER:HB2	2.11	0.49
3:I:171:LEU:HD12	3:I:172:ARG:H	1.76	0.49
2:D:234:MET:O	2:D:235:LEU:HD23	2.13	0.49
1:E:72:ASN:C	1:E:72:ASN:ND2	2.65	0.49
2:F:188:ASN:OD1	3:K:173:LEU:HD12	2.12	0.49
1:G:12:LYS:HE3	1:G:13:TYR:CZ	2.48	0.49
2:H:233:ARG:HH12	2:H:234:MET:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:HG3	1:A:433:ASP:HB3	1.95	0.49
2:B:348:GLN:OE1	2:B:348:GLN:HA	2.13	0.49
3:I:126:ILE:O	3:I:130:VAL:HG23	2.11	0.49
1:C:36:ILE:HG22	1:C:37:ASN:N	2.27	0.49
2:D:18:ASN:O	2:D:22:LYS:HG3	2.13	0.49
2:D:232:VAL:HA	2:D:236:GLN:HB3	1.94	0.49
2:D:434:VAL:HG13	2:D:436:PHE:HE1	1.77	0.49
3:J:104:LYS:HD3	3:J:112:GLU:OE2	2.12	0.49
2:F:275:GLY:O	2:F:280:LEU:HD23	2.13	0.49
1:G:12:LYS:HG3	2:H:88:LEU:HB2	1.94	0.49
2:H:357:PRO:HG3	2:H:440:PHE:CG	2.48	0.49
1:C:35:LEU:HD12	1:C:129:THR:HG23	1.94	0.49
1:C:157:GLY:HA3	1:C:485:TYR:CD1	2.47	0.49
2:F:102:PRO:HG2	2:F:105:GLU:CB	2.43	0.49
2:F:401:GLU:O	2:F:405:ARG:N	2.44	0.49
1:G:518:ASN:ND2	1:G:534:LEU:N	2.61	0.49
2:H:18:ASN:O	2:H:22:LYS:HG2	2.12	0.49
2:H:45:LEU:HD11	2:H:72:PHE:CE2	2.48	0.49
3:L:162:LEU:O	3:L:164:GLY:N	2.45	0.49
3:I:118:GLU:O	3:I:120:THR:N	2.46	0.49
1:C:131:LEU:HB3	1:C:132:PRO:CD	2.43	0.49
1:C:137:LEU:HA	1:C:398:LEU:HD23	1.95	0.49
2:F:132:ASP:HB3	2:F:157:MET:CE	2.42	0.49
3:K:118:GLU:HG2	3:K:121:ASP:CG	2.33	0.49
1:G:34:CYS:HB2	1:G:123:PHE:CD2	2.47	0.49
2:H:401:GLU:HG3	2:H:402:GLU:N	2.28	0.49
1:A:409:LYS:O	1:A:413:ILE:HG13	2.12	0.49
2:D:286:LYS:HB2	2:D:288:ILE:HG13	1.94	0.49
3:J:107:THR:HG23	3:J:109:THR:H	1.77	0.49
1:E:336:SER:OG	2:F:221:MET:HA	2.12	0.49
1:A:64:GLN:HA	1:A:83:LYS:O	2.13	0.49
1:A:164:ILE:HD11	1:A:166:ILE:HD11	1.95	0.49
2:B:418:VAL:HG22	2:B:421:GLN:HG3	1.95	0.49
1:C:220:LYS:HA	1:C:220:LYS:HE3	1.95	0.49
2:D:178:ILE:HD12	2:D:307:VAL:HG22	1.94	0.49
1:E:297:ILE:HD12	1:E:297:ILE:N	2.19	0.49
2:H:148:ILE:O	2:H:152:ARG:HG3	2.13	0.49
1:A:323:LEU:HB3	1:A:324:PRO:HD2	1.95	0.48
1:A:425:LEU:HD11	1:A:523:SER:HB2	1.95	0.48
1:C:229:THR:HG22	1:C:232:ARG:HB2	1.91	0.48
2:D:268:ALA:CB	2:D:276:VAL:HG21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LEU:CD1	1:E:383:LEU:HD22	2.39	0.48
1:G:164:ILE:HD13	1:G:515:ILE:HD12	1.95	0.48
2:H:98:ASP:OD1	2:H:101:ARG:NH1	2.46	0.48
2:H:170:ASP:O	2:H:173:SER:HB3	2.12	0.48
2:H:349:LEU:HB3	2:H:350:PRO:CD	2.42	0.48
1:A:348:GLU:HG3	1:E:115:ASN:ND2	2.27	0.48
2:B:353:ILE:CG2	2:B:355:PHE:HD1	2.23	0.48
2:D:231:TYR:C	2:D:233:ARG:N	2.64	0.48
3:J:124:GLU:HB3	3:J:152:ASP:O	2.12	0.48
1:E:12:LYS:HE3	1:E:13:TYR:CZ	2.47	0.48
1:E:158:LEU:HA	1:E:493:ILE:HG13	1.95	0.48
2:F:197:THR:CG2	2:F:198:ALA:N	2.75	0.48
2:F:322:LEU:CD1	2:F:322:LEU:C	2.82	0.48
3:K:118:GLU:O	3:K:120:THR:N	2.46	0.48
1:G:165:ILE:HG22	1:G:165:ILE:O	2.11	0.48
2:H:320:ASN:HB2	2:H:336:GLU:HA	1.95	0.48
1:A:211:HIS:HB3	1:A:335:ASP:HB3	1.96	0.48
1:A:297:ILE:HG22	1:A:298:THR:N	2.29	0.48
2:B:353:ILE:HG22	2:B:438:LEU:HB2	1.95	0.48
1:C:19:LEU:HD22	2:D:185:PHE:CE1	2.48	0.48
1:C:293:ARG:HB3	1:C:305:TRP:CD2	2.48	0.48
1:C:526:SER:O	1:C:527:GLN:HB2	2.13	0.48
2:D:207:TYR:CD1	3:J:172:ARG:HD3	2.46	0.48
2:D:225:PRO:HG3	2:D:274:ARG:O	2.13	0.48
1:E:527:GLN:CB	2:F:318:LEU:HD13	2.42	0.48
1:A:35:LEU:C	1:A:36:ILE:HD13	2.33	0.48
1:A:401:GLU:O	1:A:407:ILE:HG12	2.13	0.48
3:I:107:THR:CG2	3:I:108:LEU:N	2.76	0.48
1:C:240:LYS:O	1:C:244:ARG:HG3	2.13	0.48
2:D:208:PRO:HB2	2:D:209:PRO:HD2	1.95	0.48
1:E:220:LYS:C	1:E:222:LEU:N	2.66	0.48
1:G:218:ILE:HD11	1:G:272:VAL:HG22	1.95	0.48
2:H:56:ALA:O	2:H:103:LYS:HD3	2.12	0.48
1:A:181:GLU:O	1:A:278:THR:HB	2.13	0.48
2:B:400:ILE:H	2:B:400:ILE:CD1	2.27	0.48
2:B:417:LEU:CD1	2:B:421:GLN:HE22	2.26	0.48
1:C:190:PRO:O	1:C:194:GLU:HG3	2.13	0.48
1:C:354:ALA:HA	1:C:384:CYS:SG	2.52	0.48
1:C:481:GLU:HG2	1:C:525:MET:SD	2.53	0.48
1:C:521:ILE:HD12	1:C:532:PHE:CE1	2.49	0.48
2:D:419:ASP:HB2	2:D:440:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:CYS:HB2	1:E:123:PHE:CD2	2.48	0.48
1:E:259:PRO:CB	1:E:261:ASP:O	2.62	0.48
1:G:108:SER:HB3	1:G:111:ASN:HB3	1.94	0.48
2:H:52:LEU:HB2	2:H:138:PHE:CD2	2.48	0.48
1:A:401:GLU:OE2	1:A:534:LEU:HB2	2.13	0.48
1:E:48:ASN:HB2	1:E:502:ALA:CB	2.43	0.48
2:H:158:LEU:HD13	2:H:177:LEU:HD22	1.96	0.48
2:H:322:LEU:HD12	2:H:322:LEU:C	2.34	0.48
1:A:236:THR:O	1:A:240:LYS:HG3	2.13	0.48
2:B:198:ALA:HB3	2:B:320:ASN:ND2	2.28	0.48
2:D:87:ASN:ND2	2:D:103:LYS:HE2	2.29	0.48
2:D:249:LEU:HD11	2:D:260:ILE:HD11	1.95	0.48
1:E:183:LEU:O	1:E:184:ARG:HB2	2.14	0.48
1:E:481:GLU:OE1	2:F:29:PRO:HD2	2.13	0.48
2:H:382:THR:HA	2:H:392:LEU:HG	1.96	0.48
3:L:170:VAL:CG1	3:L:171:LEU:H	2.18	0.48
2:B:405:ARG:HB3	2:B:406:PRO:HD3	1.95	0.48
1:C:50:VAL:HG13	1:C:100:VAL:HG21	1.95	0.48
2:D:361:LEU:O	2:D:363:GLU:N	2.47	0.48
1:E:422:GLU:HG3	1:E:530:ALA:CB	2.42	0.48
1:E:435:PHE:HE1	1:E:456:LYS:HB2	1.78	0.48
2:F:231:TYR:CG	2:F:267:ARG:NH1	2.81	0.48
1:A:47:LYS:HD2	1:A:47:LYS:O	2.14	0.48
1:A:186:ASP:C	1:A:188:PRO:HD3	2.35	0.48
2:D:393:TYR:CZ	2:D:408:LEU:HD11	2.49	0.48
3:K:115:ILE:CG2	3:K:117:ILE:HD13	2.43	0.48
2:H:89:ASN:OD1	2:H:90:ARG:NH1	2.47	0.48
2:H:377:LYS:HD3	2:H:428:VAL:HG21	1.96	0.48
2:H:414:GLU:O	2:H:414:GLU:HG2	2.14	0.48
3:L:161:ILE:O	3:L:162:LEU:HD23	2.14	0.48
1:A:527:GLN:NE2	2:B:302:VAL:HG13	2.28	0.48
2:B:391:THR:O	2:B:391:THR:HG22	2.13	0.48
2:D:13:TRP:CD1	2:D:13:TRP:C	2.87	0.48
1:E:491:HIS:NE2	2:F:65:LYS:HE3	2.29	0.48
2:F:102:PRO:HG2	2:F:105:GLU:HB3	1.95	0.48
2:H:251:GLY:O	2:H:286:LYS:HD2	2.13	0.48
2:B:208:PRO:HG3	3:I:171:LEU:HD11	1.95	0.47
1:C:175:HIS:HD2	1:C:512:GLN:O	1.97	0.47
1:C:418:ASN:HD22	1:C:419:PRO:CD	2.27	0.47
2:D:73:ARG:HG3	2:D:73:ARG:NH1	2.29	0.47
3:J:115:ILE:HG23	3:J:129:ARG:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:CYS:HB2	1:E:123:PHE:CE2	2.49	0.47
1:E:187:LYS:HD2	1:E:279:THR:CG2	2.44	0.47
1:E:422:GLU:CD	1:E:422:GLU:H	2.15	0.47
2:F:158:LEU:HD12	2:F:175:VAL:HB	1.96	0.47
1:G:18:ARG:NH1	2:H:279:ARG:HG3	2.28	0.47
2:H:197:THR:HG22	2:H:198:ALA:N	2.29	0.47
1:A:40:ALA:O	1:A:43:THR:HG22	2.14	0.47
2:B:187:GLY:CA	3:I:173:LEU:HD13	2.44	0.47
2:B:403:ARG:HG3	2:B:403:ARG:HH11	1.80	0.47
1:C:168:GLU:HG2	1:C:170:PRO:HD3	1.96	0.47
1:C:264:ASN:HD22	1:C:264:ASN:N	2.10	0.47
1:C:457:LEU:C	1:C:459:SER:H	2.16	0.47
1:E:75:PHE:O	1:E:76:LEU:HD23	2.14	0.47
1:G:36:ILE:HG21	1:G:131:LEU:HD11	1.96	0.47
1:G:43:THR:HG22	1:G:44:GLU:N	2.29	0.47
1:G:120:PHE:O	1:G:148:ILE:HD13	2.14	0.47
1:G:225:TRP:CE2	1:G:234:PRO:HG3	2.49	0.47
2:H:57:GLY:HA2	2:H:91:GLN:HG2	1.96	0.47
2:H:249:LEU:HD11	2:H:260:ILE:HD11	1.95	0.47
2:B:351:GLN:H	2:B:436:PHE:HA	1.78	0.47
1:C:25:GLN:O	1:C:29:GLU:HG3	2.14	0.47
