Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:23 PM GMT

PDB ID	:	4V4O
Title	:	Crystal Structure of the Chaperonin Complex Cpn60/Cpn10/(ADP)7 from Thermus Thermophilus
Authors	:	Shimamura, T.; Koike-Takeshita, A.; Yokoyama, K.; Masui, R.; Murai, N.; Yoshida, M.; Taguchi, H.; Iwata, S.
Deposited on	:	2004-05-23
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

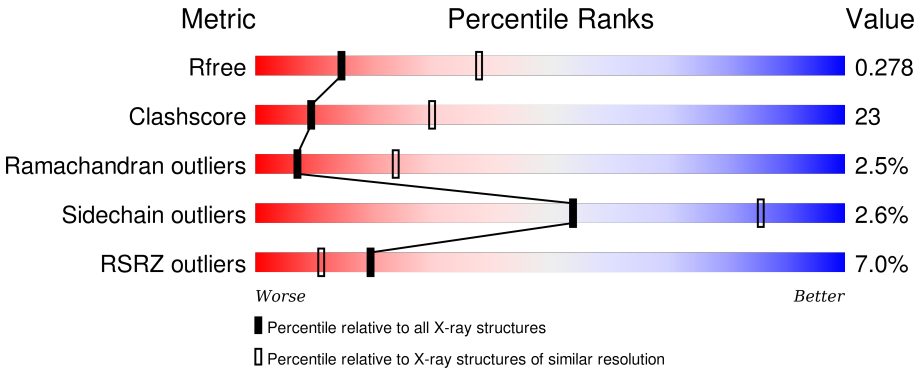
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	543	40% 54%
1	B	543	41% 53%
1	C	543	37% 56%
1	D	543	43% 50%
1	E	543	37% 55% 5%

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Mol	Chain	Length	Quality of chain
1	F	543	2% 45% 49%
1	G	543	% 39% 55%
1	H	543	3% 46% 49%
1	I	543	2% 48% 48%
1	J	543	2% 47% 48%
1	K	543	2% 47% 48%
1	L	543	2% 44% 51%
1	M	543	34% 44% 50%
1	N	543	4% 47% 48%
1	a	543	7% 93%
1	b	543	9% 93%
1	c	543	5% 92% 5%
1	d	543	2% 92% 5%
1	e	543	4% 93%
1	f	543	5% 94%
1	g	543	6% 92%
1	h	543	% 93%
1	i	543	5% 93%
1	j	543	6% 93%
1	k	543	11% 94%
1	l	543	21% 94%
1	m	543	30% 93%
1	n	543	6% 94%
2	O	100	12% 22% 65% 7%
2	P	100	7% 21% 64% 8% 6%

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Mol	Chain	Length	Quality of chain
2	Q	100	9% 8% 79% 7%
2	R	100	7% 24% 63% 9%
2	S	100	14% 19% 70% 7%
2	T	100	12% 10% 78% 7%
2	U	100	10% 14% 74% 8%
2	o	100	28% 88% 8%
2	p	100	14% 86% 10%
2	q	100	6% 79% 16%
2	r	100	9% 87% 9%
2	s	100	15% 88% 8%
2	t	100	16% 85% 11%
2	u	100	17% 84% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	H	601	-	-	-	X
5	DMS	J	601	-	-	-	X
5	DMS	L	601	-	-	-	X
5	DMS	h	601	-	-	-	X
5	DMS	i	601	-	-	-	X
5	DMS	j	601	-	-	-	X
5	DMS	k	601	-	-	-	X
5	DMS	l	601	-	-	-	X
5	DMS	m	601	-	-	-	X
5	DMS	n	701	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121267 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 cpn60(GroEL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	B	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	C	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	D	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	E	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	F	529	Total	C	N	O	S	0	0	0
			3974	2495	689	785	5			
1	G	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	H	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	I	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	J	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	K	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	L	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	M	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	N	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	a	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	b	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	d	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	e	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	f	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	g	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	h	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	i	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	j	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	k	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	l	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	m	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	n	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			

- Molecule 2 is a protein called cpn10(GroES).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	P	94	Total	C	N	O	0	0	0
			723	460	123	140			
2	Q	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	R	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	S	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	T	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	U	96	Total	C	N	O	0	0	0
			739	470	126	143			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	o	96	Total 739	C 470	N 126	O 143	0	0	0
2	p	96	Total 739	C 470	N 126	O 143	0	0	0
2	q	96	Total 739	C 470	N 126	O 143	0	0	0
2	r	96	Total 739	C 470	N 126	O 143	0	0	0
2	s	96	Total 739	C 470	N 126	O 143	0	0	0
2	t	96	Total 739	C 470	N 126	O 143	0	0	0
2	u	96	Total 739	C 470	N 126	O 143	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0
3	g	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	e	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	a	1	Total 1	Mg 1	0	0
3	c	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	f	1	Total 1	Mg 1	0	0
3	d	1	Total 1	Mg 1	0	0

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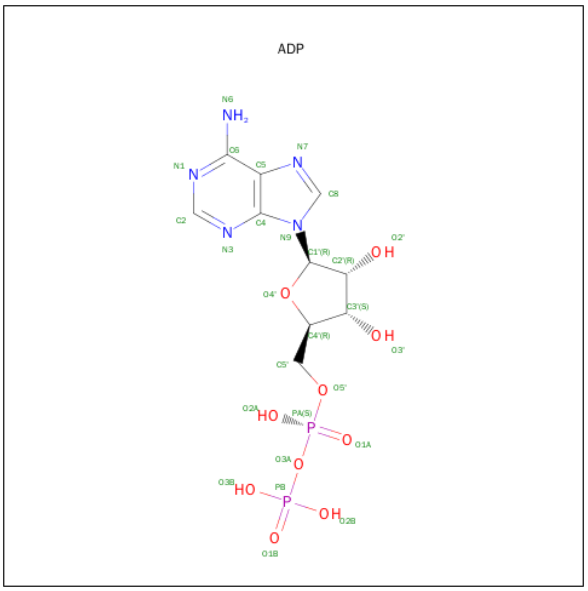
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	b	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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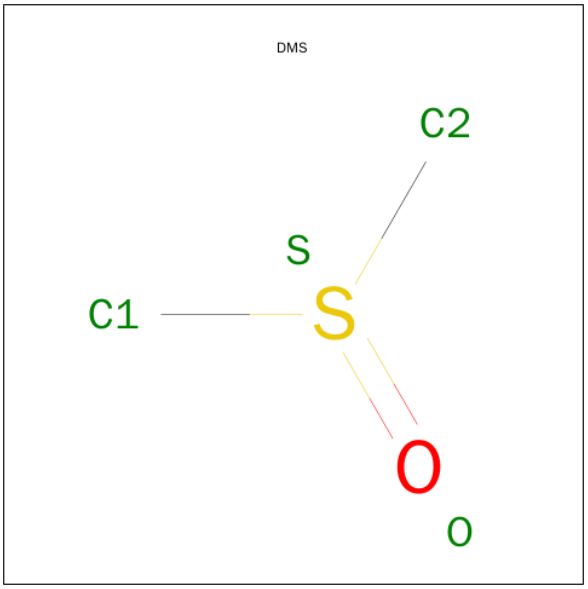
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	c	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	d	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	O	S	0	0
			4	2	1	1		
5	I	1	Total	C	O	S	0	0
			4	2	1	1		
5	J	1	Total	C	O	S	0	0
			4	2	1	1		
5	K	1	Total	C	O	S	0	0
			4	2	1	1		
5	L	1	Total	C	O	S	0	0
			4	2	1	1		
5	M	1	Total	C	O	S	0	0
			4	2	1	1		

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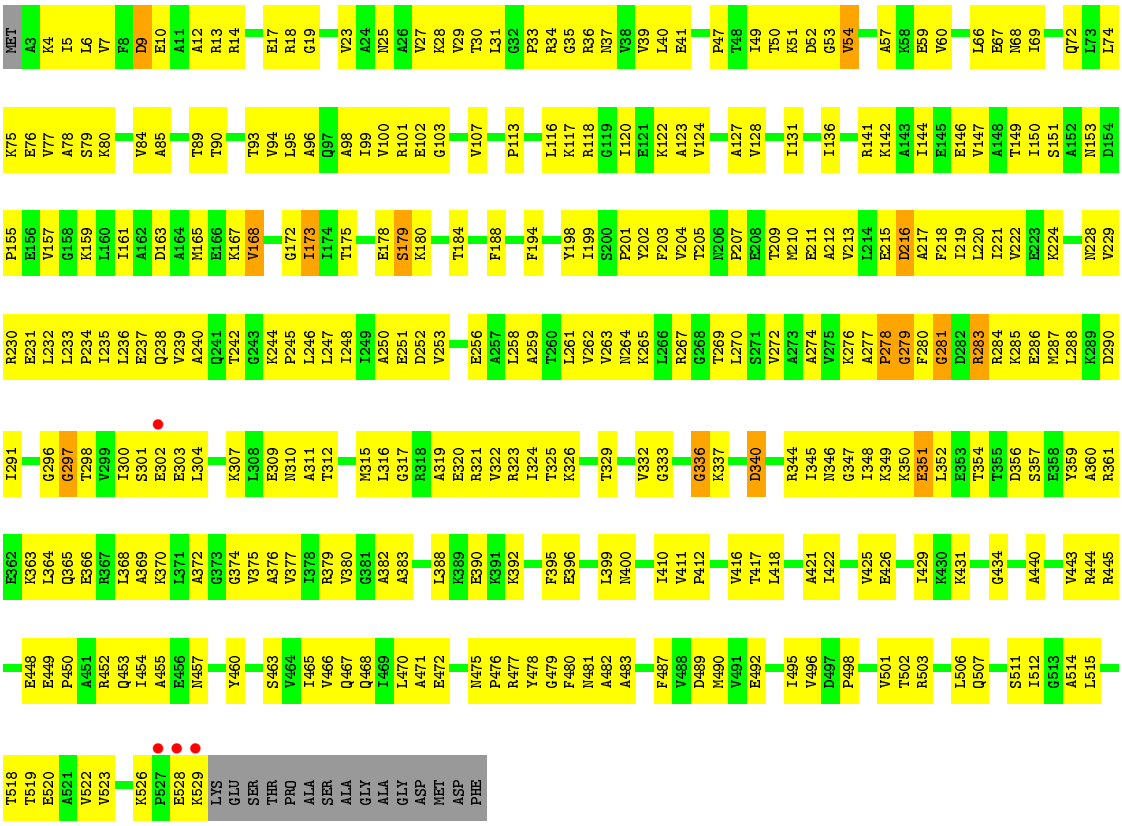
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	O	S	0	0
			4	2	1	1		
5	h	1	Total	C	O	S	0	0
			4	2	1	1		
5	i	1	Total	C	O	S	0	0
			4	2	1	1		
5	j	1	Total	C	O	S	0	0
			4	2	1	1		
5	k	1	Total	C	O	S	0	0
			4	2	1	1		
5	l	1	Total	C	O	S	0	0
			4	2	1	1		
5	m	1	Total	C	O	S	0	0
			4	2	1	1		
5	n	1	Total	C	O	S	0	0
			4	2	1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

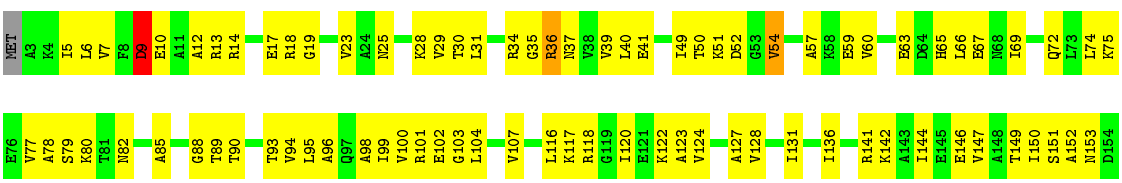
- Molecule 1: cpn60(GroEL)

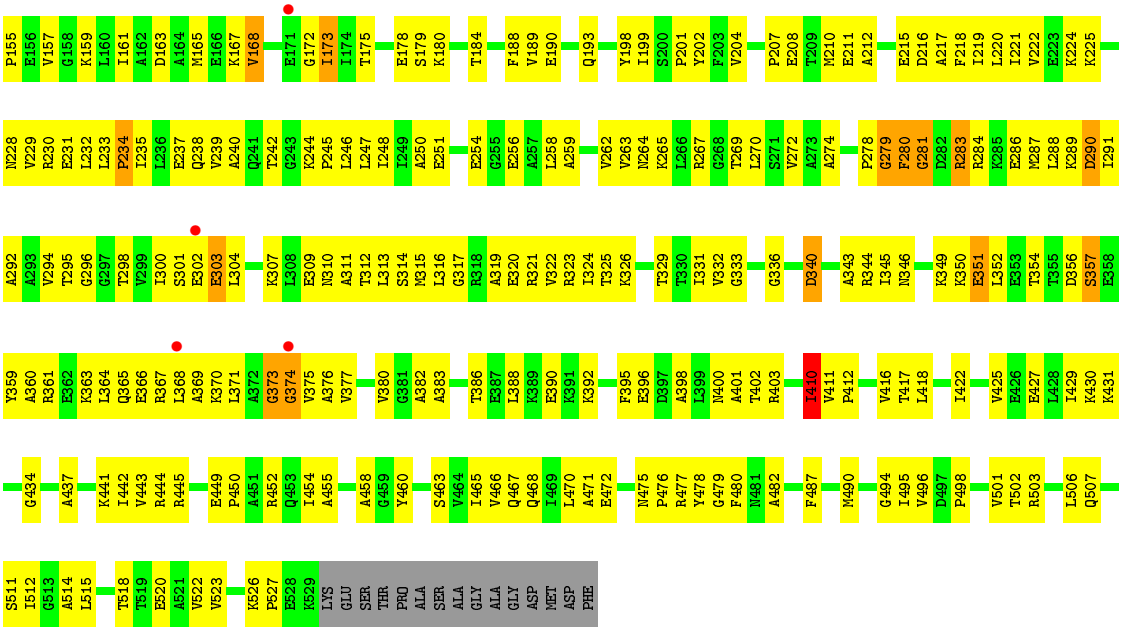
Chain A:



- Molecule 1: cpn60(GroEL)

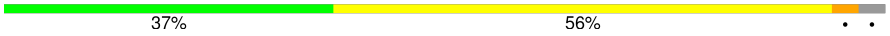
Chain B:

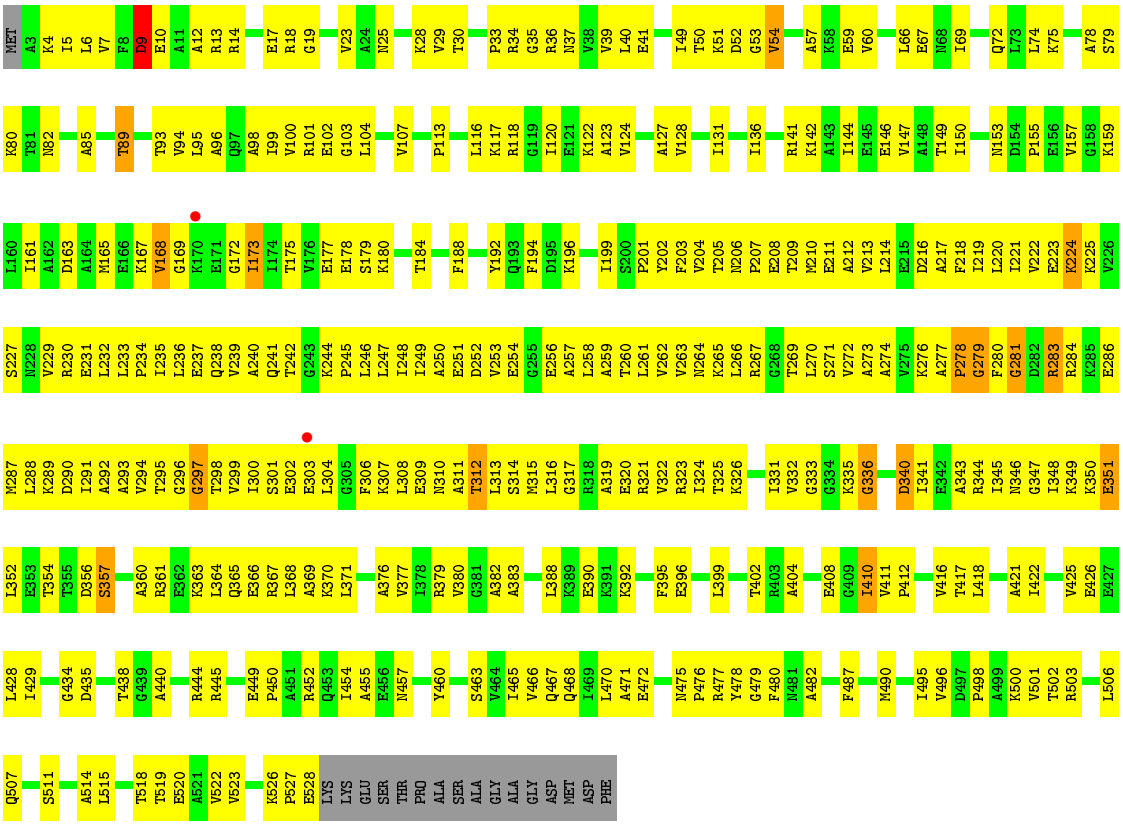




• Molecule 1: cpn60(GroEL)

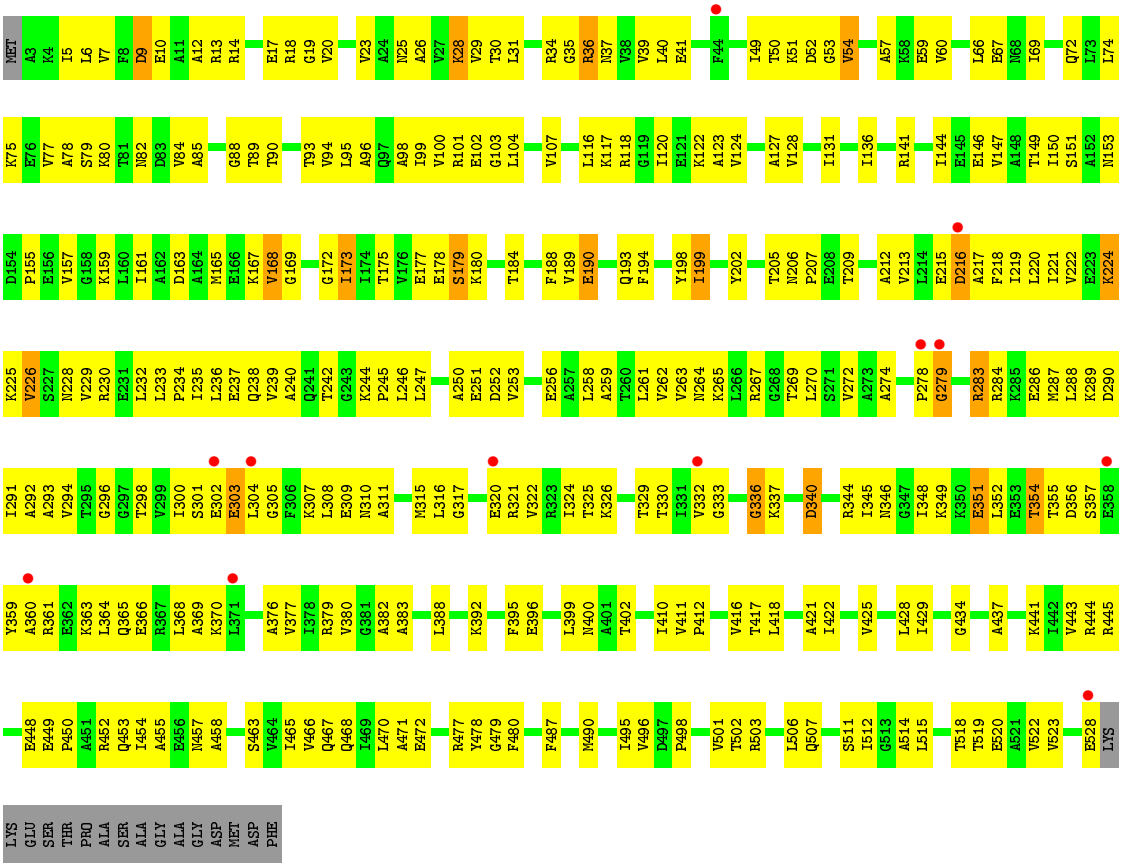
Chain C:





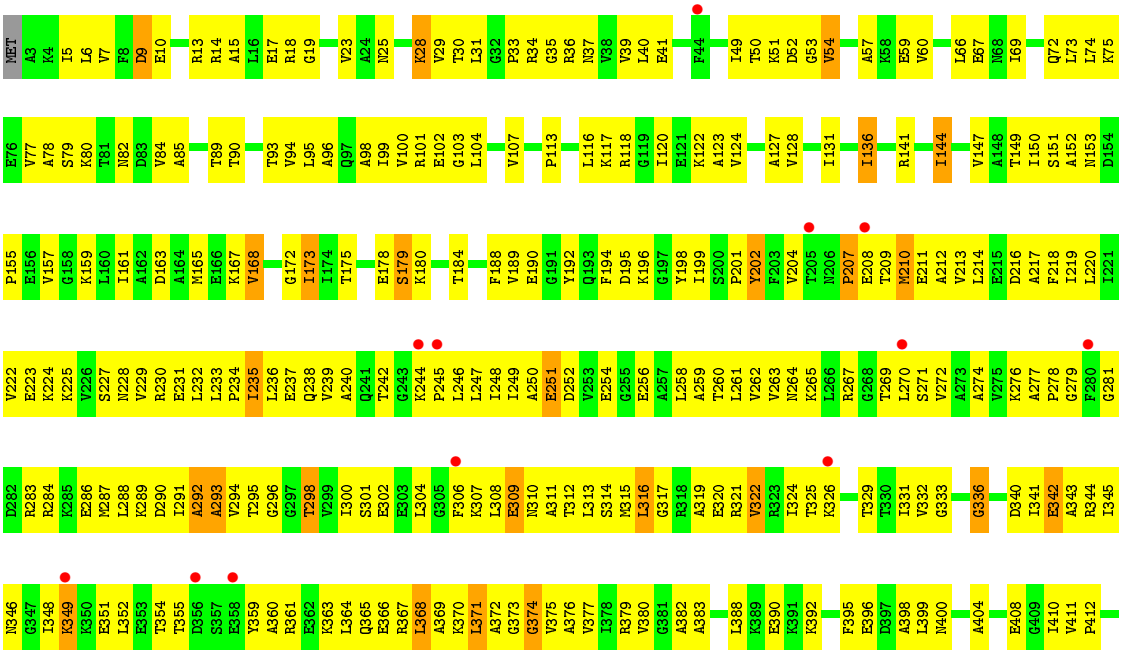
• Molecule 1: cpn60(GroEL)

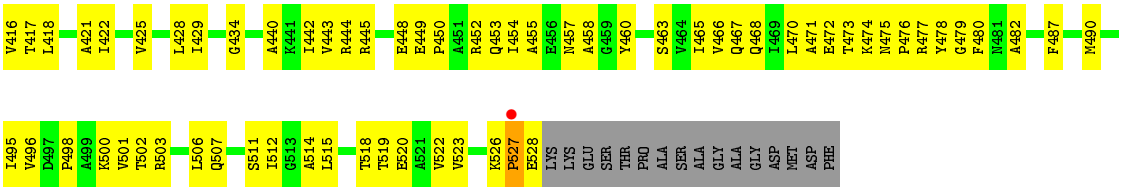
Chain D:



• Molecule 1: cpn60(GroEL)

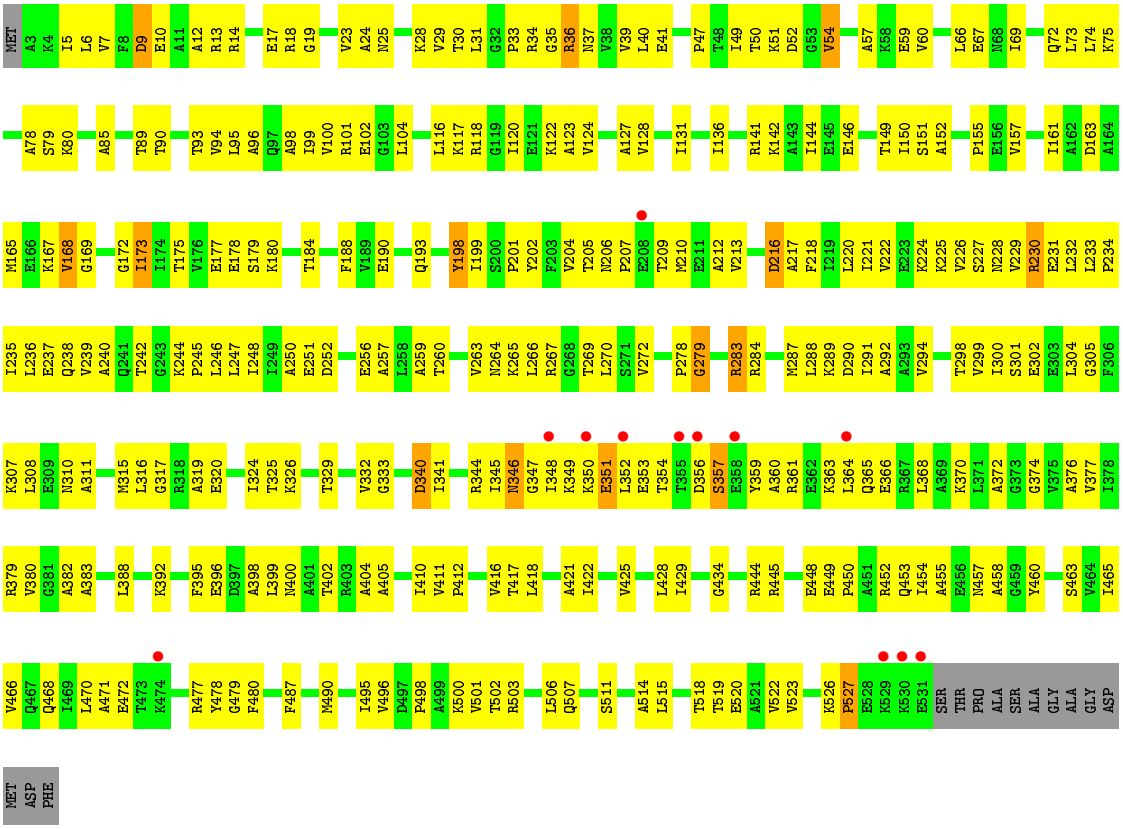
Chain E:





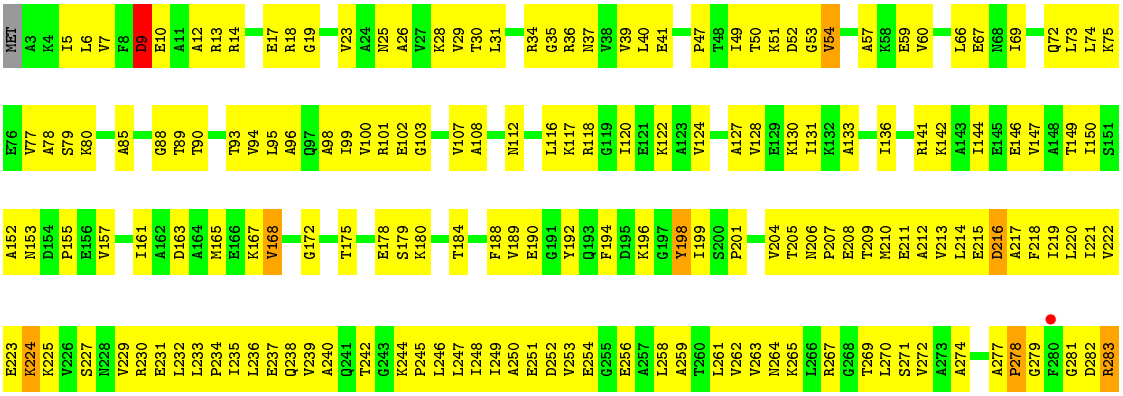
• Molecule 1: cpn60(GroEL)

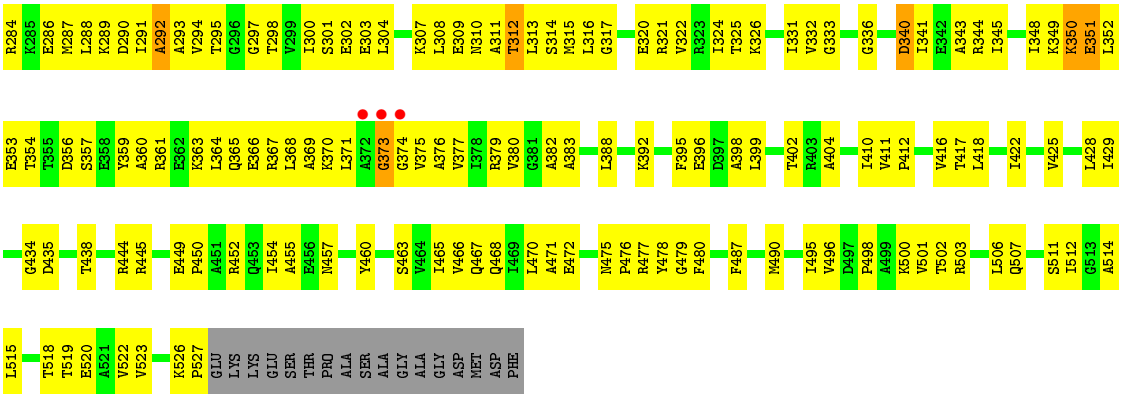
Chain F:



• Molecule 1: cpn60(GroEL)

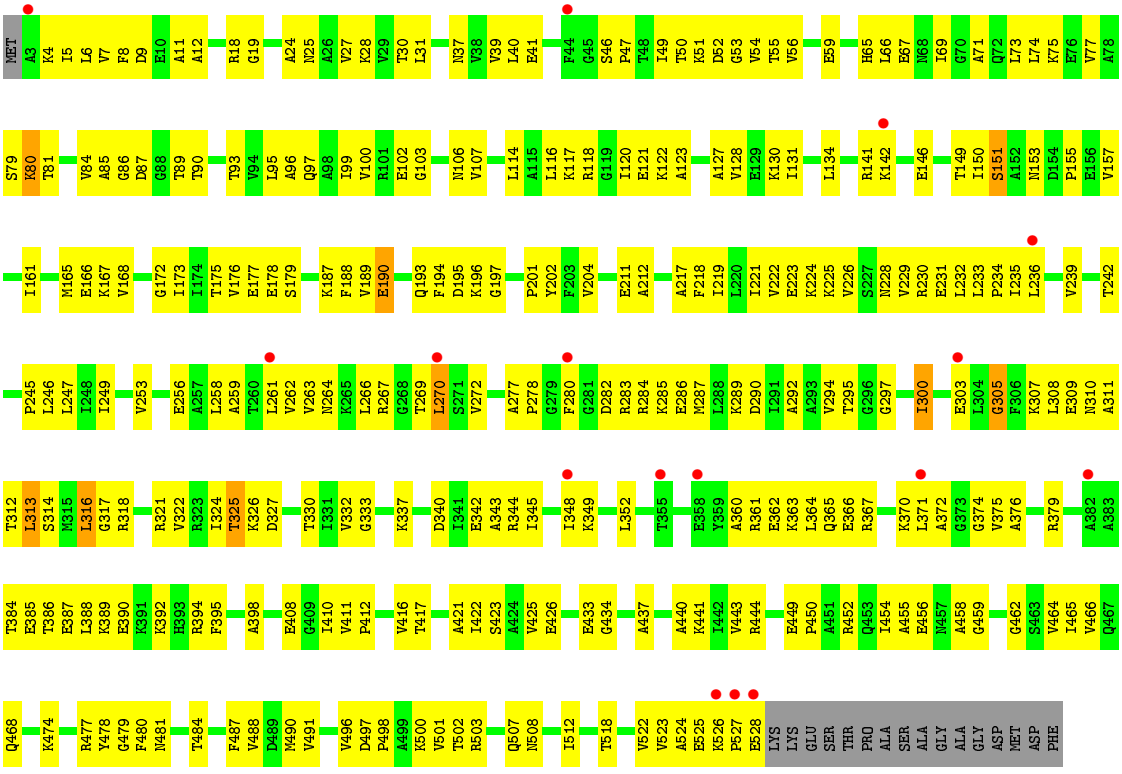
Chain G:





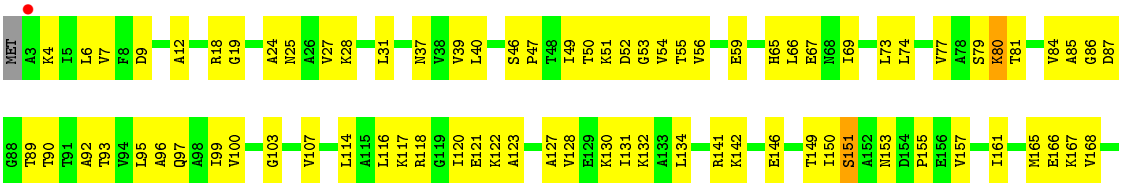
• Molecule 1: cpn60(GroEL)

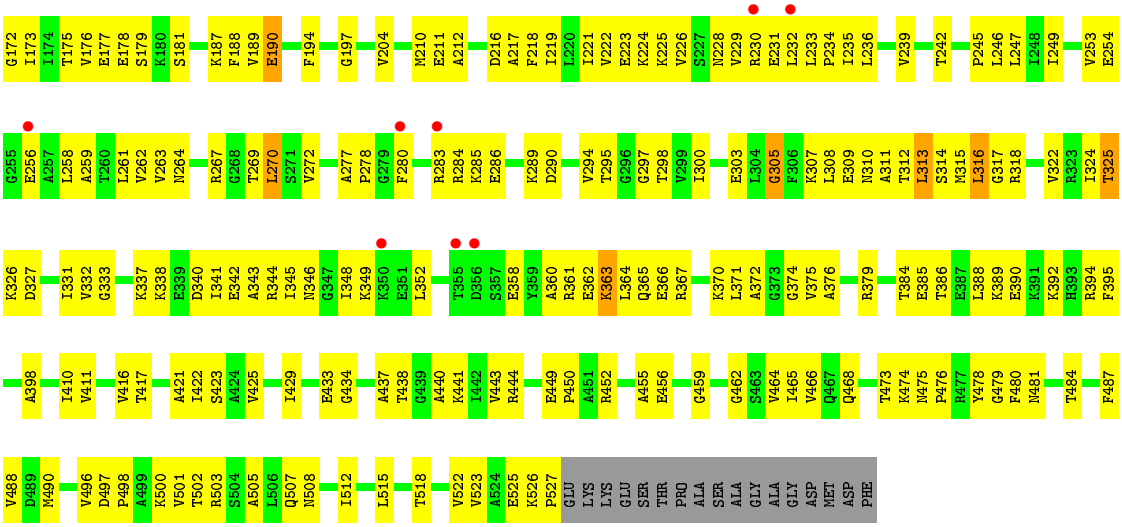
Chain H:



• Molecule 1: cpn60(GroEL)

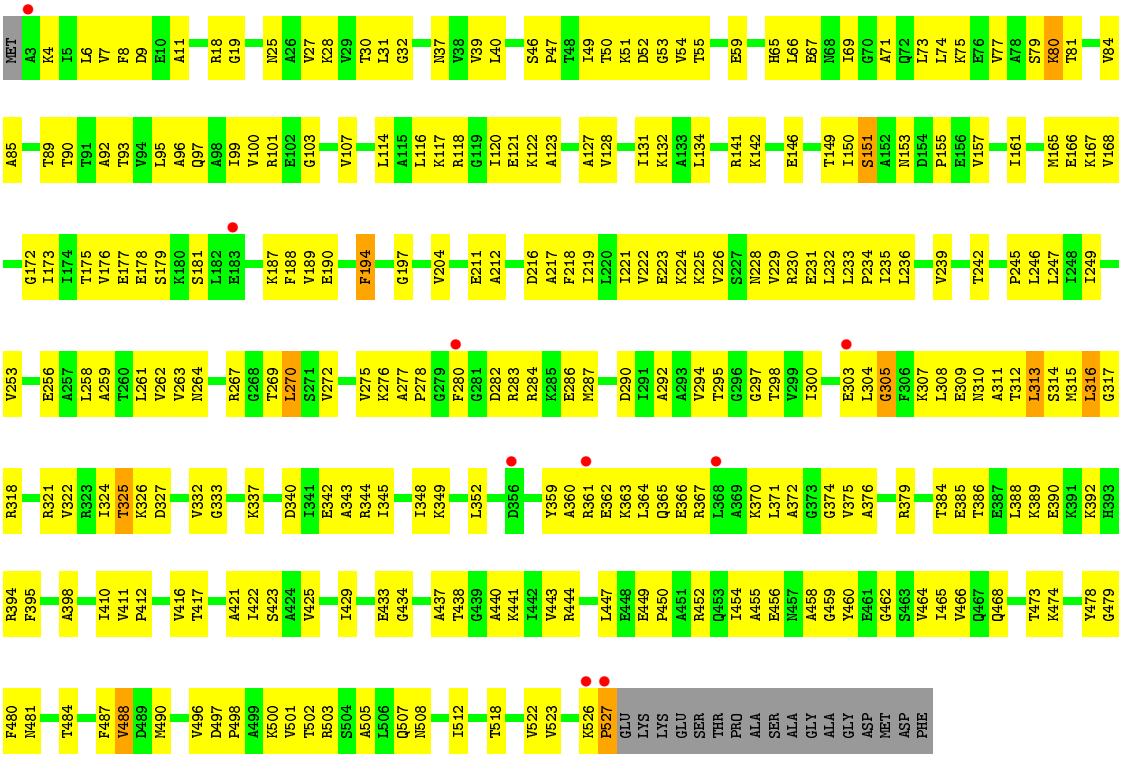
Chain I:





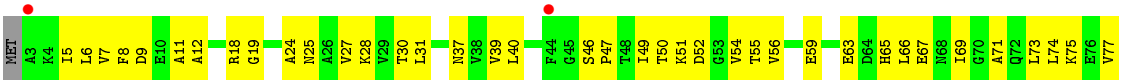
• Molecule 1: cpn60(GroEL)

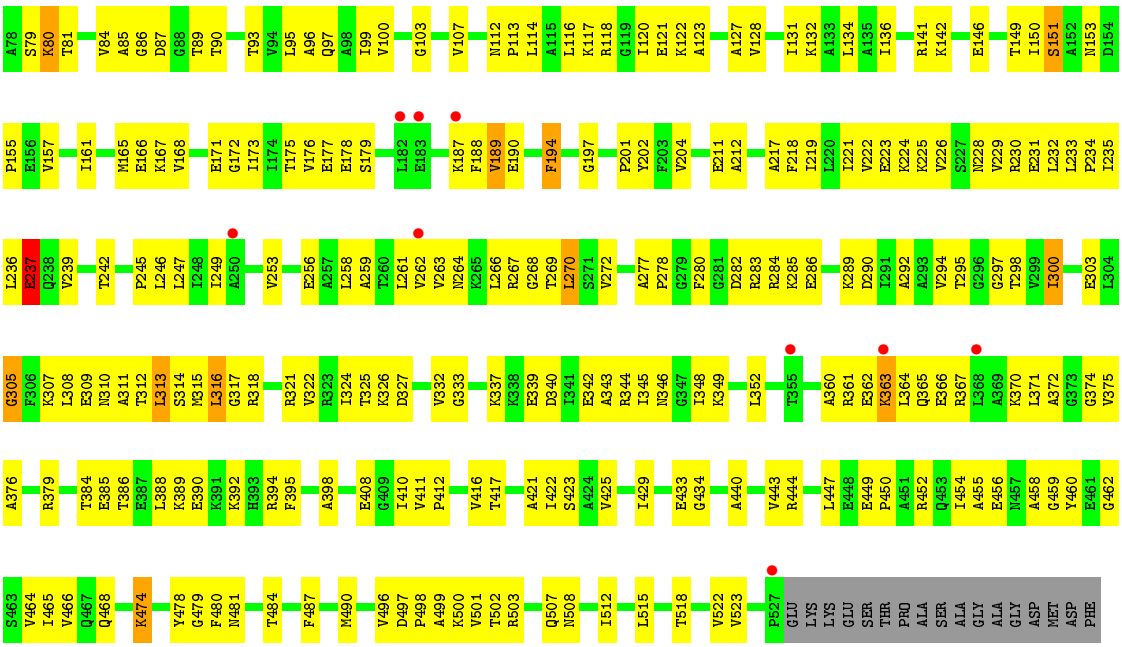
Chain J:



• Molecule 1: cpn60(GroEL)