2:D:73:ARG:HG3	2:D:73:ARG:HH11	1.78	0.47
1:E:19:LEU:HD22	2:F:185:PHE:CE1	2.48	0.47
1:E:43:THR:HG22	1:E:44:GLU:N	2.29	0.47
1:E:163:ARG:HH11	1:E:165:ILE:HG12	1.79	0.47
1:E:236:THR:HG22	1:E:237:TYR:N	2.28	0.47
2:H:267:ARG:O	2:H:267:ARG:HD3	2.14	0.47
1:A:32:HIS:HD2	1:A:56:SER:O	1.97	0.47
1:A:435:PHE:O	1:A:438:GLN:N	2.48	0.47
2:D:182:THR:CG2	2:D:183:GLU:N	2.77	0.47
2:F:231:TYR:C	2:F:233:ARG:H	2.16	0.47
2:H:190:GLN:OE1	3:L:172:ARG:NH1	2.47	0.47
2:H:423:LEU:HD12	2:H:423:LEU:N	2.29	0.47
2:B:274:ARG:HD3	1:E:62:GLY:O	2.14	0.47
2:B:421:GLN:HB2	2:B:438:LEU:HD21	1.96	0.47
1:C:130:GLN:NE2	1:C:155:THR:O	2.47	0.47
2:D:322:LEU:C	2:D:322:LEU:CD1	2.82	0.47
3:J:143:LEU:HB3	3:J:150:MET:HE1	1.97	0.47
3:J:156:ALA:O	3:J:161:ILE:HB	2.14	0.47
2:H:354:GLN:NE2	2:H:354:GLN:HA	2.29	0.47
2:H:402:GLU:HA	2:H:405:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:412:LEU:O	2:H:417:LEU:HB2	2.15	0.47
2:B:81:ASP:CB	2:B:103:LYS:HD2	2.42	0.47
1:C:248:ARG:C	1:C:250:GLY:N	2.65	0.47
1:C:484:ARG:HD2	2:D:27:SER:O	2.13	0.47
2:D:225:PRO:HB2	2:D:280:LEU:HD21	1.97	0.47
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.79	0.47
1:A:424:VAL:HA	1:A:427:LEU:HD12	1.97	0.47
1:A:516:PHE:HD2	1:A:516:PHE:H	1.62	0.47
2:B:166:ASP:O	2:B:168:VAL:N	2.45	0.47
1:C:163:ARG:NE	1:C:518:ASN:OD1	2.46	0.47
1:C:326:ARG:HG2	1:C:328:THR:HG23	1.96	0.47
2:D:152:ARG:NH2	2:D:374:LEU:O	2.48	0.47
2:D:197:THR:CG2	2:D:198:ALA:N	2.77	0.47
2:D:280:LEU:O	2:D:284:VAL:HG23	2.15	0.47
3:J:145:TYR:HB2	3:J:167:LEU:CD2	2.44	0.47
1:E:194:GLU:C	1:E:196:PHE:H	2.18	0.47
2:F:123:HIS:HB3	2:F:125:ASN:HD21	1.79	0.47
2:F:136:ARG:NH1	2:F:161:LEU:HD22	2.30	0.47
2:F:361:LEU:O	2:F:364:VAL:N	2.42	0.47
2:F:380:ALA:HB3	2:F:394:LEU:HD12	1.90	0.47
2:F:422:GLU:HA	2:F:436:PHE:O	2.15	0.47
2:F:425:VAL:O	2:F:434:VAL:HG12	2.15	0.47
1:G:97:ASN:OD1	1:G:99:ASP:HB2	2.13	0.47
1:G:158:LEU:CD2	2:H:23:PHE:CE2	2.98	0.47
1:G:184:ARG:NH2	1:G:323:LEU:O	2.47	0.47
2:H:87:ASN:HB3	2:H:91:GLN:NE2	2.29	0.47
2:H:159:ILE:HG23	2:H:162:LEU:HD12	1.96	0.47
2:H:351:GLN:HB3	2:H:436:PHE:CD2	2.50	0.47
2:H:412:LEU:CD2	2:H:438:LEU:HD21	2.44	0.47
2:H:419:ASP:HB2	2:H:440:PHE:HD1	1.79	0.47
3:L:123:VAL:HA	3:L:126:ILE:CG1	2.45	0.47
3:L:155:THR:O	3:L:158:ASP:HB2	2.14	0.47
1:A:252:LEU:C	1:A:252:LEU:HD22	2.35	0.47
1:A:467:GLU:HG2	1:A:467:GLU:O	2.15	0.47
3:I:123:VAL:O	3:I:126:ILE:N	2.45	0.47
2:D:382:THR:HG22	2:D:391:THR:HA	1.96	0.47
2:F:141:ILE:HD12	2:F:158:LEU:HD11	1.97	0.47
2:H:207:TYR:CE1	3:L:172:ARG:CD	2.97	0.47
2:H:306:GLU:O	2:H:307:VAL:C	2.53	0.47
1:A:128:ALA:HB1	1:A:131:LEU:HD12	1.97	0.47
1:A:262:GLU:HG2	1:A:265:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PHE:O	1:A:269:ILE:HG13	2.15	0.47
2:B:218:ILE:HG22	2:B:219:ALA:N	2.29	0.47
2:B:321:TYR:OH	3:I:172:ARG:CG	2.63	0.47
2:B:427:ASP:CB	2:B:429:THR:HG22	2.45	0.47
1:C:75:PHE:CD2	1:C:93:LEU:HD23	2.50	0.47
1:C:138:ARG:O	1:C:142:VAL:HG23	2.15	0.47
1:C:214:TRP:CD1	1:C:214:TRP:C	2.88	0.47
2:D:209:PRO:HG3	3:J:139:GLN:HG2	1.96	0.47
2:D:312:THR:O	2:D:313:SER:HB3	2.14	0.47
2:F:225:PRO:HG2	2:F:275:GLY:HA3	1.97	0.47
2:H:63:LEU:HD22	2:H:142:VAL:HG11	1.97	0.47
1:A:34:CYS:SG	1:A:36:ILE:CD1	3.02	0.47
1:A:262:GLU:HG2	1:A:265:PHE:CD1	2.50	0.47
1:A:489:GLU:HG2	1:A:489:GLU:O	2.14	0.47
1:A:504:GLU:O	1:A:508:ILE:HG13	2.15	0.47
1:C:307:LEU:HB3	1:C:383:LEU:HD22	1.97	0.47
1:C:401:GLU:OE1	1:C:426:TYR:OH	2.29	0.47
1:C:449:GLN:O	1:C:449:GLN:HG2	2.15	0.47
1:E:447:ASN:ND2	2:F:26:ARG:NH2	2.62	0.47
2:F:129:ASP:HB3	2:H:134:PHE:HB2	1.95	0.47
2:F:386:GLU:CB	2:F:388:LYS:HE2	2.45	0.47
1:G:180:LEU:HD12	1:G:180:LEU:N	2.19	0.47
1:A:371:ALA:O	1:A:373:GLU:N	2.47	0.46
2:B:126:LYS:O	2:B:128:GLN:N	2.48	0.46
2:B:312:THR:O	2:B:314:ALA:N	2.48	0.46
2:D:192:ILE:O	2:D:194:PRO:HD3	2.15	0.46
1:E:72:ASN:HD22	1:E:72:ASN:C	2.19	0.46
2:F:355:PHE:O	2:F:440:PHE:HA	2.16	0.46
1:G:433:ASP:O	1:G:436:HIS:HB3	2.15	0.46
1:G:510:THR:OG1	1:G:512:GLN:HB2	2.16	0.46
3:L:104:LYS:HB2	3:L:166:VAL:HG22	1.98	0.46
2:B:380:ALA:HB1	2:B:394:LEU:HD13	1.94	0.46
1:C:131:LEU:HB3	1:C:132:PRO:HD2	1.97	0.46
2:D:412:LEU:HD22	2:D:417:LEU:CD1	2.44	0.46
1:G:480:HIS:HB2	2:H:29:PRO:HG2	1.98	0.46
2:H:87:ASN:HB3	2:H:91:GLN:CD	2.35	0.46
1:C:184:ARG:HD3	1:C:279:THR:OG1	2.14	0.46
2:F:335:PHE:HE2	3:K:170:VAL:HG21	1.80	0.46
2:F:348:GLN:C	2:F:349:LEU:HD12	2.34	0.46
2:F:381:ILE:HG13	2:F:425:VAL:HG22	1.96	0.46
1:A:78:ARG:C	1:A:80:SER:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLN:O	1:A:368:ILE:N	2.47	0.46
1:A:518:ASN:HD21	1:A:534:LEU:CB	2.26	0.46
2:B:16:ARG:HH22	2:B:116:PRO:HB2	1.80	0.46
2:B:27:SER:HB3	2:B:37:PRO:CG	2.46	0.46
1:C:72:ASN:HB2	2:D:19:HIS:ND1	2.31	0.46
1:C:428:MET:HE1	1:C:479:VAL:HA	1.97	0.46
1:C:481:GLU:OE1	2:D:315:TYR:OH	2.32	0.46
1:C:489:GLU:HG2	1:C:489:GLU:O	2.16	0.46
2:D:187:GLY:CA	3:J:173:LEU:HD12	2.46	0.46
3:J:150:MET:HE2	3:J:150:MET:HB2	1.57	0.46
1:E:347:ARG:HH22	2:F:274:ARG:CD	2.15	0.46
1:G:124:THR:HG21	1:G:509:ILE:HG12	1.96	0.46
1:G:447:ASN:HA	2:H:26:ARG:HH21	1.80	0.46
2:H:257:ILE:HD13	2:H:282:GLN:HG2	1.98	0.46
3:L:151:ASN:O	3:L:153:GLU:N	2.48	0.46
2:B:207:TYR:HE2	3:I:172:ARG:HG2	1.72	0.46
3:J:105:VAL:HG11	3:J:130:VAL:HG22	1.97	0.46
2:F:106:VAL:O	2:F:109:GLU:HB3	2.16	0.46
2:F:312:THR:O	2:F:313:SER:CB	2.63	0.46
2:F:356:SER:O	2:F:358:SER:N	2.48	0.46
2:F:357:PRO:HD3	2:F:440:PHE:CG	2.51	0.46
3:K:121:ASP:HB3	3:K:125:ARG:HD2	1.98	0.46
1:G:504:GLU:OE2	1:G:507:LYS:NZ	2.42	0.46
2:B:240:GLU:O	2:B:240:GLU:CG	2.62	0.46
2:B:418:VAL:CG2	2:B:421:GLN:HG3	2.46	0.46
1:C:137:LEU:HD21	1:C:402:TYR:CG	2.51	0.46
1:C:146:SER:O	1:C:147:GLN:CB	2.61	0.46
1:C:488:ALA:HB2	2:D:22:LYS:HD2	1.98	0.46
2:D:67:LEU:O	2:D:72:PHE:HB2	2.15	0.46
1:G:386:ASN:O	1:G:387:SER:C	2.54	0.46
2:H:158:LEU:HD13	2:H:177:LEU:HB2	1.97	0.46
2:H:213:PHE:O	2:H:218:ILE:HD11	2.16	0.46
2:H:233:ARG:HG2	2:H:234:MET:N	2.31	0.46
1:A:130:GLN:HA	1:A:154:ARG:HD2	1.98	0.46
1:C:214:TRP:CD1	1:C:215:ILE:N	2.84	0.46
1:C:259:PRO:CB	1:C:262:GLU:CD	2.83	0.46
1:C:264:ASN:ND2	1:C:265:PHE:H	2.12	0.46
2:D:405:ARG:N	2:D:406:PRO:CD	2.79	0.46
2:D:419:ASP:CG	2:D:420:GLY:N	2.69	0.46
1:E:44:GLU:OE1	2:F:65:LYS:NZ	2.48	0.46
1:A:110:GLU:OE1	1:A:135:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:142:ARG:HA	3:I:142:ARG:HD3	1.82	0.46
2:D:125:ASN:N	2:D:125:ASN:ND2	2.60	0.46
3:J:135:GLY:O	3:J:137:PRO:HD3	2.16	0.46
2:F:85:VAL:HG13	2:F:86:SER:N	2.31	0.46
1:G:248:ARG:O	1:G:251:ILE:CD1	2.64	0.46
2:H:163:ASN:O	2:H:163:ASN:OD1	2.33	0.46
2:B:28:GLY:O	2:B:31:THR:HG23	2.16	0.46
2:B:349:LEU:HD23	2:B:349:LEU:N	2.30	0.46
2:D:438:LEU:HD12	2:D:439:HIS:H	1.81	0.46
1:E:301:THR:HG23	1:E:305:TRP:HB2	1.98	0.46
2:F:366:ASP:HA	2:F:369:THR:HB	1.98	0.46
1:G:157:GLY:HA3	1:G:485:TYR:CG	2.51	0.46
1:G:347:ARG:HH12	2:H:274:ARG:HD2	1.81	0.46
1:G:396:ARG:HH21	1:G:400:GLU:HB3	1.80	0.46
1:A:324:PRO:HB3	1:A:353:ASP:HB3	1.98	0.46
2:D:228:CYS:O	2:D:231:TYR:HB3	2.16	0.46
3:J:125:ARG:HG3	3:J:125:ARG:HH11	1.81	0.46
1:E:178:ASN:O	1:E:179:ALA:HB2	2.15	0.46
2:F:412:LEU:HB3	2:F:440:PHE:CZ	2.51	0.46
2:H:373:SER:OG	2:H:374:LEU:HD23	2.16	0.46
3:L:170:VAL:CG1	3:L:171:LEU:N	2.76	0.46
1:A:78:ARG:HA	1:A:81:ILE:CG1	2.46	0.45
1:A:348:GLU:O	1:A:352:LYS:HG3	2.16	0.45
1:A:490:PRO:HG3	2:B:23:PHE:HE1	1.81	0.45
1:C:119:PHE:HE1	1:C:122:ARG:NH1	2.14	0.45
1:E:49:LEU:O	1:E:52:PRO:HG2	2.14	0.45
1:E:132:PRO:O	1:E:133:GLU:C	2.54	0.45
1:G:28:LEU:HD12	1:G:28:LEU:HA	1.77	0.45
1:G:173:GLU:CG	1:G:382:LEU:HD11	2.46	0.45
2:H:75:ILE:O	2:H:120:VAL:HA	2.15	0.45
2:H:357:PRO:HD3	2:H:440:PHE:HB3	1.96	0.45
2:H:417:LEU:HD23	2:H:421:GLN:NE2	2.31	0.45
1:A:38:ALA:O	1:A:85:ARG:HD3	2.16	0.45
1:A:164:ILE:HG23	1:A:164:ILE:O	2.15	0.45
1:C:310:ALA:CB	1:C:361:VAL:HG22	2.47	0.45
2:D:76:HIS:CD2	2:D:138:PHE:HE2	2.34	0.45
1:E:181:GLU:HG3	1:E:330:PRO:HD3	1.96	0.45
2:F:32:HIS:CG	2:F:33:PRO:HD2	2.51	0.45
2:F:131:ASN:O	2:F:133:THR:N	2.49	0.45
2:F:393:TYR:CE2	2:F:408:LEU:HD11	2.52	0.45
1:G:197:GLN:C	1:G:199:TYR:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:GLN:HE22	2:H:119:ASN:ND2	2.12	0.45
2:H:158:LEU:HD12	2:H:177:LEU:HD22	1.98	0.45
2:B:130:PHE:HE2	2:D:125:ASN:OD1	1.99	0.45
2:B:217:THR:HG21	2:B:223:ARG:HH22	1.80	0.45
3:I:139:GLN:O	3:I:142:ARG:NH2	2.36	0.45
1:C:28:LEU:HD12	1:C:54:ILE:HD12	1.97	0.45
1:C:94:GLN:HE22	1:C:102:GLY:H	1.64	0.45
1:C:443:PRO:HB2	1:C:483:CYS:SG	2.56	0.45
2:D:158:LEU:CD1	2:D:177:LEU:HB2	2.46	0.45
1:E:46:LEU:HD23	1:E:93:LEU:HD13	1.97	0.45
1:E:125:VAL:HG12	1:E:126:VAL:N	2.31	0.45
2:F:13:TRP:CZ3	2:F:116:PRO:HG2	2.50	0.45
2:F:316:ILE:HD12	2:F:316:ILE:N	2.27	0.45
2:H:381:ILE:HD12	2:H:381:ILE:H	1.81	0.45
1:A:474:VAL:O	1:A:475:LYS:C	2.53	0.45
1:C:236:THR:CB	1:C:239:GLU:HG3	2.45	0.45
1:C:318:GLU:HG3	1:C:356:ALA:HB1	1.98	0.45
2:D:257:ILE:HG21	2:D:282:GLN:HG2	1.97	0.45
1:E:236:THR:C	1:E:238:LYS:H	2.20	0.45
1:E:527:GLN:OE1	2:F:302:VAL:HG13	2.16	0.45
2:F:204:LEU:HD21	2:F:375:GLN:CG	2.46	0.45
1:G:158:LEU:HA	1:G:493:ILE:HG13	1.99	0.45
1:G:214:TRP:CD1	1:G:214:TRP:C	2.90	0.45
1:G:504:GLU:O	1:G:508:ILE:HG13	2.17	0.45
3:L:103:ILE:HG22	3:L:163:GLY:O	2.17	0.45
1:A:344:ASN:HA	1:A:347:ARG:HB2	1.97	0.45
1:A:430:ARG:CZ	1:A:464:PHE:CE1	3.00	0.45
2:B:405:ARG:HG3	2:B:405:ARG:HH11	1.82	0.45
2:B:421:GLN:O	2:B:438:LEU:HD23	2.17	0.45
1:E:245:ASP:C	1:E:247:ILE:H	2.19	0.45
2:F:87:ASN:HD22	2:F:103:LYS:HE2	1.78	0.45
2:F:325:ASN:HD22	2:F:326:ASP:H	1.65	0.45
3:K:156:ALA:CA	3:K:161:ILE:HD12	2.45	0.45
1:G:172:ILE:N	1:G:172:ILE:HD12	2.32	0.45
1:G:262:GLU:HG3	1:G:264:ASN:ND2	2.32	0.45
3:L:107:THR:HG22	3:L:111:LYS:HB3	1.97	0.45
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.82	0.45
1:A:489:GLU:H	2:B:19:HIS:HD2	1.61	0.45
1:C:110:GLU:O	1:C:113:LEU:N	2.49	0.45
2:D:11:LEU:N	2:D:11:LEU:HD23	2.32	0.45
2:D:58:GLY:O	2:D:62:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:ARG:NH1	2:D:136:ARG:HG2	2.31	0.45
2:D:229:ILE:HA	2:D:264:SER:OG	2.16	0.45
2:D:270:GLN:O	2:D:272:ASN:N	2.50	0.45
1:E:286:GLU:HA	1:E:286:GLU:OE1	2.16	0.45
2:F:101:ARG:HB3	2:F:102:PRO:HD2	1.98	0.45
2:F:158:LEU:CD1	2:F:175:VAL:HB	2.47	0.45
3:K:107:THR:CG2	3:K:108:LEU:N	2.79	0.45
3:L:107:THR:HG22	3:L:111:LYS:N	2.32	0.45
2:B:25:GLU:O	2:B:37:PRO:HB3	2.16	0.45
1:C:47:LYS:HZ1	2:D:65:LYS:HE2	1.82	0.45
2:D:54:ILE:HG22	2:D:145:LEU:HD21	1.97	0.45
2:D:145:LEU:HD12	2:D:151:ARG:HG3	1.99	0.45
3:J:162:LEU:O	3:J:163:GLY:C	2.55	0.45
1:E:220:LYS:O	1:E:222:LEU:N	2.50	0.45
1:G:340:ILE:HD13	1:G:340:ILE:HA	1.86	0.45
2:H:178:ILE:HD11	2:H:310:ILE:HD13	1.96	0.45
1:A:36:ILE:HD11	1:A:60:ILE:HD12	1.99	0.45
1:A:252:LEU:C	1:A:259:PRO:CD	2.72	0.45
1:A:513:PHE:N	1:A:513:PHE:CD1	2.85	0.45
2:B:64:LEU:HB3	2:B:111:LEU:HD13	1.97	0.45
2:B:226:GLU:OE1	2:B:226:GLU:N	2.44	0.45
2:B:342:ASN:ND2	2:B:342:ASN:N	2.43	0.45
3:I:117:ILE:CG2	3:I:118:GLU:N	2.79	0.45
2:H:110:PHE:CE2	2:H:114:ARG:NH1	2.85	0.45
1:A:113:LEU:O	1:A:138:ARG:NH2	2.50	0.45
1:A:418:ASN:HB3	1:A:421:ASN:HB2	1.99	0.45
2:B:83:ILE:HB	2:B:99:ILE:HA	1.99	0.45
2:B:185:PHE:HE2	2:B:292:VAL:HG21	1.82	0.45
2:B:217:THR:CG2	2:B:223:ARG:HH22	2.30	0.45
2:B:356:SER:CA	2:B:441:THR:OG1	2.65	0.45
1:C:500:ALA:O	1:C:504:GLU:HG2	2.17	0.45
2:D:151:ARG:HG2	2:D:179:ASP:OD2	2.17	0.45
2:D:188:ASN:HA	2:D:322:LEU:O	2.17	0.45
2:F:185:PHE:HB3	2:F:326:ASP:HB3	1.98	0.45
2:B:32:HIS:CD2	2:B:34:ASP:HB2	2.52	0.45
1:C:90:MET:O	1:C:94:GLN:HB2	2.17	0.45
1:C:262:GLU:HB3	1:C:265:PHE:HB2	1.99	0.45
1:C:407:ILE:HG23	1:C:409:LYS:HG3	1.99	0.45
2:D:58:GLY:N	2:D:91:GLN:HG2	2.32	0.45
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.47	0.45
2:D:207:TYR:HE1	3:J:172:ARG:HD3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:SER:O	2:D:358:SER:N	2.50	0.45
1:E:178:ASN:ND2	3:K:136:ILE:HG12	2.32	0.45
1:E:252:LEU:O	1:E:259:PRO:CD	2.65	0.45
2:F:32:HIS:CD2	2:F:34:ASP:HB2	2.52	0.45
1:G:271:ASN:O	1:G:275:ALA:N	2.47	0.45
2:H:232:VAL:O	2:H:232:VAL:HG12	2.17	0.45
2:B:350:PRO:HB2	2:B:436:PHE:C	2.38	0.44
1:C:418:ASN:ND2	1:C:418:ASN:C	2.69	0.44
2:D:149:ILE:CD1	2:D:149:ILE:N	2.62	0.44
1:E:36:ILE:HB	1:E:128:ALA:HA	1.99	0.44
1:E:51:LEU:N	1:E:52:PRO:HD2	2.32	0.44
1:G:113:LEU:HD11	1:G:139:LEU:HB2	1.99	0.44
2:H:225:PRO:HG3	2:H:274:ARG:O	2.17	0.44
2:H:402:GLU:HG3	2:H:402:GLU:H	1.51	0.44
3:L:138:PRO:HA	3:L:141:GLN:NE2	2.31	0.44
1:A:28:LEU:CD1	1:A:509:ILE:HG21	2.44	0.44
1:A:49:LEU:C	1:A:52:PRO:HD2	2.38	0.44
1:A:376:SER:OG	1:A:379:GLU:HG3	2.18	0.44
2:B:87:ASN:ND2	2:B:103:LYS:HE3	2.33	0.44
2:B:419:ASP:HA	2:B:440:PHE:CE1	2.52	0.44
2:D:226:GLU:OE2	2:D:226:GLU:N	2.49	0.44
2:F:208:PRO:HG3	3:K:171:LEU:HD11	2.00	0.44
1:G:428:MET:O	1:G:432:VAL:HG23	2.17	0.44
3:L:123:VAL:HA	3:L:126:ILE:HG13	1.98	0.44
1:A:229:THR:O	1:A:229:THR:HG22	2.17	0.44
1:A:259:PRO:CG	1:A:262:GLU:OE1	2.65	0.44
1:A:419:PRO:HB2	1:A:475:LYS:HE3	2.00	0.44
1:C:504:GLU:HG3	1:C:516:PHE:CE2	2.51	0.44
1:E:229:THR:O	1:E:232:ARG:HG3	2.18	0.44
1:E:259:PRO:HB3	1:E:261:ASP:O	2.17	0.44
2:H:230:GLU:HA	2:H:230:GLU:OE1	2.17	0.44
2:H:230:GLU:O	2:H:234:MET:HB3	2.17	0.44
2:H:344:PRO:HD3	2:H:374:LEU:HD22	1.98	0.44
1:A:78:ARG:NH2	2:B:13:TRP:HB3	2.32	0.44
1:A:347:ARG:HH12	2:B:274:ARG:HH22	1.65	0.44
1:A:439:GLN:HE21	1:A:441:ARG:HH12	1.65	0.44
3:K:170:VAL:HG13	3:K:171:LEU:N	2.33	0.44