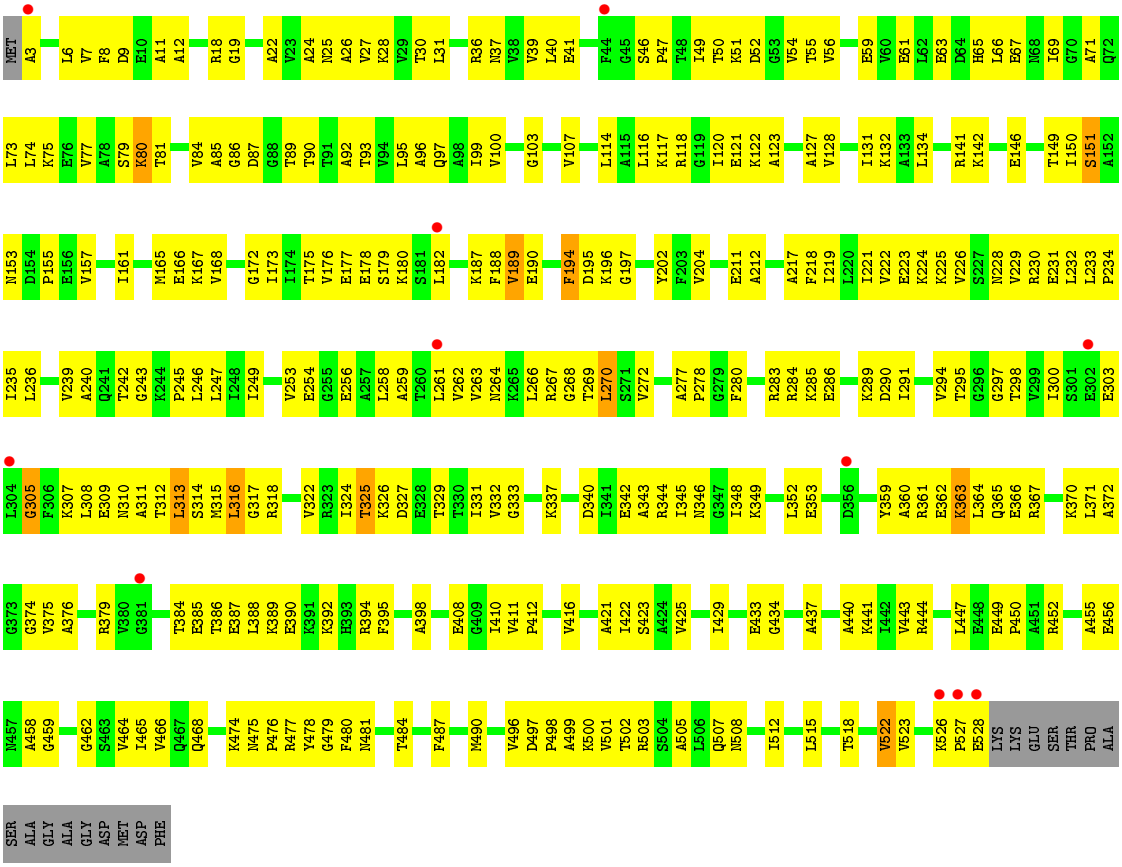
Chain K:



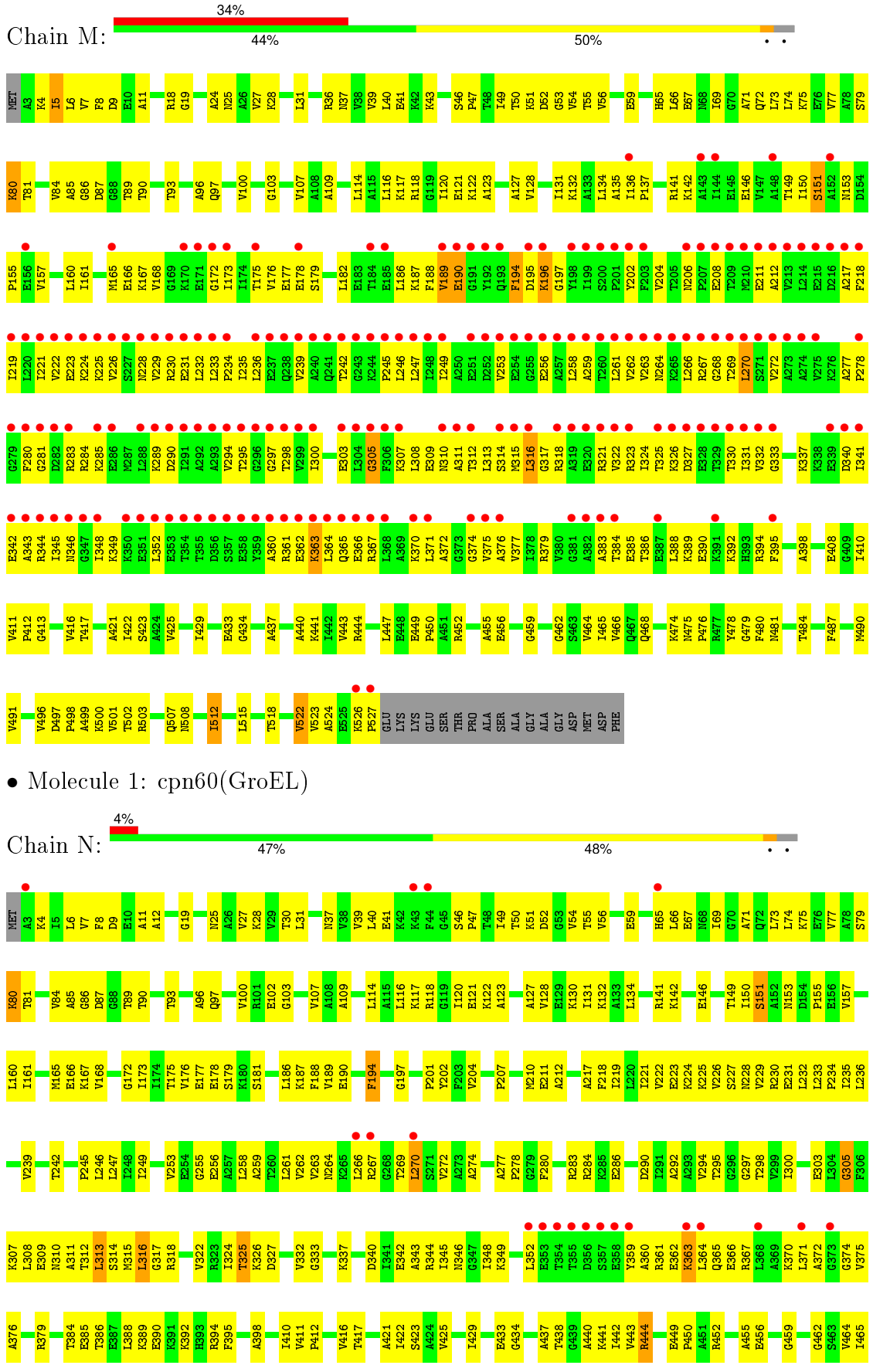


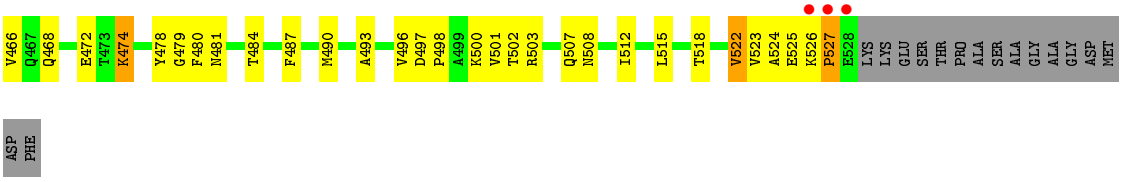
• Molecule 1: cpn60(GroEL)

Chain L:



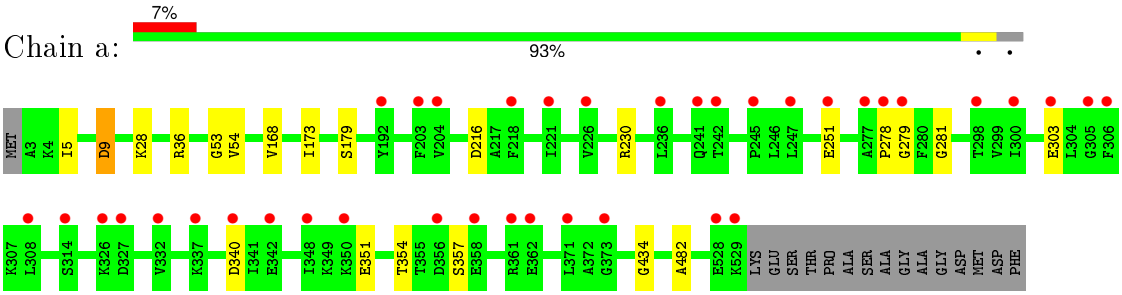
• Molecule 1: cpn60(GroEL)


Chain M:
34%
44%
50%
MET A3 K4 I5 L6 V7 F8 D9 E10 A11 R18 G19 A24 N25 A26 V27 K28 I31 R36 N37 V38 V39 I40 E41 K42 K43 S46 P47 T48 I49 T50 K51 D52 G53 V54 T55 V56 E59 H65 L66 E67 N68 I69 G70 A71 Q72 L73 L74 K75 E76 V77 A78 S79
K80 T81 V84 A85 G86 D87 G88 T89 T90 T93 A96 Q97 V100 G103 V107 A108 A109 L114 A115 L116 K117 R118 G119 I120 E121 K122 A123 A127 V128 I131 K132 A133 L134 A135 I136 P137 R141 K142 A143 I144 E145 E146 V147 A148 T149 I150 S151 A152 N153 D154
P155 E156 V157 L160 I161 M165 E166 K167 V168 G169 K170 E171 G172 I173 I174 T175 V176 E177 E178 S179 L182 E183 T184 E185 L186 K187 F188 V189 E190 F194 D195 K196 G197 Y198 I199 S200 P201 Y202 F203 V204 T205 N206 P207 E208 T209 M210 E211 A212 V213 L214 E215 D216 A217 F218
I219 L220 I221 V222 E223 K224 K225 V226 S227 N228 V229 R230 E231 L232 L233 P234 I235 L236 E237 Q238 V239 A240 Q241 T242 G243 K244 P245 L246 L247 T248 I249 A250 E251 D252 V253 E254 G255 E256 A257 I258 A259 T260 L261 V262 V263 N264 K265 I266 R267 G268 T269 L270 S271 V272 A273 A274 A277 P278 G279 F280 G281 D282 R283 R284 K285 E286 M287 L288 K289 D290 T291 A292 A293 V294 T295 G296 G297 T298 V299 I300 E303 L304 G305 F306 K307 L308 E309 N310 A311 T312 L313 S314 M315 L316 I317 R318 V322 R323 I324 T325 K326 D327 E328 T329 T330 I331 V332 G333 K337 K338 E339 D340 I341
E342 A343 R344 I345 N346 G347 I348 K349 K350 E351 L352 E353 T354 T355 D356 S357 E358 Y359 A360 R361 E362 K363 L364 Q365 E366 R367 L368 A369 K370 L371 A372 G373 G374 V375 A376 V377 I378 R379 V380 G381 A382 A383 T384 E385 T386 E387 L388 K389 E390 K391 K392 H393 R394 F395 A398 E408 G409 I410
V411 P412 G413 V416 T417 A421 I422 S423 A424 V425 I429 E433 G434 A437 A440 K441 I442 V443 R444 L447 E448 E449 P450 A451 R452 A455 E456 G459 G462 S463 V464 I465 V466 Q467 Q468 K474 N475 P476 R477 Y478 G479 F480 N481 T484 F487 M490
V491 V496 D497 P498 A499 K500 V501 T502 R503 Q507 N508 I512 L515 T518 V522 V523 A524 E525 K526 P527 GLU LYS LYS GLU SER THR PRO ALA SER ALA GLY ALA GLY ASP MET ASP PHE
• Molecule 1: cpn60(GroEL)
Chain N:
4%
47%
48%
MET A3 K4 I5 L6 V7 F8 D9 E10 A11 A12 G19 N25 A26 V27 K28 V29 T30 I31 N37 V38 V39 L40 E41 K42 K43 F44 G45 S46 P47 T48 I49 T50 K51 D52 G53 V54 T55 V56 E59 H65 L66 E67 N68 I69 G70 A71 Q72 L73 L74 K75 E76 V77 A78 S79
K80 T81 V84 A85 G86 D87 G88 T89 T90 T93 A96 Q97 V100 R101 E102 G103 V107 A108 A109 L114 A115 L116 K117 R118 G119 I120 E121 K122 A123 A127 V128 E129 K130 I131 K132 A133 L134 R141 K142 E146 T149 I150 S151 A152 N153 D154 P155 E156 V157
L160 I161 M165 E166 K167 V168 G172 I173 I174 T175 V176 E177 E178 S179 K180 S181 L186 K187 F188 V189 E190 F194 G197 P201 Y202 F203 V204 P207 M210 E211 A212 A217 F218 I219 L220 I221 V222 E223 K224 K225 V226 S227 N228 V229 R230 E231 L232 L233 P234 I235 L236
V239 T242 P245 L246 L247 T248 I249 V253 E254 G255 E256 A257 I258 A259 T260 L261 V262 V263 N264 K265 I266 R267 G268 T269 L270 S271 V272 A273 A274 A277 P278 G279 F280 R283 R284 K285 E286 D290 T291 A292 A293 V294 T295 G296 G297 T298 V299 I300 E303 L304 G305 F306
K307 L308 E309 N310 A311 T312 L313 S314 M315 L316 I317 R318 V322 R323 I324 T325 K326 D327 K337 D340 I341 E342 A343 R344 I345 N346 G347 I348 K349 L352 E353 T354 T355 D356 S357 E358 Y359 A360 R361 E362 K363 L364 Q365 E366 R367 L368 A369 K370 L371 A372 G373 G374 V375
A376 R379 T384 E385 T386 E387 L388 K389 E390 K391 K392 H393 R394 F395 A398 I410 V411 P412 V416 T417 A421 I422 S423 A424 V425 I429 E433 G434 A437 T438 G439 A440 K441 I442 V443 R444 E449 P450 A451 R452 A455 E456 G459 G462 S463 V464 I465



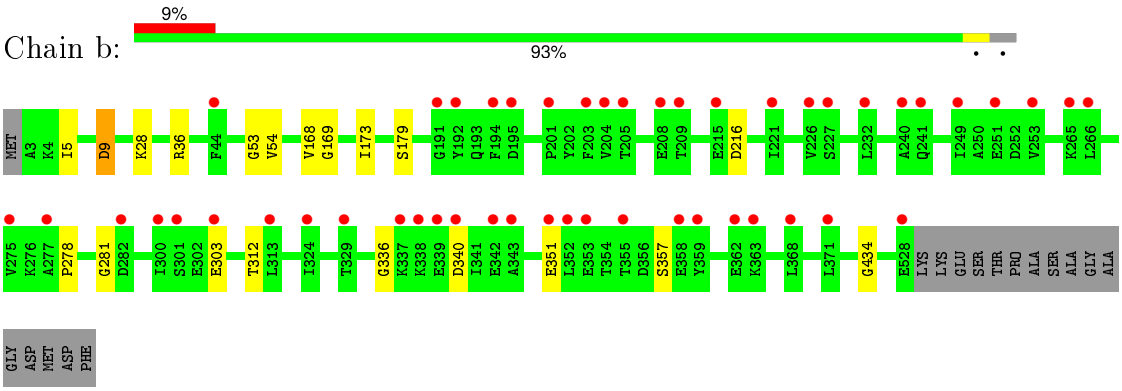
• Molecule 1: cpn60(GroEL)

Chain a:



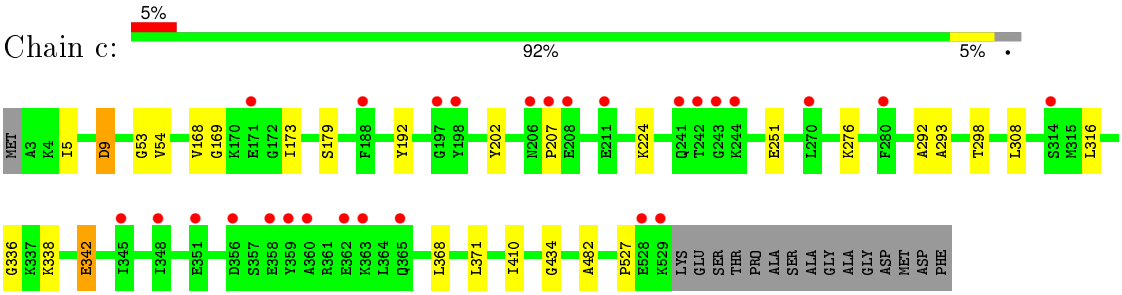
• Molecule 1: cpn60(GroEL)

Chain b:



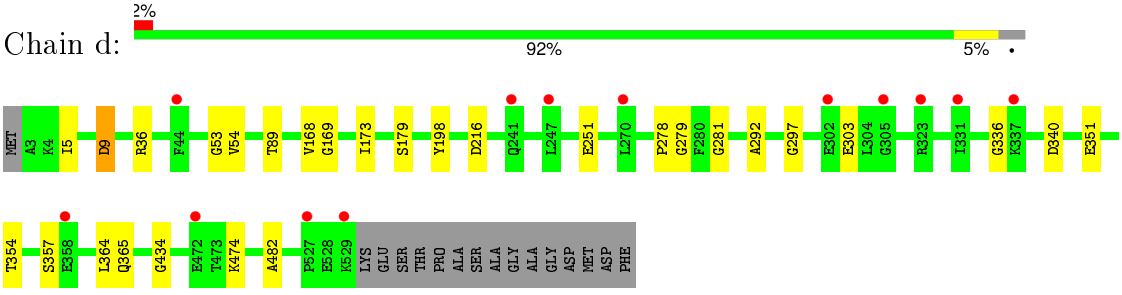
• Molecule 1: cpn60(GroEL)

Chain c:



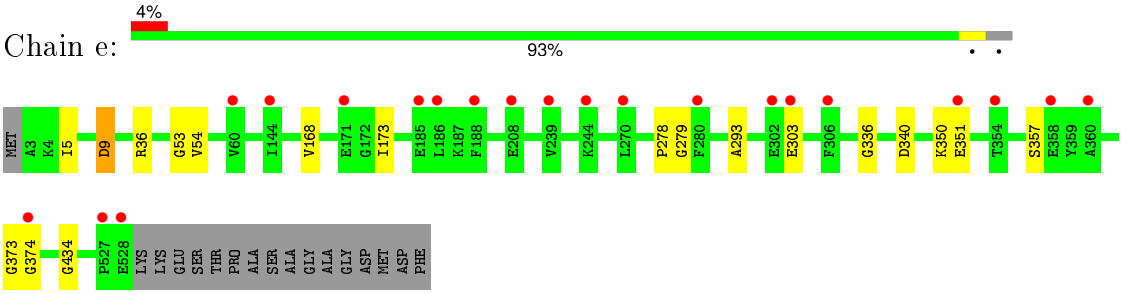
• Molecule 1: cpn60(GroEL)

Chain d:



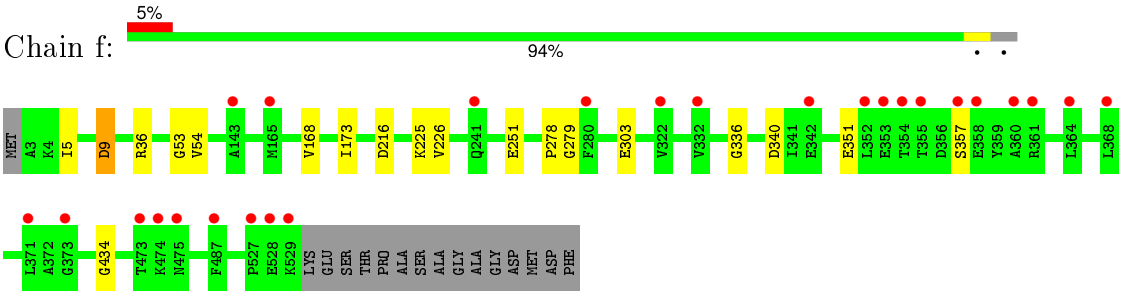
• Molecule 1: cpn60(GroEL)

Chain e:



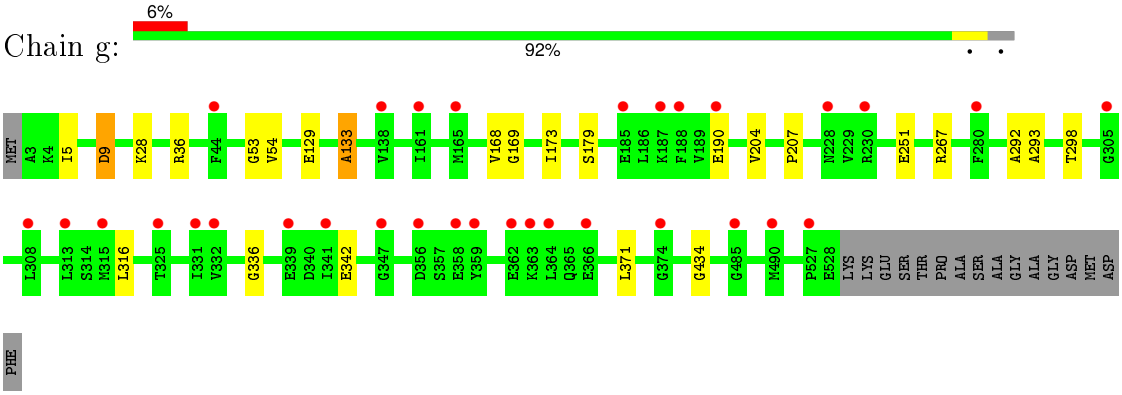
• Molecule 1: cpn60(GroEL)

Chain f:



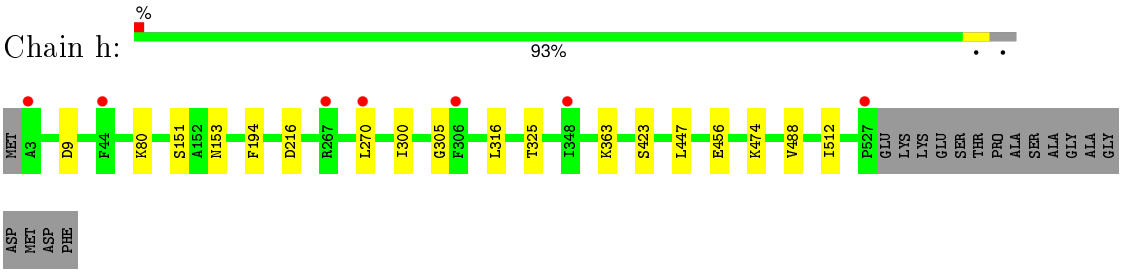
• Molecule 1: cpn60(GroEL)

Chain g:



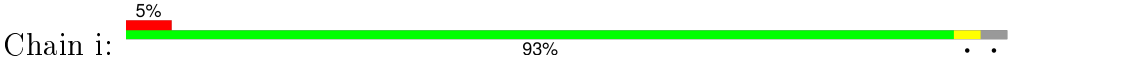
• Molecule 1: cpn60(GroEL)

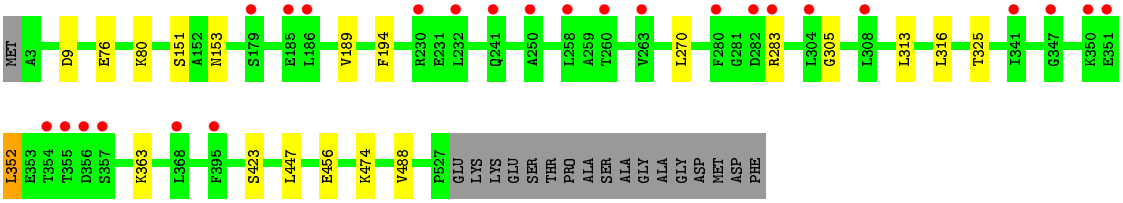
Chain h:



• Molecule 1: cpn60(GroEL)

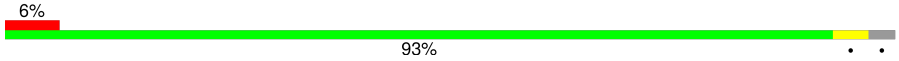
Chain i:

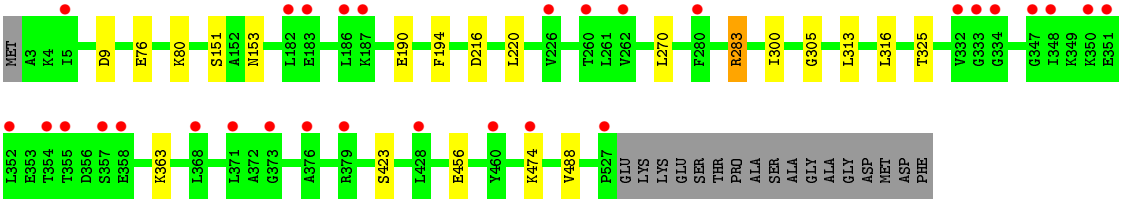




• Molecule 1: cpn60(GroEL)

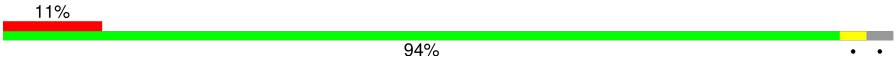
Chain j:

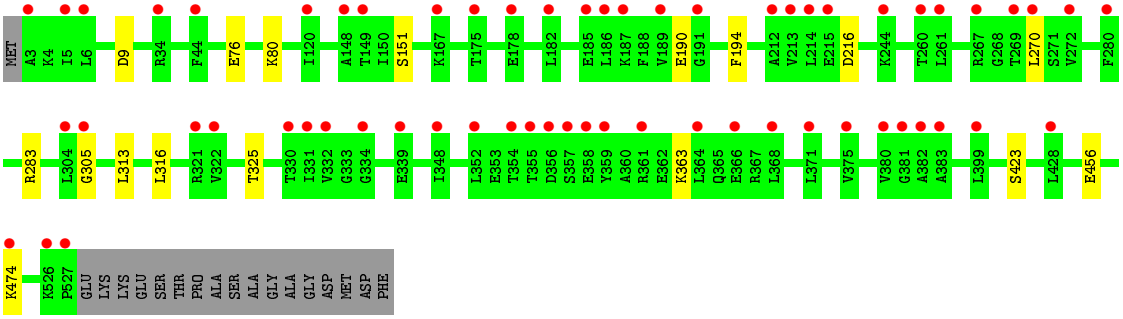




• Molecule 1: cpn60(GroEL)

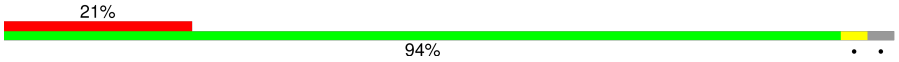
Chain k:

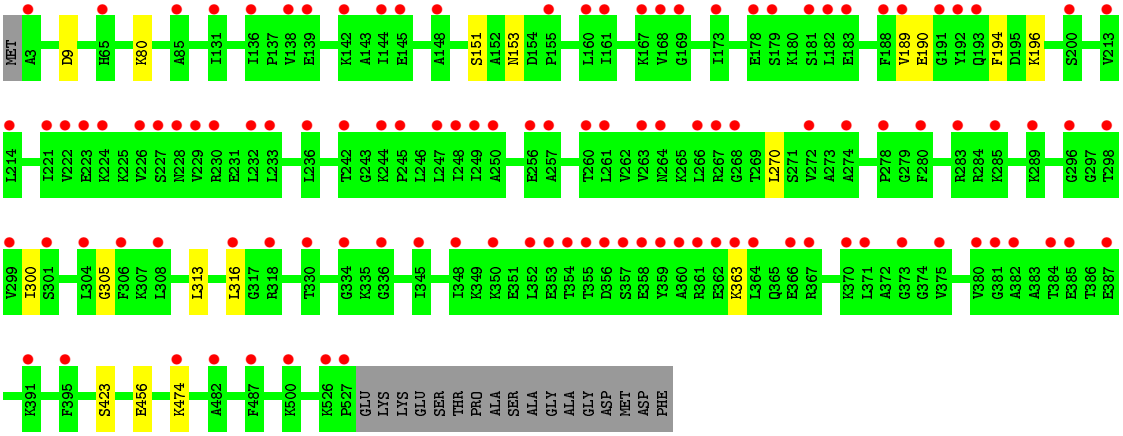




• Molecule 1: cpn60(GroEL)

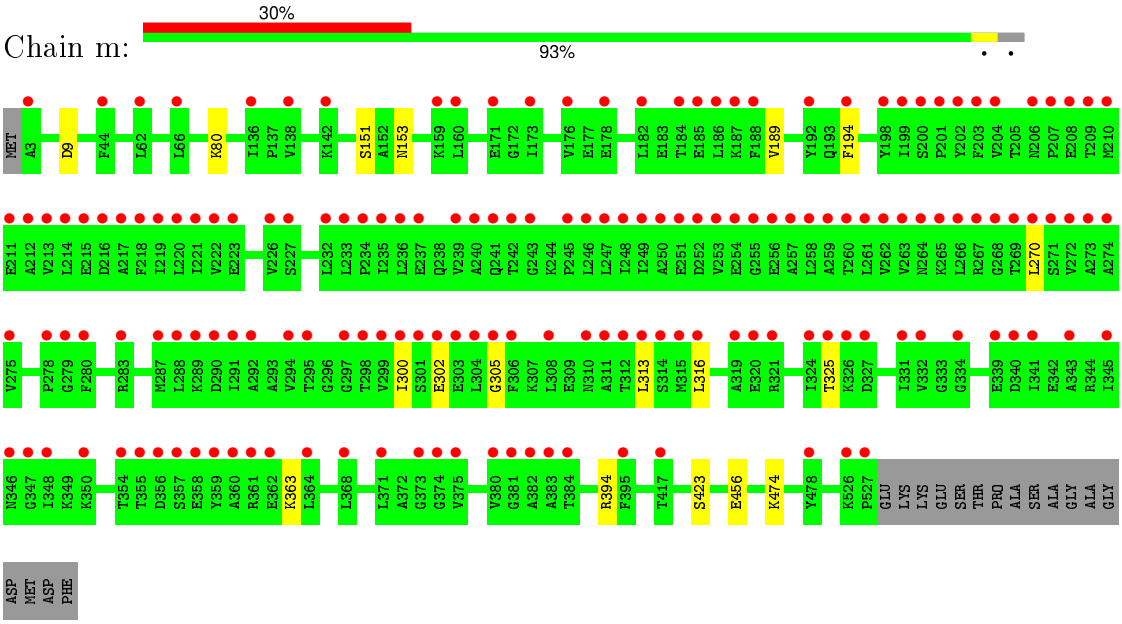
Chain l:





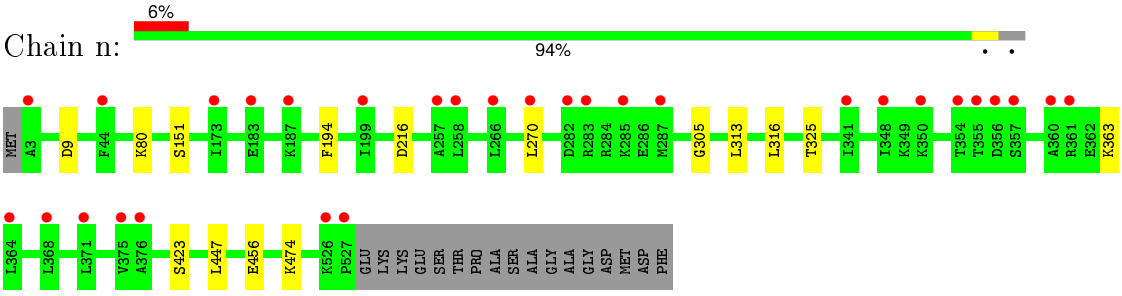
• Molecule 1: cpn60(GroEL)

Chain m:



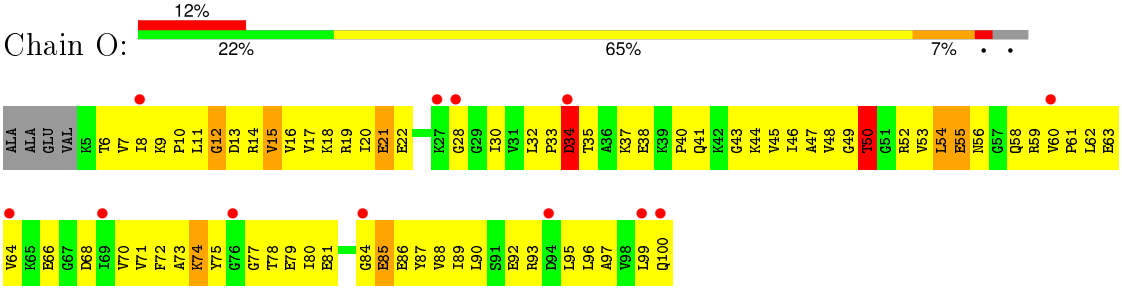
- Molecule 1: cpn60(GroEL)

Chain n:



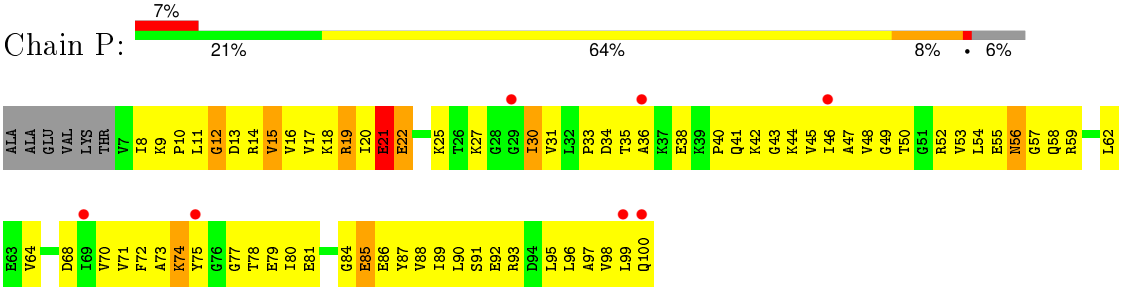
- Molecule 2: cpn10(GroES)

Chain O:



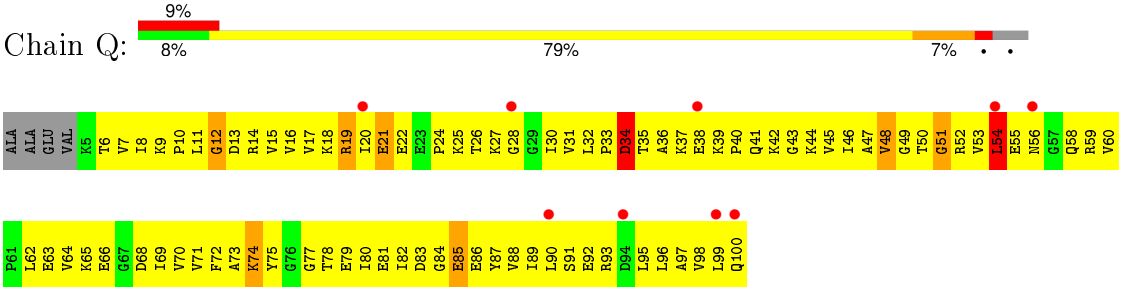
- Molecule 2: cpn10(GroES)

Chain P:



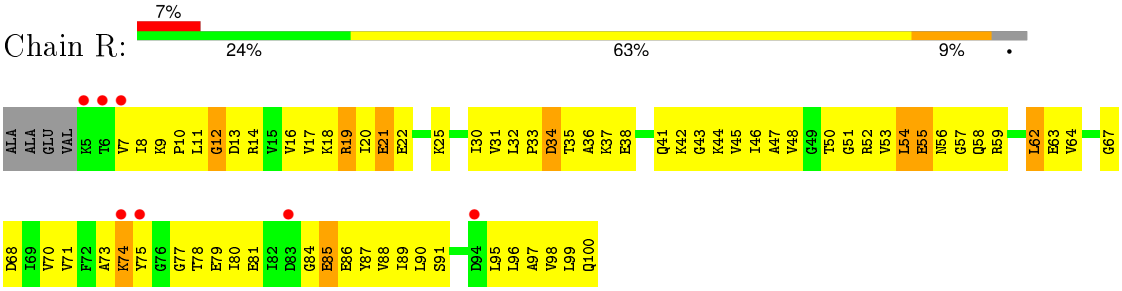
- Molecule 2: cpn10(GroES)

Chain Q:



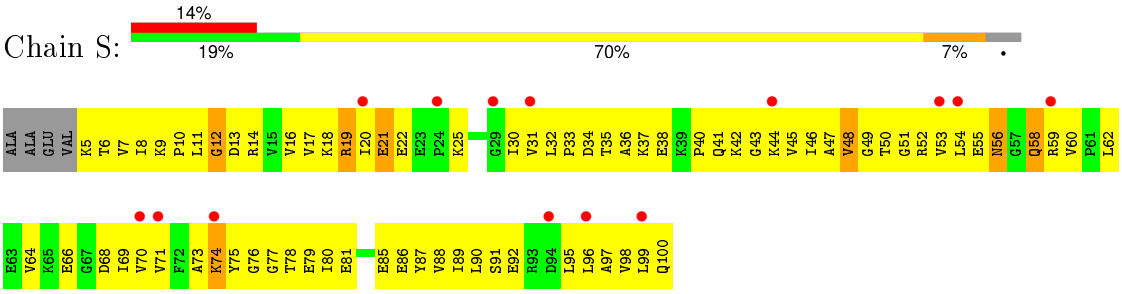
• Molecule 2: cpn10(GroES)

Chain R:



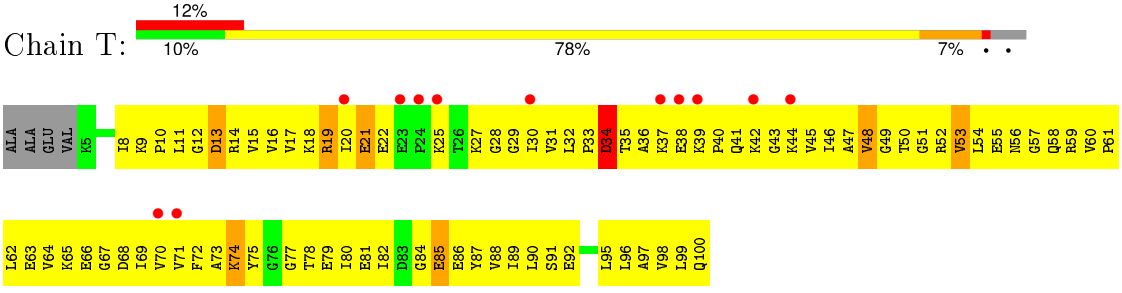
• Molecule 2: cpn10(GroES)

Chain S:



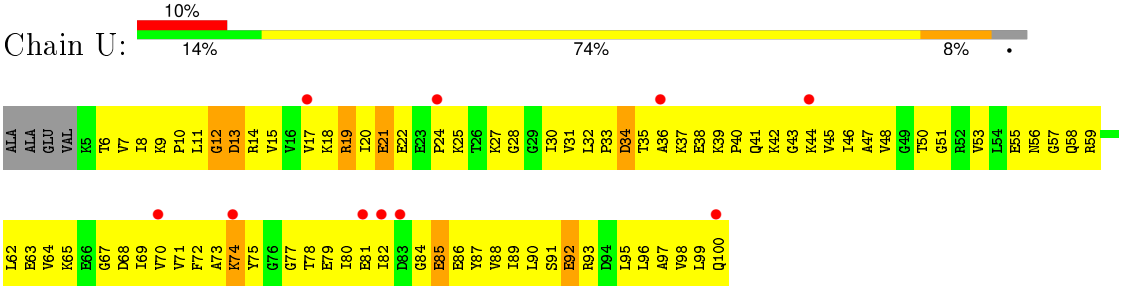
• Molecule 2: cpn10(GroES)

Chain T:



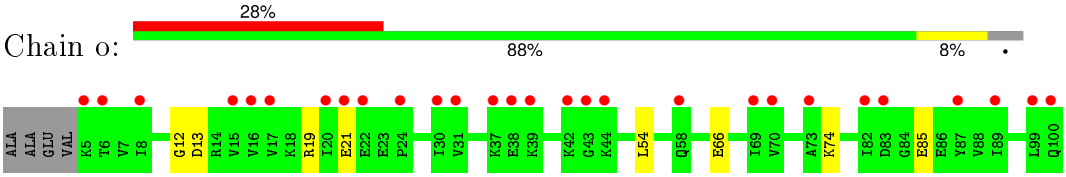
• Molecule 2: cpn10(GroES)

Chain U:



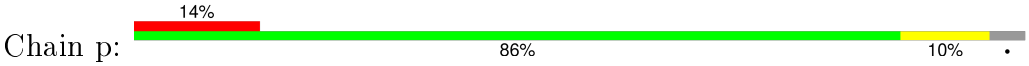
- Molecule 2: cpn10(GroES)

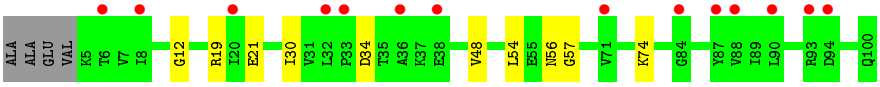
Chain o:



- Molecule 2: cpn10(GroES)

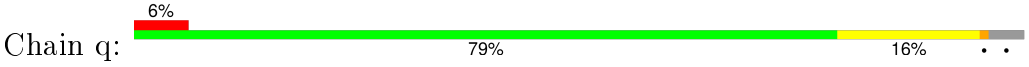
Chain p:

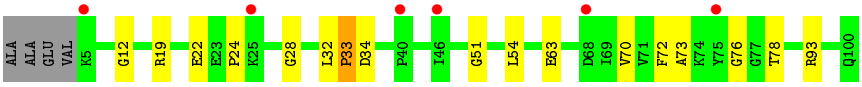




- Molecule 2: cpn10(GroES)

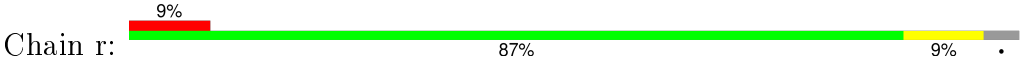
Chain q:

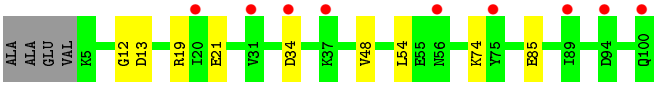




- Molecule 2: cpn10(GroES)

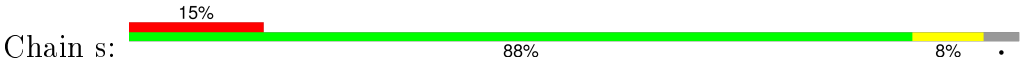
Chain r:

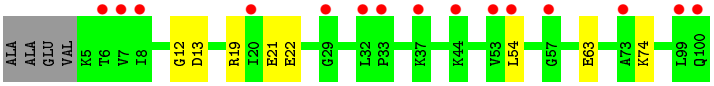




- Molecule 2: cpn10(GroES)

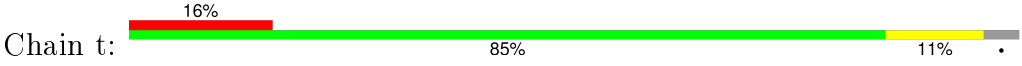
Chain s:

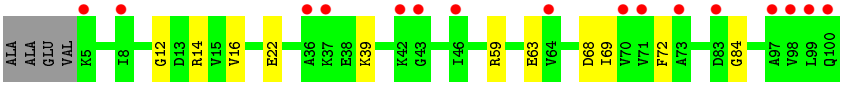




- Molecule 2: cpn10(GroES)

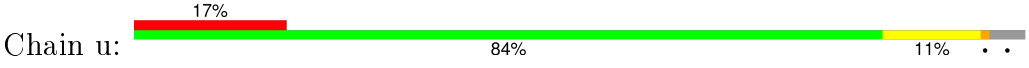
Chain t:

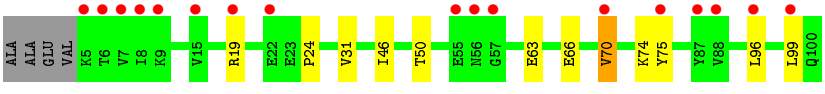




- Molecule 2: cpn10(GroES)

Chain u:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	140.38Å 156.42Å 273.15Å 82.88° 85.35° 68.52°	Depositor
Resolution (Å)	39.98 – 2.80 39.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.3 (39.98-2.80) 79.0 (39.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.279 0.239 , 0.278	Depositor DCC
R_{free} test set	12690 reflections (2.95%)	DCC
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 73.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 429625 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	121267	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/3989	0.65	0/5383
1	B	0.43	1/3989 (0.0%)	0.65	1/5383 (0.0%)
1	C	0.45	0/3980	0.67	0/5372
1	D	0.42	0/3980	0.65	1/5372 (0.0%)
1	E	0.43	0/3980	0.64	0/5372
1	F	0.39	0/4007	0.63	0/5406
1	G	0.41	0/3971	0.64	0/5360
1	H	0.36	0/3980	0.60	0/5372
1	I	0.37	0/3971	0.60	0/5360
1	J	0.40	0/3971	0.62	0/5360
1	K	0.39	1/3971 (0.0%)	0.62	0/5360
1	L	0.38	0/3980	0.60	0/5372
1	M	0.39	1/3971 (0.0%)	0.62	1/5360 (0.0%)
1	N	0.38	0/3980	0.63	1/5372 (0.0%)
1	a	0.41	0/3989	0.64	0/5383
1	b	0.40	0/3980	0.63	0/5372
1	c	0.39	0/3989	0.64	0/5383
1	d	0.39	0/3989	0.62	0/5383
1	e	0.37	0/3980	0.62	0/5372
1	f	0.34	0/3989	0.59	0/5383
1	g	0.41	1/3980 (0.0%)	0.62	1/5372 (0.0%)
1	h	0.40	0/3971	0.62	1/5360 (0.0%)
1	i	0.36	1/3971 (0.0%)	0.60	0/5360
1	j	0.35	0/3971	0.61	1/5360 (0.0%)
1	k	0.34	0/3971	0.59	0/5360
1	l	0.33	0/3971	0.59	0/5360
1	m	0.36	1/3971 (0.0%)	0.59	0/5360
1	n	0.34	0/3971	0.58	0/5360
2	O	0.40	0/746	0.68	0/1003
2	P	0.54	0/730	0.77	0/982
2	Q	0.39	0/746	0.70	2/1003 (0.2%)
2	R	0.42	0/746	0.69	0/1003

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	S	0.42	0/746	0.72	1/1003 (0.1%)
2	T	0.39	0/746	0.67	0/1003
2	U	0.46	0/746	0.72	0/1003
2	o	0.52	0/746	0.71	0/1003
2	p	0.40	0/746	0.68	0/1003
2	q	0.38	0/746	0.72	0/1003
2	r	0.41	0/746	0.67	0/1003
2	s	0.53	0/746	0.76	0/1003
2	t	0.31	0/746	0.64	0/1003
2	u	0.30	0/746	0.62	0/1003
All	All	0.39	6/121841 (0.0%)	0.63	10/164393 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	133	ALA	CA-CB	-13.30	1.24	1.52
1	m	394	ARG	CZ-NH2	-8.93	1.21	1.33
1	K	237	GLU	CD-OE1	-5.26	1.19	1.25
1	M	512	ILE	CB-CG2	5.16	1.68	1.52
1	B	410	ILE	CB-CG2	5.08	1.68	1.52
1	i	352	LEU	CG-CD2	-5.03	1.33	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	444	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	g	133	ALA	CB-CA-C	-7.31	99.13	110.10
1	j	283	ARG	CG-CD-NE	5.69	123.75	111.80
2	Q	51	GLY	N-CA-C	-5.32	99.81	113.10
1	M	512	ILE	CG1-CB-CG2	5.29	123.03	111.40
1	h	512	ILE	CG1-CB-CG2	5.25	122.96	111.40
2	Q	54	LEU	CA-CB-CG	5.18	127.20	115.30
2	S	58	GLN	CA-CB-CG	5.13	124.69	113.40
1	D	190	GLU	N-CA-C	5.08	124.71	111.00
1	B	410	ILE	CG1-CB-CG2	5.05	122.51	111.40

There are no chirality outliers.

There are no planarity outliers.

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	3956	0	4129	361	0
1	B	3956	0	4129	347	0
1	C	3947	0	4116	427	1
1	D	3947	0	4116	335	0
1	E	3947	0	4116	419	3
1	F	3974	0	4148	316	0
1	G	3938	0	4110	376	0
1	H	3947	0	4116	322	0
1	I	3938	0	4110	306	0
1	J	3938	0	4110	317	0
1	K	3938	0	4110	314	1
1	L	3947	0	4116	367	1
1	M	3938	0	4110	426	0
1	N	3947	0	4116	335	4
1	a	3956	0	4129	0	0
1	b	3947	0	4116	0	0
1	c	3956	0	4129	0	0
1	d	3956	0	4129	0	4
1	e	3947	0	4116	0	0
1	f	3956	0	4129	0	0
1	g	3947	0	4116	0	4
1	h	3938	0	4110	0	0
1	i	3938	0	4110	0	0
1	j	3938	0	4110	0	0
1	k	3938	0	4110	0	0
1	l	3938	0	4110	0	0
1	m	3938	0	4110	0	0
1	n	3938	0	4110	0	0
2	O	739	0	786	153	0
2	P	723	0	766	154	0
2	Q	739	0	786	217	0
2	R	739	0	786	137	0
2	S	739	0	786	158	0
2	T	739	0	786	196	0
2	U	739	0	786	171	0
2	o	739	0	786	0	0
2	p	739	0	786	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	q	739	0	786	0	0
2	r	739	0	786	0	0
2	s	739	0	786	0	0
2	t	739	0	786	0	0
2	u	739	0	786	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	a	1	0	0	0	0
3	b	1	0	0	0	0
3	c	1	0	0	0	0
3	d	1	0	0	0	0
3	e	1	0	0	0	0
3	f	1	0	0	0	0
3	g	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	5	0
4	F	27	0	12	2	0
4	G	27	0	12	1	0
4	a	27	0	12	0	0
4	b	27	0	12	0	0
4	c	27	0	12	0	0
4	d	27	0	12	0	0
4	e	27	0	12	0	0
4	f	27	0	12	0	0
4	g	27	0	12	0	0
5	H	4	0	6	3	0
5	I	4	0	6	0	0
5	J	4	0	6	0	0
5	K	4	0	6	0	0
5	L	4	0	6	0	0
5	M	4	0	6	0	0
5	N	4	0	6	0	0
5	h	4	0	6	0	0
5	i	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	j	4	0	6	0	0
5	k	4	0	6	0	0
5	l	4	0	6	0	0
5	m	4	0	6	0	0
5	n	4	0	6	0	0
All	All	121267	0	126522	5603	9

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 23.