1:G:320:GLN:OE1	1:G:320:GLN:HA	2.17	0.44
1:G:363:LYS:O	1:G:366:GLN:HB2	2.16	0.44
2:H:132:ASP:O	2:H:136:ARG:HG3	2.18	0.44
2:H:391:THR:O	2:H:392:LEU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:155:THR:O	3:L:158:ASP:N	2.50	0.44
2:B:399:SER:HB3	2:B:400:ILE:HD12	1.99	0.44
2:D:74:GLN:HE22	2:D:119:ASN:ND2	2.15	0.44
2:D:251:GLY:O	2:D:257:ILE:HD11	2.17	0.44
2:D:405:ARG:NH1	2:D:405:ARG:CB	2.80	0.44
1:E:194:GLU:C	1:E:196:PHE:N	2.71	0.44
2:F:261:PHE:O	2:F:264:SER:HB2	2.17	0.44
3:K:102:LEU:C	3:K:102:LEU:HD23	2.37	0.44
1:G:534:LEU:N	1:G:534:LEU:HD23	2.32	0.44
2:H:245:GLU:CG	2:H:246:GLY:N	2.80	0.44
2:H:269:SER:O	2:H:272:ASN:OD1	2.36	0.44
1:A:409:LYS:HB3	1:A:413:ILE:HD11	1.98	0.44
1:A:412:ILE:HG21	1:A:427:LEU:HD21	2.00	0.44
1:E:46:LEU:O	1:E:50:VAL:HG23	2.18	0.44
1:E:61:ASP:OD2	1:E:85:ARG:HD2	2.18	0.44
2:F:84:ASP:OD1	2:F:85:VAL:N	2.49	0.44
2:F:355:PHE:CZ	2:F:364:VAL:HG22	2.51	0.44
1:G:426:TYR:CE2	1:G:534:LEU:HD13	2.53	0.44
2:H:54:ILE:HG22	2:H:145:LEU:HD21	2.00	0.44
2:H:186:LYS:HG2	2:H:325:ASN:ND2	2.32	0.44
1:A:60:ILE:O	1:A:60:ILE:HG22	2.16	0.44
1:A:210:SER:O	1:A:211:HIS:HD2	2.01	0.44
1:A:441:ARG:HG2	1:A:441:ARG:NH1	2.32	0.44
1:C:333:ILE:O	1:C:334:ALA:HB2	2.16	0.44
1:C:368:ILE:O	1:C:368:ILE:HG22	2.17	0.44
2:D:237:TRP:CZ2	2:D:249:LEU:HA	2.53	0.44
1:E:49:LEU:C	1:E:52:PRO:HD2	2.37	0.44
1:G:283:SER:O	1:G:286:GLU:HB2	2.18	0.44
1:A:430:ARG:CZ	1:A:464:PHE:HE1	2.31	0.44
2:B:237:TRP:CE2	2:B:249:LEU:HB2	2.52	0.44
2:B:362:GLN:OE1	2:B:362:GLN:HA	2.17	0.44
2:B:386:GLU:O	2:B:387:GLY:C	2.54	0.44
2:D:327:VAL:HG23	2:D:328:ASP:N	2.33	0.44
1:E:50:VAL:HG13	1:E:100:VAL:HG21	1.99	0.44
2:F:192:ILE:O	2:F:193:LEU:HD23	2.18	0.44
1:G:222:LEU:HD13	1:G:243:PHE:CZ	2.53	0.44
2:H:213:PHE:CD1	2:H:213:PHE:N	2.79	0.44
2:H:380:ALA:O	2:H:425:VAL:HA	2.17	0.44
1:C:349:LYS:O	1:C:352:LYS:N	2.50	0.44
2:D:73:ARG:O	2:D:119:ASN:HB3	2.18	0.44
2:D:356:SER:C	2:D:358:SER:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ASN:HB3	1:E:363:LYS:HE3	1.99	0.44
2:F:53:VAL:HB	2:F:77:VAL:HG22	1.99	0.44
1:G:46:LEU:HD23	1:G:93:LEU:HD13	1.99	0.44
1:G:293:ARG:NH1	1:G:293:ARG:CG	2.77	0.44
2:H:84:ASP:OD1	2:H:86:SER:N	2.44	0.44
2:H:136:ARG:CG	2:H:161:LEU:HD22	2.48	0.44
2:H:353:ILE:HG22	2:H:355:PHE:CD1	2.53	0.44
2:H:379:PRO:HD2	2:H:395:GLN:NE2	2.33	0.44
2:H:410:LYS:CB	2:H:415:LEU:HD21	2.48	0.44
2:B:402:GLU:C	2:B:404:THR:H	2.21	0.43
1:C:61:ASP:HB3	1:C:86:ALA:HB2	2.00	0.43
2:D:29:PRO:C	2:D:31:THR:H	2.22	0.43
2:D:141:ILE:HD12	2:D:158:LEU:HD11	2.00	0.43
2:D:223:ARG:HH12	2:D:227:HIS:CE1	2.36	0.43
2:F:56:ALA:HA	2:F:60:GLY:HA3	1.99	0.43
2:F:240:GLU:O	2:F:241:GLN:C	2.56	0.43
1:G:214:TRP:CE2	1:G:271:ASN:ND2	2.86	0.43
1:G:386:ASN:O	1:G:388:ALA:N	2.51	0.43
1:G:416:MET:C	1:G:418:ASN:H	2.22	0.43
2:H:165:GLU:O	2:H:166:ASP:HB2	2.18	0.43
3:L:104:LYS:HG2	3:L:114:GLU:HG2	2.00	0.43
3:L:105:VAL:HA	3:L:167:LEU:O	2.18	0.43
1:C:34:CYS:HB2	1:C:123:PHE:CE2	2.54	0.43
1:C:56:SER:HB2	1:C:101:SER:O	2.17	0.43
1:C:65:VAL:HG22	1:C:85:ARG:HA	1.99	0.43
1:E:505:VAL:O	1:E:508:ILE:HB	2.18	0.43
2:F:377:LYS:HD2	2:F:377:LYS:O	2.18	0.43
3:K:170:VAL:HG22	3:K:171:LEU:H	1.83	0.43
1:G:226:TYR:CB	1:G:231:GLY:HA2	2.46	0.43
3:L:159:TYR:O	3:L:160:LYS:HB2	2.18	0.43
1:A:214:TRP:CD1	1:A:215:ILE:N	2.87	0.43
1:A:215:ILE:HG13	1:A:332:MET:SD	2.58	0.43
1:A:457:LEU:HD23	1:A:479:VAL:O	2.18	0.43
2:B:123:HIS:CE1	2:D:125:ASN:HD21	2.36	0.43
1:C:293:ARG:HH11	1:C:293:ARG:HG3	1.84	0.43
1:C:416:MET:HE1	1:C:424:VAL:HG12	2.01	0.43
1:C:437:LYS:HD2	1:C:437:LYS:HA	1.90	0.43
2:D:408:LEU:HD23	2:D:408:LEU:HA	1.86	0.43
2:D:412:LEU:CD1	2:D:440:PHE:HE2	2.31	0.43
1:E:314:PHE:HB2	1:E:357:VAL:HG22	1.99	0.43
1:E:411:GLU:OE1	1:E:411:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:LEU:HD22	2:F:169:LEU:HD11	2.00	0.43
2:F:367:TYR:O	2:F:371:SER:HB3	2.18	0.43
2:H:265:LEU:HD23	2:H:276:VAL:CG1	2.48	0.43
3:L:120:THR:O	3:L:120:THR:OG1	2.31	0.43
1:A:159:VAL:HG21	1:A:425:LEU:HD22	2.00	0.43
1:A:189:PHE:CE1	1:A:192:LEU:HB2	2.54	0.43
1:A:366:GLN:C	1:A:368:ILE:N	2.70	0.43
2:B:226:GLU:CG	2:B:280:LEU:HD11	2.48	0.43
1:C:349:LYS:O	1:C:350:ALA:C	2.57	0.43
2:D:98:ASP:O	2:D:99:ILE:C	2.56	0.43
2:D:106:VAL:O	2:D:109:GLU:HG2	2.18	0.43
2:F:139:HIS:O	2:F:176:PRO:HD2	2.19	0.43
1:G:47:LYS:C	1:G:47:LYS:HD2	2.39	0.43
1:G:164:ILE:HD11	1:G:508:ILE:HD11	2.00	0.43
1:G:264:ASN:N	1:G:264:ASN:HD22	2.16	0.43
1:G:264:ASN:CA	1:G:333:ILE:HD11	2.48	0.43
3:L:145:TYR:HB2	3:L:167:LEU:HD22	2.00	0.43
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.89	0.43
2:B:312:THR:C	2:B:314:ALA:N	2.72	0.43
2:D:237:TRP:O	2:D:241:GLN:HG2	2.18	0.43
2:F:249:LEU:HD13	2:F:260:ILE:HD11	1.99	0.43
1:G:516:PHE:CD2	1:G:516:PHE:N	2.86	0.43
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.85	0.43
2:B:351:GLN:N	2:B:436:PHE:HA	2.33	0.43
2:B:418:VAL:HG22	2:B:421:GLN:OE1	2.19	0.43
2:D:361:LEU:C	2:D:363:GLU:N	2.70	0.43
2:D:419:ASP:CG	2:D:420:GLY:H	2.21	0.43
3:J:123:VAL:HG13	3:J:150:MET:HE3	1.99	0.43
2:H:393:TYR:CG	2:H:394:LEU:N	2.86	0.43
2:B:249:LEU:HD12	2:B:250:ASP:N	2.33	0.43
2:B:391:THR:O	2:B:392:LEU:C	2.56	0.43
2:D:124:PHE:C	2:D:125:ASN:ND2	2.72	0.43
1:E:28:LEU:HA	1:E:28:LEU:HD12	1.81	0.43
2:F:401:GLU:O	2:F:405:ARG:HB2	2.19	0.43
2:F:412:LEU:O	2:F:417:LEU:HB2	2.18	0.43
3:L:120:THR:OG1	3:L:155:THR:OG1	2.37	0.43
2:B:253:ASP:O	2:B:256:HIS:HB2	2.19	0.43
2:B:407:ASN:HD22	2:B:415:LEU:HD13	1.83	0.43
1:E:76:LEU:HD21	1:E:89:ALA:HB2	1.99	0.43
1:G:129:THR:HA	1:G:153:CYS:O	2.19	0.43
2:H:92:PHE:CD2	2:H:92:PHE:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:348:GLN:HE21	2:H:348:GLN:C	2.22	0.43
2:B:166:ASP:C	2:B:168:VAL:H	2.22	0.43
2:B:331:TYR:CE1	3:I:110:GLY:HA2	2.54	0.43
2:D:243:PHE:N	2:D:243:PHE:CD1	2.87	0.43
1:E:396:ARG:HH21	1:E:400:GLU:HB3	1.82	0.43
1:E:421:ASN:O	1:E:424:VAL:HG22	2.19	0.43
1:E:447:ASN:ND2	2:F:26:ARG:NE	2.65	0.43
1:G:157:GLY:HA3	1:G:485:TYR:CD1	2.54	0.43
2:H:46:LEU:O	2:H:73:ARG:HB3	2.19	0.43
2:H:398:THR:O	2:H:401:GLU:HB3	2.19	0.43
1:A:225:TRP:O	1:A:229:THR:HB	2.18	0.43
1:A:364:LEU:HD12	1:A:364:LEU:HA	1.80	0.43
2:B:128:GLN:HE21	2:B:128:GLN:HB2	1.63	0.43
2:B:385:LEU:HD23	2:B:385:LEU:HA	1.53	0.43
3:I:157:ALA:C	3:I:159:TYR:H	2.22	0.43
1:C:435:PHE:CE2	1:C:439:GLN:HG3	2.54	0.43
2:D:76:HIS:CD2	2:D:138:PHE:CE2	3.07	0.43
2:D:139:HIS:O	2:D:176:PRO:HD2	2.19	0.43
2:D:325:ASN:OD1	2:D:327:VAL:HG22	2.19	0.43
2:D:422:GLU:HA	2:D:437:LYS:HA	2.01	0.43
1:E:56:SER:HB3	1:E:101:SER:HB2	2.00	0.43
1:E:214:TRP:CH2	1:E:332:MET:HG2	2.54	0.43
2:F:231:TYR:O	2:F:233:ARG:N	2.52	0.43
2:F:357:PRO:HB3	2:F:440:PHE:CZ	2.54	0.43