All (5603) 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:D:150:ILE:HD11	1:D:495:ILE:HA	1.22	1.21
1:K:283:ARG:NH2	1:K:367:ARG:HD3	2.09	1.20
1:K:283:ARG:HH21	1:K:367:ARG:CD	2.35	1.19
1:I:283:ARG:NH2	1:I:367:ARG:HD3	2.14	1.18
1:E:229:VAL:HG21	2:S:36:ALA:HB2	2.51	1.15
2:T:19:ARG:HD3	2:T:40:PRO:HG2	2.73	1.15
2:Q:70:VAL:HG12	2:Q:71:VAL:H	2.23	1.15
1:A:350:LYS:HB3	1:B:208:GLU:HG2	7.47	1.14
1:L:235:ILE:HD11	1:L:311:ALA:HB3	1.33	1.14
1:N:235:ILE:HD11	1:N:311:ALA:HB3	1.29	1.14
1:M:235:ILE:HD11	1:M:311:ALA:HB3	1.40	1.14
1:D:173:ILE:HD11	1:D:365:GLN:HG3	1.16	1.14
1:M:182:LEU:HD11	1:N:363:LYS:NZ	1.62	1.13
1:L:189:VAL:HG12	1:L:190:GLU:H	1.13	1.12
1:E:230:ARG:NH2	2:S:38:GLU:OE2	3.38	1.12
2:Q:81:GLU:HG3	2:Q:85:GLU:H	1.70	1.12
1:H:235:ILE:HD11	1:H:311:ALA:HB3	1.35	1.12
2:O:54:LEU:HD21	2:P:57:GLY:H	1.10	1.12
1:B:150:ILE:HD11	1:B:495:ILE:HA	1.33	1.12
1:I:283:ARG:HH21	1:I:367:ARG:CD	2.36	1.11
2:P:100:GLN:HB3	2:Q:7:VAL:HB	2.58	1.11
1:E:150:ILE:HD11	1:E:495:ILE:HA	1.25	1.11
1:L:182:LEU:HD11	1:M:363:LYS:NZ	1.80	1.11
1:G:150:ILE:HD11	1:G:495:ILE:HA	1.30	1.11
1:J:325:THR:HG22	1:J:327:ASP:H	1.13	1.10
2:Q:92:GLU:HA	2:Q:95:LEU:HD12	2.16	1.10
1:L:243:GLY:HA2	1:M:228:ASN:CB	1.80	1.10
1:K:235:ILE:HD11	1:K:311:ALA:HB3	1.30	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ILE:HD11	1:C:495:ILE:HA	1.19	1.10
1:H:325:THR:HG22	1:H:327:ASP:H	1.15	1.10
1:L:182:LEU:HD11	1:M:363:LYS:HZ3	1.09	1.09
1:L:243:GLY:HA2	1:M:228:ASN:HB2	1.04	1.09
1:I:283:ARG:HH11	1:I:363:LYS:HE3	1.66	1.09
1:F:150:ILE:HD11	1:F:495:ILE:HA	1.23	1.09
1:A:150:ILE:HD11	1:A:495:ILE:HA	1.28	1.08
1:I:217:ALA:HB2	1:I:245:PRO:HG2	1.41	1.08
1:M:136:ILE:HB	1:M:410:ILE:HG13	1.34	1.07
2:U:48:VAL:HG12	2:U:62:LEU:HD12	1.32	1.07
1:E:256:GLU:HB3	2:S:35:THR:HB	2.39	1.07
1:F:283:ARG:HH12	1:F:363:LYS:HD2	3.94	1.06
1:H:217:ALA:HB2	1:H:245:PRO:HG2	1.37	1.06
1:I:325:THR:HG22	1:I:327:ASP:H	1.17	1.06
1:M:189:VAL:HG12	1:M:190:GLU:H	0.95	1.06
1:N:325:THR:HG22	1:N:327:ASP:H	1.18	1.06
1:K:325:THR:HG22	1:K:327:ASP:H	1.17	1.06
1:I:235:ILE:HD11	1:I:311:ALA:HB3	1.31	1.05
1:N:189:VAL:HG11	1:N:333:GLY:HA2	1.36	1.05
1:J:217:ALA:HB2	1:J:245:PRO:HG2	1.46	1.05
1:A:168:VAL:HG12	1:A:172:GLY:HA3	1.39	1.04
2:P:48:VAL:HG12	2:P:62:LEU:HD12	1.39	1.04
2:O:48:VAL:HG12	2:O:62:LEU:HD12	1.32	1.04
1:G:168:VAL:HG12	1:G:172:GLY:HA3	1.40	1.04
1:B:229:VAL:HG21	2:P:36:ALA:HB2	1.39	1.04
1:L:325:THR:HG22	1:L:327:ASP:H	1.23	1.04
1:L:182:LEU:CD1	1:M:363:LYS:HZ3	1.74	1.04
1:E:240:ALA:HA	1:E:270:LEU:HD13	1.39	1.04
1:F:235:ILE:HD11	1:F:311:ALA:HB3	1.74	1.03
1:M:182:LEU:HD11	1:N:363:LYS:CE	1.87	1.03
1:N:50:THR:HG22	1:N:52:ASP:H	1.29	1.03
1:L:217:ALA:HB2	1:L:245:PRO:HG2	1.38	1.03
1:A:350:LYS:HB3	1:B:208:GLU:CG	8.04	1.03
1:D:168:VAL:HG12	1:D:172:GLY:HA3	1.41	1.03
1:J:283:ARG:HG3	1:J:363:LYS:NZ	3.75	1.03
1:A:237:GLU:HB3	2:O:28:GLY:HA3	2.25	1.02
1:B:251:GLU:HG3	1:B:284:ARG:HH12	1.21	1.02
1:K:283:ARG:HH21	1:K:367:ARG:HD3	1.87	1.02
1:K:332:VAL:HG22	1:K:375:VAL:HG11	1.88	1.02
1:I:189:VAL:HG12	1:I:190:GLU:H	1.32	1.02
1:J:235:ILE:HD11	1:J:311:ALA:HB3	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:VAL:HG21	1:D:66:LEU:HD11	1.42	1.02
1:L:243:GLY:CA	1:M:228:ASN:HB2	1.99	1.02
1:J:283:ARG:NH1	1:J:363:LYS:HE3	1.98	1.02
1:E:212:ALA:HB3	1:E:324:ILE:HB	2.44	1.02
1:B:343:ALA:HB2	1:C:207:PRO:HB3	1.42	1.02
2:O:84:GLY:HA3	2:U:27:LYS:HD2	2.88	1.02
1:G:283:ARG:NH1	1:G:363:LYS:HD2	3.49	1.02
1:B:168:VAL:HG12	1:B:172:GLY:HA3	1.42	1.01
1:M:217:ALA:HB2	1:M:245:PRO:HG2	1.43	1.01
1:K:217:ALA:HB2	1:K:245:PRO:HG2	1.41	1.01
1:M:325:THR:HG22	1:M:327:ASP:H	1.23	1.01
1:N:217:ALA:HB2	1:N:245:PRO:HG2	1.42	1.01
1:G:50:THR:HG22	1:G:51:LYS:H	1.26	1.01
1:F:235:ILE:HD11	1:F:311:ALA:CB	2.30	1.00
1:F:168:VAL:HG12	1:F:172:GLY:HA3	1.44	1.00
2:O:70:VAL:HG11	2:O:95:LEU:HD22	1.40	1.00
2:O:15:VAL:HG21	2:O:95:LEU:HD11	1.43	1.00
1:E:50:THR:HG22	1:E:52:ASP:H	1.26	1.00
1:B:212:ALA:HB3	1:B:324:ILE:HB	1.66	1.00
1:F:283:ARG:NH1	1:F:363:LYS:HD2	3.61	0.99
1:G:352:LEU:HD13	1:G:364:LEU:HB2	4.88	0.99
1:K:189:VAL:HG12	1:K:190:GLU:H	1.26	0.99
1:C:168:VAL:HG12	1:C:172:GLY:HA3	1.43	0.99
2:P:12:GLY:O	2:P:13:ASP:HB3	3.74	0.99
1:I:50:THR:HG22	1:I:52:ASP:H	1.23	0.99
1:L:50:THR:HG22	1:L:52:ASP:H	1.27	0.99
1:M:189:VAL:CG1	1:M:190:GLU:H	1.72	0.98
1:E:168:VAL:HG12	1:E:172:GLY:HA3	1.50	0.98
1:I:283:ARG:HH21	1:I:367:ARG:HD3	1.92	0.98
1:F:7:VAL:HG21	1:F:66:LEU:HD11	1.53	0.98
1:H:283:ARG:NH2	1:H:367:ARG:HD3	2.06	0.98
1:E:7:VAL:HG21	1:E:66:LEU:HD11	1.64	0.98
2:T:96:LEU:HA	2:U:14:ARG:HH11	1.29	0.98
1:M:323:ARG:NH2	1:M:392:LYS:HE2	1.79	0.97
2:O:48:VAL:CG1	2:O:62:LEU:HD12	2.03	0.97
1:E:352:LEU:HD13	1:E:364:LEU:HB2	1.44	0.97
1:J:50:THR:HG22	1:J:52:ASP:H	1.33	0.97
1:M:182:LEU:CD1	1:N:363:LYS:HE2	1.94	0.97
1:F:50:THR:HG22	1:F:52:ASP:H	1.44	0.97
1:A:50:THR:HG22	1:A:51:LYS:H	1.33	0.97
1:H:283:ARG:HH21	1:H:367:ARG:HD3	1.82	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:THR:HG22	1:H:52:ASP:H	1.37	0.96
1:M:178:GLU:N	1:M:321:ARG:NH1	2.13	0.96
1:M:50:THR:HG22	1:M:52:ASP:H	1.29	0.96
1:G:325:THR:HG22	1:G:326:LYS:H	1.75	0.96
1:G:50:THR:HG22	1:G:52:ASP:H	1.36	0.96
1:M:189:VAL:HG12	1:M:190:GLU:N	1.80	0.96
1:C:50:THR:HG22	1:C:51:LYS:H	1.31	0.96
1:E:50:THR:HG22	1:E:51:LYS:H	1.31	0.95
1:B:50:THR:HG22	1:B:52:ASP:H	1.34	0.95
1:H:189:VAL:HG11	1:H:333:GLY:HA2	1.47	0.95
2:R:54:LEU:HD21	2:S:55:GLU:HA	3.34	0.95
1:K:283:ARG:HH11	1:K:363:LYS:HE3	1.71	0.95
2:O:54:LEU:HD13	2:P:55:GLU:O	4.00	0.95
1:C:7:VAL:HG21	1:C:66:LEU:HD11	1.45	0.95
1:N:526:LYS:HG3	1:N:527:PRO:HD2	1.48	0.95
1:D:50:THR:HG22	1:D:52:ASP:H	1.26	0.95
1:D:212:ALA:HB3	1:D:324:ILE:HB	1.53	0.95
2:R:70:VAL:HG11	2:R:95:LEU:HD22	1.46	0.95
2:Q:70:VAL:HG11	2:Q:95:LEU:HD22	1.46	0.95
1:M:176:VAL:O	1:M:323:ARG:NH1	1.98	0.95
1:B:50:THR:HG22	1:B:51:LYS:H	1.38	0.95
1:L:410:ILE:HD12	1:L:496:VAL:HG11	1.47	0.95
1:J:189:VAL:HG12	1:J:190:GLU:H	1.31	0.95
1:E:298:THR:HG23	1:E:304:LEU:HD23	1.48	0.94
1:C:237:GLU:HB3	2:Q:28:GLY:HA3	1.48	0.94
1:D:50:THR:HG22	1:D:51:LYS:H	1.29	0.94
2:P:15:VAL:HG21	2:P:95:LEU:HD11	1.46	0.94
1:C:240:ALA:HA	1:C:270:LEU:HD13	1.98	0.94
1:F:50:THR:HG22	1:F:51:LYS:H	1.31	0.94
1:H:189:VAL:HG12	1:H:190:GLU:H	1.30	0.94
2:O:52:ARG:NH2	2:P:53:VAL:HB	1.81	0.94
1:G:235:ILE:HG12	1:G:311:ALA:HB3	2.19	0.93
2:P:70:VAL:HG11	2:P:95:LEU:HD22	1.50	0.93
1:K:50:THR:HG22	1:K:52:ASP:H	1.39	0.93
1:D:283:ARG:NH1	1:D:363:LYS:HD3	4.67	0.93
1:A:50:THR:HG22	1:A:52:ASP:H	1.29	0.93
2:Q:13:ASP:HA	2:Q:62:LEU:HD21	2.12	0.93
2:T:69:ILE:HB	2:T:99:LEU:HB2	2.38	0.93
1:J:168:VAL:HG12	1:J:172:GLY:HA3	1.51	0.93
2:S:12:GLY:O	2:S:13:ASP:HB3	1.65	0.93
1:L:270:LEU:HD22	1:L:272:VAL:HG13	1.60	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168:VAL:HG12	1:M:172:GLY:HA3	1.51	0.92
1:K:168:VAL:HG12	1:K:172:GLY:HA3	1.51	0.92
1:N:189:VAL:HG12	1:N:190:GLU:H	1.34	0.92
1:G:235:ILE:HD11	1:G:311:ALA:HB3	1.49	0.92
2:S:48:VAL:HG12	2:S:62:LEU:HD13	2.04	0.92
1:J:283:ARG:HG3	1:J:363:LYS:HZ2	3.21	0.92
1:C:325:THR:HG22	1:C:326:LYS:H	1.54	0.92
1:B:283:ARG:NH1	1:B:363:LYS:HD2	4.06	0.91
1:E:325:THR:HG22	1:E:326:LYS:H	1.32	0.91
1:M:498:PRO:HB2	1:M:501:VAL:HG23	1.62	0.91
1:C:251:GLU:HG3	1:C:284:ARG:HH12	1.33	0.91
1:E:227:SER:HB3	1:E:254:GLU:HG3	1.50	0.91
2:T:70:VAL:HG11	2:T:95:LEU:HD22	1.52	0.91
1:D:235:ILE:HG21	1:D:311:ALA:HB3	4.20	0.91
1:F:212:ALA:HB3	1:F:324:ILE:HB	1.52	0.91
1:L:234:PRO:HG3	1:L:309:GLU:HA	1.62	0.91
1:D:173:ILE:CD1	1:D:365:GLN:HG3	2.01	0.91
1:L:180:LYS:O	1:M:281:GLY:HA3	2.02	0.91
1:K:498:PRO:HB2	1:K:501:VAL:HG23	1.52	0.91
1:N:46:SER:HB2	1:N:47:PRO:HD2	1.53	0.90
1:C:312:THR:HB	1:C:315:MET:HG2	2.86	0.90
2:T:81:GLU:HA	2:T:85:GLU:O	2.02	0.90
1:A:212:ALA:HB3	1:A:324:ILE:HB	1.67	0.90
1:I:50:THR:HG22	1:I:51:LYS:H	1.36	0.90
1:N:526:LYS:CG	1:N:527:PRO:HD2	2.01	0.90
1:M:384:THR:HA	1:N:280:PHE:CE1	2.06	0.90
1:L:168:VAL:HG12	1:L:172:GLY:HA3	1.54	0.90
1:L:498:PRO:HB2	1:L:501:VAL:HG23	1.58	0.90
2:T:20:ILE:HD12	2:T:42:LYS:HG3	4.88	0.90
1:J:40:LEU:HD23	1:J:59:GLU:HG3	1.53	0.90
1:J:270:LEU:HD22	1:J:272:VAL:HG13	1.65	0.90
1:H:498:PRO:HB2	1:H:501:VAL:HG23	1.55	0.90
1:H:46:SER:HB2	1:H:47:PRO:HD2	1.60	0.90
1:J:46:SER:HB2	1:J:47:PRO:HD2	1.54	0.90
1:I:168:VAL:HG12	1:I:172:GLY:HA3	1.53	0.90
1:B:219:ILE:HD13	1:B:295:THR:HG21	2.82	0.89
1:M:182:LEU:CD1	1:N:363:LYS:CE	2.51	0.89
1:J:50:THR:HG22	1:J:51:LYS:H	1.44	0.89
1:L:180:LYS:CB	1:M:281:GLY:HA2	2.03	0.89
1:D:173:ILE:HD11	1:D:365:GLN:CG	2.02	0.89
2:P:79:GLU:O	2:P:80:ILE:HG13	2.13	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:100:GLN:HB3	2:Q:7:VAL:CB	3.54	0.89
1:H:168:VAL:HG12	1:H:172:GLY:HA3	1.53	0.89
1:A:350:LYS:CB	1:B:208:GLU:HG2	7.96	0.89
1:C:227:SER:HB3	1:C:254:GLU:HG3	2.20	0.89
1:M:410:ILE:HD12	1:M:496:VAL:HG11	1.52	0.89
2:U:74:LYS:HD2	2:U:75:TYR:N	4.79	0.89
2:P:41:GLN:OE1	2:Q:80:ILE:HG12	1.73	0.89
1:K:270:LEU:HD22	1:K:272:VAL:HG13	1.61	0.89
1:N:50:THR:HG22	1:N:51:LYS:H	1.38	0.88
1:G:283:ARG:HH12	1:G:363:LYS:HD2	3.76	0.88
2:S:5:LYS:HG2	2:S:6:THR:H	5.08	0.88
1:H:410:ILE:HD12	1:H:496:VAL:HG11	1.56	0.88
2:O:54:LEU:HD21	2:P:57:GLY:N	1.87	0.88
1:M:136:ILE:HB	1:M:410:ILE:CG1	2.02	0.88
2:Q:20:ILE:HG13	2:Q:43:GLY:HA2	1.78	0.88
1:A:7:VAL:HG21	1:A:66:LEU:HD11	1.56	0.88
2:R:13:ASP:HA	2:R:62:LEU:HD21	3.55	0.88
1:B:511:SER:O	1:B:515:LEU:HD23	1.73	0.88
1:N:283:ARG:NH1	1:N:363:LYS:HE3	1.89	0.88
1:L:182:LEU:CD1	1:M:363:LYS:NZ	2.38	0.88
1:I:385:GLU:HB2	1:J:280:PHE:CD2	2.07	0.88
1:K:179:SER:HB2	1:K:379:ARG:HB3	1.58	0.88
1:L:189:VAL:HG12	1:L:190:GLU:N	1.89	0.88
1:K:235:ILE:CD1	1:K:311:ALA:HB3	2.02	0.88
2:P:13:ASP:HA	2:P:62:LEU:HD21	2.10	0.88
1:A:235:ILE:HG21	1:A:311:ALA:HB3	3.61	0.88
1:M:372:ALA:C	1:M:374:GLY:H	1.75	0.88
1:J:189:VAL:HG11	1:J:333:GLY:HA2	1.56	0.88
1:N:410:ILE:HD12	1:N:496:VAL:HG11	1.56	0.88
1:K:234:PRO:HG3	1:K:309:GLU:HA	1.56	0.88
2:S:13:ASP:HA	2:S:62:LEU:HD21	1.55	0.88
2:S:70:VAL:HG11	2:S:95:LEU:HD22	1.56	0.88
1:L:40:LEU:HD23	1:L:59:GLU:HG3	1.54	0.88
1:E:209:THR:HG22	1:E:211:GLU:HG3	1.55	0.88
2:U:15:VAL:HG11	2:U:95:LEU:HD22	4.58	0.88
1:A:246:LEU:HB3	1:A:272:VAL:HG12	1.56	0.88
1:L:46:SER:HB2	1:L:47:PRO:HD2	1.61	0.88
1:I:345:ILE:O	1:I:348:ILE:HG22	1.74	0.88
1:M:182:LEU:HD11	1:N:363:LYS:HE2	1.51	0.87
1:L:179:SER:HB2	1:L:379:ARG:HB3	1.57	0.87
2:U:48:VAL:CG1	2:U:62:LEU:HD12	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:VAL:HG12	1:N:172:GLY:HA3	1.54	0.87
1:I:267:ARG:O	1:J:256:GLU:HG3	2.13	0.87
1:J:283:ARG:HH11	1:J:363:LYS:HE3	1.59	0.87
2:Q:32:LEU:HG	2:Q:33:PRO:HD2	1.56	0.87
1:B:7:VAL:HG21	1:B:66:LEU:HD11	1.56	0.87
1:K:46:SER:HB2	1:K:47:PRO:HD2	1.55	0.87
1:G:235:ILE:HD11	1:G:311:ALA:CB	2.04	0.87
1:L:59:GLU:O	1:M:4:LYS:HG3	1.79	0.87
1:K:50:THR:HG22	1:K:51:LYS:H	1.40	0.87
1:N:149:THR:HG23	1:N:155:PRO:HA	1.60	0.87
1:J:498:PRO:HB2	1:J:501:VAL:HG23	1.57	0.87
2:Q:81:GLU:CG	2:Q:85:GLU:H	2.43	0.87
1:L:50:THR:HG22	1:L:51:LYS:H	1.39	0.87
1:N:345:ILE:O	1:N:348:ILE:HG22	1.80	0.87
1:I:234:PRO:HG3	1:I:309:GLU:HA	1.58	0.87
1:E:246:LEU:HB3	1:E:272:VAL:HG12	1.66	0.86
1:G:7:VAL:HG21	1:G:66:LEU:HD11	1.60	0.86
1:J:345:ILE:O	1:J:348:ILE:HG22	1.75	0.86
2:P:100:GLN:CB	2:Q:7:VAL:HB	3.51	0.86
2:T:17:VAL:HG22	2:T:45:VAL:HA	3.01	0.86
1:A:237:GLU:CB	2:O:28:GLY:HA3	2.78	0.86
2:O:13:ASP:HB2	2:O:62:LEU:HD21	1.76	0.86
1:F:246:LEU:HB3	1:F:272:VAL:HG12	1.77	0.86
1:N:498:PRO:HB2	1:N:501:VAL:HG23	1.57	0.86
1:M:179:SER:HB2	1:M:379:ARG:HB3	1.57	0.86
1:D:173:ILE:HD12	1:D:366:GLU:HA	2.33	0.86
1:M:323:ARG:NH1	1:M:392:LYS:NZ	2.24	0.86
2:Q:55:GLU:HG3	2:R:55:GLU:HG2	1.58	0.86
1:M:182:LEU:CD1	1:N:363:LYS:NZ	2.39	0.86
1:J:283:ARG:HH21	1:J:367:ARG:HD3	1.92	0.86
1:C:50:THR:HG22	1:C:52:ASP:H	1.40	0.86
1:I:270:LEU:HD22	1:I:272:VAL:HG13	1.55	0.86
1:L:149:THR:HG23	1:L:155:PRO:HA	1.58	0.86
1:N:179:SER:HB2	1:N:379:ARG:HB3	1.60	0.86
2:Q:70:VAL:HG12	2:Q:71:VAL:N	2.43	0.86
2:U:70:VAL:HG11	2:U:95:LEU:HD22	1.56	0.85
2:O:54:LEU:CD2	2:P:57:GLY:H	1.87	0.85
1:I:46:SER:HB2	1:I:47:PRO:HD2	1.57	0.85
1:E:224:LYS:HE2	1:E:301:SER:HA	1.56	0.85
1:G:201:PRO:O	1:G:204:VAL:HG22	3.61	0.85
1:K:40:LEU:HD23	1:K:59:GLU:HG3	1.61	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:SER:HB2	1:H:379:ARG:HB3	1.58	0.85
1:E:235:ILE:HG12	1:E:311:ALA:HB3	1.58	0.85
1:E:289:LYS:HE3	1:F:202:TYR:OH	4.26	0.85
1:I:410:ILE:HD12	1:I:496:VAL:HG11	1.56	0.85
1:C:214:LEU:HB3	1:C:245:PRO:HB3	2.71	0.85
1:M:323:ARG:HH22	1:M:392:LYS:HE2	1.40	0.85
2:Q:81:GLU:HG3	2:Q:85:GLU:N	2.48	0.85
1:N:235:ILE:CD1	1:N:311:ALA:HB3	2.06	0.85
1:H:270:LEU:HD22	1:H:272:VAL:HG13	1.60	0.85
1:I:498:PRO:HB2	1:I:501:VAL:HG23	1.58	0.85
1:J:149:THR:HG23	1:J:155:PRO:HA	1.58	0.85
2:Q:54:LEU:HD12	2:Q:55:GLU:H	3.99	0.85
1:H:50:THR:HG22	1:H:51:LYS:H	1.48	0.85
1:M:270:LEU:HD22	1:M:272:VAL:HG13	1.56	0.85
1:E:229:VAL:HG11	2:S:32:LEU:HD22	3.23	0.84
1:K:149:THR:HG23	1:K:155:PRO:HA	1.59	0.84
1:M:50:THR:HG22	1:M:51:LYS:H	1.40	0.84
1:M:40:LEU:HD23	1:M:59:GLU:HG3	1.60	0.84
1:J:332:VAL:HG22	1:J:375:VAL:HG11	1.85	0.84
1:L:235:ILE:CD1	1:L:311:ALA:HB3	2.08	0.84
2:U:13:ASP:HB2	2:U:62:LEU:HD21	1.58	0.84
1:M:235:ILE:CD1	1:M:311:ALA:HB3	2.14	0.84
1:A:218:PHE:HB3	1:A:316:LEU:HD13	1.82	0.84
1:J:77:VAL:HG13	1:J:80:LYS:HE2	1.69	0.84
1:N:40:LEU:HD23	1:N:59:GLU:HG3	1.58	0.84
1:G:117:LYS:HG3	1:G:514:ALA:HB1	1.60	0.84
1:M:182:LEU:HD11	1:N:363:LYS:HZ1	1.37	0.84
1:L:85:ALA:HB1	1:L:501:VAL:HG22	1.60	0.84
1:H:40:LEU:HD23	1:H:59:GLU:HG3	1.59	0.84
1:G:224:LYS:HE2	1:G:301:SER:HA	6.04	0.84
1:G:209:THR:HG22	1:G:211:GLU:HG3	4.94	0.84
1:J:283:ARG:NH2	1:J:367:ARG:HD3	2.12	0.84
1:M:46:SER:HB2	1:M:47:PRO:HD2	1.59	0.84
1:L:268:GLY:O	1:M:256:GLU:HG3	1.78	0.84
1:I:179:SER:HB2	1:I:379:ARG:HB3	1.60	0.84
1:I:235:ILE:CD1	1:I:311:ALA:HB3	2.08	0.84
1:M:323:ARG:CZ	1:M:392:LYS:HE2	2.07	0.84
1:A:117:LYS:HG3	1:A:514:ALA:HB1	1.63	0.84
1:L:345:ILE:O	1:L:348:ILE:HG22	1.99	0.84
1:N:270:LEU:HD22	1:N:272:VAL:HG13	1.63	0.84
1:I:189:VAL:HG11	1:I:333:GLY:HA2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:235:ILE:CD1	1:J:311:ALA:HB3	2.08	0.84
2:P:21:GLU:O	2:P:22:GLU:O	1.95	0.83
2:R:79:GLU:O	2:R:80:ILE:HG13	2.06	0.83
1:K:345:ILE:O	1:K:348:ILE:HG22	1.79	0.83
1:E:229:VAL:CG2	2:S:36:ALA:HB2	3.47	0.83
2:Q:90:LEU:H	2:Q:90:LEU:HD23	3.75	0.83
1:N:74:LEU:HD21	1:N:93:THR:HG23	1.60	0.83
1:B:325:THR:HG22	1:B:326:LYS:H	1.48	0.83
2:S:96:LEU:CD2	2:T:14:ARG:HH12	6.59	0.83
1:M:323:ARG:CZ	1:M:392:LYS:HZ1	1.89	0.83
1:J:179:SER:HB2	1:J:379:ARG:HB3	1.61	0.83
1:A:511:SER:O	1:A:515:LEU:HD23	1.95	0.83
1:M:149:THR:HG23	1:M:155:PRO:HA	1.60	0.83
1:H:149:THR:HG23	1:H:155:PRO:HA	1.62	0.83
1:D:246:LEU:HB3	1:D:272:VAL:HG12	1.64	0.83
1:J:410:ILE:HD12	1:J:496:VAL:HG11	1.61	0.83
1:B:117:LYS:HG3	1:B:514:ALA:HB1	1.59	0.83
1:K:410:ILE:HD12	1:K:496:VAL:HG11	1.61	0.83
1:B:228:ASN:HD22	1:B:231:GLU:HG3	1.43	0.83
1:M:345:ILE:O	1:M:348:ILE:HG22	1.86	0.83
1:G:240:ALA:HA	1:G:270:LEU:HD13	1.83	0.82
1:C:117:LYS:HG3	1:C:514:ALA:HB1	1.61	0.82
1:B:246:LEU:HB3	1:B:272:VAL:HG12	1.71	0.82
1:C:218:PHE:CE1	1:C:244:LYS:HD2	5.13	0.82
1:M:178:GLU:O	1:M:321:ARG:NH2	2.12	0.82
1:F:259:ALA:O	1:F:263:VAL:HG23	1.90	0.82
1:L:180:LYS:HB2	1:M:281:GLY:HA2	1.60	0.82
1:L:37:ASN:OD1	1:M:515:LEU:HD12	1.78	0.82
2:R:100:GLN:HB3	2:S:7:VAL:HB	3.07	0.82
1:E:144:ILE:HD12	1:E:165:MET:HG2	1.62	0.82
1:F:117:LYS:HG3	1:F:514:ALA:HB1	1.63	0.82
1:M:234:PRO:HG3	1:M:309:GLU:HA	1.59	0.82
1:J:234:PRO:HG3	1:J:309:GLU:HA	1.61	0.82
1:C:312:THR:HG22	1:C:314:SER:H	2.36	0.82
1:A:66:LEU:HD22	1:A:522:VAL:HG11	1.61	0.82
1:I:149:THR:HG23	1:I:155:PRO:HA	1.59	0.82
1:A:283:ARG:NH1	1:A:363:LYS:HD2	3.64	0.82
1:M:247:LEU:HD22	1:M:322:VAL:HG11	1.62	0.82
1:H:74:LEU:HD21	1:H:93:THR:HG23	1.62	0.82
1:G:348:ILE:HD11	1:G:367:ARG:NE	2.81	0.82
1:M:136:ILE:N	1:M:410:ILE:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LEU:HB2	2:Q:30:ILE:HD11	1.61	0.81
2:Q:79:GLU:O	2:Q:80:ILE:HG13	1.78	0.81
1:C:237:GLU:CB	2:Q:28:GLY:HA3	2.09	0.81
1:I:74:LEU:HD21	1:I:93:THR:HG23	1.67	0.81
1:I:283:ARG:NH1	1:I:363:LYS:HE3	2.00	0.81
1:H:235:ILE:CD1	1:H:311:ALA:HB3	2.10	0.81
1:J:283:ARG:NH1	1:J:363:LYS:HB2	3.70	0.81
1:M:178:GLU:N	1:M:321:ARG:HH12	1.76	0.81
1:E:283:ARG:NH1	1:E:363:LYS:HD2	2.93	0.81
1:M:85:ALA:HB1	1:M:501:VAL:HG22	1.62	0.81
1:B:66:LEU:HD22	1:B:522:VAL:HG11	1.67	0.81
1:G:227:SER:HB3	1:G:254:GLU:HG3	2.30	0.81
1:I:40:LEU:HD23	1:I:59:GLU:HG3	1.60	0.81
2:T:11:LEU:O	2:T:14:ARG:HD2	3.32	0.81
1:E:66:LEU:HD22	1:E:522:VAL:HG11	1.62	0.81
1:C:224:LYS:HE2	1:C:301:SER:HA	6.04	0.81
1:M:59:GLU:O	1:N:4:LYS:HG3	2.26	0.81
1:H:345:ILE:O	1:H:348:ILE:HG22	1.80	0.81
1:E:117:LYS:HG3	1:E:514:ALA:HB1	1.62	0.81
1:B:283:ARG:HH12	1:B:363:LYS:HD2	4.28	0.81
1:G:246:LEU:HB3	1:G:272:VAL:HG12	1.61	0.81
1:N:234:PRO:HG3	1:N:309:GLU:HA	1.61	0.81
1:I:116:LEU:O	1:I:120:ILE:HG13	1.81	0.81
2:Q:44:LYS:HA	2:Q:68:ASP:O	2.05	0.81
1:K:295:THR:HG22	1:K:318:ARG:N	2.00	0.81
2:P:41:GLN:HG2	2:P:74:LYS:HB3	1.63	0.80
1:L:180:LYS:HB3	1:M:281:GLY:HA2	1.75	0.80
2:Q:92:GLU:HA	2:Q:95:LEU:CD1	2.98	0.80
1:E:301:SER:HB2	1:E:304:LEU:HB3	6.28	0.80
1:D:259:ALA:O	1:D:263:VAL:HG23	1.82	0.80
1:J:295:THR:HG22	1:J:318:ARG:N	2.00	0.80
1:F:66:LEU:HD22	1:F:522:VAL:HG11	1.63	0.80
2:Q:19:ARG:HD3	2:Q:40:PRO:HG2	2.77	0.80
2:Q:100:GLN:HB3	2:R:7:VAL:HB	1.63	0.80
1:D:117:LYS:HG3	1:D:514:ALA:HB1	1.63	0.80
1:D:50:THR:HG22	1:D:52:ASP:N	1.96	0.80
1:F:307:LYS:HE3	2:U:34:ASP:O	1.81	0.80
2:T:98:VAL:O	2:U:8:ILE:HG23	4.39	0.80
1:C:66:LEU:HD22	1:C:522:VAL:HG11	1.72	0.80
1:B:201:PRO:O	1:B:204:VAL:HG23	1.81	0.80
1:L:295:THR:HG22	1:L:318:ARG:N	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:73:ALA:O	2:Q:74:LYS:HG2	4.19	0.80
2:T:96:LEU:HD23	2:U:14:ARG:NH1	1.97	0.80
1:B:251:GLU:HG3	1:B:284:ARG:NH1	1.97	0.80
1:L:77:VAL:HG13	1:L:80:LYS:HE2	1.63	0.80
1:G:66:LEU:HD22	1:G:522:VAL:HG11	1.63	0.79
1:H:85:ALA:HB1	1:H:501:VAL:HG22	1.64	0.79
1:I:246:LEU:HB3	1:I:272:VAL:HG12	1.74	0.79
1:N:37:ASN:HD21	1:N:51:LYS:HE2	1.55	0.79
1:B:289:LYS:HE2	1:C:202:TYR:OH	1.82	0.79
1:C:150:ILE:CD1	1:C:495:ILE:HA	2.07	0.79
1:M:385:GLU:HB2	1:N:280:PHE:CE2	2.27	0.79
2:S:56:ASN:HB3	2:S:58:GLN:HG3	5.78	0.79
1:C:223:GLU:O	1:C:251:GLU:HB2	2.55	0.79
1:F:511:SER:O	1:F:515:LEU:HD23	1.86	0.79
1:M:178:GLU:C	1:M:321:ARG:HH12	1.85	0.79
1:E:98:ALA:HB2	1:E:449:GLU:HG3	1.68	0.79
1:E:149:THR:HG23	1:E:155:PRO:HA	1.65	0.79
1:D:511:SER:O	1:D:515:LEU:HD23	1.83	0.79
1:H:234:PRO:HG3	1:H:309:GLU:HA	1.66	0.79
1:A:307:LYS:HE3	2:P:34:ASP:O	1.83	0.79
2:O:45:VAL:HG21	2:O:64:VAL:HG11	1.74	0.79
1:E:50:THR:HG22	1:E:52:ASP:N	1.98	0.79
2:R:97:ALA:HA	2:S:11:LEU:CD1	2.23	0.79
1:M:362:GLU:O	1:M:365:GLN:HB2	1.92	0.79
2:P:15:VAL:HG12	2:P:45:VAL:HG13	1.63	0.78
1:L:189:VAL:CG1	1:L:190:GLU:H	1.94	0.78
1:J:74:LEU:HD21	1:J:93:THR:HG23	1.65	0.78
2:U:20:ILE:H	2:U:43:GLY:HA2	3.62	0.78
1:H:295:THR:HG22	1:H:318:ARG:N	2.01	0.78
2:S:53:VAL:HG22	2:S:59:ARG:HG2	1.99	0.78
1:D:66:LEU:HD22	1:D:522:VAL:HG11	1.64	0.78
1:J:228:ASN:HD21	1:J:230:ARG:HB3	1.49	0.78
1:I:422:ILE:HG23	1:I:444:ARG:HG3	1.66	0.78
2:Q:70:VAL:CG1	2:Q:71:VAL:H	2.79	0.78
1:B:50:THR:HG22	1:B:52:ASP:N	2.06	0.78
1:N:295:THR:HG22	1:N:318:ARG:N	1.99	0.78
1:A:285:LYS:HD3	1:B:202:TYR:OH	8.38	0.78
1:H:7:VAL:HG21	1:H:66:LEU:HD11	1.77	0.78
1:E:69:ILE:HD11	1:F:41:GLU:HB2	1.66	0.78
1:C:218:PHE:HB3	1:C:316:LEU:HD13	1.65	0.78
1:H:77:VAL:HG13	1:H:80:LYS:HE2	1.69	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:295:THR:HG22	1:I:318:ARG:N	2.01	0.78
1:M:229:VAL:HG23	1:M:256:GLU:HB3	1.65	0.78
1:E:511:SER:O	1:E:515:LEU:HD23	1.92	0.78
1:J:116:LEU:O	1:J:120:ILE:HG13	1.84	0.78
1:C:149:THR:HG23	1:C:155:PRO:HA	1.76	0.78
1:D:150:ILE:HD11	1:D:495:ILE:CA	2.10	0.78
2:O:15:VAL:HG12	2:O:45:VAL:HG13	1.66	0.78
1:H:283:ARG:HH21	1:H:367:ARG:CD	2.24	0.78
1:A:173:ILE:HD12	1:A:366:GLU:HA	1.65	0.78
1:N:362:GLU:O	1:N:365:GLN:HB2	1.83	0.78
1:F:352:LEU:HD21	1:F:364:LEU:HB2	2.01	0.78
1:C:511:SER:O	1:C:515:LEU:HD23	1.87	0.78
1:D:173:ILE:HD12	1:D:369:ALA:HB2	1.65	0.77
2:O:48:VAL:HG23	2:O:66:GLU:HG3	3.05	0.77
1:I:332:VAL:HG22	1:I:375:VAL:HG11	1.66	0.77
1:E:267:ARG:HD3	2:S:31:VAL:HG21	1.65	0.77
2:T:52:ARG:HH21	2:U:53:VAL:HB	1.49	0.77
1:K:362:GLU:O	1:K:365:GLN:HB2	1.84	0.77
1:I:228:ASN:HD21	1:I:230:ARG:HB3	1.49	0.77
1:H:267:ARG:O	1:I:256:GLU:HG3	2.08	0.77
2:R:97:ALA:HA	2:S:11:LEU:HD13	1.95	0.77
1:E:351:GLU:HG3	1:F:326:LYS:NZ	2.00	0.77
1:G:218:PHE:CE1	1:G:244:LYS:HD2	4.98	0.77
1:K:249:ILE:O	1:K:249:ILE:HG22	1.84	0.77
1:K:116:LEU:O	1:K:120:ILE:HG13	1.95	0.77
1:B:229:VAL:HG21	2:P:36:ALA:CB	2.14	0.77
1:G:312:THR:HG22	1:G:314:SER:H	2.38	0.77
1:L:116:LEU:O	1:L:120:ILE:HG13	1.98	0.77
1:L:37:ASN:HD21	1:L:51:LYS:HE2	1.50	0.77
1:H:277:ALA:HB3	1:H:284:ARG:HD2	1.71	0.77
1:C:248:ILE:HD12	1:C:261:LEU:HD21	2.51	0.77
1:N:464:VAL:HG12	1:N:468:GLN:HE21	1.48	0.77
1:F:50:THR:HG22	1:F:51:LYS:N	2.03	0.77
1:N:85:ALA:HB1	1:N:501:VAL:HG22	1.67	0.77
1:L:7:VAL:HG21	1:L:66:LEU:HD11	1.79	0.77
2:T:19:ARG:CD	2:T:40:PRO:HG2	3.36	0.77
2:Q:71:VAL:HG12	2:Q:96:LEU:HD12	2.40	0.77
1:I:85:ALA:HB1	1:I:501:VAL:HG22	1.67	0.77
1:M:307:LYS:HE3	1:M:310:ASN:ND2	2.19	0.77
1:N:235:ILE:HD11	1:N:311:ALA:CB	2.15	0.77
1:C:201:PRO:O	1:C:204:VAL:HG23	2.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:228:ASN:HD21	1:H:230:ARG:HB3	1.58	0.77
1:C:498:PRO:O	1:C:501:VAL:HG22	1.90	0.77
1:B:230:ARG:NH2	2:P:38:GLU:OE2	2.17	0.76
1:A:116:LEU:O	1:A:120:ILE:HG13	1.97	0.76
2:T:54:LEU:HD11	2:U:55:GLU:HA	1.66	0.76
1:E:247:LEU:HD22	1:E:322:VAL:HG11	1.66	0.76
1:G:301:SER:HB2	1:G:304:LEU:HB3	1.65	0.76
1:J:219:ILE:HD12	1:J:295:THR:HG23	1.72	0.76
1:N:283:ARG:HH11	1:N:363:LYS:HE3	1.50	0.76
1:M:283:ARG:NH1	1:M:363:LYS:HE3	2.00	0.76
1:K:189:VAL:HG11	1:K:333:GLY:HA2	1.66	0.76
2:R:56:ASN:HB2	2:R:58:GLN:HG3	1.99	0.76
1:D:50:THR:HG22	1:D:51:LYS:N	2.01	0.76
1:H:219:ILE:HD12	1:H:295:THR:HG23	1.67	0.76
1:K:422:ILE:HG23	1:K:444:ARG:HG3	1.67	0.76
1:L:54:VAL:HG22	1:L:89:THR:HG21	1.67	0.76
1:C:178:GLU:HG3	1:C:388:LEU:HD21	1.66	0.76
1:M:74:LEU:HD21	1:M:93:THR:HG23	1.67	0.76
1:L:235:ILE:HD11	1:L:311:ALA:CB	2.18	0.76
1:D:136:ILE:HD11	1:D:477:ARG:NH2	2.09	0.76
1:H:114:LEU:HD12	1:N:459:GLY:HA3	1.77	0.76
1:N:84:VAL:HG12	1:N:500:LYS:HE2	1.68	0.76
2:Q:16:VAL:HG12	2:Q:46:ILE:HB	2.59	0.76
1:N:189:VAL:CG1	1:N:333:GLY:HA2	2.15	0.76
1:M:295:THR:HG22	1:M:318:ARG:N	2.05	0.76
1:K:194:PHE:CD1	1:K:278:PRO:HB3	2.27	0.76
1:L:229:VAL:HG23	1:L:256:GLU:HB3	1.73	0.76
1:C:283:ARG:NH1	1:C:363:LYS:HB3	2.51	0.76
1:A:50:THR:HG22	1:A:52:ASP:N	2.01	0.76
1:M:332:VAL:HG13	1:M:377:VAL:HG21	1.68	0.76
2:Q:10:PRO:HG3	2:Q:47:ALA:O	2.06	0.76
1:E:235:ILE:HD12	1:E:311:ALA:CB	4.02	0.76
1:N:189:VAL:HG12	1:N:190:GLU:N	2.00	0.76
1:L:59:GLU:O	1:M:4:LYS:HE3	1.86	0.76
1:H:116:LEU:O	1:H:120:ILE:HG13	2.01	0.76
1:G:98:ALA:HB2	1:G:449:GLU:HG3	1.74	0.76
2:S:10:PRO:HB2	2:S:14:ARG:O	1.86	0.75
1:A:235:ILE:CG2	1:A:311:ALA:HB3	3.92	0.75
1:D:69:ILE:HD11	1:E:41:GLU:HB2	1.68	0.75
1:L:283:ARG:NH2	1:L:367:ARG:HD3	2.17	0.75
1:M:228:ASN:HD21	1:M:230:ARG:HB3	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:VAL:CG1	1:H:333:GLY:HA2	2.16	0.75
1:A:120:ILE:O	1:A:124:VAL:HG23	1.93	0.75
1:K:385:GLU:HB2	1:L:280:PHE:CE2	2.41	0.75
1:D:116:LEU:O	1:D:120:ILE:HG13	1.87	0.75
1:A:41:GLU:HB2	1:G:69:ILE:HD11	1.90	0.75
2:S:96:LEU:HA	2:T:14:ARG:CZ	3.79	0.75
2:T:96:LEU:HA	2:U:14:ARG:NH1	2.01	0.75
1:M:323:ARG:CZ	1:M:392:LYS:CE	2.64	0.75
1:N:219:ILE:HD12	1:N:295:THR:HG23	1.69	0.75
1:M:464:VAL:HG12	1:M:468:GLN:HE21	1.52	0.75
1:K:300:ILE:HG21	1:K:308:LEU:HD23	1.69	0.75
1:J:362:GLU:O	1:J:365:GLN:HB2	1.86	0.75
2:P:48:VAL:CG1	2:P:62:LEU:HD12	2.15	0.75
1:A:233:LEU:O	1:A:237:GLU:HG3	1.90	0.75
1:N:526:LYS:CD	1:N:527:PRO:HD2	2.15	0.75
1:M:361:ARG:O	1:M:365:GLN:HG2	1.89	0.75
1:B:301:SER:HB2	1:B:304:LEU:HB3	1.68	0.75
1:D:120:ILE:O	1:D:124:VAL:HG23	1.86	0.75
1:F:301:SER:HB2	1:F:304:LEU:HB3	1.67	0.75
1:K:74:LEU:HD21	1:K:93:THR:HG23	1.67	0.75
1:H:422:ILE:HG23	1:H:444:ARG:HG3	1.73	0.75
1:I:290:ASP:OD1	1:I:371:LEU:HD11	1.89	0.75
1:C:98:ALA:HB2	1:C:449:GLU:HG3	1.66	0.75
2:S:41:GLN:OE1	2:T:80:ILE:HG13	2.53	0.75
1:G:50:THR:HG22	1:G:51:LYS:N	2.01	0.75
2:R:96:LEU:O	2:S:14:ARG:HD3	2.14	0.75
1:B:498:PRO:O	1:B:501:VAL:HG22	1.87	0.75
2:Q:96:LEU:HD23	2:R:14:ARG:HH21	1.49	0.75
1:G:477:ARG:HH11	1:G:477:ARG:HG3	1.76	0.75
1:G:150:ILE:CD1	1:G:495:ILE:HA	2.15	0.75
1:D:98:ALA:HB2	1:D:449:GLU:HG3	1.73	0.75
1:G:511:SER:O	1:G:515:LEU:HD23	1.88	0.75
1:J:85:ALA:HB1	1:J:501:VAL:HG22	1.71	0.75
1:E:50:THR:HG22	1:E:51:LYS:N	2.01	0.75
1:K:189:VAL:HG12	1:K:190:GLU:N	2.01	0.75
1:H:37:ASN:HD21	1:H:51:LYS:HE2	1.51	0.75
1:B:50:THR:HG22	1:B:51:LYS:N	2.07	0.75
1:D:218:PHE:HB3	1:D:316:LEU:HD13	1.72	0.75
1:L:283:ARG:NH1	1:L:363:LYS:HE3	2.01	0.75
1:J:194:PHE:CD1	1:J:278:PRO:HB3	2.21	0.75
1:D:235:ILE:HD11	1:D:311:ALA:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:81:GLU:HA	2:U:86:GLU:HA	2.03	0.74
1:K:189:VAL:CG1	1:K:333:GLY:HA2	2.37	0.74
1:E:349:LYS:HG3	1:E:368:LEU:HD11	1.69	0.74
1:H:189:VAL:HG12	1:H:190:GLU:N	2.05	0.74
1:A:259:ALA:O	1:A:263:VAL:HG23	1.88	0.74
1:M:503:ARG:HH11	1:M:507:GLN:HE22	1.39	0.74
1:F:522:VAL:HG22	1:G:39:VAL:HB	1.79	0.74
1:J:229:VAL:HG23	1:J:256:GLU:HB3	1.69	0.74
1:E:498:PRO:O	1:E:501:VAL:HG22	1.86	0.74
1:F:98:ALA:HB2	1:F:449:GLU:HG3	1.67	0.74
1:K:7:VAL:HG21	1:K:66:LEU:HD11	1.74	0.74
1:G:178:GLU:HG3	1:G:388:LEU:HD21	1.69	0.74
1:B:150:ILE:CD1	1:B:495:ILE:HA	2.16	0.74
1:C:214:LEU:HB3	1:C:245:PRO:CB	3.04	0.74
1:F:50:THR:HG22	1:F:52:ASP:N	2.12	0.74
1:A:50:THR:HG22	1:A:51:LYS:N	2.07	0.74
1:K:37:ASN:HD21	1:K:51:LYS:HE2	1.52	0.74
1:I:229:VAL:HG23	1:I:256:GLU:HB3	1.68	0.74
1:K:212:ALA:HB3	1:K:324:ILE:HB	1.77	0.74
1:N:503:ARG:HH11	1:N:507:GLN:HE22	1.38	0.74
1:M:459:GLY:HA3	1:N:114:LEU:HD12	1.69	0.74
2:Q:96:LEU:HA	2:R:14:ARG:HE	1.53	0.74
2:Q:51:GLY:HA3	2:Q:60:VAL:O	2.69	0.74
1:I:37:ASN:HD21	1:I:51:LYS:HE2	1.59	0.74
2:R:96:LEU:HA	2:S:14:ARG:HE	1.67	0.74
1:H:246:LEU:HB3	1:H:272:VAL:HG12	1.69	0.74
1:A:72:GLN:HE22	1:A:75:LYS:NZ	2.00	0.74
1:N:229:VAL:HG23	1:N:256:GLU:HB3	1.74	0.74
1:G:229:VAL:HG21	2:U:36:ALA:HB2	1.69	0.74
1:H:229:VAL:HG23	1:H:256:GLU:HB3	1.75	0.74
1:L:180:LYS:C	1:M:281:GLY:HA3	2.11	0.74
1:K:85:ALA:HB1	1:K:501:VAL:HG22	1.70	0.74
1:K:77:VAL:HG13	1:K:80:LYS:HE2	1.69	0.74
1:B:178:GLU:HG3	1:B:388:LEU:HD21	1.69	0.74
1:M:323:ARG:NH2	1:M:392:LYS:CE	2.50	0.74
1:M:37:ASN:HD21	1:M:51:LYS:HE2	1.52	0.74
1:H:459:GLY:HA3	1:I:114:LEU:HD12	1.85	0.74
2:S:8:ILE:HG21	2:S:16:VAL:HG21	1.73	0.74
1:J:37:ASN:HD21	1:J:51:LYS:HE2	1.53	0.74
1:F:233:LEU:O	1:F:237:GLU:HG3	1.88	0.74
1:I:503:ARG:HH11	1:I:507:GLN:HE22	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:189:VAL:HG12	1:J:190:GLU:N	2.03	0.74
1:D:307:LYS:HE3	2:S:34:ASP:HB3	4.22	0.74
1:B:259:ALA:O	1:B:263:VAL:HG23	1.87	0.74
1:J:217:ALA:CB	1:J:245:PRO:HG2	2.26	0.74
1:H:232:LEU:HD22	1:H:236:LEU:HD22	1.79	0.74
1:M:136:ILE:O	1:M:410:ILE:N	2.19	0.73
2:P:96:LEU:HB3	2:Q:89:ILE:HG21	1.70	0.73
2:S:100:GLN:OE1	2:T:9:LYS:HE2	1.88	0.73
1:M:235:ILE:HD11	1:M:311:ALA:CB	2.23	0.73
1:J:283:ARG:HH21	1:J:367:ARG:HH11	3.33	0.73
1:M:77:VAL:HG13	1:M:80:LYS:HE2	1.68	0.73
1:I:77:VAL:HG13	1:I:80:LYS:HE2	1.71	0.73
1:M:323:ARG:NH1	1:M:392:LYS:HE2	2.03	0.73
1:M:246:LEU:HB3	1:M:272:VAL:HG12	1.68	0.73
1:E:120:ILE:O	1:E:124:VAL:HG23	1.99	0.73
1:I:7:VAL:HG21	1:I:66:LEU:HD11	1.69	0.73
1:G:120:ILE:O	1:G:124:VAL:HG23	1.88	0.73
2:T:32:LEU:HG	2:T:33:PRO:HD2	1.67	0.73
1:D:235:ILE:HD11	1:D:311:ALA:CB	2.18	0.73
1:M:7:VAL:HG21	1:M:66:LEU:HD11	1.70	0.73
1:H:194:PHE:CD1	1:H:278:PRO:HB3	2.32	0.73
1:B:149:THR:HG23	1:B:155:PRO:HA	1.69	0.73
1:C:136:ILE:HD11	1:C:477:ARG:NH2	2.03	0.73
1:N:50:THR:HG22	1:N:52:ASP:N	2.08	0.73
1:B:218:PHE:HB3	1:B:316:LEU:HD13	1.76	0.73
1:G:312:THR:HB	1:G:315:MET:HG2	2.57	0.73
1:K:219:ILE:HD12	1:K:295:THR:HG23	1.74	0.73
1:C:236:LEU:CB	2:Q:30:ILE:HD11	2.18	0.73
1:A:149:THR:HG23	1:A:155:PRO:HA	1.71	0.73
1:M:277:ALA:HB3	1:M:284:ARG:HD2	1.72	0.73
1:A:34:ARG:HH12	1:G:118:ARG:HH22	1.36	0.73
1:N:277:ALA:HB3	1:N:284:ARG:HD2	1.73	0.73
2:Q:18:LYS:HG2	2:Q:87:TYR:CD2	2.24	0.73
1:E:218:PHE:CE1	1:E:244:LYS:HD2	2.24	0.73
1:B:136:ILE:HD11	1:B:477:ARG:HH21	1.68	0.73
1:I:219:ILE:HD12	1:I:295:THR:HG23	1.68	0.73
1:A:98:ALA:HB2	1:A:449:GLU:HG3	1.73	0.73
1:B:98:ALA:HB2	1:B:449:GLU:HG3	1.70	0.73
1:E:150:ILE:CD1	1:E:495:ILE:HA	2.12	0.73
1:B:284:ARG:O	1:B:288:LEU:HG	2.14	0.73
2:S:13:ASP:OD1	2:S:13:ASP:O	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:422:ILE:HG23	1:M:444:ARG:HG3	1.78	0.73
1:C:120:ILE:O	1:C:124:VAL:HG23	1.89	0.73
2:O:14:ARG:HE	2:U:96:LEU:HA	1.85	0.73
1:G:50:THR:HG22	1:G:52:ASP:N	2.07	0.73
1:D:235:ILE:CG2	1:D:311:ALA:HB3	4.28	0.73
1:K:410:ILE:HB	1:K:496:VAL:CG1	2.19	0.73
1:L:194:PHE:CD1	1:L:278:PRO:HB3	2.23	0.73
1:J:300:ILE:HG21	1:J:308:LEU:HD23	1.76	0.73
1:A:237:GLU:CG	2:O:28:GLY:HA3	2.45	0.73
1:M:212:ALA:HB3	1:M:324:ILE:HB	1.71	0.73
1:N:410:ILE:HB	1:N:496:VAL:CG1	2.24	0.73
1:N:246:LEU:HB3	1:N:272:VAL:HG12	1.69	0.73
1:H:290:ASP:OD1	1:H:371:LEU:HD11	1.89	0.73
2:P:25:LYS:HG2	2:P:31:VAL:HG22	1.92	0.73
1:I:300:ILE:HG21	1:I:308:LEU:HD23	1.74	0.73
2:T:61:PRO:HG3	2:U:59:ARG:NH2	7.43	0.72
1:H:300:ILE:HG21	1:H:308:LEU:HD23	1.69	0.72
2:Q:80:ILE:HG12	2:Q:81:GLU:H	4.25	0.72
1:K:246:LEU:HB3	1:K:272:VAL:HG12	1.69	0.72
1:L:422:ILE:HG23	1:L:444:ARG:HG3	1.71	0.72
1:J:422:ILE:HG23	1:J:444:ARG:HG3	1.70	0.72
2:S:96:LEU:HD22	2:T:14:ARG:HH12	6.69	0.72
2:P:13:ASP:HB2	2:P:62:LEU:HD21	1.71	0.72
1:C:217:ALA:HB2	1:C:245:PRO:HB2	1.69	0.72
1:A:422:ILE:HG23	1:A:444:ARG:HG3	1.71	0.72
1:B:230:ARG:HH21	2:P:38:GLU:CD	1.92	0.72
1:M:189:VAL:HG11	1:M:333:GLY:HA2	1.69	0.72
1:F:235:ILE:CD1	1:F:311:ALA:HB3	2.25	0.72
2:S:14:ARG:HH11	2:S:14:ARG:HG3	1.55	0.72
2:S:5:LYS:CG	2:S:6:THR:H	4.67	0.72
1:I:74:LEU:HD12	1:I:512:ILE:HD12	1.82	0.72
1:N:361:ARG:O	1:N:365:GLN:HG2	1.92	0.72
1:N:384:THR:HG22	1:N:386:THR:H	1.54	0.72
1:H:362:GLU:O	1:H:365:GLN:HB2	1.90	0.72
1:E:229:VAL:HG21	2:S:36:ALA:CB	2.97	0.72
1:M:283:ARG:HH11	1:M:363:LYS:HE3	1.59	0.72
1:M:410:ILE:HB	1:M:496:VAL:CG1	2.19	0.72
1:H:217:ALA:CB	1:H:245:PRO:HG2	2.19	0.72
2:P:10:PRO:HB2	2:P:14:ARG:O	2.17	0.72
1:G:218:PHE:HB3	1:G:316:LEU:HD13	1.72	0.72
1:L:297:GLY:HA3	1:L:317:GLY:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:503:ARG:HH11	1:L:507:GLN:HE22	1.37	0.72
1:H:235:ILE:HD11	1:H:311:ALA:CB	2.23	0.72
2:O:81:GLU:HG3	2:O:85:GLU:H	1.55	0.72
1:H:283:ARG:HH12	1:H:364:LEU:CD1	2.33	0.72
1:G:235:ILE:CD1	1:G:311:ALA:HB3	2.20	0.72
1:N:7:VAL:HG21	1:N:66:LEU:HD11	1.70	0.72
1:I:464:VAL:HG12	1:I:468:GLN:HE21	1.55	0.72
1:J:277:ALA:HB3	1:J:284:ARG:HD2	1.74	0.72
1:C:212:ALA:HB3	1:C:324:ILE:HB	1.72	0.72
1:N:422:ILE:HG23	1:N:444:ARG:HG3	1.72	0.72
1:L:246:LEU:HB3	1:L:272:VAL:HG12	1.73	0.72
1:C:225:LYS:HG3	1:C:252:ASP:HB3	4.04	0.72
1:A:359:TYR:CE2	1:A:363:LYS:HE2	3.69	0.72
1:D:498:PRO:O	1:D:501:VAL:HG22	1.91	0.72
1:E:178:GLU:HG3	1:E:388:LEU:HD21	1.72	0.72
1:F:150:ILE:CD1	1:F:495:ILE:HA	2.11	0.72
1:C:233:LEU:O	1:C:237:GLU:HG3	1.90	0.72
1:C:235:ILE:HD11	1:C:311:ALA:HB3	1.70	0.72
1:M:219:ILE:HD12	1:M:295:THR:HG23	1.71	0.72
1:G:230:ARG:NH2	2:U:38:GLU:OE2	2.22	0.72
1:J:361:ARG:O	1:J:365:GLN:HG2	1.90	0.72
1:N:277:ALA:CB	1:N:284:ARG:HD2	2.26	0.72
2:S:73:ALA:HB1	2:S:75:TYR:CE2	2.32	0.72
1:F:498:PRO:O	1:F:501:VAL:HG22	1.89	0.72
1:L:384:THR:HG22	1:L:386:THR:H	1.55	0.72
1:E:269:THR:HG21	2:S:30:ILE:HA	1.72	0.72
1:M:224:LYS:HG2	1:M:225:LYS:N	2.05	0.72
1:K:229:VAL:HG23	1:K:256:GLU:HB3	1.75	0.72
1:N:224:LYS:HG2	1:N:225:LYS:N	2.05	0.72
1:L:228:ASN:HD21	1:L:230:ARG:HB3	1.54	0.72
1:L:74:LEU:HD21	1:L:93:THR:HG23	1.70	0.72
2:Q:70:VAL:HG11	2:Q:95:LEU:CD2	2.36	0.71
2:R:8:ILE:HG21	2:R:16:VAL:HG21	1.72	0.71
1:L:243:GLY:CA	1:M:228:ASN:CB	2.63	0.71
1:C:50:THR:HG22	1:C:51:LYS:N	2.03	0.71
1:J:74:LEU:HD12	1:J:512:ILE:CD1	2.20	0.71
1:J:267:ARG:O	1:K:256:GLU:HG3	1.95	0.71
1:F:217:ALA:HB2	1:F:245:PRO:HB2	1.72	0.71
1:L:247:LEU:HD22	1:L:322:VAL:HG11	1.80	0.71
1:K:54:VAL:HG22	1:K:89:THR:HG21	1.84	0.71
1:K:235:ILE:HD11	1:K:311:ALA:CB	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:20:ILE:HG13	2:P:43:GLY:HA2	1.71	0.71
1:M:206:ASN:ND2	1:M:389:LYS:HE2	2.05	0.71
1:H:503:ARG:HH11	1:H:507:GLN:HE22	1.37	0.71
2:T:10:PRO:HG3	2:T:47:ALA:O	1.89	0.71
2:O:54:LEU:HG	2:P:55:GLU:O	1.90	0.71
1:B:136:ILE:O	1:B:410:ILE:HG22	2.56	0.71
1:G:149:THR:HG23	1:G:155:PRO:HA	1.70	0.71
1:E:450:PRO:O	1:E:454:ILE:HG13	2.11	0.71
1:J:384:THR:HG22	1:J:386:THR:H	1.54	0.71
1:L:464:VAL:HG12	1:L:468:GLN:HE21	1.55	0.71
1:F:19:GLY:HA3	1:F:67:GLU:O	1.91	0.71
1:D:136:ILE:HD11	1:D:477:ARG:HH21	1.63	0.71
1:F:136:ILE:HD11	1:F:477:ARG:HH21	1.56	0.71
1:B:69:ILE:HD11	1:C:41:GLU:HB2	1.83	0.71
1:M:300:ILE:HG21	1:M:308:LEU:HD23	1.71	0.71
1:I:362:GLU:O	1:I:365:GLN:HB2	1.96	0.71
1:I:361:ARG:O	1:I:365:GLN:HG2	1.90	0.71
2:T:48:VAL:CG1	2:T:62:LEU:HD12	4.50	0.71
1:L:84:VAL:HG12	1:L:500:LYS:HE2	1.77	0.71
1:H:84:VAL:HG12	1:H:500:LYS:HE2	1.70	0.71
1:J:224:LYS:HG2	1:J:225:LYS:N	2.09	0.71
1:F:149:THR:HG23	1:F:155:PRO:HA	1.77	0.71
1:N:283:ARG:NH2	1:N:367:ARG:HD3	2.04	0.71
1:F:136:ILE:O	1:F:410:ILE:HG22	2.36	0.71
1:J:283:ARG:HG3	1:J:363:LYS:HZ1	3.43	0.71
1:L:410:ILE:HB	1:L:496:VAL:CG1	2.21	0.71
1:L:74:LEU:HD12	1:L:512:ILE:HD12	1.72	0.71
1:G:498:PRO:O	1:G:501:VAL:HG22	1.92	0.71
1:H:224:LYS:HG2	1:H:225:LYS:N	2.08	0.71
1:J:232:LEU:HD22	1:J:236:LEU:HD22	1.71	0.71
1:B:229:VAL:HG12	1:B:233:LEU:HD11	1.85	0.71
1:I:189:VAL:HG12	1:I:190:GLU:N	2.07	0.71
1:J:189:VAL:CG1	1:J:333:GLY:HA2	2.28	0.71
1:L:283:ARG:HH12	1:L:364:LEU:HD12	1.56	0.71
2:T:100:GLN:HE22	2:U:9:LYS:NZ	6.51	0.71
1:L:182:LEU:HD11	1:M:363:LYS:HZ1	1.92	0.71
1:L:50:THR:HG22	1:L:52:ASP:N	2.05	0.71
1:E:222:VAL:HG22	1:E:300:ILE:HD12	2.45	0.71
1:K:224:LYS:HG2	1:K:225:LYS:N	2.06	0.71
2:R:73:ALA:HB1	2:R:75:TYR:CE2	2.36	0.71
1:K:283:ARG:NH1	1:K:363:LYS:HE3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HB2	2:O:30:ILE:HD11	1.90	0.71
1:I:50:THR:HG22	1:I:52:ASP:N	2.04	0.71
1:F:118:ARG:HH22	1:G:34:ARG:HH12	1.41	0.71
1:N:228:ASN:HD21	1:N:230:ARG:HB3	1.56	0.71
1:D:382:ALA:HB3	1:D:388:LEU:HB2	1.75	0.71
1:I:224:LYS:HG2	1:I:225:LYS:N	2.07	0.71
1:A:350:LYS:O	1:B:208:GLU:HA	7.27	0.71
2:O:79:GLU:HG2	2:O:88:VAL:HG22	1.95	0.71
2:R:56:ASN:ND2	2:S:55:GLU:O	3.30	0.71
1:M:116:LEU:O	1:M:120:ILE:HG13	1.91	0.71
1:J:7:VAL:HG21	1:J:66:LEU:HD11	1.73	0.71
1:L:277:ALA:HB3	1:L:284:ARG:HD2	1.77	0.71
2:P:13:ASP:OD2	2:P:92:GLU:HB2	1.91	0.70
1:L:217:ALA:CB	1:L:245:PRO:HG2	2.20	0.70
1:B:219:ILE:HD13	1:B:295:THR:CG2	3.16	0.70
1:D:50:THR:CG2	1:D:52:ASP:H	2.03	0.70
1:F:229:VAL:HG12	1:F:233:LEU:HD11	1.71	0.70
1:A:366:GLU:O	1:A:370:LYS:HG3	1.98	0.70
1:K:247:LEU:HD22	1:K:322:VAL:HG11	1.92	0.70
1:K:464:VAL:HG12	1:K:468:GLN:HE21	1.56	0.70
2:R:20:ILE:HG13	2:R:43:GLY:HA2	1.74	0.70
1:L:224:LYS:HG2	1:L:225:LYS:N	2.06	0.70
1:D:118:ARG:HH22	1:E:34:ARG:HH12	1.50	0.70
2:O:97:ALA:HA	2:P:11:LEU:HG	1.86	0.70
2:Q:26:THR:HG22	2:Q:32:LEU:HD21	5.62	0.70
1:M:323:ARG:NH1	1:M:392:LYS:CE	2.53	0.70
1:J:410:ILE:HB	1:J:496:VAL:CG1	2.23	0.70
1:K:228:ASN:HD21	1:K:230:ARG:HB3	1.55	0.70
1:A:69:ILE:HD11	1:B:41:GLU:HB2	1.72	0.70
1:K:84:VAL:HG12	1:K:500:LYS:HE2	1.72	0.70
2:T:100:GLN:OXT	2:U:6:THR:HG23	2.75	0.70
2:P:48:VAL:HG12	2:P:62:LEU:HD13	2.52	0.70
1:C:246:LEU:HB3	1:C:272:VAL:HG12	1.72	0.70
1:J:246:LEU:HB3	1:J:272:VAL:HG12	1.73	0.70
1:K:361:ARG:O	1:K:365:GLN:HG2	1.91	0.70
2:Q:89:ILE:HG22	2:Q:89:ILE:O	2.20	0.70
1:C:247:LEU:HD22	1:C:322:VAL:HG11	2.34	0.70
1:F:85:ALA:HB1	1:F:501:VAL:HG12	1.84	0.70
1:H:384:THR:HG22	1:H:386:THR:H	1.55	0.70
1:N:290:ASP:OD1	1:N:371:LEU:HD11	1.93	0.70
1:A:368:LEU:O	1:A:368:LEU:HD12	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:384:THR:HG22	1:M:386:THR:H	1.58	0.70
1:K:277:ALA:HB3	1:K:284:ARG:HD2	1.76	0.70
1:J:290:ASP:OD1	1:J:371:LEU:HD11	1.91	0.70
1:D:284:ARG:O	1:D:288:LEU:HG	1.91	0.70
2:Q:58:GLN:HG2	2:Q:59:ARG:N	4.93	0.70
1:A:118:ARG:HH22	1:B:34:ARG:HH12	1.59	0.70
1:L:526:LYS:CD	1:L:527:PRO:HD2	2.21	0.70
1:G:284:ARG:O	1:G:288:LEU:HG	1.91	0.70
1:N:194:PHE:CD1	1:N:278:PRO:HB3	2.26	0.70
2:Q:8:ILE:HD12	2:Q:8:ILE:N	2.07	0.70
1:D:366:GLU:O	1:D:370:LYS:HG3	1.91	0.70
1:N:116:LEU:O	1:N:120:ILE:HG13	1.92	0.70
1:M:84:VAL:HG12	1:M:500:LYS:HE2	1.78	0.70
1:J:464:VAL:HG12	1:J:468:GLN:HE21	1.56	0.70
2:S:20:ILE:HG13	2:S:43:GLY:HA2	1.79	0.70
1:N:77:VAL:HG13	1:N:80:LYS:HE2	1.74	0.70
1:J:74:LEU:HD12	1:J:512:ILE:HD12	1.72	0.70
1:C:352:LEU:HD23	1:C:364:LEU:HD12	2.63	0.70
1:H:212:ALA:HB3	1:H:324:ILE:HB	1.75	0.70
1:L:361:ARG:O	1:L:365:GLN:HG2	1.98	0.70
1:A:526:LYS:HD3	1:A:529:LYS:CE	2.22	0.70
1:D:522:VAL:HG22	1:E:39:VAL:HB	1.74	0.70
1:B:422:ILE:HG23	1:B:444:ARG:HG3	1.77	0.70
1:D:234:PRO:O	1:D:238:GLN:HG3	1.91	0.70
1:D:23:VAL:HG22	1:D:60:VAL:HG11	1.72	0.70
1:B:352:LEU:HD21	1:B:364:LEU:HB2	1.73	0.70
1:M:283:ARG:NH2	1:M:367:ARG:HD3	2.08	0.69
1:C:224:LYS:H	1:C:224:LYS:HD2	4.45	0.69
1:D:94:VAL:HG12	1:D:449:GLU:HB3	1.74	0.69
1:I:277:ALA:HB3	1:I:284:ARG:HD2	1.74	0.69
1:G:373:GLY:O	1:G:375:VAL:N	2.25	0.69
1:J:283:ARG:HH11	1:J:363:LYS:CE	2.55	0.69
1:L:212:ALA:HB3	1:L:324:ILE:HB	1.81	0.69
1:I:84:VAL:HG12	1:I:500:LYS:HE2	1.74	0.69
1:C:422:ILE:HG23	1:C:444:ARG:HG3	1.79	0.69
1:C:348:ILE:HD12	1:C:367:ARG:NE	4.54	0.69
1:M:323:ARG:CZ	1:M:392:LYS:NZ	2.53	0.69
1:C:352:LEU:HD21	1:C:364:LEU:HB2	1.90	0.69
1:F:120:ILE:O	1:F:124:VAL:HG23	1.98	0.69
1:I:54:VAL:HG22	1:I:89:THR:HG21	1.74	0.69
1:L:277:ALA:CB	1:L:284:ARG:HD2	2.30	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:384:THR:HG22	1:I:386:THR:H	1.56	0.69
1:D:96:ALA:O	1:D:100:VAL:HG23	2.16	0.69
1:M:54:VAL:HG22	1:M:89:THR:HG21	1.73	0.69
1:J:249:ILE:O	1:J:249:ILE:HG22	2.01	0.69
1:B:136:ILE:HD11	1:B:477:ARG:NH2	2.16	0.69
1:I:217:ALA:CB	1:I:245:PRO:HG2	2.23	0.69
2:Q:19:ARG:HB3	2:Q:40:PRO:HB2	3.79	0.69
1:E:515:LEU:HD12	1:F:49:ILE:HG21	1.73	0.69
1:E:116:LEU:O	1:E:120:ILE:HG13	2.04	0.69
1:J:54:VAL:HG22	1:J:89:THR:HG21	1.81	0.69
1:F:234:PRO:O	1:F:238:GLN:HG3	1.92	0.69
2:S:48:VAL:CG1	2:S:62:LEU:HD13	2.93	0.69
1:I:235:ILE:HD11	1:I:311:ALA:CB	2.17	0.69
1:D:50:THR:HG21	1:D:52:ASP:HB3	1.75	0.69
1:H:410:ILE:HB	1:H:496:VAL:CG1	2.23	0.69
1:L:219:ILE:HD12	1:L:295:THR:HG23	1.74	0.69
1:C:136:ILE:HD11	1:C:477:ARG:HH21	1.57	0.69
1:J:264:ASN:HB3	1:J:269:THR:HB	1.73	0.69
1:A:233:LEU:HD23	2:O:30:ILE:HG21	2.22	0.69
2:S:10:PRO:HG3	2:S:47:ALA:O	1.93	0.69
1:L:234:PRO:CG	1:L:309:GLU:HA	2.27	0.69
1:L:269:THR:HA	1:M:256:GLU:CG	2.23	0.69
1:A:363:LYS:C	1:A:365:GLN:H	2.23	0.69
1:H:277:ALA:CB	1:H:284:ARG:HD2	2.25	0.69
1:N:212:ALA:HB3	1:N:324:ILE:HB	1.78	0.69
1:A:178:GLU:HG3	1:A:388:LEU:HD21	1.83	0.69
2:U:77:GLY:HA3	2:U:90:LEU:HD23	1.75	0.69
1:H:264:ASN:HB3	1:H:269:THR:HB	1.78	0.69
1:D:149:THR:HG23	1:D:155:PRO:HA	1.73	0.69
1:E:229:VAL:HG11	2:S:32:LEU:CD2	3.68	0.69
2:R:13:ASP:HB2	2:R:62:LEU:HD11	1.75	0.69
2:R:81:GLU:HG3	2:R:85:GLU:H	1.58	0.69
1:C:298:THR:HG23	1:C:304:LEU:CD1	7.70	0.69
1:I:410:ILE:HB	1:I:496:VAL:CG1	2.23	0.69
1:H:283:ARG:NH1	1:H:363:LYS:HE3	2.07	0.69
1:D:222:VAL:HG22	1:D:300:ILE:HD12	1.94	0.69
1:G:224:LYS:HB3	1:G:302:GLU:OE1	1.92	0.69
1:A:498:PRO:O	1:A:501:VAL:HG22	1.93	0.69
1:L:360:ALA:O	1:L:363:LYS:HG3	2.57	0.69
1:M:277:ALA:CB	1:M:284:ARG:HD2	2.26	0.69
1:M:268:GLY:HA3	1:N:227:SER:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:GLY:C	1:E:284:ARG:HB3	2.70	0.68
1:M:307:LYS:HE3	1:M:310:ASN:HD21	1.75	0.68
1:F:345:ILE:HG23	1:F:368:LEU:HD13	1.77	0.68
1:E:235:ILE:O	1:E:239:VAL:HG23	1.92	0.68
1:M:366:GLU:O	1:M:370:LYS:HG3	1.94	0.68
1:I:325:THR:HG22	1:I:327:ASP:N	2.01	0.68
1:H:283:ARG:HG2	1:H:363:LYS:HZ2	1.89	0.68
1:J:50:THR:HG22	1:J:52:ASP:N	2.12	0.68
1:N:526:LYS:HG3	1:N:527:PRO:CD	2.21	0.68
1:K:384:THR:HG22	1:K:386:THR:H	1.59	0.68
1:G:72:GLN:HE22	1:G:75:LYS:NZ	1.91	0.68
1:A:325:THR:HG22	1:A:326:LYS:H	1.65	0.68
1:C:307:LYS:HB3	1:C:310:ASN:HD22	1.71	0.68
1:L:290:ASP:OD1	1:L:371:LEU:HD11	1.93	0.68
1:G:259:ALA:O	1:G:263:VAL:HG23	1.94	0.68
1:B:118:ARG:HH22	1:C:34:ARG:HH12	1.48	0.68
1:E:527:PRO:O	1:E:528:GLU:HB2	1.93	0.68
2:O:9:LYS:HB2	2:U:98:VAL:O	2.14	0.68
1:F:136:ILE:HD11	1:F:477:ARG:NH2	2.12	0.68
1:H:283:ARG:HH11	1:H:363:LYS:HE3	1.58	0.68
1:K:408:GLU:OE2	1:K:500:LYS:HG3	2.55	0.68
1:D:352:LEU:HD21	1:D:364:LEU:HB2	1.76	0.68
1:C:118:ARG:HH22	1:D:34:ARG:HH12	1.38	0.68
1:G:212:ALA:HB3	1:G:324:ILE:HB	1.73	0.68
1:F:279:GLY:C	1:F:284:ARG:HB3	2.13	0.68
1:F:72:GLN:HE22	1:F:75:LYS:NZ	1.90	0.68
1:B:235:ILE:HD11	1:B:316:LEU:HD21	1.75	0.68
2:U:73:ALA:HB1	2:U:75:TYR:CE2	2.29	0.68
2:U:74:LYS:NZ	2:U:75:TYR:HB3	6.45	0.68
1:G:223:GLU:O	1:G:251:GLU:HB2	2.56	0.68
1:I:59:GLU:O	1:J:4:LYS:HG3	1.92	0.68
1:D:279:GLY:C	1:D:284:ARG:HB3	2.14	0.68
1:C:450:PRO:O	1:C:454:ILE:HG13	1.94	0.68
1:G:189:VAL:CG1	1:G:190:GLU:N	2.56	0.68
1:H:464:VAL:HG12	1:H:468:GLN:HE21	1.58	0.68
2:O:14:ARG:HH11	2:O:14:ARG:HG3	1.57	0.68
2:O:10:PRO:HB2	2:O:14:ARG:O	2.24	0.68
1:A:150:ILE:CD1	1:A:495:ILE:HA	2.19	0.68
1:B:246:LEU:HB3	1:B:272:VAL:CG1	2.43	0.68
1:C:326:LYS:HD3	1:C:326:LYS:O	4.53	0.68
1:E:325:THR:HG22	1:E:326:LYS:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:VAL:HG12	1:M:224:LYS:H	1.58	0.68
1:I:352:LEU:HD23	1:I:364:LEU:HD22	5.53	0.68
1:E:136:ILE:HD11	1:E:477:ARG:HH21	1.99	0.68
2:P:12:GLY:O	2:P:13:ASP:CB	3.84	0.68
2:P:13:ASP:OD1	2:P:92:GLU:HB3	5.11	0.68
1:H:283:ARG:HH12	1:H:364:LEU:HD12	1.64	0.68
1:A:202:TYR:OH	1:G:289:LYS:HE2	1.94	0.68
1:N:247:LEU:HD22	1:N:322:VAL:HG11	1.78	0.68
1:I:366:GLU:O	1:I:370:LYS:HG3	1.94	0.68
1:F:263:VAL:O	1:F:267:ARG:HB2	2.15	0.68
2:R:98:VAL:HG23	2:S:11:LEU:HD11	2.25	0.68
1:G:258:LEU:HA	1:G:261:LEU:HD12	2.28	0.68
2:U:32:LEU:HD12	2:U:36:ALA:HB1	5.18	0.68
1:C:72:GLN:HE22	1:C:75:LYS:NZ	1.90	0.68
1:C:96:ALA:O	1:C:100:VAL:HG23	1.92	0.68
1:E:307:LYS:HB3	1:E:310:ASN:HD22	1.58	0.68
2:R:80:ILE:HG22	2:R:81:GLU:N	2.17	0.68
1:A:150:ILE:HD11	1:A:495:ILE:CA	2.17	0.68
1:F:270:LEU:HG	1:F:272:VAL:HG13	1.76	0.68
1:B:522:VAL:HG22	1:C:39:VAL:HB	1.82	0.68
1:G:222:VAL:HA	1:G:300:ILE:HB	2.22	0.68
1:H:103:GLY:O	1:H:107:VAL:HG23	2.09	0.68
2:P:80:ILE:HG22	2:P:81:GLU:N	2.09	0.68
1:C:236:LEU:HB2	2:Q:30:ILE:CD1	2.23	0.68
1:E:50:THR:CG2	1:E:52:ASP:H	2.04	0.68
2:S:5:LYS:HG2	2:S:6:THR:N	4.73	0.68
1:A:263:VAL:O	1:A:267:ARG:HB2	3.07	0.68
1:H:222:VAL:HG12	1:H:224:LYS:H	1.64	0.68
1:B:373:GLY:O	1:B:375:VAL:N	2.27	0.68
1:F:69:ILE:HD11	1:G:41:GLU:HB2	1.75	0.68
2:O:20:ILE:HG13	2:O:43:GLY:HA2	1.76	0.67
1:H:222:VAL:HG12	1:H:223:GLU:N	2.12	0.67
1:E:422:ILE:HG23	1:E:444:ARG:HG3	1.80	0.67
1:E:264:ASN:OD1	2:S:30:ILE:HG23	1.94	0.67
2:T:99:LEU:O	2:T:100:GLN:HG3	5.15	0.67
2:U:10:PRO:HB2	2:U:14:ARG:O	1.95	0.67
1:K:232:LEU:HD22	1:K:236:LEU:HD22	1.76	0.67
1:N:300:ILE:HG21	1:N:308:LEU:HD23	1.75	0.67
1:K:503:ARG:HH11	1:K:507:GLN:HE22	1.42	0.67
1:E:256:GLU:OE1	2:S:36:ALA:HA	1.94	0.67
2:U:8:ILE:HD12	2:U:8:ILE:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:234:PRO:CG	1:I:309:GLU:HA	2.25	0.67
1:B:189:VAL:CG1	1:B:190:GLU:N	2.57	0.67
1:H:96:ALA:O	1:H:100:VAL:HG23	2.00	0.67
1:I:459:GLY:HA3	1:J:114:LEU:HD12	1.74	0.67
1:L:300:ILE:HG21	1:L:308:LEU:HD23	1.81	0.67
2:P:38:GLU:OE1	2:P:74:LYS:NZ	2.27	0.67
2:R:14:ARG:HH11	2:R:14:ARG:HG3	1.73	0.67
1:C:345:ILE:CG1	1:C:368:LEU:HD23	6.98	0.67
1:K:74:LEU:HD12	1:K:512:ILE:HD12	1.77	0.67
1:B:228:ASN:ND2	1:B:231:GLU:HG3	2.09	0.67
1:K:277:ALA:CB	1:K:284:ARG:HD2	2.28	0.67
1:G:94:VAL:HG12	1:G:449:GLU:HB3	1.82	0.67
1:H:361:ARG:O	1:H:365:GLN:HG2	2.01	0.67
2:S:80:ILE:HG22	2:S:81:GLU:N	2.09	0.67
1:G:422:ILE:HG23	1:G:444:ARG:HG3	1.75	0.67
1:A:301:SER:HB2	1:A:304:LEU:HB3	1.77	0.67
2:Q:15:VAL:HG12	2:Q:16:VAL:H	3.96	0.67
2:Q:79:GLU:C	2:Q:80:ILE:HG13	2.15	0.67
1:A:136:ILE:HD11	1:A:477:ARG:HH21	1.67	0.67
1:J:219:ILE:HD12	1:J:295:THR:CG2	2.26	0.67
1:J:277:ALA:CB	1:J:284:ARG:HD2	2.27	0.67
1:N:222:VAL:HG12	1:N:224:LYS:H	1.64	0.67
1:I:194:PHE:CD1	1:I:278:PRO:HB3	2.30	0.67
1:J:157:VAL:HG21	1:J:395:PHE:CE2	2.32	0.67
1:L:372:ALA:O	1:L:374:GLY:N	2.26	0.67
1:G:225:LYS:HG3	1:G:252:ASP:HB3	3.99	0.67
1:D:515:LEU:HD12	1:E:49:ILE:HG21	2.10	0.67
1:K:222:VAL:HG12	1:K:223:GLU:N	2.13	0.67
1:H:249:ILE:HG22	1:H:249:ILE:O	1.93	0.67
2:U:81:GLU:HG3	2:U:85:GLU:H	1.59	0.67
1:A:50:THR:CG2	1:A:52:ASP:H	2.07	0.67
1:D:325:THR:HG22	1:D:326:LYS:H	1.60	0.67
1:G:217:ALA:HB2	1:G:245:PRO:HB2	1.89	0.67
1:L:503:ARG:NH1	1:L:507:GLN:HE22	1.93	0.67
1:K:222:VAL:HG12	1:K:224:LYS:H	1.68	0.67
1:C:19:GLY:HA3	1:C:67:GLU:O	1.95	0.67
1:M:157:VAL:HG21	1:M:395:PHE:CE2	2.32	0.67
1:A:455:ALA:HB1	1:A:465:ILE:HD12	1.76	0.67
2:O:10:PRO:HG3	2:O:47:ALA:O	2.19	0.67
2:Q:55:GLU:CG	2:R:55:GLU:HG2	2.24	0.67
1:C:78:ALA:O	1:C:89:THR:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:CG2	1:B:52:ASP:H	2.11	0.67
1:L:180:LYS:O	1:M:281:GLY:CA	2.61	0.67
1:I:385:GLU:HB2	1:J:280:PHE:CE2	2.30	0.67
1:A:279:GLY:C	1:A:284:ARG:HB3	2.16	0.67
1:I:74:LEU:HD12	1:I:512:ILE:CD1	2.30	0.67
2:P:8:ILE:HD12	2:P:8:ILE:N	2.10	0.67
1:N:249:ILE:O	1:N:249:ILE:HG22	1.94	0.67
1:F:96:ALA:O	1:F:100:VAL:HG23	1.94	0.67
1:K:290:ASP:OD1	1:K:371:LEU:HD11	1.98	0.67
2:T:22:GLU:OE1	2:T:37:LYS:HB3	5.70	0.67
2:R:10:PRO:HG3	2:R:47:ALA:O	2.26	0.67
1:B:325:THR:HG22	1:B:326:LYS:N	2.11	0.67
2:U:51:GLY:HA2	2:U:62:LEU:HD21	3.35	0.67
1:B:240:ALA:HA	1:B:270:LEU:HD13	2.00	0.67
1:N:217:ALA:CB	1:N:245:PRO:HG2	2.24	0.67
1:E:351:GLU:HG3	1:F:326:LYS:HZ1	1.59	0.67
1:F:50:THR:CG2	1:F:52:ASP:H	2.18	0.67
1:C:50:THR:HG22	1:C:52:ASP:N	2.10	0.67
1:M:234:PRO:CG	1:M:309:GLU:HA	2.24	0.67
1:F:173:ILE:HD12	1:F:366:GLU:HA	2.02	0.67
1:B:235:ILE:HD12	1:B:311:ALA:CB	2.49	0.66
1:L:40:LEU:HD23	1:L:59:GLU:CG	2.25	0.66
1:H:31:LEU:HD13	1:H:90:THR:HG22	1.76	0.66
2:R:48:VAL:HG12	2:R:62:LEU:CD1	4.45	0.66
1:G:116:LEU:O	1:G:120:ILE:HG13	1.95	0.66
1:L:408:GLU:OE2	1:L:500:LYS:HG3	1.94	0.66
1:C:184:THR:HG23	1:C:380:VAL:HA	1.77	0.66
2:O:73:ALA:HB1	2:O:75:TYR:CE2	2.35	0.66
1:E:72:GLN:HE22	1:E:75:LYS:NZ	2.02	0.66
1:H:524:ALA:HA	1:N:41:GLU:HG2	1.77	0.66
2:T:98:VAL:C	2:U:8:ILE:HG23	5.22	0.66
2:U:53:VAL:HG22	2:U:59:ARG:HG2	1.77	0.66
1:H:234:PRO:CG	1:H:309:GLU:HA	2.32	0.66
1:B:85:ALA:HB1	1:B:501:VAL:HG12	1.78	0.66
1:E:96:ALA:O	1:E:100:VAL:HG23	2.19	0.66
1:N:157:VAL:HG21	1:N:395:PHE:CZ	2.30	0.66
2:O:54:LEU:CD2	2:P:57:GLY:N	2.53	0.66
1:E:290:ASP:HB3	1:E:371:LEU:HD21	1.77	0.66
1:K:234:PRO:CG	1:K:309:GLU:HA	2.23	0.66
1:H:74:LEU:HD12	1:H:512:ILE:CD1	2.29	0.66
1:H:54:VAL:HG22	1:H:89:THR:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:ILE:HD11	1:G:331:ILE:HD11	2.64	0.66
1:M:290:ASP:OD1	1:M:371:LEU:HD11	1.96	0.66
1:D:150:ILE:CD1	1:D:495:ILE:HA	2.14	0.66
1:J:40:LEU:HD23	1:J:59:GLU:CG	2.25	0.66
1:K:385:GLU:HB2	1:L:280:PHE:CD2	2.31	0.66
1:D:72:GLN:HE22	1:D:75:LYS:NZ	2.01	0.66
1:N:219:ILE:HD12	1:N:295:THR:CG2	2.25	0.66
1:F:455:ALA:HB1	1:F:465:ILE:HD12	1.81	0.66
1:I:219:ILE:HD12	1:I:295:THR:CG2	2.26	0.66
1:A:240:ALA:HA	1:A:270:LEU:HD13	1.96	0.66
2:T:20:ILE:HG13	2:T:43:GLY:HA2	1.76	0.66
2:S:96:LEU:HD23	2:T:14:ARG:HH12	5.70	0.66
1:C:277:ALA:HB1	1:C:284:ARG:HD2	2.87	0.66
1:M:323:ARG:NH1	1:M:392:LYS:HZ1	1.89	0.66
1:K:410:ILE:HB	1:K:496:VAL:HG11	1.78	0.66
1:E:94:VAL:CG1	1:E:449:GLU:HB3	2.25	0.66
1:D:233:LEU:O	1:D:237:GLU:HG3	2.17	0.66
1:A:19:GLY:HA3	1:A:67:GLU:O	2.00	0.66
1:J:212:ALA:HB3	1:J:324:ILE:HB	1.77	0.66
1:E:228:ASN:HD22	1:E:231:GLU:HG3	4.48	0.66
1:J:103:GLY:O	1:J:107:VAL:HG23	1.96	0.66
2:Q:17:VAL:HG12	2:Q:45:VAL:HA	4.97	0.66
2:U:45:VAL:HG21	2:U:64:VAL:HG11	1.77	0.66
1:E:50:THR:HG21	1:E:52:ASP:HB3	1.76	0.66
1:C:325:THR:HG22	1:C:326:LYS:N	2.15	0.66
1:A:246:LEU:HB3	1:A:272:VAL:CG1	2.25	0.66
1:D:94:VAL:CG1	1:D:449:GLU:HB3	2.25	0.66
1:G:382:ALA:HB3	1:G:388:LEU:HB2	1.77	0.66
1:L:372:ALA:C	1:L:374:GLY:H	2.00	0.66
1:E:217:ALA:HB2	1:E:245:PRO:HB2	1.78	0.65
1:G:325:THR:HG22	1:G:326:LYS:N	2.28	0.65
1:L:180:LYS:CB	1:M:281:GLY:CA	2.74	0.65
1:L:264:ASN:HB3	1:L:269:THR:HB	1.81	0.65
1:E:94:VAL:HG12	1:E:449:GLU:HB3	1.79	0.65
1:B:120:ILE:O	1:B:124:VAL:HG23	2.00	0.65
1:D:178:GLU:HG3	1:D:388:LEU:HD21	1.83	0.65
1:B:455:ALA:HB1	1:B:465:ILE:HD12	1.76	0.65
1:A:298:THR:HB	1:A:315:MET:HB2	1.85	0.65
1:B:23:VAL:HG22	1:B:60:VAL:HG11	1.78	0.65
1:J:459:GLY:HA3	1:K:114:LEU:HD12	1.76	0.65
2:Q:92:GLU:CA	2:Q:95:LEU:HD12	3.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:LYS:C	1:D:365:GLN:H	2.23	0.65
1:N:283:ARG:HD3	1:N:363:LYS:HE3	1.78	0.65
2:P:10:PRO:HG3	2:P:47:ALA:O	1.96	0.65
1:B:290:ASP:O	1:B:294:VAL:HG23	1.96	0.65
1:L:50:THR:HG22	1:L:51:LYS:N	2.12	0.65
1:M:383:ALA:O	1:N:280:PHE:CD1	2.50	0.65
1:C:259:ALA:O	1:C:263:VAL:HG23	1.99	0.65
1:F:94:VAL:CG1	1:F:449:GLU:HB3	2.25	0.65
1:F:116:LEU:O	1:F:120:ILE:HG13	2.03	0.65
1:K:264:ASN:HB3	1:K:269:THR:HB	1.82	0.65
1:E:199:ILE:HG13	1:E:274:ALA:O	1.96	0.65
2:O:8:ILE:HD12	2:O:8:ILE:N	2.10	0.65
1:J:50:THR:HG22	1:J:51:LYS:N	2.17	0.65
1:A:522:VAL:HG22	1:B:39:VAL:HB	1.78	0.65
1:K:232:LEU:HD21	1:K:236:LEU:HD13	1.75	0.65
1:F:94:VAL:HG12	1:F:449:GLU:HB3	1.79	0.65
2:P:73:ALA:HB1	2:P:75:TYR:CE2	2.31	0.65
1:N:283:ARG:HG2	1:N:363:LYS:HZ2	1.59	0.65
1:M:283:ARG:NH1	1:M:363:LYS:HG3	2.33	0.65
1:H:325:THR:HG22	1:H:327:ASP:N	2.00	0.65
2:R:53:VAL:HG22	2:R:59:ARG:HG2	1.78	0.65
1:G:94:VAL:CG1	1:G:449:GLU:HB3	2.28	0.65
2:S:52:ARG:NH2	2:T:53:VAL:HB	3.58	0.65
1:I:462:GLY:O	1:I:466:VAL:HG23	1.97	0.65
1:B:320:GLU:HB3	1:B:333:GLY:HA3	1.77	0.65
1:K:157:VAL:HG21	1:K:395:PHE:CE2	2.31	0.65
1:E:259:ALA:O	1:E:263:VAL:HG23	1.97	0.65
1:J:283:ARG:HH12	1:J:364:LEU:HD12	1.61	0.65
1:B:279:GLY:C	1:B:284:ARG:HB3	2.37	0.65
1:A:50:THR:HG21	1:A:52:ASP:HB3	1.81	0.65
1:K:40:LEU:HD23	1:K:59:GLU:CG	2.29	0.65
1:N:157:VAL:HG21	1:N:395:PHE:CE2	2.32	0.65
1:E:373:GLY:O	1:E:375:VAL:N	2.69	0.65
1:J:84:VAL:HG12	1:J:500:LYS:HE2	1.84	0.65
1:J:325:THR:HG22	1:J:327:ASP:N	1.98	0.65
2:Q:58:GLN:HG2	2:Q:59:ARG:H	4.89	0.65
1:L:366:GLU:O	1:L:370:LYS:HG3	1.97	0.65
1:A:94:VAL:CG1	1:A:449:GLU:HB3	2.26	0.65
1:J:340:ASP:O	1:J:343:ALA:HB3	2.05	0.65
1:D:19:GLY:HA3	1:D:67:GLU:O	2.01	0.65
1:K:96:ALA:O	1:K:100:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:GLU:OE1	2:S:35:THR:HG22	4.13	0.65
2:R:45:VAL:HG21	2:R:64:VAL:HG11	1.79	0.65
2:O:48:VAL:HG13	2:O:62:LEU:HD12	2.08	0.65
2:Q:52:ARG:HH11	2:Q:52:ARG:HG2	4.30	0.65
1:K:217:ALA:CB	1:K:245:PRO:HG2	2.25	0.65
1:D:50:THR:CG2	1:D:51:LYS:H	2.08	0.65
1:K:74:LEU:HD12	1:K:512:ILE:CD1	2.31	0.65
1:H:290:ASP:O	1:H:294:VAL:HG23	2.11	0.65
2:U:10:PRO:HG3	2:U:47:ALA:O	1.97	0.65
2:O:54:LEU:HD11	2:P:57:GLY:H	3.22	0.65
2:Q:58:GLN:CG	2:Q:59:ARG:H	4.87	0.65
1:G:50:THR:CG2	1:G:52:ASP:H	2.10	0.65
1:C:522:VAL:HG22	1:D:39:VAL:HB	1.94	0.65
1:D:54:VAL:HG22	1:D:89:THR:HG21	1.78	0.65
2:S:62:LEU:H	2:S:62:LEU:HD12	3.53	0.65
2:S:52:ARG:O	2:S:52:ARG:HG3	1.95	0.65
1:E:207:PRO:HG2	1:E:208:GLU:H	1.60	0.65
2:Q:91:SER:CB	2:Q:93:ARG:HH11	4.06	0.65
1:B:363:LYS:C	1:B:365:GLN:H	1.98	0.65
2:Q:33:PRO:C	2:Q:35:THR:H	2.15	0.65
1:M:177:GLU:HB3	1:M:321:ARG:NH1	2.12	0.65
1:J:187:LYS:NZ	1:J:379:ARG:HG3	2.12	0.65
1:A:307:LYS:HB2	1:A:310:ASN:HD22	1.97	0.65
1:C:263:VAL:O	1:C:267:ARG:HB2	1.96	0.65
1:L:290:ASP:N	1:L:344:ARG:HH12	1.95	0.65
1:M:249:ILE:HG22	1:M:249:ILE:O	1.97	0.65
1:L:340:ASP:O	1:L:343:ALA:HB3	1.96	0.65
1:G:96:ALA:O	1:G:100:VAL:HG23	1.97	0.65
1:B:224:LYS:HB3	1:B:302:GLU:OE1	1.98	0.65
1:N:232:LEU:HD23	1:N:232:LEU:O	1.97	0.65
1:M:194:PHE:CD1	1:M:278:PRO:HB3	2.32	0.65
1:J:503:ARG:HH11	1:J:507:GLN:HE22	1.46	0.65
1:B:450:PRO:O	1:B:454:ILE:HG13	2.15	0.65
2:T:79:GLU:C	2:T:80:ILE:HD12	2.49	0.65
1:G:136:ILE:HD11	1:G:477:ARG:HH21	1.61	0.65
1:F:218:PHE:HB3	1:F:316:LEU:HD13	1.80	0.65
1:M:217:ALA:CB	1:M:245:PRO:HG2	2.25	0.65
1:F:236:LEU:HB2	2:T:30:ILE:HD11	1.79	0.65
1:H:168:VAL:HG11	1:H:173:ILE:H	1.62	0.65
1:A:515:LEU:HD12	1:B:49:ILE:HG21	1.77	0.65