1:G:31:ALA:HB3	1:G:54:ILE:HD11	2.01	0.43
1:G:110:GLU:OE2	1:G:138:ARG:NH1	2.52	0.43
2:H:200:ILE:HD13	3:L:172:ARG:NH2	2.34	0.43
2:H:233:ARG:HG2	2:H:233:ARG:HH11	1.84	0.43
1:A:139:LEU:HD12	1:A:143:LEU:HG	2.01	0.42
1:A:140:ALA:CB	1:A:398:LEU:HD23	2.48	0.42
1:A:181:GLU:OE1	1:A:330:PRO:HD3	2.19	0.42
1:A:279:THR:O	1:A:280:GLN:HB2	2.17	0.42
1:A:430:ARG:O	1:A:433:ASP:HB2	2.19	0.42
1:A:481:GLU:O	1:A:484:ARG:HB3	2.18	0.42
1:A:518:ASN:HD21	1:A:534:LEU:CA	2.31	0.42
2:B:156:GLY:HA3	2:B:430:THR:CG2	2.49	0.42
2:B:217:THR:CB	2:B:223:ARG:NH2	2.79	0.42
2:B:356:SER:HA	2:B:441:THR:H	1.84	0.42
3:I:170:VAL:CG1	3:I:171:LEU:N	2.82	0.42
1:C:474:VAL:O	1:C:475:LYS:C	2.57	0.42
2:D:90:ARG:HG2	2:D:90:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:351:GLN:O	2:D:436:PHE:HA	2.19	0.42
2:D:390:ARG:CG	2:D:391:THR:N	2.80	0.42
1:E:120:PHE:HA	1:E:123:PHE:CD1	2.54	0.42
1:E:190:PRO:O	1:E:191:GLU:C	2.58	0.42
2:F:256:HIS:CD2	2:F:256:HIS:N	2.87	0.42
2:F:405:ARG:N	2:F:406:PRO:CD	2.82	0.42
1:G:171:VAL:HG12	1:G:391:ARG:O	2.19	0.42
2:H:272:ASN:OD1	2:H:272:ASN:N	2.49	0.42
1:A:171:VAL:HG13	1:A:391:ARG:HB2	2.01	0.42
1:A:248:ARG:O	1:A:251:ILE:HG13	2.20	0.42
1:A:260:GLU:O	1:A:261:ASP:OD1	2.37	0.42
1:A:403:GLY:HA3	1:A:406:THR:OG1	2.19	0.42
2:B:151:ARG:HH11	2:B:151:ARG:HG3	1.83	0.42
1:C:25:GLN:HE21	1:C:29:GLU:CG	2.31	0.42
1:C:409:LYS:O	1:C:410:ASP:C	2.56	0.42
2:D:405:ARG:HB3	2:D:406:PRO:HD3	2.00	0.42
1:E:279:THR:O	1:E:280:GLN:HB2	2.20	0.42
2:F:148:ILE:O	2:F:152:ARG:HG3	2.20	0.42
1:G:193:ARG:C	1:G:195:HIS:N	2.73	0.42
1:G:447:ASN:ND2	2:H:26:ARG:HE	2.17	0.42
2:H:226:GLU:OE1	2:H:226:GLU:N	2.53	0.42
1:A:238:LYS:O	1:A:238:LYS:HD3	2.19	0.42
1:A:396:ARG:NH2	1:A:406:THR:O	2.47	0.42
1:A:518:ASN:CG	1:A:519:THR:N	2.65	0.42
2:B:221:MET:HB3	2:B:221:MET:HE2	1.91	0.42
2:B:415:LEU:HB2	2:B:417:LEU:HD23	2.01	0.42
2:B:417:LEU:HD22	2:B:417:LEU:N	2.35	0.42
2:D:286:LYS:O	2:D:287:ARG:C	2.57	0.42
2:D:321:TYR:OH	3:J:172:ARG:HA	2.20	0.42
2:D:399:SER:HB2	2:D:403:ARG:HH12	1.83	0.42
1:E:48:ASN:O	1:E:52:PRO:HG3	2.19	0.42
1:A:225:TRP:CE2	1:A:234:PRO:HG3	2.54	0.42
1:C:71:GLY:HA3	2:D:16:ARG:O	2.19	0.42
1:C:354:ALA:O	1:C:380:LEU:HD21	2.18	0.42
1:C:377:GLU:O	1:C:381:LYS:HG2	2.19	0.42
1:C:446:SER:HB2	1:C:449:GLN:CB	2.50	0.42
2:F:204:LEU:HD21	2:F:375:GLN:HG2	2.01	0.42
1:G:236:THR:O	1:G:240:LYS:HG3	2.19	0.42
1:G:318:GLU:OE1	1:G:360:HIS:NE2	2.52	0.42
1:G:484:ARG:NH1	2:H:315:TYR:CZ	2.88	0.42
1:G:514:VAL:HB	2:H:328:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HD13	1:A:398:LEU:HB2	2.01	0.42
2:B:230:GLU:CD	2:B:233:ARG:HH12	2.22	0.42
1:C:160:GLY:HA3	1:C:497:LEU:HD11	2.01	0.42
1:C:299:LYS:HA	1:C:368:ILE:CG2	2.43	0.42
2:D:32:HIS:HB3	2:D:313:SER:O	2.19	0.42
3:J:137:PRO:HA	3:J:138:PRO:HD3	1.89	0.42
2:H:260:ILE:O	2:H:264:SER:HB2	2.20	0.42
1:A:89:ALA:O	1:A:90:MET:C	2.58	0.42
3:I:103:ILE:HD11	3:I:117:ILE:CD1	2.49	0.42
2:D:217:THR:CG2	2:D:223:ARG:HH22	2.33	0.42
1:E:352:LYS:O	1:E:355:ALA:N	2.52	0.42
1:E:504:GLU:O	1:E:508:ILE:HG13	2.20	0.42
2:H:169:LEU:HD12	2:H:170:ASP:N	2.34	0.42
2:H:423:LEU:HD11	2:H:438:LEU:HB2	2.02	0.42
1:A:236:THR:HB	1:A:239:GLU:H	1.85	0.42
1:A:318:GLU:OE1	1:A:318:GLU:N	2.50	0.42
3:I:102:LEU:O	3:I:102:LEU:CG	2.67	0.42
1:C:416:MET:CE	1:C:419:PRO:HA	2.50	0.42
2:D:316:ILE:HA	2:D:317:PRO:HD3	1.84	0.42
3:J:169:LEU:HD23	3:J:169:LEU:HA	1.87	0.42
1:E:211:HIS:HE1	2:F:221:MET:CE	2.33	0.42
1:E:259:PRO:HB2	1:E:261:ASP:O	2.20	0.42
1:G:53:GLY:O	1:G:54:ILE:C	2.58	0.42
1:G:214:TRP:H	1:G:332:MET:HE2	1.85	0.42
1:G:299:LYS:HA	1:G:368:ILE:HG21	2.01	0.42
2:H:425:VAL:O	2:H:434:VAL:HG12	2.19	0.42
3:L:154:LYS:HB3	3:L:158:ASP:OD1	2.19	0.42
1:A:307:LEU:HD21	1:A:375:ILE:HG21	2.02	0.42
2:B:351:GLN:HB3	2:B:436:PHE:CD1	2.54	0.42
3:I:137:PRO:O	3:I:140:GLN:HG2	2.20	0.42
1:C:252:LEU:HA	1:C:252:LEU:HD23	1.77	0.42
2:D:316:ILE:H	2:D:316:ILE:CD1	2.32	0.42
2:D:359:ALA:HB1	2:D:363:GLU:CD	2.40	0.42
1:E:428:MET:CE	1:E:479:VAL:HA	2.50	0.42
2:F:127:ILE:O	2:F:135:TYR:OH	2.38	0.42
2:F:212:ASN:HD22	2:F:212:ASN:HA	1.58	0.42
2:F:217:THR:CG2	2:F:223:ARG:NH2	2.79	0.42
3:K:107:THR:HB	3:K:111:LYS:HB3	2.02	0.42
1:G:225:TRP:CD1	1:G:225:TRP:C	2.92	0.42
1:G:311:LEU:HD21	1:G:387:SER:HB2	2.02	0.42
2:H:30:PHE:N	2:H:30:PHE:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:356:SER:OG	2:H:358:SER:HB3	2.19	0.42
1:A:96:LEU:HD23	2:B:95:ARG:NH2	2.34	0.42
1:A:457:LEU:HD22	1:A:483:CYS:SG	2.60	0.42
2:B:52:LEU:HD11	2:B:78:ILE:HG13	2.02	0.42
2:B:357:PRO:O	2:B:411:THR:HB	2.20	0.42
2:B:381:ILE:CG2	2:B:423:LEU:HD22	2.50	0.42
2:B:417:LEU:HD12	2:B:421:GLN:HE22	1.84	0.42
1:C:189:PHE:O	1:C:192:LEU:N	2.52	0.42
1:C:359:ASN:O	1:C:363:LYS:HG3	2.20	0.42
1:C:446:SER:HB2	1:C:449:GLN:HE21	1.84	0.42
2:D:46:LEU:HB3	2:D:73:ARG:NH1	2.34	0.42
2:D:412:LEU:HD12	2:D:440:PHE:HE2	1.84	0.42
1:E:214:TRP:CZ3	1:E:332:MET:HG2	2.54	0.42
1:E:396:ARG:HD3	1:E:534:LEU:O	2.20	0.42
2:F:393:TYR:HD1	2:F:404:THR:OG1	2.03	0.42
1:G:185:LEU:O	1:G:188:PRO:HD3	2.19	0.42
1:G:282:PRO:HG2	1:G:285:ILE:HD13	2.02	0.42
1:G:323:LEU:HB3	1:G:324:PRO:HD2	2.02	0.42
2:H:178:ILE:N	2:H:178:ILE:CD1	2.82	0.42
1:A:78:ARG:HB2	1:A:81:ILE:HD11	2.02	0.42
2:B:178:ILE:HD12	2:B:178:ILE:N	2.34	0.42
2:B:419:ASP:OD1	2:B:440:PHE:CD1	2.62	0.42
2:B:441:THR:O	2:B:442:SER:OXT	2.38	0.42
2:D:237:TRP:C	2:D:239:LYS:H	2.23	0.42
1:E:215:ILE:HD12	1:E:342:LEU:HD21	2.01	0.42
2:F:52:LEU:HD11	2:F:78:ILE:HG13	2.01	0.42
1:G:362:ALA:O	1:G:366:GLN:HG3	2.20	0.42
1:G:481:GLU:OE1	1:G:481:GLU:HA	2.20	0.42
2:H:193:LEU:HD23	2:H:193:LEU:HA	1.74	0.42
2:H:318:LEU:O	2:H:319:ASN:C	2.55	0.42
1:A:42:GLY:HA2	1:A:129:THR:HG21	2.02	0.41
1:A:84:ASN:HB3	1:A:87:GLU:HB3	2.02	0.41
3:I:107:THR:CG2	3:I:109:THR:HG23	2.50	0.41
1:C:143:LEU:HD22	1:C:148:ILE:CB	2.45	0.41
1:C:157:GLY:HA3	1:C:485:TYR:CG	2.55	0.41
1:C:340:ILE:CD1	2:D:271:TYR:O	2.68	0.41
2:D:64:LEU:HB3	2:D:111:LEU:HD13	2.02	0.41
1:E:43:THR:CG2	1:E:44:GLU:N	2.83	0.41
1:E:240:LYS:HG2	1:E:276:LEU:CD1	2.49	0.41
2:F:154:ILE:O	2:F:154:ILE:HG13	2.20	0.41
2:F:243:PHE:O	2:F:247:VAL:HG21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:135:GLY:O	3:L:137:PRO:HD3	2.20	0.41
1:A:416:MET:CE	1:A:424:VAL:HG22	2.50	0.41
1:A:426:TYR:O	1:A:429:LEU:HB2	2.19	0.41
1:A:514:VAL:HB	2:B:328:ASP:HA	2.01	0.41
2:B:339:ARG:NH2	2:B:346:CYS:O	2.44	0.41
1:C:39:THR:O	1:C:43:THR:HB	2.19	0.41
1:C:329:ILE:HB	1:C:330:PRO:HD2	2.02	0.41
1:E:187:LYS:N	1:E:188:PRO:CD	2.82	0.41
1:E:282:PRO:HG2	1:E:388:ALA:HB1	2.03	0.41
2:F:75:ILE:O	2:F:120:VAL:HA	2.19	0.41
2:F:143:CYS:HB2	2:F:179:ASP:HA	2.01	0.41