1:N:222:VAL:HG12	1:N:223:GLU:N	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:ALA:O	1:G:75:LYS:HD3	1.97	0.65
1:D:298:THR:HB	1:D:315:MET:HB2	1.87	0.65
1:L:157:VAL:HG21	1:L:395:PHE:CE2	2.32	0.65
2:T:49:GLY:O	2:T:62:LEU:HD11	1.96	0.64
2:T:77:GLY:HA3	2:T:90:LEU:HD23	1.79	0.64
1:E:265:LYS:NZ	1:E:271:SER:HB2	2.11	0.64
1:M:503:ARG:NH1	1:M:507:GLN:HE22	1.98	0.64
1:F:366:GLU:O	1:F:370:LYS:HG3	2.03	0.64
1:H:524:ALA:HB1	1:N:41:GLU:OE2	1.96	0.64
1:F:450:PRO:O	1:F:454:ILE:HG13	2.22	0.64
1:H:167:LYS:HD2	1:H:188:PHE:CZ	2.32	0.64
2:T:45:VAL:HG21	2:T:64:VAL:HG11	1.79	0.64
1:E:366:GLU:O	1:E:370:LYS:HG3	2.46	0.64
2:S:45:VAL:HG21	2:S:64:VAL:HG11	1.78	0.64
1:H:187:LYS:NZ	1:H:379:ARG:HG3	2.11	0.64
1:K:295:THR:HG22	1:K:317:GLY:C	2.18	0.64
1:A:127:ALA:O	1:A:131:ILE:HG13	2.07	0.64
1:L:74:LEU:HD12	1:L:512:ILE:CD1	2.26	0.64
1:G:455:ALA:HB1	1:G:465:ILE:HD12	1.89	0.64
1:B:175:THR:HB	1:B:377:VAL:HG22	2.02	0.64
1:M:173:ILE:HD11	1:M:370:LYS:HB3	1.78	0.64
1:G:277:ALA:HB1	1:G:284:ARG:HD2	2.65	0.64
1:B:50:THR:CG2	1:B:51:LYS:H	2.16	0.64
1:L:79:SER:C	1:L:81:THR:H	2.01	0.64
2:S:8:ILE:HD12	2:S:8:ILE:N	2.13	0.64
1:E:141:ARG:NH2	1:E:163:ASP:OD1	2.30	0.64
1:C:69:ILE:HD11	1:D:41:GLU:HB2	1.88	0.64
1:B:234:PRO:O	1:B:238:GLN:HG3	1.96	0.64
2:Q:15:VAL:HG12	2:Q:16:VAL:N	4.35	0.64
1:B:50:THR:HG21	1:B:52:ASP:HB3	1.80	0.64
1:L:39:VAL:C	1:L:40:LEU:HD12	2.17	0.64
1:N:187:LYS:NZ	1:N:379:ARG:HG3	2.18	0.64
1:J:232:LEU:HD21	1:J:236:LEU:HD13	1.80	0.64
1:I:222:VAL:HG12	1:I:224:LYS:H	1.63	0.64
1:N:31:LEU:HD13	1:N:90:THR:HG22	1.80	0.64
1:H:157:VAL:HG21	1:H:395:PHE:CE2	2.33	0.64
1:J:312:THR:C	1:J:314:SER:H	2.05	0.64
1:I:157:VAL:HG21	1:I:395:PHE:CE2	2.34	0.64
1:D:320:GLU:HB3	1:D:333:GLY:HA3	1.87	0.64
1:H:332:VAL:HG22	1:H:375:VAL:HG11	1.80	0.64
2:T:96:LEU:HB3	2:U:89:ILE:HG21	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:50:THR:HG22	1:N:51:LYS:N	2.10	0.64
1:G:326:LYS:O	1:G:326:LYS:HD3	4.64	0.64
1:N:40:LEU:HD23	1:N:59:GLU:CG	2.27	0.64
1:H:74:LEU:HA	1:H:512:ILE:HD11	1.79	0.64
2:O:56:ASN:HD21	2:P:56:ASN:HB3	1.63	0.64
1:K:103:GLY:O	1:K:107:VAL:HG23	2.02	0.64
1:D:359:TYR:CZ	1:D:363:LYS:HE3	2.52	0.64
2:P:13:ASP:O	2:P:13:ASP:OD1	3.12	0.64
2:O:77:GLY:HA3	2:O:90:LEU:HD23	1.86	0.64
1:M:345:ILE:O	1:M:349:LYS:HG3	1.98	0.64
1:N:234:PRO:CG	1:N:309:GLU:HA	2.28	0.64
1:C:85:ALA:HB1	1:C:501:VAL:HG12	1.86	0.64
1:B:94:VAL:CG1	1:B:449:GLU:HB3	2.27	0.64
1:M:175:THR:HG21	1:M:177:GLU:OE2	2.12	0.64
1:I:503:ARG:NH1	1:I:507:GLN:HE22	1.95	0.64
1:L:222:VAL:HG12	1:L:223:GLU:N	2.13	0.64
2:P:100:GLN:HB2	2:Q:9:LYS:HE2	1.80	0.64
1:I:212:ALA:HB3	1:I:324:ILE:HB	1.79	0.64
1:E:248:ILE:HD12	1:E:261:LEU:HD21	1.79	0.64
1:J:234:PRO:CG	1:J:309:GLU:HA	2.29	0.64
1:C:94:VAL:CG1	1:C:449:GLU:HB3	2.30	0.64
1:C:116:LEU:O	1:C:120:ILE:HG13	1.97	0.64
1:I:222:VAL:HG12	1:I:223:GLU:N	2.11	0.64
1:I:277:ALA:CB	1:I:284:ARG:HD2	2.29	0.64
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.80	0.64
1:E:233:LEU:O	1:E:237:GLU:HG3	2.33	0.64
2:Q:54:LEU:CD1	2:Q:55:GLU:H	3.79	0.64
1:D:304:LEU:CD1	1:E:262:VAL:HG11	2.27	0.64
1:I:189:VAL:CG1	1:I:333:GLY:HA2	2.26	0.64
1:G:348:ILE:HD11	1:G:367:ARG:HE	2.32	0.64
1:L:65:HIS:O	1:L:69:ILE:HG13	1.98	0.64
1:E:320:GLU:HB3	1:E:333:GLY:HA3	4.01	0.64
2:O:32:LEU:HG	2:O:33:PRO:HD2	4.04	0.64
1:F:23:VAL:HG22	1:F:60:VAL:HG11	1.85	0.64
1:I:247:LEU:HD22	1:I:322:VAL:HG11	1.82	0.64
1:E:298:THR:HB	1:E:315:MET:HB2	4.37	0.64
1:K:168:VAL:HG11	1:K:173:ILE:H	1.63	0.64
1:K:297:GLY:HA3	1:K:317:GLY:H	1.63	0.64
1:N:264:ASN:HB3	1:N:269:THR:HB	1.80	0.64
1:E:416:VAL:HG21	1:E:490:MET:HG3	1.90	0.63
1:G:136:ILE:O	1:G:410:ILE:HG22	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ILE:HD11	1:F:495:ILE:CA	2.14	0.63
1:A:237:GLU:HB3	2:O:28:GLY:CA	2.97	0.63
1:C:50:THR:HG21	1:C:52:ASP:HB3	1.82	0.63
1:J:345:ILE:O	1:J:349:LYS:HG3	2.06	0.63
2:S:100:GLN:OE1	2:T:9:LYS:CE	2.46	0.63
1:B:319:ALA:HB1	1:B:332:VAL:O	2.43	0.63
1:K:157:VAL:HG21	1:K:395:PHE:CZ	2.33	0.63
1:J:167:LYS:HD2	1:J:188:PHE:CZ	2.36	0.63
1:M:167:LYS:HD2	1:M:188:PHE:CZ	2.32	0.63
1:I:352:LEU:HD11	1:I:365:GLN:HE22	2.79	0.63
2:Q:62:LEU:H	2:Q:62:LEU:HD12	1.63	0.63
2:T:14:ARG:HG2	2:T:14:ARG:HH11	2.75	0.63
1:A:210:MET:HE1	1:G:343:ALA:HA	1.80	0.63
1:D:78:ALA:O	1:D:89:THR:HG22	2.06	0.63
1:J:411:VAL:O	1:J:496:VAL:HG13	2.05	0.63
1:L:222:VAL:HG12	1:L:224:LYS:H	1.62	0.63
1:H:247:LEU:HD22	1:H:322:VAL:HG11	1.80	0.63
1:H:157:VAL:HG21	1:H:395:PHE:CZ	2.34	0.63
1:G:19:GLY:HA3	1:G:67:GLU:O	2.03	0.63
1:L:312:THR:C	1:L:314:SER:H	2.01	0.63
1:K:340:ASP:O	1:K:343:ALA:HB3	2.04	0.63
1:N:340:ASP:O	1:N:343:ALA:HB3	2.10	0.63
1:I:232:LEU:HD21	1:I:236:LEU:HD13	1.79	0.63
1:F:422:ILE:HG23	1:F:444:ARG:HG3	1.82	0.63
2:P:81:GLU:HG3	2:P:85:GLU:H	1.63	0.63
2:P:15:VAL:CG2	2:P:95:LEU:HD11	2.26	0.63
1:L:410:ILE:CD1	1:L:496:VAL:HG11	2.27	0.63
1:D:222:VAL:O	1:D:250:ALA:HA	1.97	0.63
1:A:287:MET:O	1:A:291:ILE:HG13	2.29	0.63
1:K:167:LYS:HD2	1:K:188:PHE:CZ	2.34	0.63
1:E:235:ILE:HD12	1:E:311:ALA:HB1	3.93	0.63
2:T:61:PRO:HG3	2:U:59:ARG:HH21	7.08	0.63
1:J:283:ARG:CG	1:J:363:LYS:NZ	2.89	0.63
1:C:280:PHE:O	1:C:283:ARG:HB3	3.84	0.63
1:E:294:VAL:HA	1:E:341:ILE:HD11	1.79	0.63
1:K:50:THR:HG22	1:K:52:ASP:N	2.15	0.63
1:M:39:VAL:O	1:N:522:VAL:HA	2.13	0.63
1:F:290:ASP:O	1:F:294:VAL:HG23	1.98	0.63
1:B:19:GLY:HA3	1:B:67:GLU:O	1.98	0.63
1:I:167:LYS:HD2	1:I:188:PHE:CZ	2.34	0.63
1:M:173:ILE:HD11	1:M:370:LYS:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:18:LYS:HG2	2:P:87:TYR:CD2	3.78	0.63
2:O:81:GLU:HA	2:O:86:GLU:HA	1.81	0.63
1:M:219:ILE:HB	1:M:295:THR:HG21	1.81	0.63
1:I:168:VAL:HG11	1:I:173:ILE:H	1.63	0.63
1:J:410:ILE:HB	1:J:496:VAL:HG11	1.79	0.63
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.92	0.63
1:N:337:LYS:HB2	1:N:340:ASP:OD2	1.98	0.63
1:E:19:GLY:HA3	1:E:67:GLU:O	1.97	0.63
1:L:103:GLY:O	1:L:107:VAL:HG23	2.15	0.63
1:I:352:LEU:HD11	1:I:365:GLN:NE2	2.70	0.63
2:Q:45:VAL:HG21	2:Q:64:VAL:HG11	1.80	0.63
2:O:45:VAL:HG21	2:O:64:VAL:CG1	2.32	0.63
2:S:96:LEU:HB3	2:T:89:ILE:HD13	1.81	0.63
2:T:62:LEU:HD12	2:T:62:LEU:H	1.63	0.63
1:N:189:VAL:CG1	1:N:190:GLU:H	2.10	0.63
1:G:294:VAL:HA	1:G:341:ILE:HD11	2.62	0.63
1:E:223:GLU:O	1:E:251:GLU:HB2	1.98	0.63
1:E:289:LYS:CE	1:F:202:TYR:OH	3.43	0.63
1:N:410:ILE:HB	1:N:496:VAL:HG11	1.85	0.63
1:K:219:ILE:HD12	1:K:295:THR:CG2	2.32	0.63
1:J:222:VAL:HG12	1:J:224:LYS:H	1.66	0.63
1:J:290:ASP:N	1:J:344:ARG:HH12	2.09	0.63
1:L:362:GLU:O	1:L:365:GLN:HB2	2.04	0.63
1:J:157:VAL:HG21	1:J:395:PHE:CZ	2.35	0.63
1:B:298:THR:HB	1:B:315:MET:HB2	1.78	0.63
2:Q:17:VAL:HG12	2:Q:44:LYS:O	3.57	0.63
1:D:283:ARG:HH11	1:D:363:LYS:HD3	5.15	0.63
2:T:99:LEU:HD23	2:U:8:ILE:CD1	8.23	0.63
2:T:100:GLN:HE22	2:U:9:LYS:HZ2	7.08	0.63
1:M:168:VAL:HG11	1:M:173:ILE:H	1.64	0.63
1:G:290:ASP:HB3	1:G:371:LEU:HD21	2.25	0.63
1:A:235:ILE:O	1:A:239:VAL:HG23	2.46	0.63
1:M:157:VAL:HG21	1:M:395:PHE:CZ	2.36	0.63
1:N:54:VAL:HG22	1:N:89:THR:HG21	1.87	0.63
1:K:290:ASP:O	1:K:294:VAL:HG23	1.99	0.63
2:Q:45:VAL:HG12	2:Q:46:ILE:N	2.68	0.63
2:Q:77:GLY:HA3	2:Q:90:LEU:HB3	4.17	0.63
2:R:18:LYS:HG2	2:R:87:TYR:CD2	2.34	0.63
1:G:287:MET:O	1:G:290:ASP:HB2	2.18	0.63
1:H:283:ARG:HG2	1:H:363:LYS:NZ	2.44	0.63
1:M:178:GLU:HB3	1:M:388:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:74:LEU:HD12	1:N:512:ILE:CD1	2.29	0.63
1:C:98:ALA:HB2	1:C:449:GLU:CG	2.28	0.63
1:A:94:VAL:HG12	1:A:449:GLU:HB3	1.83	0.63
1:L:157:VAL:HG21	1:L:395:PHE:CZ	2.34	0.63
1:D:345:ILE:HG23	1:D:368:LEU:HD13	1.87	0.63
1:N:178:GLU:HB3	1:N:388:LEU:HD21	1.81	0.63
2:R:48:VAL:HG13	2:R:62:LEU:HD23	1.79	0.63
1:I:50:THR:HG22	1:I:51:LYS:N	2.10	0.63
1:H:40:LEU:HD23	1:H:59:GLU:CG	2.29	0.63
1:G:85:ALA:HB1	1:G:501:VAL:HG12	1.84	0.63
1:L:232:LEU:HD22	1:L:236:LEU:HD22	1.82	0.63
1:K:178:GLU:HB3	1:K:388:LEU:HD21	1.81	0.63
2:U:80:ILE:HG22	2:U:81:GLU:N	2.14	0.62
1:C:168:VAL:HG12	1:C:168:VAL:O	1.99	0.62
1:A:39:VAL:HB	1:G:522:VAL:HG22	1.81	0.62
1:N:307:LYS:HE3	1:N:310:ASN:ND2	2.14	0.62
2:S:81:GLU:HG3	2:S:85:GLU:H	1.64	0.62
1:J:247:LEU:HD22	1:J:322:VAL:HG11	1.80	0.62
1:E:411:VAL:HB	1:E:412:PRO:HD2	1.98	0.62
1:F:298:THR:HB	1:F:315:MET:HB2	1.81	0.62
1:D:450:PRO:O	1:D:454:ILE:HG13	1.98	0.62
1:E:118:ARG:HH22	1:F:34:ARG:HH12	1.52	0.62
1:E:263:VAL:O	1:E:267:ARG:HB2	3.26	0.62
2:Q:41:GLN:HG2	2:Q:74:LYS:HB3	1.81	0.62
1:E:264:ASN:CG	2:S:30:ILE:HG23	2.19	0.62
1:F:246:LEU:HB3	1:F:272:VAL:CG1	2.58	0.62
1:E:283:ARG:NH2	1:E:366:GLU:OE1	2.32	0.62
2:R:54:LEU:CD2	2:S:55:GLU:HA	4.12	0.62
1:C:224:LYS:HB3	1:C:302:GLU:OE1	1.99	0.62
1:K:187:LYS:NZ	1:K:379:ARG:HG3	2.14	0.62
1:K:408:GLU:O	1:K:499:ALA:HB3	2.44	0.62
1:B:72:GLN:HE22	1:B:75:LYS:NZ	2.00	0.62
1:L:175:THR:HG21	1:L:177:GLU:OE2	2.03	0.62
1:J:465:ILE:HD13	1:J:480:PHE:CE1	2.34	0.62
2:R:13:ASP:CA	2:R:62:LEU:HD21	3.73	0.62
1:A:352:LEU:HD21	1:A:364:LEU:HB2	1.81	0.62
2:S:41:GLN:HG2	2:S:74:LYS:HB3	1.89	0.62
2:Q:50:THR:O	2:Q:51:GLY:O	4.09	0.62
1:M:206:ASN:HD21	1:M:389:LYS:CD	2.12	0.62
1:H:496:VAL:HG12	1:H:497:ASP:H	1.71	0.62
1:C:124:VAL:O	1:C:128:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:503:ARG:NH1	1:H:507:GLN:HE22	1.97	0.62
1:F:416:VAL:HG21	1:F:490:MET:HG3	1.96	0.62
2:T:60:VAL:HG13	2:T:61:PRO:HD2	3.28	0.62
1:E:265:LYS:HZ2	1:E:271:SER:HB2	1.64	0.62
1:M:50:THR:HG22	1:M:51:LYS:N	2.14	0.62
1:J:297:GLY:HA3	1:J:317:GLY:H	1.75	0.62
1:C:199:ILE:HG13	1:C:274:ALA:O	2.06	0.62
1:E:382:ALA:HB3	1:E:388:LEU:HB2	1.83	0.62
1:L:195:ASP:O	1:L:196:LYS:HD3	2.53	0.62
1:B:366:GLU:O	1:B:370:LYS:HG3	2.01	0.62
1:E:136:ILE:HD11	1:E:477:ARG:NH2	2.28	0.62
1:C:209:THR:HB	1:C:211:GLU:HG2	4.05	0.62
1:G:50:THR:HG21	1:G:52:ASP:HB3	1.83	0.62
1:F:168:VAL:O	1:F:168:VAL:HG12	2.00	0.62
1:I:187:LYS:NZ	1:I:379:ARG:HG3	2.14	0.62
1:G:256:GLU:HB3	2:U:35:THR:HB	1.81	0.62
1:A:416:VAL:HG21	1:A:490:MET:HG3	1.81	0.62
1:E:455:ALA:HB1	1:E:465:ILE:HD12	1.81	0.62
1:C:175:THR:HB	1:C:377:VAL:HG22	1.80	0.62
2:R:48:VAL:HG12	2:R:62:LEU:HD13	4.19	0.62
2:T:99:LEU:HA	2:U:8:ILE:HG12	6.49	0.62
1:E:85:ALA:HB1	1:E:501:VAL:HG12	1.82	0.62
1:L:178:GLU:HB3	1:L:388:LEU:HD21	1.83	0.62
1:D:422:ILE:HG23	1:D:444:ARG:HG3	1.82	0.62
1:I:175:THR:HG21	1:I:177:GLU:OE2	2.00	0.62
2:Q:97:ALA:HA	2:R:9:LYS:O	2.73	0.62
1:N:366:GLU:O	1:N:370:LYS:HG3	2.13	0.62
2:P:45:VAL:HG21	2:P:64:VAL:HG11	1.80	0.62
1:H:360:ALA:HA	1:H:363:LYS:HG3	3.61	0.62
1:A:50:THR:CG2	1:A:51:LYS:H	2.11	0.62
1:J:168:VAL:HG11	1:J:173:ILE:H	1.63	0.62
1:B:94:VAL:HG12	1:B:449:GLU:HB3	1.80	0.62
1:J:222:VAL:HG12	1:J:223:GLU:N	2.17	0.62
1:G:247:LEU:HD22	1:G:322:VAL:HG11	2.16	0.62
1:D:57:ALA:O	1:D:75:LYS:HD3	1.99	0.62
1:I:232:LEU:HD22	1:I:236:LEU:HD22	1.84	0.62
1:G:411:VAL:HB	1:G:412:PRO:HD2	1.81	0.62
2:P:77:GLY:HA3	2:P:90:LEU:HD23	1.82	0.62
1:K:312:THR:C	1:K:314:SER:H	2.07	0.62
2:Q:80:ILE:HG12	2:Q:81:GLU:N	4.61	0.62
2:U:10:PRO:C	2:U:11:LEU:HD22	4.59	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:PHE:HA	2:T:34:ASP:OD2	3.50	0.62
1:G:235:ILE:CG1	1:G:311:ALA:HB3	2.36	0.62
1:G:224:LYS:HD2	1:G:224:LYS:H	4.42	0.62
1:G:248:ILE:HD12	1:G:261:LEU:HD21	2.43	0.62
1:L:283:ARG:HH11	1:L:363:LYS:HE3	1.64	0.62
1:J:290:ASP:O	1:J:294:VAL:HG23	1.99	0.62
1:L:526:LYS:CG	1:L:527:PRO:HD2	2.29	0.62
1:I:226:VAL:HG11	1:I:232:LEU:HD12	1.81	0.62
1:F:411:VAL:HB	1:F:412:PRO:HD2	1.87	0.62
1:M:465:ILE:HD13	1:M:480:PHE:CE1	2.44	0.62
1:B:141:ARG:NH2	1:B:163:ASP:OD1	2.42	0.62
2:U:13:ASP:CB	2:U:62:LEU:HD21	2.30	0.62
1:C:229:VAL:HG23	1:C:256:GLU:HG3	2.28	0.62
1:M:187:LYS:NZ	1:M:379:ARG:HG3	2.14	0.62
1:N:503:ARG:NH1	1:N:507:GLN:HE22	1.98	0.62
1:F:368:LEU:O	1:F:368:LEU:HD12	2.01	0.62
1:E:57:ALA:O	1:E:75:LYS:HD3	2.08	0.62
2:R:25:LYS:HG2	2:R:31:VAL:HG22	2.16	0.62
1:L:462:GLY:O	1:L:466:VAL:HG23	2.00	0.62
1:A:450:PRO:O	1:A:454:ILE:HG13	2.10	0.62
1:L:96:ALA:O	1:L:100:VAL:HG23	2.12	0.62
2:U:92:GLU:HA	2:U:95:LEU:HD12	1.79	0.62
1:N:189:VAL:HG11	1:N:333:GLY:CA	2.23	0.62
2:O:84:GLY:CA	2:U:27:LYS:HD3	2.30	0.62
1:E:54:VAL:HG22	1:E:89:THR:HG21	1.82	0.62
1:E:352:LEU:HD21	1:E:364:LEU:HB2	3.79	0.62
1:G:234:PRO:O	1:G:238:GLN:HG3	2.00	0.62
1:B:382:ALA:HB3	1:B:388:LEU:HB2	1.81	0.62
2:S:77:GLY:HA3	2:S:90:LEU:HD23	1.86	0.62
1:K:465:ILE:HD13	1:K:480:PHE:CE1	2.35	0.62
1:I:340:ASP:O	1:I:343:ALA:HB3	1.99	0.62
1:E:348:ILE:HD11	1:E:367:ARG:NE	2.14	0.62
2:T:15:VAL:HG23	2:T:15:VAL:O	2.99	0.61
2:T:15:VAL:O	2:T:17:VAL:HG23	4.36	0.61
1:M:283:ARG:HG2	1:M:363:LYS:HZ2	1.64	0.61
1:B:343:ALA:HB2	1:C:207:PRO:CB	2.26	0.61
1:L:180:LYS:HB3	1:M:281:GLY:N	2.15	0.61
1:H:219:ILE:HD12	1:H:295:THR:CG2	2.30	0.61
1:K:74:LEU:HA	1:K:512:ILE:CD1	2.35	0.61
1:C:352:LEU:CD2	1:C:364:LEU:HB2	2.68	0.61
1:H:195:ASP:O	1:H:196:LYS:HD3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HG23	1:A:256:GLU:OE2	2.00	0.61
1:H:178:GLU:HB3	1:H:388:LEU:HD21	1.82	0.61
1:I:264:ASN:HB3	1:I:269:THR:HB	1.81	0.61
1:I:178:GLU:HB3	1:I:388:LEU:HD21	1.83	0.61
2:S:25:LYS:HG2	2:S:31:VAL:HG22	1.82	0.61
2:S:96:LEU:O	2:T:14:ARG:HD3	2.16	0.61
1:M:283:ARG:HD3	1:M:363:LYS:NZ	2.15	0.61
1:H:283:ARG:HD3	1:H:363:LYS:NZ	2.47	0.61
1:L:7:VAL:HG12	1:L:12:ALA:HB2	1.82	0.61
1:C:94:VAL:HG12	1:C:449:GLU:HB3	1.81	0.61
2:U:8:ILE:HG22	2:U:9:LYS:N	2.76	0.61
1:M:50:THR:HG22	1:M:52:ASP:N	2.09	0.61
2:R:73:ALA:O	2:R:75:TYR:N	2.36	0.61
1:I:157:VAL:HG21	1:I:395:PHE:CZ	2.35	0.61
1:I:249:ILE:O	1:I:249:ILE:HG22	2.00	0.61
1:L:167:LYS:HD2	1:L:188:PHE:CZ	2.37	0.61
1:J:178:GLU:HB3	1:J:388:LEU:HD21	1.82	0.61
1:B:345:ILE:HG23	1:B:368:LEU:HD13	1.87	0.61
1:M:96:ALA:O	1:M:100:VAL:HG23	2.07	0.61
1:D:416:VAL:HG21	1:D:490:MET:HG3	1.85	0.61
2:Q:16:VAL:HG12	2:Q:46:ILE:HD12	5.83	0.61
1:L:189:VAL:HG11	1:L:333:GLY:HA2	1.81	0.61
2:T:8:ILE:CD1	2:T:82:ILE:HD11	4.57	0.61
2:U:13:ASP:OD1	2:U:93:ARG:HG2	7.01	0.61
1:C:416:VAL:HG21	1:C:490:MET:HG3	1.81	0.61
1:C:270:LEU:HG	1:C:272:VAL:HG13	1.80	0.61
1:G:52:ASP:OD1	1:G:54:VAL:HG23	2.01	0.61
1:M:229:VAL:HG23	1:M:256:GLU:CB	2.29	0.61
1:B:189:VAL:HG11	1:B:193:GLN:HG2	3.20	0.61
1:F:178:GLU:HG3	1:F:388:LEU:HD21	1.82	0.61
1:A:30:THR:O	1:A:35:GLY:HA3	2.09	0.61
1:M:195:ASP:O	1:M:196:LYS:HD3	2.00	0.61
1:I:410:ILE:HB	1:I:496:VAL:HG11	1.82	0.61
1:I:290:ASP:N	1:I:344:ARG:HH12	2.00	0.61
1:N:232:LEU:HD22	1:N:236:LEU:HD22	1.87	0.61
1:M:264:ASN:HB3	1:M:269:THR:HB	1.83	0.61
2:T:41:GLN:HG2	2:T:42:LYS:HE3	9.44	0.61
2:Q:78:THR:HG22	2:Q:79:GLU:N	2.36	0.61
1:A:233:LEU:HD23	2:O:30:ILE:HD13	1.82	0.61
1:L:49:ILE:HG21	1:M:515:LEU:HD21	1.82	0.61
2:O:52:ARG:HH21	2:P:53:VAL:HB	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:ASN:OD1	1:L:515:LEU:HD12	2.19	0.61
1:L:187:LYS:NZ	1:L:379:ARG:HG3	2.17	0.61
1:M:222:VAL:HG12	1:M:223:GLU:N	2.16	0.61
1:K:408:GLU:OE1	1:K:500:LYS:HA	2.51	0.61
1:H:157:VAL:O	1:H:161:ILE:HG13	2.03	0.61
1:H:452:ARG:HH11	1:H:452:ARG:HG2	1.65	0.61
1:A:23:VAL:HG22	1:A:60:VAL:HG11	1.83	0.61
1:B:526:LYS:HG3	1:B:527:PRO:HD2	2.31	0.61
1:I:283:ARG:HH12	1:I:364:LEU:HD12	1.64	0.61
2:P:22:GLU:OE2	2:P:38:GLU:O	2.19	0.61
2:Q:91:SER:HB3	2:Q:93:ARG:HH11	3.56	0.61
1:A:136:ILE:HD11	1:A:477:ARG:NH2	2.16	0.61
1:C:235:ILE:CD1	1:C:311:ALA:HB3	2.30	0.61
1:C:382:ALA:HB3	1:C:388:LEU:HB2	1.84	0.61
1:N:290:ASP:N	1:N:344:ARG:HH12	2.01	0.61
1:I:96:ALA:O	1:I:100:VAL:HG23	2.07	0.61
1:H:218:PHE:CE1	1:H:242:THR:HG21	2.35	0.61
1:C:455:ALA:HB1	1:C:465:ILE:HD12	1.83	0.61
1:N:167:LYS:HD2	1:N:188:PHE:CZ	2.35	0.61
2:T:10:PRO:HB3	2:T:16:VAL:HG23	2.49	0.61
1:M:283:ARG:HH12	1:M:364:LEU:HD12	1.69	0.61
1:A:237:GLU:CD	2:O:28:GLY:HA3	2.21	0.61
1:C:348:ILE:CD1	1:C:367:ARG:NE	3.72	0.61
1:M:219:ILE:HD12	1:M:295:THR:CG2	2.32	0.61
1:N:65:HIS:O	1:N:69:ILE:HG13	2.12	0.61
1:L:345:ILE:O	1:L:349:LYS:HG3	2.04	0.61
1:A:85:ALA:HB1	1:A:501:VAL:HG12	1.83	0.61
1:D:175:THR:HB	1:D:377:VAL:HG22	1.83	0.61
1:L:465:ILE:HD13	1:L:480:PHE:CE1	2.39	0.61
1:K:218:PHE:CE1	1:K:242:THR:HG21	2.44	0.61
2:Q:41:GLN:HG3	2:Q:72:PHE:O	4.66	0.61
1:A:228:ASN:HD21	1:A:230:ARG:HB2	1.85	0.61
1:C:368:LEU:O	1:C:368:LEU:HD12	2.00	0.61
1:E:522:VAL:HG22	1:F:39:VAL:HB	1.81	0.61
1:F:50:THR:CG2	1:F:51:LYS:H	2.11	0.61
1:F:78:ALA:O	1:F:89:THR:HG22	2.00	0.61
1:A:235:ILE:HD12	1:A:311:ALA:CB	2.31	0.61
1:N:168:VAL:HG11	1:N:173:ILE:H	1.66	0.61
1:M:40:LEU:HD23	1:M:59:GLU:CG	2.32	0.61
1:I:229:VAL:HG23	1:I:256:GLU:CB	2.30	0.61
2:T:66:GLU:HG2	2:T:67:GLY:N	3.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:VAL:HB	1:B:412:PRO:HD2	1.90	0.61
1:C:411:VAL:HB	1:C:412:PRO:HD2	1.83	0.61
1:N:283:ARG:NH1	1:N:363:LYS:HG3	2.15	0.61
2:O:11:LEU:O	2:O:12:GLY:C	2.39	0.61
2:T:10:PRO:HB2	2:T:14:ARG:HB2	2.63	0.61
1:C:50:THR:CG2	1:C:51:LYS:H	2.10	0.61
1:L:168:VAL:HG11	1:L:173:ILE:H	1.67	0.61
1:I:40:LEU:HD23	1:I:59:GLU:CG	2.30	0.61
1:J:295:THR:HG22	1:J:317:GLY:C	2.24	0.61
1:D:98:ALA:HB2	1:D:449:GLU:CG	2.31	0.61
1:D:18:ARG:HD2	1:D:67:GLU:OE2	2.01	0.61
1:C:251:GLU:HA	1:C:277:ALA:HB2	2.91	0.60
1:C:265:LYS:NZ	1:C:271:SER:HB2	3.31	0.60
1:C:283:ARG:HH12	1:C:363:LYS:HB3	2.21	0.60
1:M:178:GLU:H	1:M:321:ARG:NH1	1.95	0.60
1:H:50:THR:HG22	1:H:51:LYS:N	2.18	0.60
1:G:235:ILE:HG12	1:G:311:ALA:CB	2.96	0.60
1:L:180:LYS:O	1:M:280:PHE:C	2.40	0.60
1:D:85:ALA:HB1	1:D:501:VAL:HG12	1.82	0.60
2:U:24:PRO:HB2	2:U:37:LYS:HZ1	5.54	0.60
2:S:100:GLN:HB2	2:T:9:LYS:HE3	3.60	0.60
1:N:224:LYS:HG2	1:N:225:LYS:H	1.66	0.60
1:G:222:VAL:O	1:G:250:ALA:HA	2.01	0.60
1:E:348:ILE:HD11	1:E:367:ARG:HE	1.65	0.60
1:D:6:LEU:HD22	1:D:523:VAL:HG22	1.82	0.60
2:O:9:LYS:HE2	2:U:100:GLN:HB2	1.82	0.60
1:K:345:ILE:HG22	1:K:349:LYS:HE3	1.83	0.60
1:H:458:ALA:O	1:I:114:LEU:HD12	2.49	0.60
1:H:290:ASP:N	1:H:344:ARG:HH12	1.99	0.60
1:K:503:ARG:NH1	1:K:507:GLN:HE22	2.04	0.60
1:M:232:LEU:HD22	1:M:236:LEU:HD22	1.83	0.60
2:R:45:VAL:O	2:R:46:ILE:HD13	2.01	0.60
1:A:350:LYS:O	1:B:208:GLU:CA	7.70	0.60
1:M:410:ILE:HB	1:M:496:VAL:HG11	1.82	0.60
2:Q:54:LEU:HD12	2:Q:55:GLU:N	4.56	0.60
1:C:300:ILE:O	1:C:300:ILE:HG22	2.01	0.60
2:Q:26:THR:HG22	2:Q:32:LEU:CD2	5.10	0.60
1:M:295:THR:HG22	1:M:317:GLY:C	2.25	0.60
1:G:50:THR:CG2	1:G:51:LYS:H	2.06	0.60
1:F:54:VAL:HG22	1:F:89:THR:HG21	1.83	0.60
1:E:98:ALA:HB2	1:E:449:GLU:CG	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:280:PHE:CD2	1:N:385:GLU:HB2	2.90	0.60
1:D:287:MET:O	1:D:291:ILE:HG13	2.01	0.60
1:D:455:ALA:HB1	1:D:465:ILE:HD12	1.87	0.60
1:E:23:VAL:HG22	1:E:60:VAL:HG11	1.82	0.60
1:F:184:THR:HG23	1:F:380:VAL:HA	1.82	0.60
1:A:184:THR:HG23	1:A:380:VAL:HA	2.02	0.60
2:Q:96:LEU:HA	2:R:14:ARG:NE	2.16	0.60
2:T:80:ILE:HG22	2:T:81:GLU:N	2.19	0.60
1:I:189:VAL:CG1	1:I:190:GLU:H	2.14	0.60
1:H:283:ARG:HD3	1:H:363:LYS:HZ1	2.10	0.60
1:M:178:GLU:OE1	1:M:323:ARG:NH2	2.33	0.60
1:E:345:ILE:HD11	1:E:368:LEU:HD23	1.82	0.60
2:T:25:LYS:HG2	2:T:31:VAL:HG22	1.83	0.60
1:H:219:ILE:HB	1:H:295:THR:HG21	1.84	0.60
1:I:229:VAL:CG2	1:I:256:GLU:HB3	2.31	0.60
1:K:263:VAL:O	1:K:267:ARG:HB2	2.01	0.60
1:M:268:GLY:O	1:N:227:SER:OG	2.18	0.60
1:M:218:PHE:CE1	1:M:242:THR:HG21	2.39	0.60
2:Q:70:VAL:HG11	2:Q:95:LEU:HD23	2.59	0.60
1:A:233:LEU:HA	2:O:30:ILE:CD1	2.62	0.60
2:O:80:ILE:HG22	2:O:81:GLU:N	2.15	0.60
1:E:360:ALA:O	1:E:364:LEU:HG	2.01	0.60
1:D:235:ILE:CD1	1:D:311:ALA:HB3	2.29	0.60
1:L:180:LYS:HB3	1:M:281:GLY:CA	2.31	0.60
1:K:224:LYS:HG2	1:K:225:LYS:H	1.66	0.60
1:G:222:VAL:HG22	1:G:300:ILE:HD12	1.82	0.60
1:M:290:ASP:N	1:M:344:ARG:HH12	2.02	0.60
1:H:312:THR:C	1:H:314:SER:H	2.05	0.60
1:H:337:LYS:HB2	1:H:340:ASP:OD2	2.02	0.60
2:Q:58:GLN:CG	2:Q:59:ARG:N	4.83	0.60
1:H:50:THR:HG22	1:H:52:ASP:N	2.16	0.60
1:L:526:LYS:HG3	1:L:527:PRO:HD2	1.82	0.60
1:F:382:ALA:HB3	1:F:388:LEU:HB2	1.83	0.60
1:I:465:ILE:HD13	1:I:480:PHE:CE1	2.36	0.60
1:K:28:LYS:NZ	1:K:97:GLN:HE22	2.09	0.60
1:K:366:GLU:O	1:K:370:LYS:HG3	2.08	0.60
2:Q:73:ALA:HB1	2:Q:75:TYR:CE2	2.37	0.60
2:U:13:ASP:C	2:U:13:ASP:OD1	2.40	0.60
1:C:54:VAL:HG22	1:C:89:THR:HG21	1.84	0.60
1:H:189:VAL:CG1	1:H:190:GLU:H	2.11	0.60
1:J:229:VAL:HG23	1:J:256:GLU:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:74:LEU:HA	1:I:512:ILE:HD11	1.84	0.60
1:C:501:VAL:HG23	1:C:502:THR:N	2.17	0.60
1:D:127:ALA:O	1:D:131:ILE:HG13	2.05	0.60
1:G:263:VAL:HG13	1:G:267:ARG:NH1	3.99	0.60
1:N:79:SER:C	1:N:81:THR:H	2.06	0.60
1:I:31:LEU:HD13	1:I:90:THR:HG22	1.87	0.60
2:U:13:ASP:CG	2:U:92:GLU:HB3	2.98	0.60
2:U:20:ILE:CG1	2:U:44:LYS:HG3	4.68	0.60
1:N:74:LEU:HA	1:N:512:ILE:HD11	1.84	0.60
1:G:98:ALA:HB2	1:G:449:GLU:CG	2.39	0.60
1:G:23:VAL:HG22	1:G:60:VAL:HG11	1.83	0.60
1:C:404:ALA:HB1	1:C:500:LYS:HB3	1.82	0.60
1:I:79:SER:C	1:I:81:THR:H	2.07	0.60
1:H:527:PRO:O	1:H:528:GLU:HG2	2.02	0.60
1:H:175:THR:HG21	1:H:177:GLU:OE2	2.09	0.60
2:Q:62:LEU:O	2:Q:64:VAL:N	2.57	0.60
1:M:182:LEU:HD12	1:N:363:LYS:HE2	1.82	0.60
1:E:234:PRO:O	1:E:238:GLN:HG3	2.09	0.60
2:S:96:LEU:CD2	2:T:14:ARG:NH1	6.06	0.60
1:E:225:LYS:HG3	1:E:252:ASP:HB3	1.84	0.60
1:E:251:GLU:HA	1:E:277:ALA:HB2	1.83	0.60
1:C:298:THR:HG23	1:C:304:LEU:HD12	8.55	0.60
1:F:98:ALA:HB2	1:F:449:GLU:CG	2.33	0.60
1:K:79:SER:C	1:K:81:THR:H	2.05	0.60
1:K:229:VAL:HG23	1:K:256:GLU:CB	2.35	0.60
1:H:316:LEU:CD2	1:H:316:LEU:H	2.15	0.60
1:D:30:THR:O	1:D:35:GLY:HA3	2.12	0.60
1:D:150:ILE:CD1	1:D:496:VAL:H	2.14	0.60
2:S:41:GLN:HE21	2:S:74:LYS:HG2	2.24	0.60
2:T:55:GLU:CD	2:U:55:GLU:HB3	3.99	0.60
2:P:92:GLU:HA	2:P:95:LEU:HD12	2.08	0.60
1:F:233:LEU:HD23	2:T:30:ILE:HD13	1.84	0.60
1:M:74:LEU:HA	1:M:512:ILE:CD1	2.59	0.60
1:K:74:LEU:HA	1:K:512:ILE:HD11	2.00	0.60
1:N:465:ILE:HD13	1:N:480:PHE:CE1	2.36	0.60
1:F:224:LYS:HB3	1:F:302:GLU:OE1	2.14	0.60
2:Q:96:LEU:HD23	2:R:14:ARG:NH2	2.16	0.59
1:E:258:LEU:HA	1:E:261:LEU:HD12	1.83	0.59
1:E:246:LEU:HB3	1:E:272:VAL:CG1	2.54	0.59
1:F:218:PHE:O	1:F:246:LEU:HD12	2.19	0.59
1:F:325:THR:HG22	1:F:326:LYS:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG22	1:A:300:ILE:HD12	1.95	0.59
1:M:372:ALA:C	1:M:374:GLY:N	2.48	0.59
1:M:229:VAL:CG2	1:M:256:GLU:HB3	2.32	0.59
1:H:232:LEU:HD21	1:H:236:LEU:HD13	1.84	0.59
1:L:526:LYS:HD2	1:L:527:PRO:HD2	1.84	0.59
1:J:65:HIS:HD2	1:J:527:PRO:HG3	2.71	0.59
1:H:6:LEU:HD23	1:H:523:VAL:HG22	1.90	0.59
1:J:218:PHE:CE1	1:J:242:THR:HG21	2.40	0.59
1:M:410:ILE:CD1	1:M:496:VAL:HG11	2.29	0.59
1:L:410:ILE:HB	1:L:496:VAL:HG11	1.83	0.59
1:C:258:LEU:HA	1:C:261:LEU:HD12	2.54	0.59
1:J:157:VAL:O	1:J:161:ILE:HG13	2.06	0.59
1:L:157:VAL:O	1:L:161:ILE:HG13	2.06	0.59
1:I:157:VAL:O	1:I:161:ILE:HG13	2.01	0.59
1:L:232:LEU:HD21	1:L:236:LEU:HD13	1.84	0.59
1:M:390:GLU:OE1	1:M:394:ARG:NH1	2.35	0.59
2:Q:81:GLU:OE2	2:Q:84:GLY:HA2	2.95	0.59
2:T:8:ILE:HD12	2:T:8:ILE:N	2.17	0.59
1:B:416:VAL:HG21	1:B:490:MET:HG3	1.96	0.59
1:A:231:GLU:O	1:A:234:PRO:HD2	2.99	0.59
1:C:237:GLU:CG	2:Q:28:GLY:HA3	2.31	0.59
2:U:41:GLN:HG2	2:U:74:LYS:HB3	1.83	0.59
1:J:233:LEU:N	1:J:234:PRO:HD2	2.17	0.59
1:C:498:PRO:HG2	1:C:501:VAL:CG2	2.41	0.59
1:G:267:ARG:HG3	1:G:267:ARG:HH11	4.49	0.59
1:J:226:VAL:HG11	1:J:232:LEU:HD12	1.99	0.59
1:N:290:ASP:O	1:N:294:VAL:HG23	2.04	0.59
1:D:290:ASP:O	1:D:294:VAL:HG23	2.02	0.59
1:I:372:ALA:C	1:I:374:GLY:H	2.22	0.59
1:A:175:THR:HB	1:A:377:VAL:HG22	1.86	0.59
2:R:8:ILE:N	2:R:8:ILE:HD12	2.19	0.59
1:N:283:ARG:HH12	1:N:364:LEU:HD12	1.67	0.59
2:S:96:LEU:HB3	2:T:89:ILE:HG21	1.84	0.59
2:T:8:ILE:H	2:T:8:ILE:HD12	1.67	0.59
2:U:78:THR:HG22	2:U:80:ILE:HD11	1.94	0.59
2:U:79:GLU:C	2:U:80:ILE:HD12	2.51	0.59
1:M:136:ILE:HD11	1:M:491:VAL:CG2	2.33	0.59
2:P:18:LYS:HE3	2:P:86:GLU:O	2.58	0.59
1:E:213:VAL:O	1:E:214:LEU:HD23	2.02	0.59
1:K:189:VAL:CG1	1:K:190:GLU:H	2.08	0.59
1:M:177:GLU:HB3	1:M:321:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:LEU:HA	1:J:512:ILE:CD1	2.41	0.59
1:N:295:THR:HG22	1:N:317:GLY:C	2.26	0.59
1:L:229:VAL:HG23	1:L:256:GLU:CB	2.35	0.59
1:B:116:LEU:O	1:B:120:ILE:HG13	2.01	0.59
1:G:127:ALA:O	1:G:131:ILE:HG13	2.02	0.59
1:J:458:ALA:O	1:K:114:LEU:HD12	2.02	0.59
1:J:28:LYS:NZ	1:J:97:GLN:HE22	1.99	0.59
1:L:118:ARG:O	1:L:122:LYS:HG3	2.02	0.59
1:L:31:LEU:HD13	1:L:90:THR:HG22	1.86	0.59
1:N:218:PHE:CE1	1:N:242:THR:HG21	2.38	0.59
2:S:96:LEU:HD23	2:T:14:ARG:NH1	5.17	0.59
2:T:96:LEU:O	2:T:97:ALA:HB2	2.41	0.59
2:O:6:THR:HG23	2:U:100:GLN:OXT	5.07	0.59
2:T:97:ALA:HB1	2:U:8:ILE:CG2	3.86	0.59
1:M:410:ILE:HB	1:M:496:VAL:HG12	1.84	0.59
1:I:325:THR:CG2	1:I:327:ASP:H	2.05	0.59
1:C:201:PRO:O	1:C:204:VAL:CG2	2.99	0.59
1:E:224:LYS:HB3	1:E:302:GLU:OE1	8.22	0.59
1:H:295:THR:HG22	1:H:317:GLY:C	2.21	0.59
1:H:79:SER:C	1:H:81:THR:H	2.05	0.59
1:J:337:LYS:HB2	1:J:340:ASP:OD2	2.07	0.59
1:L:232:LEU:O	1:L:232:LEU:HD23	2.03	0.59
1:M:226:VAL:HG11	1:M:232:LEU:HD12	1.88	0.59
1:G:30:THR:O	1:G:35:GLY:HA3	2.02	0.59
1:K:128:VAL:HA	1:K:131:ILE:HD12	1.83	0.59
1:K:283:ARG:HH12	1:K:364:LEU:HD12	1.66	0.59
1:B:136:ILE:HB	1:B:410:ILE:HG22	1.84	0.59
1:G:352:LEU:HD21	1:G:365:GLN:HG2	6.09	0.59
1:H:410:ILE:HB	1:H:496:VAL:HG11	1.83	0.59
1:M:74:LEU:HD12	1:M:512:ILE:CD1	2.32	0.59
1:K:267:ARG:HG2	1:L:256:GLU:CD	2.23	0.59
1:F:301:SER:HB2	1:F:304:LEU:CB	2.33	0.59
1:C:57:ALA:O	1:C:75:LYS:HD3	2.02	0.59
1:K:290:ASP:N	1:K:344:ARG:HH12	2.00	0.59
2:U:81:GLU:HA	2:U:85:GLU:O	2.02	0.59
1:E:281:GLY:O	1:E:284:ARG:HG2	2.02	0.59
1:D:325:THR:HG22	1:D:326:LYS:N	2.18	0.59
2:S:12:GLY:O	2:S:13:ASP:CB	2.45	0.59
1:G:225:LYS:HD3	1:G:254:GLU:CD	3.25	0.59
1:L:295:THR:HG22	1:L:317:GLY:C	2.23	0.59
1:D:501:VAL:HG23	1:D:502:THR:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:VAL:O	1:F:128:VAL:HG23	2.16	0.59
1:A:382:ALA:HB3	1:A:388:LEU:HB2	1.85	0.59
1:F:284:ARG:O	1:F:288:LEU:HG	2.03	0.59
1:N:226:VAL:HG11	1:N:232:LEU:HD12	2.29	0.59
1:M:232:LEU:HD21	1:M:236:LEU:HD13	1.88	0.59
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.96	0.59
1:H:65:HIS:O	1:H:69:ILE:HG13	2.13	0.59
1:G:136:ILE:HD11	1:G:477:ARG:NH2	2.21	0.59
1:C:235:ILE:HD11	1:C:311:ALA:CB	2.33	0.59
1:E:283:ARG:NH1	1:E:363:LYS:HB3	2.17	0.59
2:T:25:LYS:HA	2:T:30:ILE:O	2.75	0.59
1:G:242:THR:HG22	1:G:244:LYS:HG3	2.85	0.59
1:C:498:PRO:HG2	1:C:501:VAL:HG22	1.94	0.59
1:B:57:ALA:O	1:B:75:LYS:HD3	2.12	0.59
1:D:224:LYS:HB3	1:D:302:GLU:OE1	2.03	0.59
2:T:8:ILE:CG2	2:T:16:VAL:HG21	2.60	0.59
1:G:279:GLY:C	1:G:284:ARG:HB3	2.22	0.59