2:F:320:ASN:HB2	2:F:336:GLU:HA	2.02	0.41
3:K:123:VAL:HG13	3:K:150:MET:HE2	2.02	0.41
1:G:196:PHE:O	1:G:199:TYR:HB2	2.20	0.41
1:G:238:LYS:O	1:G:241:GLU:HB3	2.20	0.41
1:G:264:ASN:HD22	1:G:265:PHE:N	2.18	0.41
2:H:148:ILE:CG1	3:L:174:ARG:HG2	2.46	0.41
3:L:106:LYS:CG	3:L:112:GLU:HG2	2.49	0.41
3:L:123:VAL:HG23	3:L:154:LYS:O	2.20	0.41
3:L:151:ASN:C	3:L:153:GLU:H	2.23	0.41
2:B:132:ASP:O	2:B:134:PHE:N	2.53	0.41
2:B:207:TYR:CE2	3:I:172:ARG:CG	2.91	0.41
2:B:325:ASN:HD22	2:B:326:ASP:N	2.18	0.41
2:D:90:ARG:HG3	2:D:91:GLN:HG3	2.02	0.41
2:D:277:THR:HG22	2:D:279:ARG:H	1.85	0.41
2:F:357:PRO:HD3	2:F:440:PHE:CD2	2.54	0.41
1:A:186:ASP:OD2	1:A:187:LYS:N	2.53	0.41
1:C:212:THR:HA	1:C:213:PRO:HD3	1.94	0.41
1:E:364:LEU:HD12	1:E:364:LEU:HA	1.84	0.41
2:F:241:GLN:CB	2:F:245:GLU:HA	2.51	0.41
1:G:333:ILE:CG2	2:H:223:ARG:NH1	2.83	0.41
2:H:217:THR:HG21	2:H:223:ARG:NE	2.31	0.41
2:H:220:SER:O	2:H:222:PRO:CD	2.68	0.41
2:H:427:ASP:OD2	2:H:428:VAL:N	2.49	0.41
1:C:47:LYS:NZ	2:D:65:LYS:HE2	2.36	0.41
1:C:245:ASP:O	1:C:249:GLN:HG3	2.21	0.41
1:C:314:PHE:HZ	1:C:353:ASP:OD2	2.04	0.41
2:D:268:ALA:O	2:D:273:ILE:N	2.53	0.41
2:D:418:VAL:CG2	2:D:421:GLN:NE2	2.80	0.41
3:J:125:ARG:HG3	3:J:125:ARG:NH1	2.35	0.41
1:E:311:LEU:HD22	1:E:383:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:344:ASN:O	1:G:348:GLU:HB2	2.20	0.41
2:H:354:GLN:NE2	2:H:439:HIS:HB3	2.34	0.41
3:L:155:THR:HG22	3:L:158:ASP:CG	2.41	0.41
1:A:154:ARG:HG2	1:A:154:ARG:NH1	2.36	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.84	0.41
1:A:335:ASP:O	1:A:336:SER:C	2.59	0.41
1:A:428:MET:SD	1:A:461:LEU:HD22	2.61	0.41
2:B:434:VAL:HG22	2:B:436:PHE:CE1	2.55	0.41
3:I:117:ILE:HD13	3:I:126:ILE:HG12	2.03	0.41
1:C:40:ALA:O	1:C:43:THR:HG22	2.21	0.41
1:E:241:GLU:OE1	1:E:244:ARG:HD2	2.21	0.41
1:E:419:PRO:HB2	1:E:475:LYS:HE3	2.03	0.41
1:E:501:ALA:O	1:E:505:VAL:HG23	2.20	0.41
2:F:79:ASP:OD2	2:F:81:ASP:HB2	2.20	0.41
2:F:271:TYR:O	2:F:272:ASN:OD1	2.37	0.41
1:G:282:PRO:HG2	1:G:285:ILE:HB	2.02	0.41
1:G:497:LEU:HD12	1:G:497:LEU:HA	1.92	0.41
2:H:35:PHE:O	2:H:36:GLU:HG2	2.19	0.41
2:H:249:LEU:CD2	2:H:260:ILE:HD11	2.50	0.41
2:H:349:LEU:O	2:H:350:PRO:O	2.38	0.41
3:L:125:ARG:C	3:L:127:LYS:N	2.72	0.41
1:A:37:ASN:HB2	1:A:129:THR:O	2.21	0.41
1:A:297:ILE:N	1:A:297:ILE:CD1	2.76	0.41
2:B:50:LYS:H	2:B:139:HIS:CD2	2.38	0.41
1:C:499:GLY:O	2:D:294:SER:HB2	2.20	0.41
2:D:228:CYS:SG	2:D:267:ARG:HG2	2.61	0.41
2:D:385:LEU:O	2:D:387:GLY:N	2.52	0.41
1:E:318:GLU:HG3	1:E:356:ALA:HB1	2.02	0.41
2:F:136:ARG:HH11	2:F:136:ARG:HG3	1.85	0.41
2:F:261:PHE:CZ	2:F:265:LEU:HD11	2.55	0.41
1:G:15:ARG:HA	1:G:15:ARG:HD3	1.92	0.41
1:G:311:LEU:HD12	1:G:311:LEU:HA	1.83	0.41
1:G:333:ILE:CG2	2:H:223:ARG:HH12	2.34	0.41
1:G:333:ILE:HD13	1:G:333:ILE:HG21	1.74	0.41
2:H:204:LEU:HG	2:H:204:LEU:O	2.20	0.41
1:A:97:ASN:HB3	1:A:100:VAL:HG23	2.02	0.41
1:A:261:ASP:O	1:A:262:GLU:CG	2.69	0.41
1:A:353:ASP:O	1:A:357:VAL:HG23	2.20	0.41
1:A:359:ASN:HD22	1:A:359:ASN:HA	1.60	0.41
2:B:309:LYS:HD3	2:B:317:PRO:HA	2.03	0.41
3:I:102:LEU:O	3:I:163:GLY:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:PHE:HB3	1:C:312:LYS:HD2	2.03	0.41
1:C:481:GLU:HG3	1:C:485:TYR:CE2	2.56	0.41
2:D:231:TYR:HD1	2:D:235:LEU:HD12	1.85	0.41
2:D:333:TYR:CE2	2:D:335:PHE:HB3	2.56	0.41
1:E:518:ASN:CB	1:E:533:GLN:HA	2.50	0.41
2:F:209:PRO:HG2	3:K:139:GLN:O	2.20	0.41
2:F:247:VAL:HA	2:F:248:PRO:HD3	1.81	0.41
1:G:66:SER:N	1:G:69:ASP:HB2	2.35	0.41
1:G:248:ARG:O	1:G:251:ILE:HD12	2.21	0.41
3:L:131:GLU:O	3:L:131:GLU:HG2	2.19	0.41
1:A:165:ILE:C	1:A:166:ILE:HG13	2.40	0.41
2:B:16:ARG:NH2	2:B:116:PRO:HB2	2.36	0.41
1:C:120:PHE:O	1:C:122:ARG:N	2.54	0.41
1:C:158:LEU:HD12	1:C:525:MET:HG2	2.01	0.41
1:C:163:ARG:HH12	1:C:165:ILE:HG12	1.81	0.41
1:C:293:ARG:HB3	1:C:305:TRP:CE3	2.55	0.41
2:D:141:ILE:HD12	2:D:158:LEU:CD2	2.41	0.41
2:D:186:LYS:C	3:J:173:LEU:HD13	2.41	0.41
2:D:213:PHE:HB2	2:D:218:ILE:HD11	2.02	0.41
1:E:35:LEU:HD12	1:E:36:ILE:N	2.36	0.41
1:E:45:ILE:CG1	1:E:498:GLY:HA2	2.49	0.41
1:E:241:GLU:O	1:E:244:ARG:HB2	2.21	0.41
1:E:274:THR:O	1:E:276:LEU:N	2.54	0.41
2:F:74:GLN:NE2	2:F:74:GLN:HA	2.36	0.41
2:F:410:LYS:HD3	2:F:415:LEU:HG	2.03	0.41
1:G:72:ASN:C	1:G:72:ASN:ND2	2.74	0.41
1:G:422:GLU:O	1:G:424:VAL:N	2.54	0.41
2:H:171:PRO:C	2:H:173:SER:H	2.24	0.41
2:H:385:LEU:CD1	2:H:390:ARG:HD3	2.51	0.41
3:L:106:LYS:HB2	3:L:168:HIS:CD2	2.55	0.41
3:L:120:THR:OG1	3:L:155:THR:CB	2.68	0.41
1:A:213:PRO:HG3	1:A:334:ALA:CB	2.50	0.41
1:A:510:THR:O	1:A:511:LYS:HB2	2.21	0.41
2:B:257:ILE:HG22	2:B:278:TYR:CE1	2.56	0.41
3:I:102:LEU:O	3:I:102:LEU:HG	2.21	0.41
1:C:9:LYS:HE2	1:C:9:LYS:HB3	1.90	0.41
2:D:15:GLY:O	2:D:17:TRP:N	2.54	0.41
2:D:32:HIS:CE1	2:D:33:PRO:HD2	2.56	0.41
2:D:140:ILE:HG22	2:D:141:ILE:N	2.35	0.41
2:D:150:ALA:O	2:D:154:ILE:HG22	2.21	0.41
2:D:249:LEU:CD1	2:D:260:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:ASP:OD1	2:D:255:GLU:HB2	2.20	0.41
2:D:356:SER:C	2:D:358:SER:N	2.75	0.41
2:D:405:ARG:NH1	2:D:405:ARG:HB3	2.35	0.41
1:E:245:ASP:C	1:E:247:ILE:N	2.74	0.41
1:E:474:VAL:O	1:E:475:LYS:C	2.59	0.41
2:F:321:TYR:OH	3:K:172:ARG:HG3	2.21	0.41
3:K:101:MET:HE3	3:K:117:ILE:HG22	2.02	0.41
3:K:131:GLU:CD	3:K:138:PRO:HD3	2.41	0.41
1:G:286:GLU:OE1	1:G:286:GLU:HA	2.20	0.41
1:G:437:LYS:HA	1:G:437:LYS:HD2	1.90	0.41
1:G:512:GLN:C	1:G:513:PHE:CD1	2.94	0.41
2:H:64:LEU:HD11	2:H:77:VAL:HG21	2.03	0.41
2:H:115:VAL:HA	2:H:116:PRO:HD2	1.88	0.41
2:H:233:ARG:NH1	2:H:233:ARG:HG2	2.35	0.41
2:H:241:GLN:HA	2:H:242:PRO:HD3	1.57	0.41
2:H:352:ASN:HD22	2:H:439:HIS:CD2	2.39	0.41
1:A:140:ALA:HB3	1:A:398:LEU:HD23	2.03	0.40
1:A:371:ALA:C	1:A:373:GLU:N	2.75	0.40
1:A:424:VAL:HG11	1:A:478:TYR:CD1	2.56	0.40
2:B:265:LEU:HD13	1:E:66:SER:HA	2.02	0.40
1:C:302:PRO:O	1:C:304:PHE:N	2.54	0.40
1:E:528:THR:HG22	2:F:334:THR:OG1	2.20	0.40
2:F:95:ARG:HB2	2:F:97:LYS:HG2	2.03	0.40
2:F:219:ALA:HB2	2:F:231:TYR:CD1	2.56	0.40
2:F:356:SER:C	2:F:358:SER:N	2.75	0.40
1:A:248:ARG:HH11	1:A:248:ARG:HG3	1.87	0.40
1:A:430:ARG:NH2	1:A:464:PHE:HE1	2.18	0.40
1:C:9:LYS:HA	1:C:12:LYS:HB3	2.03	0.40
1:C:190:PRO:HG2	1:C:191:GLU:OE2	2.21	0.40
2:D:323:VAL:HG21	3:J:170:VAL:HG23	2.03	0.40
1:E:129:THR:HA	1:E:153:CYS:O	2.21	0.40
1:E:201:LEU:H	1:E:201:LEU:HG	1.34	0.40
1:E:241:GLU:OE1	1:E:241:GLU:HA	2.21	0.40
1:E:434:ARG:HD3	1:E:460:CYS:O	2.21	0.40
2:F:195:GLY:HA2	2:F:339:ARG:NH2	2.35	0.40
2:H:143:CYS:HB3	2:H:179:ASP:OD2	2.20	0.40
1:A:51:LEU:N	1:A:52:PRO:HD2	2.36	0.40
2:B:87:ASN:ND2	2:B:103:LYS:CE	2.85	0.40
2:B:355:PHE:CE2	2:B:363:GLU:O	2.74	0.40
1:C:161:TYR:OH	1:C:163:ARG:HB2	2.21	0.40
1:C:261:ASP:O	1:C:262:GLU:OE2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:GLY:O	2:D:16:ARG:C	2.59	0.40
2:F:65:LYS:HE2	2:F:65:LYS:HB3	1.91	0.40
1:G:66:SER:H	1:G:69:ASP:HB2	1.86	0.40
1:G:111:ASN:O	1:G:114:ASP:HB3	2.22	0.40
1:G:158:LEU:HA	1:G:158:LEU:HD13	1.83	0.40
1:G:243:PHE:CE2	1:G:247:ILE:HD11	2.56	0.40
2:H:28:GLY:O	2:H:31:THR:HG22	2.22	0.40
1:C:215:ILE:HG13	1:C:332:MET:CE	2.52	0.40
1:C:361:VAL:CG1	1:C:375:ILE:HD12	2.51	0.40
1:C:419:PRO:O	1:C:424:VAL:HG11	2.21	0.40
2:D:170:ASP:OD2	2:D:172:SER:HB2	2.21	0.40
2:D:270:GLN:C	2:D:272:ASN:N	2.75	0.40
2:D:351:GLN:HG2	2:D:352:ASN:N	2.36	0.40
1:E:33:VAL:HG12	1:E:34:CYS:N	2.36	0.40
1:E:90:MET:O	1:E:94:GLN:HB2	2.20	0.40
1:E:189:PHE:CE1	1:E:349:LYS:HB2	2.56	0.40
1:E:236:THR:C	1:E:238:LYS:N	2.74	0.40
1:E:266:GLU:C	1:E:268:ALA:H	2.23	0.40
1:G:65:VAL:HG23	1:G:83:LYS:O	2.21	0.40
1:G:441:ARG:NH2	1:G:453:ASP:OD2	2.55	0.40
2:H:302:VAL:HG11	2:H:322:LEU:HD23	2.04	0.40
1:A:192:LEU:HD11	1:A:196:PHE:CZ	2.57	0.40
1:A:215:ILE:HD11	1:A:332:MET:CE	2.51	0.40
1:A:454:ILE:HG21	1:A:480:HIS:CE1	2.56	0.40
2:B:243:PHE:N	2:B:243:PHE:CD1	2.90	0.40
1:C:309:ARG:HH11	1:C:309:ARG:HG3	1.86	0.40
2:D:21:LYS:O	2:D:25:GLU:HG3	2.22	0.40
2:D:94:PHE:N	2:D:94:PHE:CD2	2.87	0.40
2:D:325:ASN:HD21	2:D:327:VAL:CG2	2.29	0.40
2:D:355:PHE:CZ	2:D:364:VAL:HA	2.57	0.40
1:E:7:LEU:O	1:E:7:LEU:HD23	2.20	0.40
1:E:229:THR:HG22	1:E:232:ARG:HB2	2.04	0.40
1:E:251:ILE:HG13	1:E:251:ILE:H	1.44	0.40
2:F:335:PHE:CZ	3:K:144:ILE:HD13	2.57	0.40
2:F:351:GLN:HB2	2:F:436:PHE:HD2	1.77	0.40
1:G:251:ILE:C	1:G:252:LEU:O	2.58	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	513/531 (97%)	433 (84%)	64 (12%)	16 (3%)	4	19
1	C	512/531 (96%)	432 (84%)	59 (12%)	21 (4%)	3	14
1	E	511/531 (96%)	447 (88%)	46 (9%)	18 (4%)	3	17
1	G	502/531 (94%)	434 (86%)	54 (11%)	14 (3%)	5	21
2	B	430/434 (99%)	362 (84%)	56 (13%)	12 (3%)	5	21
2	D	429/434 (99%)	347 (81%)	62 (14%)	20 (5%)	2	12
2	F	429/434 (99%)	362 (84%)	51 (12%)	16 (4%)	3	16
2	H	429/434 (99%)	344 (80%)	60 (14%)	25 (6%)	1	8
3	I	81/88 (92%)	71 (88%)	5 (6%)	5 (6%)	1	7
3	J	75/88 (85%)	66 (88%)	7 (9%)	2 (3%)	5	21
3	K	75/88 (85%)	63 (84%)	8 (11%)	4 (5%)	2	10
3	L	76/88 (86%)	60 (79%)	12 (16%)	4 (5%)	2	10
All	All	4062/4212 (96%)	3421 (84%)	484 (12%)	157 (4%)	3	15

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	LYS
2	B	116	PRO
2	B	127	ILE
2	B	241	GLN
2	B	387	GLY
1	C	253	LYS
2	D	13	TRP
2	D	16	ARG
2	D	41	SER
2	D	92	PHE
2	D	116	PRO
2	D	320	ASN

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Mol	Chain	Res	Type
1	E	253	LYS
1	E	275	ALA
1	E	276	LEU
2	F	116	PRO
2	F	132	ASP
2	F	375	GLN
1	G	276	LEU
2	H	116	PRO
2	H	132	ASP
2	H	242	PRO
2	H	320	ASN
2	H	350	PRO
2	H	377	LYS
2	H	396	SER
3	L	163	GLY
1	A	228	GLU
1	A	336	SER
1	A	367	SER
1	A	450	VAL
3	I	147	GLY
3	I	163	GLY
1	C	36	ILE
1	C	79	SER
1	C	249	GLN
1	C	275	ALA
1	C	451	GLU
2	D	270	GLN
2	D	271	TYR
1	E	195	HIS
1	E	200	ASP
1	E	280	GLN
2	F	320	ASN
1	G	171	VAL
1	G	335	ASP
1	G	451	GLU
1	G	453	ASP
1	G	475	LYS
2	H	88	LEU
2	H	244	GLY
2	H	319	ASN
2	H	362	GLN
2	H	399	SER

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Mol	Chain	Res	Type
2	H	407	ASN
3	L	119	PRO
1	A	90	MET
1	A	106	GLU
1	A	280	GLN
2	B	92	PHE
2	B	133	THR
2	B	313	SER
2	B	403	ARG
3	I	119	PRO
3	I	158	ASP
1	C	121	CYS
1	C	252	LEU
1	C	475	LYS
1	C	518	ASN
2	D	29	PRO
2	D	30	PHE
2	D	237	TRP
2	D	362	GLN
1	E	134	SER
1	E	229	THR
1	E	249	GLN
1	E	264	ASN
1	E	318	GLU
1	E	336	SER
2	F	183	GLU
2	F	232	VAL
2	F	396	SER
2	F	410	LYS
3	K	119	PRO
3	K	152	ASP
1	G	452	GLU
2	H	194	PRO
2	H	232	VAL
2	H	239	LYS
2	H	265	LEU
2	H	345	ALA
2	H	357	PRO
3	L	152	ASP
1	A	79	SER
1	A	198	SER
1	A	230	ASN

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Mol	Chain	Res	Type
1	A	435	PHE
2	B	361	LEU
3	I	146	SER
1	C	72	ASN
1	C	147	GLN
1	C	251	ILE
2	D	34	ASP
2	D	183	GLU
2	D	412	LEU
3	J	163	GLY
1	E	38	ALA
1	E	106	GLU
2	F	88	LEU
2	F	194	PRO
2	F	211	VAL
2	F	216	ALA
2	F	357	PRO
1	G	198	SER
1	G	275	ALA
1	G	387	SER
2	H	31	THR
2	H	374	LEU
2	H	388	LYS
1	A	249	GLN
2	B	242	PRO
1	C	106	GLU
1	C	303	SER
1	C	397	SER
2	D	241	GLN
1	E	190	PRO
2	F	92	PHE
3	K	108	LEU
3	K	175	GLY
1	G	250	GLY
2	H	261	PHE
1	A	372	PRO
2	B	348	GLN
1	C	259	PRO
1	E	221	TYR
1	E	228	GLU
1	G	407	ILE
1	C	109	PRO

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Mol	Chain	Res	Type
2	D	357	PRO
2	F	144	GLY
1	C	407	ILE
2	D	232	VAL
1	E	213	PRO
1	G	423	ILE
2	H	405	ARG
1	C	450	VAL
2	D	211	VAL
1	G	419	PRO
2	H	238	PRO
1	A	333	ILE
1	A	443	PRO
2	B	167	GLY
1	C	60	ILE
2	D	194	PRO
3	L	175	GLY
3	J	119	PRO
2	F	229	ILE

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	449/462 (97%)	424 (94%)	25 (6%)	21	49
1	C	448/462 (97%)	425 (95%)	23 (5%)	24	53
1	E	448/462 (97%)	417 (93%)	31 (7%)	15	42
1	G	442/462 (96%)	419 (95%)	23 (5%)	23	52
2	B	378/382 (99%)	349 (92%)	29 (8%)	13	38
2	D	378/382 (99%)	352 (93%)	26 (7%)	15	42
2	F	377/382 (99%)	350 (93%)	27 (7%)	14	40
2	H	375/382 (98%)	348 (93%)	27 (7%)	14	40
3	I	73/74 (99%)	67 (92%)	6 (8%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	68/74 (92%)	66 (97%)	2 (3%)	42	70
3	K	68/74 (92%)	62 (91%)	6 (9%)	10	32
3	L	68/74 (92%)	67 (98%)	1 (2%)	65	83
All	All	3572/3672 (97%)	3346 (94%)	226 (6%)	18	45

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	39	THR
1	A	43	THR
1	A	69	ASP
1	A	72	ASN
1	A	90	MET
1	A	147	GLN
1	A	171	VAL
1	A	208	ASP
1	A	214	TRP
1	A	245	ASP
1	A	252	LEU
1	A	262	GLU
1	A	264	ASN
1	A	277	ASN
1	A	335	ASP
1	A	364	LEU
1	A	368	ILE
1	A	395	CYS
1	A	407	ILE
1	A	418	ASN
1	A	437	LYS
1	A	439	GLN
1	A	477	ASP
1	A	480	HIS
2	B	97	LYS
2	B	114	ARG
2	B	116	PRO
2	B	118	CYS
2	B	128	GLN
2	B	132	ASP
2	B	137	GLN
2	B	149	ILE

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Mol	Chain	Res	Type
2	B	154	ILE
2	B	197	THR
2	B	217	THR
2	B	218	ILE
2	B	233	ARG
2	B	274	ARG
2	B	316	ILE
2	B	321	TYR
2	B	325	ASN
2	B	327	VAL
2	B	342	ASN
2	B	353	ILE
2	B	360	LYS
2	B	363	GLU
2	B	364	VAL
2	B	382	THR
2	B	392	LEU
2	B	412	LEU
2	B	414	GLU
2	B	430	THR
2	B	442	SER
3	I	97	SER
3	I	101	MET
3	I	102	LEU
3	I	107	THR
3	I	144	ILE
3	I	170	VAL
1	C	10	GLU
1	C	14	ASP
1	C	34	CYS
1	C	37	ASN
1	C	39	THR
1	C	112	LEU
1	C	171	VAL
1	C	191	GLU
1	C	214	TRP
1	C	251	ILE
1	C	264	ASN
1	C	274	THR
1	C	277	ASN
1	C	293	ARG
1	C	297	ILE

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Mol	Chain	Res	Type
1	C	311	LEU
1	C	328	THR
1	C	353	ASP
1	C	396	ARG
1	C	418	ASN
1	C	422	GLU
1	C	439	GLN
1	C	517	ASN
2	D	11	LEU
2	D	13	TRP
2	D	14	GLU
2	D	77	VAL
2	D	82	THR
2	D	97	LYS
2	D	111	LEU
2	D	113	ASP
2	D	114	ARG