1:I:307:LYS:HE3	1:I:310:ASN:ND2	2.24	0.59
1:G:301:SER:HB2	1:G:304:LEU:CB	2.31	0.59
1:I:74:LEU:HA	1:I:512:ILE:CD1	2.32	0.59
1:B:498:PRO:HG2	1:B:501:VAL:CG2	2.32	0.59
1:N:229:VAL:HG23	1:N:256:GLU:CB	2.34	0.59
1:L:226:VAL:HG11	1:L:232:LEU:HD12	1.84	0.59
1:H:303:GLU:C	1:H:305:GLY:H	2.08	0.59
2:T:54:LEU:HD13	2:U:57:GLY:HA2	5.13	0.59
2:U:84:GLY:O	2:U:85:GLU:HG3	2.03	0.59
1:C:218:PHE:HE1	1:C:244:LYS:HD2	4.36	0.59
1:H:283:ARG:NH1	1:H:363:LYS:HG3	2.17	0.59
1:F:50:THR:HG21	1:F:52:ASP:HB3	1.83	0.59
1:L:180:LYS:C	1:M:281:GLY:CA	2.71	0.59
1:K:345:ILE:O	1:K:349:LYS:HG3	2.07	0.59
1:E:501:VAL:HG23	1:E:502:THR:N	2.22	0.59
1:L:74:LEU:HA	1:L:512:ILE:CD1	2.32	0.59
1:G:207:PRO:HG2	1:G:208:GLU:H	2.62	0.59
1:M:303:GLU:C	1:M:305:GLY:H	2.10	0.59
1:F:157:VAL:HG22	1:F:395:PHE:CZ	2.37	0.59
1:N:175:THR:HG21	1:N:177:GLU:OE2	2.02	0.59
1:L:182:LEU:HD12	1:M:363:LYS:NZ	2.18	0.58
1:C:230:ARG:O	1:C:234:PRO:HD2	2.03	0.58
1:M:297:GLY:HA3	1:M:317:GLY:H	1.73	0.58
1:L:47:PRO:HB3	1:M:69:ILE:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:HG22	1:G:304:LEU:O	4.50	0.58
1:M:74:LEU:HA	1:M:512:ILE:HD11	2.31	0.58
1:L:359:TYR:O	1:L:363:LYS:HG2	2.54	0.58
1:A:96:ALA:O	1:A:100:VAL:HG23	2.07	0.58
1:J:79:SER:C	1:J:81:THR:H	2.08	0.58
1:B:40:LEU:HD13	1:B:59:GLU:HG3	1.94	0.58
2:R:81:GLU:HA	2:R:86:GLU:HA	1.85	0.58
2:T:81:GLU:HG3	2:T:85:GLU:H	1.67	0.58
1:C:278:PRO:O	1:C:279:GLY:O	2.21	0.58
1:B:247:LEU:HD13	1:B:324:ILE:HD11	1.85	0.58
1:C:349:LYS:C	1:C:351:GLU:H	2.06	0.58
1:F:237:GLU:CG	2:T:28:GLY:HA3	2.32	0.58
1:K:496:VAL:HG12	1:K:497:ASP:H	1.68	0.58
2:S:56:ASN:N	2:S:56:ASN:OD1	2.35	0.58
1:H:118:ARG:O	1:H:122:LYS:HG3	2.02	0.58
1:L:283:ARG:HH21	1:L:367:ARG:CD	2.42	0.58
1:J:118:ARG:O	1:J:122:LYS:HG3	2.08	0.58
2:S:52:ARG:HH21	2:T:53:VAL:HB	2.98	0.58
1:D:141:ARG:NH2	1:D:163:ASP:OD1	2.29	0.58
1:J:217:ALA:HB2	1:J:245:PRO:CG	2.35	0.58
1:A:236:LEU:HB2	2:O:30:ILE:CD1	2.55	0.58
2:S:49:GLY:O	2:S:62:LEU:HD11	2.46	0.58
1:I:345:ILE:O	1:I:349:LYS:HG3	2.11	0.58
1:D:263:VAL:O	1:D:267:ARG:HB2	2.10	0.58
1:A:501:VAL:HG23	1:A:502:THR:N	2.20	0.58
1:B:124:VAL:O	1:B:128:VAL:HG23	2.03	0.58
1:B:127:ALA:O	1:B:131:ILE:HG13	2.14	0.58
1:B:501:VAL:HG23	1:B:502:THR:N	2.20	0.58
1:C:136:ILE:CD1	1:C:477:ARG:HH21	2.16	0.58
1:L:224:LYS:HG2	1:L:225:LYS:H	1.68	0.58
1:K:175:THR:HG21	1:K:177:GLU:OE2	2.03	0.58
2:Q:34:ASP:OD1	2:Q:34:ASP:N	2.35	0.58
1:H:106:ASN:HD21	5:H:601:DMS:H11	1.68	0.58
2:S:96:LEU:HD23	2:T:14:ARG:HH22	4.48	0.58
2:O:14:ARG:HE	2:U:96:LEU:HD23	1.68	0.58
1:I:297:GLY:HA3	1:I:317:GLY:H	1.70	0.58
1:K:50:THR:HG22	1:K:51:LYS:N	2.14	0.58
1:H:411:VAL:O	1:H:496:VAL:HG13	2.13	0.58
1:N:258:LEU:O	1:N:262:VAL:HG23	2.03	0.58
1:B:498:PRO:HG2	1:B:501:VAL:HG22	1.84	0.58
1:L:290:ASP:O	1:L:294:VAL:HG23	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:65:HIS:O	1:J:69:ILE:HG13	2.12	0.58
1:N:103:GLY:O	1:N:107:VAL:HG23	2.04	0.58
1:M:79:SER:C	1:M:81:THR:H	2.06	0.58
1:A:320:GLU:HB3	1:A:333:GLY:HA3	1.87	0.58
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.90	0.58
1:M:31:LEU:HD13	1:M:90:THR:HG22	1.84	0.58
2:U:20:ILE:HG13	2:U:43:GLY:HA2	1.86	0.58
1:G:283:ARG:NH2	1:G:366:GLU:OE2	3.05	0.58
1:B:54:VAL:HG22	1:B:89:THR:HG21	1.86	0.58
1:E:301:SER:HB2	1:E:304:LEU:CB	6.29	0.58
1:H:496:VAL:HG12	1:H:497:ASP:N	2.20	0.58
1:N:345:ILE:O	1:N:349:LYS:HG3	2.12	0.58
1:M:345:ILE:HG22	1:M:349:LYS:HE3	1.85	0.58
1:J:503:ARG:NH1	1:J:507:GLN:HE22	2.04	0.58
1:J:81:THR:OG1	1:J:508:ASN:ND2	2.35	0.58
1:J:175:THR:HG21	1:J:177:GLU:OE2	2.07	0.58
1:L:36:ARG:HB3	1:M:518:THR:O	2.04	0.58
1:I:312:THR:C	1:I:314:SER:H	2.07	0.58
1:H:258:LEU:O	1:H:262:VAL:HG23	2.14	0.58
1:K:258:LEU:O	1:K:262:VAL:HG23	2.09	0.58
1:M:283:ARG:CZ	1:M:363:LYS:HG3	2.90	0.58
1:C:298:THR:HB	1:C:315:MET:HB2	1.84	0.58
1:E:18:ARG:HD2	1:E:67:GLU:OE2	2.04	0.58
1:E:175:THR:HB	1:E:377:VAL:HG22	1.95	0.58
2:O:34:ASP:OD1	2:O:34:ASP:N	2.31	0.58
1:K:6:LEU:HD23	1:K:523:VAL:HG22	1.96	0.58
1:J:96:ALA:O	1:J:100:VAL:HG23	2.03	0.58
1:A:372:ALA:C	1:A:374:GLY:N	2.78	0.58
1:B:218:PHE:HE1	1:B:244:LYS:HB2	1.95	0.58
1:B:222:VAL:O	1:B:250:ALA:HA	2.10	0.58
2:U:74:LYS:HZ1	2:U:75:TYR:HB3	6.60	0.58
1:G:283:ARG:HH22	1:G:366:GLU:CD	3.51	0.58
1:E:283:ARG:HH12	1:E:363:LYS:HD2	3.08	0.58
1:E:326:LYS:O	1:E:326:LYS:HD3	2.03	0.58
1:L:234:PRO:HG3	1:L:309:GLU:CA	2.37	0.58
1:I:263:VAL:O	1:I:267:ARG:HB2	2.03	0.58
1:L:219:ILE:HB	1:L:295:THR:HG21	1.87	0.58
1:C:253:VAL:HG21	1:C:274:ALA:HB1	1.85	0.58
1:H:229:VAL:HG23	1:H:256:GLU:CB	2.33	0.58
1:I:103:GLY:O	1:I:107:VAL:HG23	2.06	0.58
1:M:337:LYS:HB2	1:M:340:ASP:OD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:259:ALA:O	1:M:263:VAL:HG23	2.03	0.58
2:T:81:GLU:HA	2:T:86:GLU:HA	1.84	0.58
1:H:325:THR:CG2	1:H:327:ASP:H	2.05	0.58
1:I:295:THR:HG22	1:I:317:GLY:C	2.24	0.58
1:A:236:LEU:CB	2:O:30:ILE:HD11	2.57	0.58
1:G:78:ALA:O	1:G:89:THR:HG22	2.04	0.58
1:J:189:VAL:CG1	1:J:190:GLU:H	2.12	0.58
1:I:234:PRO:HG3	1:I:309:GLU:CA	2.33	0.58
2:Q:11:LEU:O	2:Q:12:GLY:C	2.40	0.58
1:G:501:VAL:HG23	1:G:502:THR:N	2.21	0.58
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.97	0.58
1:G:392:LYS:O	1:G:396:GLU:HG3	2.04	0.58
1:G:88:GLY:HA2	4:G:602:ADP:O2B	2.03	0.58
1:L:249:ILE:O	1:L:249:ILE:HG22	2.02	0.58
1:D:101:ARG:HG3	1:D:102:GLU:N	2.19	0.58
1:B:95:LEU:O	1:B:99:ILE:HG13	2.25	0.58
1:D:411:VAL:HB	1:D:412:PRO:HD2	1.89	0.58
2:R:17:VAL:HG12	2:R:18:LYS:N	2.18	0.58
1:N:283:ARG:CZ	1:N:363:LYS:HG3	2.33	0.58
1:C:237:GLU:HB3	2:Q:28:GLY:CA	2.27	0.58
1:B:168:VAL:O	1:B:168:VAL:HG12	2.11	0.58
1:E:289:LYS:HE3	1:F:202:TYR:CZ	5.03	0.58
1:M:37:ASN:OD1	1:N:515:LEU:HD12	2.03	0.58
1:B:78:ALA:O	1:B:89:THR:HG22	2.04	0.58
1:L:233:LEU:N	1:L:234:PRO:HD2	2.25	0.58
1:A:124:VAL:O	1:A:128:VAL:HG23	2.02	0.58
1:D:229:VAL:HG21	2:R:36:ALA:HB2	1.86	0.58
1:K:157:VAL:O	1:K:161:ILE:HG13	2.03	0.58
1:J:303:GLU:C	1:J:305:GLY:H	2.07	0.58
1:G:450:PRO:O	1:G:454:ILE:HG13	2.04	0.58
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.89	0.58
2:T:18:LYS:HZ1	2:T:85:GLU:CD	2.06	0.58
1:B:300:ILE:O	1:B:300:ILE:HG22	2.02	0.58
1:C:290:ASP:HB3	1:C:371:LEU:HD21	1.89	0.58
1:F:325:THR:HG22	1:F:326:LYS:N	2.19	0.58
2:T:32:LEU:HB3	2:T:36:ALA:HB3	3.85	0.58
1:C:326:LYS:HD3	1:C:326:LYS:C	4.40	0.58
1:N:410:ILE:HB	1:N:496:VAL:HG12	1.90	0.58
1:K:234:PRO:HG3	1:K:309:GLU:CA	2.32	0.58
1:K:219:ILE:HB	1:K:295:THR:HG21	1.90	0.58
1:J:316:LEU:H	1:J:316:LEU:CD2	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:LEU:HD22	1:G:523:VAL:HG22	1.86	0.58
1:G:199:ILE:HG13	1:G:274:ALA:O	2.15	0.58
1:D:235:ILE:CG1	1:D:311:ALA:HB3	2.33	0.57
1:M:385:GLU:N	1:N:280:PHE:CE2	2.72	0.57
1:C:225:LYS:HD3	1:C:254:GLU:CD	3.31	0.57
1:H:345:ILE:O	1:H:349:LYS:HG3	2.04	0.57
1:M:157:VAL:O	1:M:161:ILE:HG13	2.05	0.57
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.88	0.57
1:L:218:PHE:CE1	1:L:242:THR:HG21	2.43	0.57
1:I:303:GLU:C	1:I:305:GLY:H	2.08	0.57
1:M:462:GLY:O	1:M:466:VAL:HG23	2.03	0.57
2:U:78:THR:HG22	2:U:80:ILE:CD1	2.46	0.57
1:C:150:ILE:HD11	1:C:495:ILE:CA	2.12	0.57
1:I:219:ILE:HB	1:I:295:THR:HG21	1.85	0.57
2:P:79:GLU:C	2:P:80:ILE:HG13	2.74	0.57
1:G:341:ILE:C	1:G:343:ALA:H	3.24	0.57
1:E:343:ALA:HA	1:F:210:MET:HE3	2.34	0.57
1:J:307:LYS:HB3	1:J:309:GLU:OE1	2.15	0.57
1:L:54:VAL:HG22	1:L:89:THR:CG2	2.32	0.57
1:M:332:VAL:CG1	1:M:377:VAL:HG21	2.34	0.57
1:E:127:ALA:O	1:E:131:ILE:HG13	2.11	0.57
1:A:57:ALA:O	1:A:75:LYS:HD3	2.03	0.57
1:N:157:VAL:O	1:N:161:ILE:HG13	2.05	0.57
1:B:366:GLU:O	1:B:369:ALA:HB3	2.03	0.57
1:L:316:LEU:CD2	1:L:316:LEU:H	2.18	0.57
1:N:303:GLU:C	1:N:305:GLY:H	2.09	0.57
1:G:231:GLU:HA	1:G:309:GLU:HB3	2.16	0.57
1:I:130:LYS:HD3	1:I:142:LYS:NZ	29.77	0.57
1:L:303:GLU:C	1:L:305:GLY:H	2.08	0.57
1:H:372:ALA:C	1:H:374:GLY:H	2.19	0.57
2:U:17:VAL:HG21	2:U:70:VAL:HG21	3.98	0.57
1:L:219:ILE:HD12	1:L:295:THR:CG2	2.34	0.57
1:G:263:VAL:O	1:G:267:ARG:HB2	2.04	0.57
1:J:259:ALA:O	1:J:263:VAL:HG23	2.17	0.57
1:J:385:GLU:HB2	1:K:280:PHE:CD2	2.48	0.57
1:F:57:ALA:O	1:F:75:LYS:HD3	2.10	0.57
1:A:101:ARG:HG3	1:A:102:GLU:N	2.26	0.57
2:R:21:GLU:H	2:R:21:GLU:CD	2.07	0.57
2:Q:46:ILE:O	2:Q:66:GLU:HG3	3.29	0.57
1:E:312:THR:HG22	1:E:314:SER:H	1.69	0.57
2:O:54:LEU:HD11	2:P:55:GLU:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:GLN:HB3	1:C:313:LEU:HG	2.09	0.57
1:C:264:ASN:OD1	1:C:269:THR:HG21	2.35	0.57
1:M:178:GLU:CA	1:M:321:ARG:HH12	2.17	0.57
1:G:218:PHE:O	1:G:246:LEU:HD12	2.57	0.57
1:N:74:LEU:HD12	1:N:512:ILE:HD12	1.87	0.57
1:L:337:LYS:HB2	1:L:340:ASP:OD2	2.04	0.57
1:K:316:LEU:CD2	1:K:316:LEU:H	2.22	0.57
1:B:96:ALA:O	1:B:100:VAL:HG23	2.03	0.57
2:P:13:ASP:HB2	2:P:62:LEU:CD2	2.34	0.57
2:P:79:GLU:HG2	2:P:88:VAL:HG22	2.02	0.57
1:C:203:PHE:CD1	1:C:273:ALA:HA	2.74	0.57
1:E:352:LEU:HD21	1:E:365:GLN:HG2	1.87	0.57
1:L:410:ILE:HB	1:L:496:VAL:HG12	1.86	0.57
1:A:218:PHE:O	1:A:246:LEU:HD12	2.38	0.57
1:N:74:LEU:HA	1:N:512:ILE:CD1	2.34	0.57
1:H:74:LEU:HA	1:H:512:ILE:CD1	2.33	0.57
1:N:232:LEU:HD21	1:N:236:LEU:HD13	1.89	0.57
1:M:41:GLU:OE2	1:N:524:ALA:HB1	2.05	0.57
1:G:184:THR:HG23	1:G:380:VAL:HA	1.86	0.57
1:I:352:LEU:HD23	1:I:364:LEU:CD2	6.04	0.57
2:P:71:VAL:CG1	2:Q:80:ILE:HD13	2.35	0.57
2:T:8:ILE:HG21	2:T:16:VAL:HG21	1.86	0.57
1:B:219:ILE:N	1:B:317:GLY:O	2.52	0.57
1:H:360:ALA:O	1:H:364:LEU:HD13	2.23	0.57
1:A:288:LEU:HD23	1:A:291:ILE:HD12	2.53	0.57
1:C:136:ILE:HB	1:C:410:ILE:HG22	1.89	0.57
1:D:230:ARG:HA	1:D:233:LEU:HD12	2.09	0.57
1:A:325:THR:HG22	1:A:326:LYS:N	2.20	0.57
1:B:18:ARG:HD2	1:B:67:GLU:OE2	2.05	0.57
2:T:56:ASN:O	2:T:58:GLN:HG3	2.04	0.57
1:C:30:THR:O	1:C:35:GLY:HA3	2.08	0.57
1:G:175:THR:HB	1:G:377:VAL:HG22	1.86	0.57
2:U:15:VAL:HG11	2:U:95:LEU:CD2	4.72	0.57
1:G:251:GLU:HA	1:G:277:ALA:HB2	2.84	0.57
1:A:235:ILE:HD12	1:A:311:ALA:HB1	1.87	0.57
1:L:360:ALA:HA	1:L:363:LYS:HG3	2.93	0.57
1:H:256:GLU:HG3	1:N:267:ARG:O	2.04	0.57
1:G:130:LYS:O	1:G:133:ALA:HB3	2.59	0.57
1:H:465:ILE:HD13	1:H:480:PHE:CE1	2.40	0.57
2:Q:48:VAL:CG1	2:Q:62:LEU:HD12	4.49	0.57
2:R:81:GLU:HA	2:R:85:GLU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:46:ILE:HD12	2:U:87:TYR:CE2	5.83	0.57
1:M:283:ARG:CD	1:M:363:LYS:HZ2	2.17	0.57
1:M:496:VAL:HG12	1:M:497:ASP:H	1.69	0.57
1:A:168:VAL:HG12	1:A:168:VAL:O	2.05	0.57
2:Q:54:LEU:HD11	2:R:57:GLY:CA	2.34	0.57
1:G:168:VAL:HG12	1:G:168:VAL:O	2.05	0.57
1:J:235:ILE:HD11	1:J:311:ALA:CB	2.26	0.57
1:C:229:VAL:HG23	1:C:256:GLU:OE2	2.03	0.57
1:C:294:VAL:HG23	1:C:295:THR:HG23	5.95	0.57
1:E:225:LYS:HD3	1:E:254:GLU:CD	2.25	0.57
1:F:233:LEU:HD21	2:T:32:LEU:HD21	5.24	0.57
1:N:496:VAL:HG12	1:N:497:ASP:H	1.71	0.57
1:J:307:LYS:HE3	1:J:310:ASN:ND2	2.23	0.57
1:N:233:LEU:N	1:N:234:PRO:HD2	2.20	0.57
1:D:128:VAL:HG13	1:D:503:ARG:HG3	1.85	0.57
1:B:349:LYS:C	1:B:351:GLU:H	2.07	0.57
1:K:459:GLY:HA3	1:L:114:LEU:HD12	2.00	0.57
1:M:263:VAL:O	1:M:267:ARG:HB2	2.04	0.57
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.91	0.57
2:T:73:ALA:HB1	2:T:75:TYR:CE2	2.39	0.57
1:G:233:LEU:O	1:G:237:GLU:HG3	2.04	0.57
2:R:34:ASP:HA	2:R:37:LYS:HE2	1.85	0.57
1:N:421:ALA:O	1:N:425:VAL:HG23	2.05	0.57
1:G:40:LEU:HD13	1:G:59:GLU:HG3	1.87	0.57
2:Q:17:VAL:O	2:Q:87:TYR:HB3	2.05	0.57
2:R:17:VAL:O	2:R:87:TYR:HB3	2.05	0.57
2:T:10:PRO:HB2	2:T:14:ARG:O	2.04	0.57
2:T:13:ASP:HA	2:T:62:LEU:HD21	1.87	0.57
2:U:20:ILE:HD11	2:U:44:LYS:HG3	3.36	0.57
1:B:235:ILE:HD12	1:B:311:ALA:HB1	2.00	0.57
1:D:247:LEU:HD22	1:D:322:VAL:HG11	2.00	0.57
1:L:40:LEU:N	1:L:40:LEU:HD12	2.19	0.57
1:G:224:LYS:CE	1:G:301:SER:HA	6.89	0.57
1:M:74:LEU:HD12	1:M:512:ILE:HD12	2.03	0.57
1:J:263:VAL:O	1:J:267:ARG:HB2	2.08	0.57
1:G:231:GLU:O	1:G:309:GLU:HA	2.41	0.57
1:M:146:GLU:O	1:M:150:ILE:HG13	2.05	0.57
1:G:452:ARG:NH1	1:G:463:SER:HA	2.19	0.57
1:E:101:ARG:HG3	1:E:102:GLU:N	2.21	0.57
1:D:80:LYS:HE2	1:E:383:ALA:O	2.04	0.57
1:J:127:ALA:O	1:J:131:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:LYS:HE2	1:F:383:ALA:O	2.41	0.57
1:B:199:ILE:HG13	1:B:274:ALA:O	2.05	0.57
2:T:48:VAL:HG12	2:T:62:LEU:HD12	4.06	0.57
1:B:136:ILE:CD1	1:B:477:ARG:HH21	2.27	0.57
1:M:360:ALA:O	1:M:363:LYS:HG2	2.22	0.57
1:C:290:ASP:O	1:C:294:VAL:HG23	2.04	0.57
1:E:78:ALA:O	1:E:89:THR:HG22	2.08	0.57
1:H:283:ARG:HD3	1:H:363:LYS:HE3	1.87	0.57
1:F:228:ASN:HD21	1:F:230:ARG:HB2	1.90	0.57
1:I:233:LEU:N	1:I:234:PRO:HD2	2.23	0.57
1:K:410:ILE:HB	1:K:496:VAL:HG12	1.88	0.57
1:H:74:LEU:HD12	1:H:512:ILE:HD12	1.87	0.57
1:H:345:ILE:HG22	1:H:349:LYS:HE3	1.86	0.57
1:A:98:ALA:HB2	1:A:449:GLU:CG	2.38	0.57
1:K:222:VAL:HG12	1:K:223:GLU:H	1.74	0.57
1:C:101:ARG:HG3	1:C:102:GLU:N	2.25	0.57
1:D:452:ARG:NH1	1:D:463:SER:HA	2.23	0.57
1:N:127:ALA:O	1:N:131:ILE:HG13	2.04	0.57
1:C:445:ARG:CZ	1:C:452:ARG:HH21	2.18	0.57
1:F:101:ARG:HG3	1:F:102:GLU:N	2.20	0.57
2:R:77:GLY:HA3	2:R:90:LEU:HD23	2.04	0.57
2:P:27:LYS:HD3	2:Q:84:GLY:HA3	1.86	0.56
1:N:50:THR:CG2	1:N:51:LYS:H	2.18	0.56
1:B:359:TYR:CZ	1:B:363:LYS:HE3	2.40	0.56
1:C:207:PRO:HG2	1:C:208:GLU:H	3.91	0.56
1:C:220:LEU:HG	1:C:222:VAL:HG23	1.87	0.56
1:H:283:ARG:HH22	1:H:364:LEU:HA	1.70	0.56
1:G:201:PRO:O	1:G:204:VAL:HG23	2.05	0.56
1:J:496:VAL:HG12	1:J:497:ASP:H	1.70	0.56
1:E:144:ILE:CD1	1:E:165:MET:HG2	2.34	0.56
1:N:316:LEU:CD2	1:N:316:LEU:H	2.19	0.56
1:K:127:ALA:O	1:K:131:ILE:HG13	2.09	0.56
1:N:452:ARG:HG2	1:N:452:ARG:HH11	1.77	0.56
1:G:95:LEU:O	1:G:99:ILE:HG13	2.05	0.56
1:N:96:ALA:O	1:N:100:VAL:HG23	2.09	0.56
1:D:136:ILE:CD1	1:D:477:ARG:HH21	2.19	0.56
1:M:283:ARG:HD3	1:M:363:LYS:HZ2	1.69	0.56
1:M:65:HIS:O	1:M:69:ILE:HG13	2.05	0.56
1:N:307:LYS:HE3	1:N:310:ASN:HD21	1.71	0.56
1:L:229:VAL:CG2	1:L:256:GLU:HB3	2.41	0.56
2:O:44:LYS:HA	2:O:68:ASP:O	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:GLU:OE2	1:B:430:LYS:HD2	2.05	0.56
1:H:25:ASN:HA	1:H:28:LYS:HE2	1.90	0.56
1:G:416:VAL:HG21	1:G:490:MET:HG3	1.86	0.56
2:Q:26:THR:HG21	2:Q:30:ILE:HB	3.63	0.56
1:G:283:ARG:O	1:G:287:MET:HG3	2.05	0.56
1:E:289:LYS:NZ	1:F:202:TYR:CE2	5.41	0.56
1:L:307:LYS:HE3	1:L:310:ASN:ND2	2.25	0.56
1:L:307:LYS:HB3	1:L:309:GLU:OE1	2.08	0.56
1:L:180:LYS:HB3	1:M:281:GLY:H	1.68	0.56
1:C:298:THR:HG23	1:C:304:LEU:HD13	7.84	0.56
1:M:208:GLU:OE1	1:M:389:LYS:HD3	2.05	0.56
1:N:410:ILE:CD1	1:N:496:VAL:HG11	2.34	0.56
1:J:410:ILE:HB	1:J:496:VAL:HG12	1.92	0.56
1:K:136:ILE:HB	1:K:410:ILE:HG13	2.52	0.56
1:M:234:PRO:HG3	1:M:309:GLU:CA	2.33	0.56
2:S:100:GLN:CG	2:T:9:LYS:HE2	2.35	0.56
1:F:128:VAL:HG13	1:F:503:ARG:HG3	1.92	0.56
1:I:54:VAL:HG22	1:I:89:THR:CG2	2.35	0.56
1:A:301:SER:HB2	1:A:304:LEU:CB	2.35	0.56
1:M:312:THR:C	1:M:314:SER:H	2.12	0.56
2:O:50:THR:O	2:O:50:THR:HG23	2.05	0.56
1:K:372:ALA:C	1:K:374:GLY:H	2.08	0.56
1:J:6:LEU:HD23	1:J:523:VAL:HG22	1.85	0.56
1:D:286:GLU:OE1	1:D:344:ARG:NH2	2.62	0.56
1:M:6:LEU:HD23	1:M:523:VAL:HG22	1.87	0.56
2:Q:80:ILE:HG22	2:Q:81:GLU:N	2.20	0.56
1:A:345:ILE:HG23	1:A:368:LEU:HD13	1.93	0.56
1:F:359:TYR:CE1	1:F:363:LYS:HE2	2.66	0.56
1:C:348:ILE:CG2	1:C:368:LEU:HG	5.90	0.56
2:Q:26:THR:O	2:Q:27:LYS:HB2	4.81	0.56
2:O:52:ARG:HH21	2:P:53:VAL:CG1	2.18	0.56
1:A:235:ILE:HG21	1:A:311:ALA:CB	4.34	0.56
1:K:307:LYS:HB3	1:K:309:GLU:OE1	2.12	0.56
1:L:59:GLU:OE1	1:M:4:LYS:NZ	2.35	0.56
1:M:258:LEU:O	1:M:262:VAL:HG23	2.06	0.56
1:G:298:THR:HB	1:G:315:MET:HB2	1.88	0.56
1:J:496:VAL:HG12	1:J:497:ASP:N	2.20	0.56
1:K:496:VAL:HG12	1:K:497:ASP:N	2.21	0.56
1:M:233:LEU:N	1:M:234:PRO:HD2	2.21	0.56
1:K:7:VAL:HG12	1:K:12:ALA:HB2	1.87	0.56
1:H:106:ASN:HD21	5:H:601:DMS:C1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.87	0.56
1:B:101:ARG:HG3	1:B:102:GLU:N	2.23	0.56
1:B:147:VAL:CG2	1:B:410:ILE:HD11	2.35	0.56
1:E:50:THR:CG2	1:E:51:LYS:H	2.09	0.56
1:C:168:VAL:CG1	1:C:172:GLY:HA3	2.27	0.56
2:O:52:ARG:NH2	2:P:53:VAL:CB	2.65	0.56
1:K:233:LEU:N	1:K:234:PRO:HD2	2.23	0.56
1:M:408:GLU:O	1:M:499:ALA:HB3	2.36	0.56
1:D:229:VAL:HG11	2:R:32:LEU:CD2	2.35	0.56
1:E:228:ASN:ND2	1:E:231:GLU:HG3	3.90	0.56
1:K:452:ARG:HH11	1:K:452:ARG:HG2	1.75	0.56
1:C:520:GLU:HB3	1:D:29:VAL:HG11	1.88	0.56
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.90	0.56
1:J:31:LEU:HD13	1:J:90:THR:HG22	1.87	0.56
1:G:101:ARG:HG3	1:G:102:GLU:N	2.23	0.56
1:B:219:ILE:HG22	1:B:221:ILE:HG13	1.86	0.56
1:C:235:ILE:O	1:C:239:VAL:HG23	2.15	0.56
1:B:215:GLU:OE1	1:B:321:ARG:HG3	2.67	0.56
1:E:341:ILE:C	1:E:343:ALA:H	2.08	0.56
1:E:349:LYS:C	1:E:351:GLU:H	2.85	0.56
1:E:361:ARG:O	1:E:365:GLN:HB2	3.14	0.56
1:J:229:VAL:CG2	1:J:256:GLU:HB3	2.36	0.56
1:N:307:LYS:HB3	1:N:309:GLU:OE1	2.06	0.56
1:L:283:ARG:HH12	1:L:364:LEU:CD1	2.18	0.56
1:K:54:VAL:HG22	1:K:89:THR:CG2	2.45	0.56
1:G:465:ILE:HD13	1:G:480:PHE:CE2	2.41	0.56
1:L:459:GLY:HA3	1:M:114:LEU:HD12	1.91	0.56
1:L:452:ARG:HH11	1:L:452:ARG:HG2	1.72	0.56
1:I:218:PHE:CE1	1:I:242:THR:HG21	2.42	0.56
1:B:452:ARG:NH1	1:B:463:SER:HA	2.21	0.56
2:O:18:LYS:HG2	2:O:87:TYR:CD2	2.40	0.56
1:H:363:LYS:O	1:H:366:GLU:HG2	2.16	0.56
1:G:326:LYS:C	1:G:326:LYS:HD3	4.37	0.56
1:F:237:GLU:OE1	2:T:27:LYS:HG3	2.61	0.56
2:R:100:GLN:CG	2:S:9:LYS:HE2	5.41	0.56
1:D:235:ILE:O	1:D:239:VAL:HG23	2.30	0.56
1:C:178:GLU:CG	1:C:388:LEU:HD21	2.36	0.56
1:H:224:LYS:HG2	1:H:225:LYS:H	1.72	0.56
1:I:224:LYS:HG2	1:I:225:LYS:H	1.73	0.56
1:F:127:ALA:O	1:F:131:ILE:HG13	2.15	0.56
1:K:118:ARG:O	1:K:122:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:41:GLN:HG2	2:R:74:LYS:HB3	1.99	0.56
1:I:283:ARG:HH12	1:I:363:LYS:HG3	2.28	0.56
2:Q:18:LYS:HE3	2:Q:86:GLU:O	2.05	0.56
1:K:307:LYS:HE3	1:K:310:ASN:ND2	2.21	0.56
1:H:218:PHE:HE1	1:H:242:THR:HG21	1.70	0.56
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.88	0.56
1:K:31:LEU:HD13	1:K:90:THR:HG22	1.89	0.56
1:C:23:VAL:HG22	1:C:60:VAL:HG11	1.86	0.56
1:H:421:ALA:O	1:H:425:VAL:HG23	2.11	0.56
2:R:79:GLU:C	2:R:80:ILE:HG13	2.75	0.56
2:T:62:LEU:O	2:T:64:VAL:N	2.68	0.56
2:T:95:LEU:O	2:U:14:ARG:NH1	2.38	0.56
2:T:97:ALA:HB1	2:U:8:ILE:HG22	3.39	0.56
1:M:283:ARG:CG	1:M:363:LYS:HZ2	2.18	0.56
1:E:52:ASP:OD1	1:E:54:VAL:HG23	2.09	0.56
1:K:411:VAL:O	1:K:496:VAL:HG13	2.09	0.56
1:L:283:ARG:HG2	1:L:363:LYS:HZ2	1.70	0.56
1:D:230:ARG:O	1:D:234:PRO:HD2	2.18	0.56
1:A:332:VAL:HG12	1:A:333:GLY:N	2.21	0.56
1:D:189:VAL:HG13	1:D:193:GLN:HG2	1.86	0.56
1:J:197:GLY:HA3	1:J:325:THR:O	2.06	0.56
1:G:345:ILE:HG23	1:G:368:LEU:HD13	1.87	0.56
1:G:345:ILE:HG23	1:G:368:LEU:CD1	2.36	0.56
1:F:51:LYS:NZ	4:F:602:ADP:O1A	2.86	0.56
1:E:306:PHE:CE2	1:E:315:MET:SD	2.99	0.56
1:J:345:ILE:HG22	1:J:349:LYS:HE3	1.95	0.56
1:H:59:GLU:O	1:I:4:LYS:HG3	2.07	0.56
1:A:361:ARG:O	1:A:365:GLN:HB2	2.06	0.56
1:A:72:GLN:HE22	1:A:75:LYS:HZ1	1.76	0.56
1:D:445:ARG:CZ	1:D:452:ARG:HH21	2.24	0.56
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.73	0.56
1:M:452:ARG:HG2	1:M:452:ARG:HH11	1.73	0.56
1:D:199:ILE:HG13	1:D:274:ALA:O	2.06	0.56
1:E:445:ARG:CZ	1:E:452:ARG:HH21	2.31	0.56
1:I:25:ASN:HA	1:I:28:LYS:HE2	1.87	0.56
1:A:452:ARG:NH1	1:A:463:SER:HA	2.21	0.56
2:O:41:GLN:HG2	2:O:74:LYS:HB3	2.08	0.56
1:C:526:LYS:HG3	1:C:527:PRO:HD2	2.13	0.56
2:Q:8:ILE:HG21	2:Q:16:VAL:HG21	1.87	0.55
1:F:150:ILE:CD1	1:F:496:VAL:H	2.19	0.55
1:N:219:ILE:HB	1:N:295:THR:HG21	1.91	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:SER:HB2	1:B:304:LEU:CB	2.34	0.55
1:M:290:ASP:O	1:M:294:VAL:HG23	2.07	0.55
1:M:118:ARG:O	1:M:122:LYS:HG3	2.14	0.55
1:I:316:LEU:CD2	1:I:316:LEU:H	2.21	0.55
1:L:421:ALA:O	1:L:425:VAL:HG23	2.15	0.55
1:F:201:PRO:O	1:F:204:VAL:HG23	2.05	0.55
2:R:78:THR:HG22	2:R:79:GLU:N	2.21	0.55
1:E:235:ILE:HD12	1:E:311:ALA:HB3	3.82	0.55
1:N:50:THR:CG2	1:N:52:ASP:H	2.14	0.55
1:D:52:ASP:OD1	1:D:54:VAL:HG23	2.15	0.55
1:B:98:ALA:HB2	1:B:449:GLU:CG	2.34	0.55
1:C:307:LYS:HE3	1:C:309:GLU:OE1	2.05	0.55
1:C:465:ILE:HD13	1:C:480:PHE:CD2	2.42	0.55
1:B:520:GLU:HB3	1:C:29:VAL:HG11	2.01	0.55
1:H:128:VAL:HA	1:H:131:ILE:HD12	1.94	0.55
1:M:103:GLY:O	1:M:107:VAL:HG23	2.06	0.55
1:E:267:ARG:HG3	1:E:267:ARG:HH11	1.71	0.55
1:N:283:ARG:HD3	1:N:363:LYS:NZ	2.45	0.55
1:F:237:GLU:HB3	2:T:28:GLY:HA3	1.87	0.55
1:N:229:VAL:CG2	1:N:256:GLU:HB3	2.40	0.55
1:B:178:GLU:CG	1:B:388:LEU:HD21	2.36	0.55
1:C:127:ALA:O	1:C:131:ILE:HG13	2.06	0.55
1:H:222:VAL:HG12	1:H:223:GLU:H	1.73	0.55
1:C:72:GLN:HE22	1:C:75:LYS:HZ1	1.52	0.55
1:M:232:LEU:O	1:M:232:LEU:HD23	2.11	0.55
1:D:199:ILE:O	1:D:199:ILE:HG22	2.06	0.55
1:B:230:ARG:HA	1:B:233:LEU:HD12	2.07	0.55
1:K:325:THR:HG22	1:K:327:ASP:N	2.02	0.55
2:P:45:VAL:HG21	2:P:64:VAL:CG1	2.43	0.55
1:B:283:ARG:O	1:B:287:MET:HG3	2.06	0.55
1:G:349:LYS:C	1:G:351:GLU:H	2.10	0.55
1:H:366:GLU:O	1:H:370:LYS:HG3	2.06	0.55
2:S:11:LEU:O	2:S:13:ASP:N	2.39	0.55
1:A:222:VAL:O	1:A:250:ALA:HA	2.08	0.55
1:I:290:ASP:O	1:I:294:VAL:HG23	2.07	0.55
1:F:501:VAL:HG23	1:F:502:THR:N	2.22	0.55
1:E:425:VAL:O	1:E:429:ILE:HG13	2.23	0.55
1:F:14:ARG:NH1	1:M:109:ALA:HA	2.22	0.55
1:K:283:ARG:HG2	1:K:363:LYS:HZ2	1.77	0.55
2:Q:65:LYS:HG3	2:Q:68:ASP:OD1	4.31	0.55
2:O:9:LYS:O	2:U:97:ALA:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:96:LEU:HD23	2:U:14:ARG:HH11	1.71	0.55
2:Q:33:PRO:O	2:Q:35:THR:N	2.48	0.55
1:B:212:ALA:CB	1:B:324:ILE:HB	2.56	0.55
2:O:52:ARG:HG3	2:O:52:ARG:O	2.12	0.55
1:H:426:GLU:OE1	1:H:444:ARG:NH1	2.56	0.55
1:J:54:VAL:HG22	1:J:89:THR:CG2	2.41	0.55
2:P:56:ASN:N	2:P:56:ASN:OD1	2.39	0.55
1:D:465:ILE:HD13	1:D:480:PHE:CE2	2.50	0.55
1:L:25:ASN:HA	1:L:28:LYS:HE2	1.92	0.55
1:I:283:ARG:NH1	1:I:363:LYS:HG3	2.53	0.55
2:R:10:PRO:C	2:R:11:LEU:HD12	5.14	0.55
1:D:168:VAL:O	1:D:168:VAL:HG12	2.07	0.55
1:B:220:LEU:HD13	1:B:235:ILE:CD1	2.36	0.55
1:B:235:ILE:O	1:B:239:VAL:HG23	2.10	0.55
1:E:247:LEU:HD13	1:E:324:ILE:HD11	1.98	0.55
1:E:294:VAL:HA	1:E:341:ILE:CD1	2.35	0.55
1:N:496:VAL:HG12	1:N:497:ASP:N	2.21	0.55
1:I:496:VAL:HG12	1:I:497:ASP:N	2.23	0.55
1:C:142:LYS:HE2	1:C:146:GLU:OE2	2.11	0.55
1:I:232:LEU:HD23	1:I:232:LEU:O	2.07	0.55
1:G:472:GLU:HB3	1:G:478:TYR:CD2	2.52	0.55
1:L:6:LEU:HD23	1:L:523:VAL:HG22	1.94	0.55
1:D:161:ILE:HD12	1:D:399:LEU:CD2	2.44	0.55
2:Q:72:PHE:CD2	2:Q:72:PHE:N	3.02	0.55
2:R:8:ILE:HD12	2:R:8:ILE:H	2.23	0.55
1:M:182:LEU:CD1	1:N:363:LYS:HZ3	2.17	0.55
1:M:496:VAL:HG12	1:M:497:ASP:N	2.22	0.55
1:E:354:THR:HG22	1:E:354:THR:O	2.07	0.55
1:A:78:ALA:O	1:A:89:THR:HG22	2.10	0.55
1:C:50:THR:CG2	1:C:52:ASP:H	2.15	0.55
1:L:41:GLU:HB3	1:M:69:ILE:HD11	1.88	0.55
1:H:307:LYS:HB3	1:H:309:GLU:OE1	2.08	0.55
1:C:526:LYS:CG	1:C:527:PRO:HD2	2.74	0.55
1:D:144:ILE:CD1	1:D:165:MET:HG2	2.37	0.55
1:C:354:THR:HG22	1:C:354:THR:O	2.25	0.55
1:K:518:THR:O	1:K:518:THR:HG22	2.07	0.55
1:E:30:THR:O	1:E:35:GLY:HA3	2.06	0.55
1:E:520:GLU:HB3	1:F:29:VAL:HG11	1.91	0.55
1:F:320:GLU:HB3	1:F:333:GLY:HA3	1.88	0.55
1:D:95:LEU:O	1:D:99:ILE:HG13	2.07	0.55
1:I:360:ALA:O	1:I:364:LEU:HD13	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:80:ILE:CG2	2:R:81:GLU:N	2.76	0.55
1:E:218:PHE:HB3	1:E:316:LEU:HD13	2.55	0.55
1:F:136:ILE:CD1	1:F:477:ARG:HH21	2.20	0.55
2:P:85:GLU:HA	2:P:85:GLU:OE1	2.05	0.55
1:A:234:PRO:HG2	1:A:309:GLU:HA	2.37	0.55
1:E:277:ALA:HB1	1:E:284:ARG:HD2	1.88	0.55
1:N:345:ILE:HG22	1:N:349:LYS:HE3	1.99	0.55
1:C:267:ARG:HH11	1:C:267:ARG:HG3	4.48	0.55
1:M:224:LYS:HG2	1:M:225:LYS:H	1.70	0.55
1:A:411:VAL:HB	1:A:412:PRO:HD2	1.94	0.55
1:A:369:ALA:HB1	1:A:375:VAL:CG2	2.96	0.55
2:P:100:GLN:OXT	2:Q:7:VAL:N	2.92	0.55
1:D:173:ILE:HD12	1:D:366:GLU:CA	3.11	0.55
2:P:11:LEU:O	2:P:12:GLY:C	2.45	0.55
1:G:168:VAL:HG21	1:G:376:ALA:HB2	1.92	0.55
1:A:228:ASN:HD22	1:A:231:GLU:HG3	1.72	0.55
1:A:207:PRO:HB3	1:G:343:ALA:HB2	1.88	0.55
1:G:354:THR:O	1:G:354:THR:HG22	2.22	0.55
1:E:222:VAL:HA	1:E:300:ILE:HB	1.88	0.55
1:N:518:THR:O	1:N:518:THR:HG22	2.05	0.55
1:C:52:ASP:OD1	1:C:54:VAL:HG23	2.07	0.55
1:D:217:ALA:HB2	1:D:245:PRO:HB2	1.89	0.55
1:F:307:LYS:HB2	1:F:310:ASN:HD22	1.87	0.55
1:H:307:LYS:HE3	1:H:310:ASN:ND2	2.21	0.55
1:C:199:ILE:HG23	1:C:276:LYS:HZ2	5.44	0.55
1:I:118:ARG:O	1:I:122:LYS:HG3	2.07	0.55
1:D:307:LYS:HB2	1:D:310:ASN:HD22	1.71	0.55
1:G:189:VAL:HG13	1:G:190:GLU:N	2.21	0.55
1:C:18:ARG:HD2	1:C:67:GLU:OE2	2.07	0.55
1:K:218:PHE:HE1	1:K:242:THR:HG21	1.81	0.55
1:D:6:LEU:CD2	1:D:523:VAL:HG22	2.37	0.55
1:M:316:LEU:H	1:M:316:LEU:CD2	2.20	0.55
1:F:225:LYS:O	1:F:226:VAL:HG23	2.30	0.55
1:E:157:VAL:HG22	1:E:395:PHE:CZ	2.41	0.55
1:F:452:ARG:NH1	1:F:463:SER:HA	2.23	0.55
1:B:230:ARG:O	1:B:234:PRO:HD2	2.08	0.55
2:T:11:LEU:C	2:T:14:ARG:HD2	3.01	0.55
1:F:235:ILE:CG1	1:F:311:ALA:HB3	2.37	0.55
1:A:233:LEU:CD2	2:O:30:ILE:HG21	2.66	0.55
1:M:178:GLU:N	1:M:321:ARG:HH11	2.02	0.55
1:G:325:THR:CG2	1:G:326:LYS:H	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:410:ILE:HB	1:I:496:VAL:HG12	1.89	0.55
1:G:246:LEU:HB3	1:G:272:VAL:CG1	2.35	0.55
1:D:124:VAL:O	1:D:128:VAL:HG23	2.10	0.55
1:G:178:GLU:CG	1:G:388:LEU:HD21	2.36	0.55
1:L:226:VAL:CG1	1:L:232:LEU:HD12	2.40	0.55
1:D:465:ILE:HD13	1:D:480:PHE:CD2	2.52	0.55
1:K:24:ALA:O	1:K:28:LYS:HG2	2.07	0.55
1:N:312:THR:C	1:N:314:SER:H	2.10	0.55
1:M:117:LYS:O	1:M:121:GLU:HG3	2.16	0.55
2:Q:73:ALA:O	2:Q:75:TYR:N	2.40	0.54
1:M:136:ILE:HD11	1:M:491:VAL:HG21	1.97	0.54
2:P:70:VAL:HG11	2:P:95:LEU:CD2	2.30	0.54
1:D:301:SER:HB2	1:D:304:LEU:HB2	1.89	0.54
1:C:366:GLU:O	1:C:370:LYS:HG3	2.06	0.54
1:H:360:ALA:O	1:H:363:LYS:HG2	2.07	0.54
1:F:230:ARG:HA	1:F:233:LEU:HD12	1.88	0.54
1:I:496:VAL:HG12	1:I:497:ASP:H	1.74	0.54
1:J:226:VAL:CG1	1:J:232:LEU:HD12	2.48	0.54
1:J:232:LEU:HD23	1:J:236:LEU:HB2	1.88	0.54
1:F:284:ARG:HG3	1:F:284:ARG:HH11	1.71	0.54
1:L:372:ALA:C	1:L:374:GLY:N	2.60	0.54
1:L:518:THR:O	1:L:518:THR:HG22	2.07	0.54
1:J:490:MET:CE	1:J:490:MET:HA	2.37	0.54
1:D:417:THR:HG23	1:D:418:LEU:HD12	2.00	0.54
1:C:144:ILE:HD12	1:C:165:MET:HG2	2.22	0.54
2:T:48:VAL:CG1	2:T:62:LEU:CD1	3.99	0.54
1:D:168:VAL:HG21	1:D:376:ALA:HB2	1.88	0.54
1:C:222:VAL:O	1:C:250:ALA:HA	2.07	0.54
1:G:366:GLU:O	1:G:370:LYS:HG3	2.07	0.54
1:F:230:ARG:O	1:F:234:PRO:HD2	2.08	0.54
2:O:60:VAL:HG21	2:P:53:VAL:HG11	1.89	0.54
1:H:410:ILE:HB	1:H:496:VAL:HG12	1.88	0.54
1:A:284:ARG:O	1:A:288:LEU:HG	2.07	0.54
1:N:297:GLY:HA3	1:N:317:GLY:H	1.75	0.54
2:R:20:ILE:CG1	2:R:43:GLY:HA2	2.40	0.54