2	D	116	PRO
2	D	125	ASN
2	D	128	GLN
2	D	132	ASP
2	D	142	VAL
2	D	149	ILE
2	D	196	MET
2	D	201	GLU
2	D	223	ARG
2	D	316	ILE
2	D	322	LEU
2	D	323	VAL
2	D	362	GLN
2	D	388	LYS
2	D	401	GLU
2	D	407	ASN
2	D	441	THR
3	J	108	LEU
3	J	155	THR
1	E	39	THR
1	E	43	THR
1	E	72	ASN
1	E	79	SER
1	E	101	SER
1	E	201	LEU

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Mol	Chain	Res	Type
1	E	211	HIS
1	E	226	TYR
1	E	229	THR
1	E	242	ASP
1	E	251	ILE
1	E	253	LYS
1	E	262	GLU
1	E	264	ASN
1	E	265	PHE
1	E	277	ASN
1	E	292	ASP
1	E	293	ARG
1	E	297	ILE
1	E	309	ARG
1	E	364	LEU
1	E	410	ASP
1	E	418	ASN
1	E	422	GLU
1	E	424	VAL
1	E	452	GLU
1	E	497	LEU
1	E	516	PHE
1	E	517	ASN
1	E	518	ASN
1	E	533	GLN
2	F	31	THR
2	F	38	SER
2	F	82	THR
2	F	95	ARG
2	F	110	PHE
2	F	111	LEU
2	F	114	ARG
2	F	116	PRO
2	F	118	CYS
2	F	125	ASN
2	F	128	GLN
2	F	149	ILE
2	F	182	THR
2	F	194	PRO
2	F	212	ASN
2	F	241	GLN
2	F	292	VAL

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Mol	Chain	Res	Type
2	F	316	ILE
2	F	319	ASN
2	F	322	LEU
2	F	325	ASN
2	F	342	ASN
2	F	355	PHE
2	F	361	LEU
2	F	374	LEU
2	F	397	VAL
2	F	430	THR
3	K	101	MET
3	K	115	ILE
3	K	117	ILE
3	K	155	THR
3	K	170	VAL
3	K	173	LEU
1	G	33	VAL
1	G	43	THR
1	G	72	ASN
1	G	73	ASN
1	G	79	SER
1	G	90	MET
1	G	154	ARG
1	G	163	ARG
1	G	186	ASP
1	G	189	PHE
1	G	214	TRP
1	G	220	LYS
1	G	264	ASN
1	G	277	ASN
1	G	293	ARG
1	G	300	GLN
1	G	318	GLU
1	G	343	GLN
1	G	385	SER
1	G	410	ASP
1	G	492	THR
1	G	503	GLN
1	G	516	PHE
2	H	14	GLU
2	H	49	CYS
2	H	82	THR

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Mol	Chain	Res	Type
2	H	105	GLU
2	H	111	LEU
2	H	114	ARG
2	H	116	PRO
2	H	128	GLN
2	H	132	ASP
2	H	139	HIS
2	H	154	ILE
2	H	182	THR
2	H	201	GLU
2	H	213	PHE
2	H	224	LEU
2	H	316	ILE
2	H	323	VAL
2	H	325	ASN
2	H	348	GLN
2	H	350	PRO
2	H	360	LYS
2	H	366	ASP
2	H	374	LEU
2	H	402	GLU
2	H	403	ARG
2	H	405	ARG
2	H	430	THR
3	L	150	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	ASN
1	A	72	ASN
1	A	111	ASN
1	A	147	GLN
1	A	169	HIS
1	A	178	ASN
1	A	197	GLN
1	A	211	HIS
1	A	224	GLN
1	A	264	ASN
1	A	277	ASN
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	418	ASN
1	A	439	GLN
1	A	480	HIS
1	A	512	GLN
1	A	518	ASN
2	B	19	HIS
2	B	66	ASN
2	B	74	GLN
2	B	137	GLN
2	B	210	GLN
2	B	236	GLN
2	B	319	ASN
2	B	325	ASN
2	B	342	ASN
2	B	351	GLN
2	B	389	ASN
2	B	395	GLN
2	B	407	ASN
3	I	140	GLN
1	C	37	ASN
1	C	197	GLN
1	C	224	GLN
1	C	230	ASN
1	C	264	ASN
1	C	320	GLN
1	C	322	ASN
1	C	344	ASN
1	C	359	ASN
1	C	386	ASN
1	C	418	ASN
1	C	436	HIS
1	C	439	GLN
1	C	447	ASN
1	C	512	GLN
1	C	517	ASN
2	D	18	ASN
2	D	74	GLN
2	D	125	ASN
2	D	128	GLN
2	D	131	ASN
2	D	139	HIS

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Mol	Chain	Res	Type
2	D	210	GLN
2	D	236	GLN
2	D	270	GLN
2	D	325	ASN
2	D	348	GLN
2	D	362	GLN
2	D	421	GLN
2	D	432	GLN
1	E	72	ASN
1	E	115	ASN
1	E	178	ASN
1	E	197	GLN
1	E	211	HIS
1	E	264	ASN
1	E	271	ASN
1	E	277	ASN
1	E	359	ASN
1	E	370	GLN
1	E	418	ASN
1	E	436	HIS
1	E	439	GLN
1	E	447	ASN
1	E	466	GLN
1	E	518	ASN
2	F	18	ASN
2	F	19	HIS
2	F	32	HIS
2	F	74	GLN
2	F	125	ASN
2	F	128	GLN
2	F	131	ASN
2	F	212	ASN
2	F	236	GLN
2	F	241	GLN
2	F	319	ASN
2	F	320	ASN
2	F	325	ASN
2	F	342	ASN
2	F	351	GLN
2	F	362	GLN
2	F	370	ASN
2	F	395	GLN

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Mol	Chain	Res	Type
2	F	407	ASN
1	G	37	ASN
1	G	64	GLN
1	G	72	ASN
1	G	197	GLN
1	G	230	ASN
1	G	264	ASN
1	G	271	ASN
1	G	277	ASN
1	G	300	GLN
1	G	322	ASN
1	G	343	GLN
1	G	344	ASN
1	G	359	ASN
1	G	366	GLN
1	G	386	ASN
1	G	438	GLN
1	G	439	GLN
1	G	447	ASN
1	G	518	ASN
1	G	527	GLN
2	H	18	ASN
2	H	19	HIS
2	H	32	HIS
2	H	74	GLN
2	H	87	ASN
2	H	125	ASN
2	H	128	GLN
2	H	131	ASN
2	H	163	ASN
2	H	236	GLN
2	H	258	GLN
2	H	325	ASN
2	H	348	GLN
2	H	351	GLN
2	H	352	ASN
2	H	354	GLN
2	H	362	GLN
2	H	395	GLN
2	H	407	ASN
3	L	141	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	517/531 (97%)	-0.10	5 (0%)	82	63	46, 76, 107, 130	0
1	C	516/531 (97%)	-0.03	7 (1%)	75	53	53, 82, 116, 140	0
1	E	515/531 (96%)	-0.06	8 (1%)	72	49	36, 62, 128, 141	0
1	G	508/531 (95%)	-0.05	10 (1%)	65	41	44, 71, 135, 147	0
2	B	432/434 (99%)	-0.02	13 (3%)	50	25	46, 68, 122, 131	0
2	D	431/434 (99%)	0.17	10 (2%)	60	36	47, 85, 118, 131	0
2	F	431/434 (99%)	0.09	16 (3%)	41	20	41, 70, 121, 134	0
2	H	431/434 (99%)	0.07	15 (3%)	44	22	45, 79, 127, 140	0
3	I	85/88 (96%)	0.03	1 (1%)	79	58	54, 77, 99, 110	0
3	J	77/88 (87%)	0.29	2 (2%)	56	30	58, 90, 106, 116	0
3	K	77/88 (87%)	-0.03	0	100	100	56, 81, 99, 104	0
3	L	78/88 (88%)	0.21	0	100	100	70, 105, 125, 129	0
All	All	4098/4212 (97%)	0.01	87 (2%)	63	39	36, 76, 122, 147	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	HIS	5.1
1	G	252	LEU	4.6
2	D	243	PHE	4.2
1	E	260	GLU	3.7
2	B	392	LEU	3.7
1	E	253	LYS	3.5
2	B	442	SER	3.5
2	F	243	PHE	3.5
1	G	251	ILE	3.5
2	H	404	THR	3.4
2	B	408	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	242	PRO	3.4
2	F	441	THR	3.3
2	H	385	LEU	3.3
1	A	260	GLU	3.3
2	B	413	LYS	3.1
1	A	252	LEU	3.1
2	F	242	PRO	3.1
2	H	408	LEU	3.1
3	I	99	GLY	3.1
1	G	217	ILE	3.0
1	C	259	PRO	3.0
2	F	412	LEU	3.0
2	D	385	LEU	2.9
1	E	261	ASP	2.9
2	H	236	GLN	2.9
2	F	417	LEU	2.9
2	H	441	THR	2.8
2	D	244	GLY	2.8
2	B	351	GLN	2.8
2	H	239	LYS	2.8
2	D	390	ARG	2.8
2	H	243	PHE	2.8
1	C	209	HIS	2.8
1	G	249	GLN	2.7
1	G	250	GLY	2.7
2	H	391	THR	2.7
1	G	246	LEU	2.6
2	F	383	ALA	2.6
2	B	211	VAL	2.6
2	B	394	LEU	2.6
2	F	360	LYS	2.5
1	C	278	THR	2.5
1	G	265	PHE	2.5
3	J	117	ILE	2.4
1	A	7	LEU	2.4
1	C	253	LYS	2.4
1	E	248	ARG	2.4
2	H	388	LYS	2.4
1	G	212	THR	2.4
1	E	200	ASP	2.4
2	B	381	ILE	2.4
3	J	103	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	252	LEU	2.3
1	G	272	VAL	2.3
2	D	394	LEU	2.3
2	H	393	TYR	2.3
1	G	247	ILE	2.3
2	F	247	VAL	2.3
2	B	438	LEU	2.3
2	F	394	LEU	2.3
1	C	210	SER	2.3
2	H	359	ALA	2.3
1	E	259	PRO	2.2
1	C	260	GLU	2.2
2	H	365	LEU	2.2
1	A	115	ASN	2.2
2	F	385	LEU	2.2
2	F	418	VAL	2.2
2	B	385	LEU	2.2
2	D	382	THR	2.2
2	D	423	LEU	2.2
2	B	353	ILE	2.1
2	F	244	GLY	2.1
2	D	294	SER	2.1
1	E	251	ILE	2.1
2	H	394	LEU	2.1
2	D	239	LYS	2.1
2	F	248	PRO	2.1
2	B	412	LEU	2.1
1	C	370	GLN	2.1
2	H	354	GLN	2.0
2	F	440	PHE	2.0
2	B	423	LEU	2.0
2	F	392	LEU	2.0
2	H	437	LYS	2.0
2	F	246	GLY	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 monosaccharides 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, 95th 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
4	ZN	B	1	1/1	0.99	0.14	70,70,70,70	0
4	ZN	F	4	1/1	0.99	0.14	67,67,67,67	0
4	ZN	H	2	1/1	0.99	0.15	84,84,84,84	0
4	ZN	D	3	1/1	1.00	0.13	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.