1:J:218:PHE:HE1	1:J:242:THR:HG21	1.74	0.54
1:K:175:THR:HG22	1:K:176:VAL:N	2.22	0.54
1:K:6:LEU:CD2	1:K:523:VAL:HG22	2.47	0.54
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.88	0.54
1:L:258:LEU:O	1:L:262:VAL:HG23	2.11	0.54
1:G:526:LYS:HG3	1:G:527:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:332:VAL:HG22	1:N:375:VAL:HG11	1.92	0.54
1:F:520:GLU:HB3	1:G:29:VAL:HG11	1.89	0.54
1:C:204:VAL:HG11	1:C:210:MET:HA	2.79	0.54
1:D:218:PHE:HE1	1:D:244:LYS:HB2	1.73	0.54
1:D:270:LEU:HG	1:D:272:VAL:HG13	1.94	0.54
1:I:345:ILE:HG22	1:I:349:LYS:HE3	1.97	0.54
1:G:238:GLN:HB3	1:G:313:LEU:HG	2.14	0.54
1:L:297:GLY:HA3	1:L:317:GLY:N	2.20	0.54
1:E:124:VAL:O	1:E:128:VAL:HG23	2.18	0.54
1:K:229:VAL:CG2	1:K:256:GLU:HB3	2.40	0.54
1:D:229:VAL:HG12	1:D:233:LEU:HD11	2.07	0.54
1:A:141:ARG:NH2	1:A:163:ASP:OD1	2.47	0.54
1:G:350:LYS:O	1:G:353:GLU:HG2	3.35	0.54
1:J:123:ALA:HB2	1:J:440:ALA:HA	1.92	0.54
2:R:85:GLU:OE1	2:R:85:GLU:HA	2.08	0.54
2:O:11:LEU:HD11	2:U:98:VAL:HG23	3.18	0.54
1:J:283:ARG:HD3	1:J:363:LYS:NZ	2.22	0.54
1:C:229:VAL:HG12	1:C:233:LEU:HG	2.23	0.54
1:A:220:LEU:HG	1:A:222:VAL:HG23	2.08	0.54
1:L:41:GLU:HB3	1:M:69:ILE:CD1	2.38	0.54
1:L:63:GLU:OE2	1:M:526:LYS:HE2	2.08	0.54
1:M:459:GLY:CA	1:N:114:LEU:HD12	2.37	0.54
1:A:72:GLN:NE2	1:A:75:LYS:NZ	2.68	0.54
1:H:459:GLY:CA	1:I:114:LEU:HD12	2.64	0.54
1:C:147:VAL:CG2	1:C:410:ILE:HD11	2.37	0.54
2:O:22:GLU:N	2:O:22:GLU:OE1	2.35	0.54
1:N:360:ALA:O	1:N:364:LEU:HD12	2.29	0.54
1:N:360:ALA:O	1:N:363:LYS:HG2	2.06	0.54
2:U:12:GLY:HA2	2:U:51:GLY:N	5.09	0.54
1:L:240:ALA:O	1:M:228:ASN:OD1	2.25	0.54
1:J:366:GLU:O	1:J:370:LYS:HG3	2.17	0.54
1:J:128:VAL:HA	1:J:131:ILE:HD12	1.92	0.54
1:F:6:LEU:HD22	1:F:523:VAL:HG22	1.96	0.54
2:Q:15:VAL:CG1	2:Q:45:VAL:HG13	3.78	0.54
1:E:219:ILE:N	1:E:317:GLY:O	2.41	0.54
2:U:71:VAL:O	2:U:95:LEU:HD12	7.76	0.54
1:B:150:ILE:HG22	1:B:151:SER:N	2.53	0.54
1:G:341:ILE:O	1:G:345:ILE:HG22	5.26	0.54
1:K:410:ILE:CD1	1:K:496:VAL:HG11	2.38	0.54
1:J:219:ILE:O	1:J:221:ILE:HG13	2.24	0.54
1:B:173:ILE:HD12	1:B:366:GLU:HA	6.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:445:ARG:CZ	1:G:452:ARG:HH21	2.25	0.54
1:B:468:GLN:O	1:B:471:ALA:HB3	2.22	0.54
1:I:204:VAL:HG13	1:I:211:GLU:O	2.15	0.54
1:I:258:LEU:O	1:I:262:VAL:HG23	2.10	0.54
2:T:41:GLN:HG2	2:T:74:LYS:HB3	1.90	0.54
1:C:361:ARG:O	1:C:365:GLN:HB2	2.08	0.54
1:H:37:ASN:OD1	1:I:515:LEU:HD12	2.35	0.54
1:C:50:THR:HA	1:C:390:GLU:OE1	2.17	0.54
1:D:240:ALA:HA	1:D:270:LEU:HD13	1.90	0.54
1:H:410:ILE:CD1	1:H:496:VAL:HG11	2.35	0.54
1:A:365:GLN:OE1	1:A:365:GLN:HA	2.08	0.54
1:L:69:ILE:O	1:L:73:LEU:HB2	2.15	0.54
2:U:24:PRO:HB2	2:U:37:LYS:NZ	5.60	0.54
1:N:263:VAL:O	1:N:267:ARG:HB2	2.08	0.54
1:K:81:THR:OG1	1:K:508:ASN:ND2	2.59	0.54
1:M:41:GLU:HG2	1:N:524:ALA:HA	1.90	0.54
1:I:283:ARG:HG2	1:I:363:LYS:NZ	2.33	0.54
2:T:78:THR:HG22	2:T:80:ILE:HD11	2.00	0.54
2:U:18:LYS:HG2	2:U:87:TYR:CD2	2.43	0.54
1:B:416:VAL:HG21	1:B:479:GLY:HA3	1.88	0.54
1:C:416:VAL:HG21	1:C:479:GLY:HA3	2.01	0.54
1:J:283:ARG:HH21	1:J:367:ARG:CD	2.34	0.54
1:J:360:ALA:O	1:J:363:LYS:HG3	2.53	0.54
1:B:218:PHE:CE1	1:B:244:LYS:HB2	2.68	0.54
2:Q:33:PRO:C	2:Q:35:THR:N	2.73	0.54
1:E:31:LEU:HB2	1:E:90:THR:HG21	1.89	0.54
1:E:325:THR:CG2	1:E:326:LYS:H	2.14	0.54
1:D:246:LEU:HB3	1:D:272:VAL:CG1	2.34	0.54
1:I:410:ILE:CD1	1:I:496:VAL:HG11	2.35	0.54
1:C:263:VAL:HG13	1:C:267:ARG:NH1	3.85	0.54
1:H:226:VAL:HG11	1:H:232:LEU:HD12	1.89	0.54
1:G:124:VAL:O	1:G:128:VAL:HG23	2.08	0.54
1:J:222:VAL:HG12	1:J:223:GLU:H	1.84	0.54
1:C:360:ALA:O	1:C:364:LEU:HG	2.07	0.54
1:M:218:PHE:HB3	1:M:316:LEU:HG	1.89	0.54
1:D:472:GLU:HB3	1:D:478:TYR:CD2	2.43	0.54
1:M:141:ARG:NH1	1:M:166:GLU:HG3	2.23	0.54
2:T:20:ILE:HD12	2:T:42:LYS:CG	4.09	0.54
2:P:100:GLN:OE1	2:Q:9:LYS:CE	2.56	0.54
1:N:325:THR:HG22	1:N:327:ASP:N	2.04	0.54
1:E:247:LEU:HD22	1:E:322:VAL:CG1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:VAL:HG21	1:F:376:ALA:HB2	1.94	0.54
1:L:50:THR:CG2	1:L:51:LYS:H	2.19	0.54
1:A:37:ASN:ND2	1:G:518:THR:OG1	2.46	0.54
1:F:232:LEU:HB3	1:F:236:LEU:CD1	2.38	0.54
2:T:25:LYS:HD3	2:T:29:GLY:O	2.54	0.54
2:O:63:GLU:OE2	2:P:50:THR:HG21	2.85	0.54
2:R:100:GLN:OE1	2:S:9:LYS:HE2	4.76	0.54
1:M:208:GLU:OE1	1:M:389:LYS:CD	2.55	0.54
1:A:251:GLU:O	1:A:252:ASP:HB2	2.29	0.54
1:N:411:VAL:O	1:N:496:VAL:HG13	2.13	0.54
1:G:261:LEU:O	1:G:265:LYS:HB2	2.08	0.54
1:M:307:LYS:HB3	1:M:309:GLU:OE1	2.08	0.54
1:M:54:VAL:HG22	1:M:89:THR:CG2	2.37	0.54
1:J:316:LEU:O	1:J:316:LEU:HD23	2.08	0.54
1:K:303:GLU:C	1:K:305:GLY:H	2.11	0.54
2:P:52:ARG:O	2:P:52:ARG:HG3	2.22	0.54
1:J:283:ARG:CG	1:J:363:LYS:HZ1	2.48	0.54
1:L:345:ILE:HG22	1:L:349:LYS:HE3	1.89	0.54
1:J:232:LEU:HD23	1:J:232:LEU:O	2.08	0.54
2:S:80:ILE:CG2	2:S:81:GLU:N	2.71	0.54
1:I:226:VAL:CG1	1:I:232:LEU:HD12	2.38	0.54
1:L:218:PHE:HB3	1:L:316:LEU:HG	1.92	0.54
1:J:6:LEU:CD2	1:J:523:VAL:HG22	2.38	0.54
1:C:173:ILE:HD12	1:C:369:ALA:HB2	1.89	0.54
1:I:518:THR:HG22	1:I:518:THR:O	2.09	0.54
1:H:151:SER:HB2	1:H:398:ALA:HA	1.92	0.54
1:L:204:VAL:HG13	1:L:211:GLU:O	2.07	0.54
1:I:352:LEU:HD21	1:I:365:GLN:HE22	1.73	0.53
2:Q:79:GLU:HB2	2:Q:87:TYR:O	4.49	0.53
1:N:360:ALA:O	1:N:364:LEU:CD1	2.62	0.53
2:O:13:ASP:CB	2:O:62:LEU:HD21	2.40	0.53
2:O:55:GLU:HG3	2:P:55:GLU:OE1	3.85	0.53
1:F:235:ILE:HG12	1:F:311:ALA:HB3	1.90	0.53
1:M:247:LEU:HD22	1:M:322:VAL:CG1	2.36	0.53
1:G:54:VAL:HG22	1:G:89:THR:HG21	1.94	0.53
1:D:261:LEU:O	1:D:265:LYS:HB2	2.77	0.53
1:K:40:LEU:HD12	1:K:40:LEU:N	2.28	0.53
1:J:74:LEU:HA	1:J:512:ILE:HD11	2.00	0.53
1:C:515:LEU:HD12	1:D:49:ILE:HG21	2.05	0.53
2:O:8:ILE:HG21	2:O:16:VAL:HG21	1.90	0.53
1:L:455:ALA:HB1	1:L:465:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:226:VAL:CG1	1:M:232:LEU:HD12	2.39	0.53
1:I:452:ARG:HH11	1:I:452:ARG:HG2	1.73	0.53
1:M:135:ALA:O	1:M:137:PRO:HD3	2.08	0.53
1:A:6:LEU:HD22	1:A:523:VAL:HG22	1.95	0.53
1:L:142:LYS:O	1:L:146:GLU:HG3	2.09	0.53
2:S:44:LYS:HA	2:S:68:ASP:O	2.08	0.53
1:A:219:ILE:HG22	1:A:221:ILE:HG13	1.90	0.53
2:R:11:LEU:O	2:R:12:GLY:C	2.46	0.53
2:R:13:ASP:OD1	2:R:13:ASP:C	2.68	0.53
2:O:62:LEU:C	2:O:64:VAL:H	2.14	0.53
2:S:96:LEU:HD23	2:T:14:ARG:NH2	3.78	0.53
1:A:230:ARG:O	1:A:234:PRO:HD2	2.09	0.53
1:B:284:ARG:HG3	1:B:284:ARG:HH11	4.04	0.53
1:B:287:MET:O	1:B:290:ASP:HB2	2.09	0.53
2:T:34:ASP:N	2:T:34:ASP:OD1	2.36	0.53
1:K:168:VAL:HG12	1:K:172:GLY:CA	2.33	0.53
1:B:515:LEU:HD12	1:C:49:ILE:HG21	1.90	0.53
1:N:234:PRO:HG3	1:N:309:GLU:CA	2.36	0.53
1:C:128:VAL:HG13	1:C:503:ARG:HG3	1.93	0.53
1:L:74:LEU:HA	1:L:512:ILE:HD11	1.93	0.53
1:C:466:VAL:HG12	1:C:470:LEU:HD12	1.99	0.53
2:O:8:ILE:H	2:O:8:ILE:HD12	1.74	0.53
1:H:526:LYS:HG3	1:H:527:PRO:HD2	1.90	0.53
1:J:175:THR:HG22	1:J:176:VAL:N	2.25	0.53
1:C:173:ILE:HD12	1:C:369:ALA:CB	2.38	0.53
1:I:95:LEU:O	1:I:99:ILE:HG13	2.08	0.53
1:H:95:LEU:HD21	1:H:450:PRO:HG2	2.05	0.53
1:B:30:THR:O	1:B:35:GLY:HA3	2.15	0.53
2:Q:48:VAL:HG12	2:Q:62:LEU:HD12	4.03	0.53
2:Q:78:THR:CG2	2:Q:79:GLU:N	2.93	0.53
2:O:18:LYS:HE3	2:O:86:GLU:O	2.09	0.53
1:G:293:ALA:O	1:G:336:GLY:HA3	2.52	0.53
1:L:496:VAL:HG12	1:L:497:ASP:N	2.26	0.53
1:M:372:ALA:O	1:M:374:GLY:N	2.38	0.53
1:K:39:VAL:C	1:K:40:LEU:HD12	2.39	0.53
1:H:233:LEU:N	1:H:234:PRO:HD2	2.22	0.53
1:H:229:VAL:CG2	1:H:256:GLU:HB3	2.38	0.53
1:G:144:ILE:HD12	1:G:165:MET:HG2	1.91	0.53
1:H:142:LYS:O	1:H:146:GLU:HG3	2.13	0.53
2:U:44:LYS:HA	2:U:68:ASP:O	2.08	0.53
1:C:341:ILE:C	1:C:343:ALA:H	3.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:GLU:OE2	1:G:326:LYS:NZ	2.23	0.53
1:I:411:VAL:O	1:I:496:VAL:HG13	2.09	0.53
1:H:458:ALA:O	1:I:114:LEU:CD1	3.02	0.53
1:J:224:LYS:HG2	1:J:225:LYS:H	1.73	0.53
2:R:33:PRO:C	2:R:35:THR:H	2.20	0.53
1:C:465:ILE:HD13	1:C:480:PHE:CE2	2.42	0.53
1:F:445:ARG:CZ	1:F:452:ARG:HH21	2.22	0.53
1:D:258:LEU:O	1:D:262:VAL:HG23	2.28	0.53
2:R:52:ARG:HG3	2:R:52:ARG:O	2.09	0.53
1:F:141:ARG:NH2	1:F:163:ASP:OD1	2.45	0.53
1:E:189:VAL:CG1	1:E:190:GLU:N	2.70	0.53
1:N:6:LEU:HD23	1:N:523:VAL:HG22	1.91	0.53
1:I:151:SER:HB2	1:I:398:ALA:HA	1.90	0.53
1:C:340:ASP:O	1:C:344:ARG:HB2	2.09	0.53
1:F:222:VAL:HG22	1:F:300:ILE:HD12	1.91	0.53
2:U:18:LYS:O	2:U:19:ARG:C	2.72	0.53
2:O:54:LEU:CD1	2:P:57:GLY:H	3.53	0.53
1:B:220:LEU:HD23	1:B:248:ILE:HG23	2.37	0.53
1:E:278:PRO:HG3	1:E:291:ILE:HD11	1.90	0.53
1:F:349:LYS:C	1:F:351:GLU:H	2.11	0.53
1:D:198:TYR:O	1:D:198:TYR:HD1	1.92	0.53
1:L:411:VAL:O	1:L:496:VAL:HG13	2.20	0.53
1:E:304:LEU:O	1:F:259:ALA:HB1	5.12	0.53
2:P:53:VAL:HG22	2:P:59:ARG:HE	1.74	0.53
1:K:226:VAL:HG11	1:K:232:LEU:HD12	1.95	0.53
1:H:263:VAL:O	1:H:267:ARG:HB2	2.09	0.53
2:S:8:ILE:CG2	2:S:16:VAL:HG21	2.49	0.53
1:A:202:TYR:CE1	1:G:289:LYS:NZ	2.71	0.53
1:E:465:ILE:HD13	1:E:480:PHE:CE2	2.51	0.53
1:N:316:LEU:HD23	1:N:316:LEU:O	2.09	0.53
1:K:421:ALA:O	1:K:425:VAL:HG23	2.08	0.53
1:B:184:THR:HG23	1:B:380:VAL:HA	1.96	0.53
1:A:258:LEU:O	1:A:262:VAL:HG23	2.23	0.53
1:E:392:LYS:O	1:E:396:GLU:HG3	2.11	0.53
1:B:392:LYS:O	1:B:396:GLU:HG3	2.21	0.53
1:D:477:ARG:HH11	1:D:477:ARG:HG3	1.74	0.53
1:D:150:ILE:CD1	1:D:496:VAL:N	2.72	0.53
1:B:233:LEU:O	1:B:237:GLU:HG3	2.10	0.53
1:G:235:ILE:O	1:G:239:VAL:HG23	2.44	0.53
1:J:219:ILE:HB	1:J:295:THR:HG21	1.91	0.53
1:H:458:ALA:C	1:I:114:LEU:CD1	3.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:VAL:HG12	1:L:223:GLU:H	1.77	0.53
1:N:218:PHE:HE1	1:N:242:THR:HG21	1.72	0.53
1:H:201:PRO:O	1:H:204:VAL:HG23	2.08	0.53
1:B:144:ILE:HD12	1:B:165:MET:HG2	1.89	0.53
1:C:418:LEU:HD12	1:C:418:LEU:H	1.79	0.53
1:E:201:PRO:O	1:E:204:VAL:HG22	2.09	0.53
1:G:150:ILE:CD1	1:G:496:VAL:H	2.39	0.53
1:F:410:ILE:HD11	1:F:496:VAL:HG21	1.96	0.53
1:A:136:ILE:O	1:A:410:ILE:HG22	2.27	0.53
1:F:240:ALA:HA	1:F:270:LEU:HD13	1.90	0.53
1:B:287:MET:O	1:B:291:ILE:HG13	2.36	0.53
1:N:40:LEU:HD12	1:N:40:LEU:N	2.31	0.53
1:A:149:THR:HG23	1:A:155:PRO:CA	2.43	0.53
1:B:189:VAL:HG13	1:B:190:GLU:N	2.24	0.53
1:K:218:PHE:HB3	1:K:316:LEU:HG	1.90	0.53
1:K:25:ASN:HA	1:K:28:LYS:HE2	1.90	0.53
1:L:28:LYS:NZ	1:L:97:GLN:HE22	2.07	0.53
1:K:142:LYS:O	1:K:146:GLU:HG3	2.09	0.53
1:C:192:TYR:CD2	1:C:192:TYR:C	3.40	0.53
2:P:21:GLU:CD	2:P:21:GLU:H	2.46	0.53
1:E:238:GLN:HB3	1:E:313:LEU:HG	1.90	0.53
2:T:92:GLU:HA	2:T:95:LEU:HD12	1.99	0.53
1:D:301:SER:HB2	1:D:304:LEU:CB	2.38	0.53
1:E:168:VAL:HG12	1:E:168:VAL:O	2.09	0.53
1:M:323:ARG:HH12	1:M:392:LYS:HE2	1.69	0.53
1:E:368:LEU:O	1:E:368:LEU:HD12	5.50	0.53
1:E:224:LYS:HD2	1:E:224:LYS:H	1.74	0.53
1:A:270:LEU:HG	1:A:272:VAL:HG13	2.04	0.53
1:K:259:ALA:O	1:K:263:VAL:HG23	2.28	0.53
1:J:194:PHE:CG	1:J:278:PRO:HB3	2.44	0.53
1:G:72:GLN:HE22	1:G:75:LYS:HZ3	1.57	0.53
1:K:337:LYS:HB2	1:K:340:ASP:OD2	2.12	0.53
1:I:6:LEU:HD23	1:I:523:VAL:HG22	1.90	0.53
1:D:289:LYS:O	1:D:292:ALA:HB3	2.37	0.53
1:L:259:ALA:O	1:L:263:VAL:HG23	2.08	0.53
1:L:263:VAL:O	1:L:267:ARG:HB2	2.14	0.53
1:N:28:LYS:NZ	1:N:97:GLN:HE22	2.07	0.53
1:A:520:GLU:HB3	1:B:29:VAL:HG11	1.92	0.53
1:I:363:LYS:O	1:I:366:GLU:HG2	2.15	0.53
1:B:228:ASN:HD21	1:B:230:ARG:HB2	1.74	0.53
1:E:321:ARG:O	1:E:322:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:HB3	1:C:209:THR:OG1	2.08	0.53
1:C:234:PRO:O	1:C:238:GLN:HG3	2.28	0.53
2:O:81:GLU:HA	2:O:85:GLU:O	2.09	0.53
1:C:168:VAL:HG21	1:C:376:ALA:HB2	1.95	0.53
1:E:287:MET:O	1:E:290:ASP:HB2	2.08	0.53
1:E:294:VAL:HG23	1:E:295:THR:N	2.24	0.53
1:M:383:ALA:HB1	1:N:359:TYR:OH	2.08	0.53
1:N:118:ARG:O	1:N:122:LYS:HG3	2.13	0.53
1:G:229:VAL:HG23	1:G:256:GLU:HG3	2.04	0.53
1:E:466:VAL:HG12	1:E:470:LEU:HD12	1.91	0.53
1:N:226:VAL:CG1	1:N:232:LEU:HD12	2.75	0.53
1:A:445:ARG:CZ	1:A:452:ARG:HH21	2.33	0.53
2:P:44:LYS:HA	2:P:68:ASP:O	2.09	0.53
1:E:372:ALA:O	1:E:374:GLY:N	4.33	0.53
1:N:141:ARG:NH1	1:N:166:GLU:HG3	2.24	0.53
1:K:283:ARG:NH2	1:K:367:ARG:CD	2.80	0.53
1:N:283:ARG:HG2	1:N:363:LYS:NZ	2.24	0.53
1:A:168:VAL:HG21	1:A:376:ALA:HB2	1.94	0.53
2:P:13:ASP:CB	2:P:62:LEU:HD21	2.37	0.53
2:Q:53:VAL:HG22	2:Q:59:ARG:HG2	1.91	0.53
1:D:7:VAL:HG21	1:D:66:LEU:CD1	2.29	0.53
1:B:7:VAL:HG12	1:B:12:ALA:HB2	1.91	0.53
1:B:360:ALA:O	1:B:364:LEU:HG	2.09	0.53
1:J:117:LYS:O	1:J:121:GLU:HG3	2.09	0.53
1:F:416:VAL:HG21	1:F:479:GLY:HA3	1.93	0.53
1:A:229:VAL:HG23	1:A:256:GLU:CD	2.29	0.53
1:D:184:THR:HG23	1:D:380:VAL:HA	1.90	0.53
1:L:239:VAL:HG22	1:L:313:LEU:CD1	2.44	0.53
1:C:320:GLU:HB3	1:C:333:GLY:HA3	1.91	0.53
2:Q:81:GLU:CD	2:Q:84:GLY:HA2	3.42	0.52
2:T:52:ARG:NH2	2:U:53:VAL:HB	2.21	0.52
1:E:147:VAL:CG2	1:E:410:ILE:HD11	2.38	0.52
1:J:283:ARG:HG2	1:J:363:LYS:HZ2	1.74	0.52
1:B:235:ILE:HD12	1:B:311:ALA:HB3	2.25	0.52
1:C:347:GLY:O	1:C:351:GLU:HB2	2.08	0.52
1:C:128:VAL:HA	1:C:131:ILE:HD12	1.91	0.52
1:D:368:LEU:HD12	1:D:368:LEU:O	2.09	0.52
1:B:368:LEU:HD12	1:B:368:LEU:O	2.20	0.52
1:M:142:LYS:O	1:M:146:GLU:HG3	2.08	0.52
2:O:53:VAL:HG22	2:O:59:ARG:HG2	1.90	0.52
1:M:421:ALA:O	1:M:425:VAL:HG23	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:THR:HB	1:F:377:VAL:HG22	1.91	0.52
1:I:283:ARG:HD3	1:I:363:LYS:NZ	2.25	0.52
1:B:263:VAL:HG21	2:P:33:PRO:HB3	3.12	0.52
1:D:363:LYS:C	1:D:365:GLN:N	2.86	0.52
2:T:63:GLU:HB3	2:U:11:LEU:CD1	5.11	0.52
1:M:228:ASN:HB3	1:M:231:GLU:HG2	1.96	0.52
1:F:235:ILE:HD11	1:F:311:ALA:HB1	2.49	0.52
1:F:52:ASP:OD1	1:F:54:VAL:HG23	2.09	0.52
2:S:10:PRO:C	2:S:11:LEU:HD12	2.30	0.52
1:L:39:VAL:O	1:M:522:VAL:HA	2.35	0.52
1:A:363:LYS:HA	1:A:366:GLU:HG2	2.70	0.52
1:L:283:ARG:HD3	1:L:363:LYS:NZ	2.24	0.52
1:H:458:ALA:C	1:I:114:LEU:HD12	2.81	0.52
1:I:7:VAL:HG12	1:I:12:ALA:HB2	1.96	0.52
1:J:458:ALA:O	1:K:114:LEU:CD1	2.56	0.52
1:B:345:ILE:HG23	1:B:368:LEU:CD1	2.39	0.52
1:B:307:LYS:HD3	1:B:309:GLU:OE2	2.09	0.52
1:F:340:ASP:O	1:F:344:ARG:HB2	2.10	0.52
1:F:40:LEU:HD13	1:F:59:GLU:HG3	1.96	0.52
2:R:14:ARG:HH11	2:R:14:ARG:CG	2.37	0.52
2:Q:52:ARG:NH2	2:R:53:VAL:HB	2.24	0.52
1:F:518:THR:OG1	1:G:37:ASN:ND2	2.41	0.52
1:I:50:THR:CG2	1:I:51:LYS:H	2.16	0.52
1:E:278:PRO:CG	1:E:291:ILE:HD11	2.39	0.52
1:H:40:LEU:HD12	1:H:40:LEU:N	2.30	0.52
1:G:253:VAL:HG12	1:G:258:LEU:HB2	1.91	0.52
1:G:258:LEU:O	1:G:262:VAL:HG23	2.09	0.52
1:A:128:VAL:HG13	1:A:503:ARG:HG3	1.90	0.52
2:S:17:VAL:O	2:S:87:TYR:HB3	2.29	0.52
1:H:175:THR:HG22	1:H:176:VAL:N	2.25	0.52
1:N:131:ILE:HD13	1:N:502:THR:HG22	1.92	0.52
1:I:218:PHE:HB3	1:I:316:LEU:HG	1.93	0.52
1:F:222:VAL:O	1:F:250:ALA:HA	2.10	0.52
1:G:425:VAL:O	1:G:429:ILE:HG13	2.17	0.52
1:N:151:SER:HB2	1:N:398:ALA:HA	1.91	0.52
1:J:142:LYS:O	1:J:146:GLU:HG3	2.10	0.52
2:T:38:GLU:OE1	2:T:74:LYS:NZ	2.34	0.52
2:Q:16:VAL:CG1	2:Q:46:ILE:HB	3.35	0.52
1:A:347:GLY:O	1:A:351:GLU:HB2	2.27	0.52
1:M:283:ARG:HH22	1:M:364:LEU:HA	1.87	0.52
1:A:150:ILE:HG22	1:A:151:SER:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:THR:HG22	1:F:244:LYS:HG2	2.32	0.52
1:K:168:VAL:HG11	1:K:173:ILE:N	2.24	0.52
1:L:41:GLU:OE2	1:M:65:HIS:ND1	2.42	0.52
1:G:348:ILE:CD1	1:G:367:ARG:NE	3.45	0.52
1:H:297:GLY:HA3	1:H:317:GLY:H	1.74	0.52
1:D:498:PRO:HG2	1:D:501:VAL:HG22	2.06	0.52
1:A:466:VAL:HG12	1:A:470:LEU:HD12	1.91	0.52
1:J:526:LYS:CD	1:J:527:PRO:HD2	2.40	0.52
1:L:458:ALA:O	1:M:114:LEU:HD12	2.09	0.52
1:N:141:ARG:HH11	1:N:166:GLU:HG3	1.74	0.52
1:A:396:GLU:O	1:A:400:ASN:ND2	2.63	0.52
1:N:123:ALA:HB2	1:N:440:ALA:HA	1.94	0.52
1:K:283:ARG:HG2	1:K:363:LYS:NZ	2.34	0.52
1:I:283:ARG:HH11	1:I:363:LYS:CE	2.60	0.52
2:U:45:VAL:HG22	2:U:70:VAL:HG13	5.25	0.52
1:F:7:VAL:HG12	1:F:12:ALA:HB2	1.90	0.52
1:L:168:VAL:HG12	1:L:172:GLY:CA	2.36	0.52
1:G:214:LEU:HB3	1:G:245:PRO:CB	2.99	0.52
1:H:234:PRO:HG3	1:H:309:GLU:CA	2.41	0.52
1:K:352:LEU:HD21	1:K:365:GLN:HE22	1.87	0.52
1:L:363:LYS:O	1:L:366:GLU:HG2	2.16	0.52
1:A:118:ARG:O	1:A:122:LYS:HG3	2.10	0.52
1:D:348:ILE:HG21	1:D:364:LEU:O	2.17	0.52
2:P:8:ILE:HG21	2:P:16:VAL:HG21	1.91	0.52
1:E:448:GLU:OE1	1:E:452:ARG:NH2	2.43	0.52
1:F:144:ILE:CD1	1:F:165:MET:HG2	2.40	0.52
1:F:25:ASN:HA	1:F:28:LYS:HG2	1.94	0.52
1:L:151:SER:HB2	1:L:398:ALA:HA	1.91	0.52
1:N:283:ARG:HD3	1:N:363:LYS:HZ1	2.23	0.52
1:E:416:VAL:HG21	1:E:479:GLY:HA3	1.94	0.52
1:A:207:PRO:CB	1:G:343:ALA:HB2	2.41	0.52
1:N:168:VAL:HG12	1:N:172:GLY:CA	2.37	0.52
1:F:305:GLY:HA2	2:U:33:PRO:HB2	3.08	0.52
1:L:175:THR:HG22	1:L:176:VAL:N	2.25	0.52
1:H:218:PHE:HB3	1:H:316:LEU:HG	1.91	0.52
1:C:452:ARG:NH1	1:C:463:SER:HA	2.25	0.52
1:D:293:ALA:HB1	1:D:340:ASP:HB3	1.92	0.52
1:D:157:VAL:HG22	1:D:395:PHE:CZ	2.45	0.52
1:M:141:ARG:HH11	1:M:166:GLU:HG3	1.74	0.52
1:D:349:LYS:C	1:D:351:GLU:H	2.19	0.52
1:L:141:ARG:NH1	1:L:166:GLU:HG3	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:99:LEU:HD21	2:R:8:ILE:HG13	6.42	0.52
2:O:48:VAL:CG1	2:O:62:LEU:CD1	2.83	0.52
2:T:69:ILE:HB	2:T:99:LEU:HD12	5.07	0.52
1:M:168:VAL:HG11	1:M:173:ILE:N	2.25	0.52
2:R:50:THR:CG2	2:R:59:ARG:HD3	2.40	0.52
1:D:304:LEU:HD11	1:E:262:VAL:HG11	1.90	0.52
1:B:232:LEU:O	1:B:235:ILE:HG22	2.09	0.52
1:G:361:ARG:O	1:G:365:GLN:HB2	2.08	0.52
2:S:45:VAL:HG21	2:S:64:VAL:CG1	2.39	0.52
1:E:209:THR:CG2	1:E:211:GLU:HG3	2.32	0.52
1:A:363:LYS:C	1:A:365:GLN:N	2.84	0.52
1:E:131:ILE:HD13	1:E:502:THR:HG22	1.92	0.52
1:H:54:VAL:HG22	1:H:89:THR:CG2	2.39	0.52
1:D:466:VAL:HG12	1:D:470:LEU:HD12	1.92	0.52
1:K:458:ALA:O	1:L:114:LEU:HD12	2.15	0.52
1:K:131:ILE:HD13	1:K:502:THR:HG22	2.06	0.52
1:N:175:THR:HG22	1:N:176:VAL:N	2.25	0.52
1:L:141:ARG:HH11	1:L:166:GLU:HG3	1.77	0.52
1:J:258:LEU:O	1:J:262:VAL:HG23	2.14	0.52
1:A:277:ALA:HB1	1:A:278:PRO:HD2	1.91	0.52
1:G:468:GLN:O	1:G:471:ALA:HB3	2.17	0.52
2:U:15:VAL:HG23	2:U:47:ALA:O	5.83	0.52
1:C:201:PRO:O	1:C:203:PHE:N	3.29	0.52
1:H:283:ARG:NH2	1:H:367:ARG:CD	2.73	0.52
1:C:7:VAL:HG12	1:C:12:ALA:HB2	1.92	0.52
1:I:168:VAL:HG12	1:I:172:GLY:CA	2.35	0.52
1:H:7:VAL:HG12	1:H:12:ALA:HB2	1.92	0.52
2:Q:39:LYS:HB3	2:Q:40:PRO:HD2	2.79	0.52
1:G:289:LYS:HB2	1:G:344:ARG:NH2	2.88	0.52
1:B:345:ILE:HG22	1:B:346:ASN:N	2.25	0.52
2:T:56:ASN:O	2:T:58:GLN:N	2.43	0.52
1:G:237:GLU:CD	2:U:28:GLY:HA3	3.90	0.52
1:C:144:ILE:CD1	1:C:165:MET:HG2	2.55	0.52
1:H:518:THR:O	1:H:518:THR:HG22	2.10	0.52
1:J:462:GLY:O	1:J:466:VAL:HG23	2.09	0.52
1:B:157:VAL:HG22	1:B:395:PHE:CZ	2.48	0.52
1:C:141:ARG:NH2	1:C:163:ASP:OD1	2.43	0.52
1:C:10:GLU:N	1:C:13:ARG:HH12	2.28	0.52
1:N:372:ALA:C	1:N:374:GLY:H	2.16	0.52
2:T:21:GLU:H	2:T:21:GLU:CD	2.13	0.52
1:N:283:ARG:NH2	1:N:367:ARG:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:8:ILE:HG22	2:T:16:VAL:HG21	2.60	0.52
2:T:90:LEU:HD12	2:T:90:LEU:N	4.13	0.52
2:O:96:LEU:O	2:P:14:ARG:HD3	2.09	0.52
1:C:220:LEU:HD13	1:C:235:ILE:CD1	3.01	0.52
1:C:283:ARG:NH1	1:C:363:LYS:HD2	3.24	0.52
1:C:290:ASP:OD2	1:C:371:LEU:HD11	2.10	0.52
1:L:180:LYS:O	1:M:281:GLY:N	2.43	0.52
1:A:235:ILE:HD11	1:A:316:LEU:HD21	1.91	0.52
1:A:39:VAL:HG23	1:G:519:THR:HG23	2.08	0.52
1:M:39:VAL:C	1:M:40:LEU:HD12	2.30	0.52
1:H:292:ALA:HB1	1:H:297:GLY:O	2.09	0.52
1:G:118:ARG:O	1:G:122:LYS:HG3	2.13	0.52
1:J:114:LEU:O	1:J:118:ARG:HG3	2.27	0.52
1:J:177:GLU:HB3	1:J:321:ARG:NH1	2.31	0.52
1:B:445:ARG:CZ	1:B:452:ARG:HH21	2.28	0.52
1:E:452:ARG:NH1	1:E:463:SER:HA	2.24	0.52
1:F:30:THR:O	1:F:35:GLY:HA3	2.10	0.52
1:D:416:VAL:HG21	1:D:479:GLY:HA3	1.92	0.52
2:T:13:ASP:OD1	2:T:13:ASP:C	2.48	0.52
1:C:265:LYS:HD3	1:C:272:VAL:H	2.26	0.52
1:C:235:ILE:HD12	1:C:311:ALA:HB1	3.95	0.52
1:E:284:ARG:O	1:E:288:LEU:HG	2.13	0.52
1:E:294:VAL:HG23	1:E:295:THR:HG23	1.92	0.52
2:T:32:LEU:HD13	2:T:36:ALA:HB1	4.90	0.52
1:L:168:VAL:CG1	1:L:173:ILE:H	2.26	0.52
1:J:40:LEU:N	1:J:40:LEU:HD12	2.25	0.52
1:I:307:LYS:HB3	1:I:309:GLU:OE1	2.10	0.52
1:L:79:SER:O	1:L:81:THR:N	2.43	0.52
1:I:142:LYS:O	1:I:146:GLU:HG3	2.08	0.52
1:I:6:LEU:CD2	1:I:523:VAL:HG22	2.40	0.52
1:A:392:LYS:O	1:A:396:GLU:HG3	2.09	0.52
1:F:144:ILE:HD12	1:F:165:MET:HG2	1.92	0.52
1:E:418:LEU:HD12	1:E:418:LEU:H	1.75	0.52
1:N:142:LYS:O	1:N:146:GLU:HG3	2.10	0.52
1:A:356:ASP:O	1:A:357:SER:C	2.50	0.52
1:K:141:ARG:HH11	1:K:166:GLU:HG3	1.75	0.52
1:K:141:ARG:NH1	1:K:166:GLU:HG3	2.25	0.52
1:K:283:ARG:HH22	1:K:364:LEU:HA	1.84	0.51
1:E:256:GLU:OE1	2:S:35:THR:O	3.36	0.51
2:U:46:ILE:O	2:U:46:ILE:HG22	2.28	0.51
2:U:62:LEU:C	2:U:64:VAL:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:CD1	1:A:477:ARG:HH21	2.23	0.51
1:A:150:ILE:CD1	1:A:496:VAL:H	2.27	0.51
1:C:283:ARG:O	1:C:287:MET:HG3	2.10	0.51
1:K:189:VAL:HG12	1:K:333:GLY:HA2	2.35	0.51
1:H:168:VAL:CG1	1:H:173:ILE:H	2.24	0.51
1:B:304:LEU:O	1:C:263:VAL:HG22	4.24	0.51
1:B:465:ILE:HD13	1:B:480:PHE:CE2	2.44	0.51
1:J:84:VAL:O	1:J:84:VAL:HG12	2.11	0.51
1:H:452:ARG:NH1	1:H:452:ARG:HG2	2.24	0.51
1:H:316:LEU:O	1:H:316:LEU:HD23	2.12	0.51
1:D:101:ARG:CG	1:D:102:GLU:N	2.73	0.51
1:L:6:LEU:CD2	1:L:523:VAL:HG22	2.49	0.51
1:D:144:ILE:HD12	1:D:165:MET:HG2	1.91	0.51
1:I:65:HIS:O	1:I:69:ILE:HG13	2.11	0.51
1:H:481:ASN:HD21	1:H:484:THR:HG23	1.75	0.51
1:E:184:THR:HG23	1:E:380:VAL:HA	1.91	0.51
1:I:131:ILE:HD13	1:I:502:THR:HG22	1.92	0.51
1:N:437:ALA:O	1:N:441:LYS:HG3	2.09	0.51
1:E:235:ILE:HD11	1:E:316:LEU:HD21	7.03	0.51
2:T:99:LEU:HD23	2:U:8:ILE:HD11	8.00	0.51
1:M:411:VAL:O	1:M:496:VAL:HG13	2.11	0.51
2:O:93:ARG:O	2:P:14:ARG:NH2	2.50	0.51
1:M:175:THR:HG22	1:M:176:VAL:N	2.26	0.51
1:K:168:VAL:HG21	1:K:376:ALA:HB2	1.93	0.51
1:E:326:LYS:HD3	1:E:326:LYS:C	2.30	0.51
1:G:248:ILE:CD1	1:G:261:LEU:HD21	2.65	0.51
1:K:295:THR:HG22	1:K:317:GLY:HA3	1.92	0.51
1:J:295:THR:HG22	1:J:317:GLY:HA3	2.02	0.51
1:K:194:PHE:CG	1:K:278:PRO:HB3	2.50	0.51
1:D:498:PRO:HG2	1:D:501:VAL:CG2	2.52	0.51
2:R:33:PRO:HG2	2:R:36:ALA:HB2	2.29	0.51
1:F:361:ARG:O	1:F:365:GLN:HB2	2.16	0.51
1:G:25:ASN:HA	1:G:28:LYS:HG2	1.92	0.51
1:A:224:LYS:HB3	1:A:302:GLU:OE1	2.13	0.51
1:I:141:ARG:NH1	1:I:166:GLU:HG3	2.27	0.51
2:O:78:THR:HG22	2:O:80:ILE:HD11	1.92	0.51
1:H:283:ARG:CG	1:H:363:LYS:NZ	3.05	0.51
1:M:178:GLU:C	1:M:321:ARG:NH1	2.61	0.51
1:E:209:THR:HG22	1:E:211:GLU:CG	2.36	0.51
1:G:213:VAL:O	1:G:214:LEU:HD23	2.64	0.51
1:N:222:VAL:HG12	1:N:223:GLU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:408:GLU:HB2	1:L:500:LYS:HB2	2.04	0.51
1:A:202:TYR:CZ	1:G:289:LYS:NZ	2.72	0.51
1:H:6:LEU:CD2	1:H:523:VAL:HG22	2.41	0.51
1:D:289:LYS:NZ	1:E:202:TYR:CE1	2.77	0.51
1:C:10:GLU:N	1:C:13:ARG:NH1	2.69	0.51
1:L:128:VAL:HA	1:L:131:ILE:HD12	1.95	0.51
1:J:518:THR:HG22	1:J:518:THR:O	2.12	0.51
1:H:141:ARG:NH1	1:H:166:GLU:HG3	2.25	0.51
1:B:10:GLU:N	1:B:13:ARG:NH1	2.58	0.51
1:C:6:LEU:HD22	1:C:523:VAL:HG22	1.91	0.51
2:R:71:VAL:HG23	2:R:99:LEU:HD13	2.08	0.51
1:J:421:ALA:O	1:J:425:VAL:HG23	2.11	0.51
1:M:481:ASN:HD21	1:M:484:THR:HG23	1.74	0.51
2:T:14:ARG:HG2	2:T:14:ARG:NH1	3.13	0.51
1:A:234:PRO:O	1:A:238:GLN:HG3	2.13	0.51
1:B:246:LEU:CB	1:B:272:VAL:HG12	2.49	0.51
1:A:52:ASP:OD1	1:A:54:VAL:HG23	2.10	0.51
2:R:100:GLN:OE1	2:S:9:LYS:CE	3.95	0.51
1:L:179:SER:CB	1:L:379:ARG:HB3	2.37	0.51
1:J:410:ILE:CD1	1:J:496:VAL:HG11	2.39	0.51
1:E:498:PRO:HG2	1:E:501:VAL:CG2	2.40	0.51
1:F:18:ARG:HD2	1:F:67:GLU:OE2	2.10	0.51
1:D:229:VAL:HG21	2:R:36:ALA:CB	2.39	0.51
1:H:525:GLU:N	1:N:41:GLU:OE2	2.37	0.51
1:E:465:ILE:HD13	1:E:480:PHE:CD2	2.50	0.51
1:H:127:ALA:O	1:H:131:ILE:HG13	2.14	0.51
1:N:25:ASN:HA	1:N:28:LYS:HE2	1.91	0.51
1:I:128:VAL:HA	1:I:131:ILE:HD12	1.94	0.51
1:K:151:SER:HB2	1:K:398:ALA:HA	1.94	0.51
1:C:457:ASN:N	1:C:457:ASN:HD22	2.08	0.51
1:I:416:VAL:HG21	1:I:479:GLY:HA3	1.98	0.51
2:T:48:VAL:HG13	2:T:62:LEU:HD13	4.02	0.51
2:P:17:VAL:HG12	2:P:18:LYS:N	2.24	0.51
1:C:235:ILE:HD12	1:C:311:ALA:CB	3.88	0.51
1:C:251:GLU:HG3	1:C:284:ARG:NH1	2.13	0.51
1:I:168:VAL:CG1	1:I:173:ILE:H	2.24	0.51
1:K:297:GLY:HA3	1:K:317:GLY:N	2.26	0.51
1:A:131:ILE:HD13	1:A:502:THR:HG22	1.91	0.51
1:E:128:VAL:HG13	1:E:503:ARG:HG3	1.96	0.51
1:H:232:LEU:HD23	1:H:232:LEU:O	2.10	0.51
2:S:73:ALA:O	2:S:75:TYR:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:TYR:OH	1:G:289:LYS:CE	2.58	0.51
1:I:175:THR:HG22	1:I:176:VAL:N	2.27	0.51
1:H:340:ASP:O	1:H:343:ALA:HB3	2.09	0.51
1:I:455:ALA:HB1	1:I:465:ILE:HD12	2.01	0.51
1:G:231:GLU:HB3	1:G:308:LEU:HB3	2.32	0.51
1:F:101:ARG:CG	1:F:102:GLU:N	2.73	0.51
1:M:6:LEU:CD2	1:M:523:VAL:HG22	2.41	0.51
1:I:421:ALA:O	1:I:425:VAL:HG23	2.20	0.51
1:J:151:SER:HB2	1:J:398:ALA:HA	1.92	0.51
1:E:256:GLU:O	2:S:33:PRO:HG2	4.15	0.51
1:E:267:ARG:CD	2:S:31:VAL:HG21	2.36	0.51
2:P:41:GLN:HE21	2:P:74:LYS:HG2	1.76	0.51
2:O:46:ILE:O	2:O:46:ILE:HG22	2.25	0.51
2:T:54:LEU:HD21	2:T:60:VAL:HG21	4.02	0.51
1:G:416:VAL:HG21	1:G:479:GLY:HA3	1.94	0.51
1:J:168:VAL:HG11	1:J:173:ILE:N	2.26	0.51
1:D:220:LEU:HG	1:D:222:VAL:HG23	1.97	0.51
1:D:242:THR:HG22	1:D:244:LYS:HG2	1.94	0.51
1:C:224:LYS:CE	1:C:301:SER:HA	6.88	0.51
2:Q:20:ILE:HG13	2:Q:43:GLY:CA	2.58	0.51
1:G:348:ILE:HD11	1:G:367:ARG:CZ	3.08	0.51
1:B:128:VAL:HG13	1:B:503:ARG:HG3	1.94	0.51
1:B:466:VAL:HG12	1:B:470:LEU:HD12	1.96	0.51
1:N:54:VAL:HG22	1:N:89:THR:CG2	2.47	0.51
1:G:144:ILE:CD1	1:G:165:MET:HG2	2.40	0.51
1:I:127:ALA:O	1:I:131:ILE:HG13	2.10	0.51
1:M:127:ALA:O	1:M:131:ILE:HG13	2.10	0.51
1:M:151:SER:HB2	1:M:398:ALA:HA	1.92	0.51
1:B:286:GLU:OE1	1:B:344:ARG:NH2	2.42	0.51
1:D:136:ILE:O	1:D:410:ILE:HG22	2.34	0.51
2:Q:96:LEU:O	2:R:14:ARG:HD3	2.11	0.51
1:D:359:TYR:CE1	1:D:363:LYS:HE2	2.45	0.51
1:N:283:ARG:HH21	1:N:367:ARG:CD	2.24	0.51
2:T:45:VAL:HG21	2:T:64:VAL:CG1	2.40	0.51
2:P:80:ILE:HG22	2:P:81:GLU:H	1.76	0.51
1:C:292:ALA:O	1:C:293:ALA:C	2.78	0.51
1:F:202:TYR:CD2	1:F:266:LEU:HD11	2.54	0.51
1:L:496:VAL:HG12	1:L:497:ASP:H	1.80	0.51
2:S:53:VAL:HG22	2:S:59:ARG:CG	2.73	0.51
1:I:222:VAL:HG12	1:I:223:GLU:H	1.75	0.51
1:K:177:GLU:HB3	1:K:321:ARG:NH1	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:44:LYS:HA	2:R:68:ASP:O	2.11	0.51
1:A:468:GLN:O	1:A:471:ALA:HB3	2.11	0.51
2:U:17:VAL:HG13	2:U:44:LYS:N	2.89	0.51
1:M:136:ILE:HD11	1:M:491:VAL:HG22	1.91	0.51
2:O:100:GLN:CG	2:P:9:LYS:HE2	2.77	0.51
1:C:232:LEU:O	1:C:235:ILE:HG22	5.35	0.51
1:I:141:ARG:HH11	1:I:166:GLU:HG3	1.77	0.51
1:E:10:GLU:N	1:E:13:ARG:NH1	2.59	0.51
1:F:80:LYS:HE2	1:G:383:ALA:O	2.22	0.51
1:G:14:ARG:NH1	1:G:17:GLU:OE1	2.44	0.51
1:B:258:LEU:O	1:B:262:VAL:HG23	2.45	0.51
2:P:98:VAL:O	2:Q:9:LYS:HB2	2.11	0.51
2:T:79:GLU:O	2:T:80:ILE:HG13	2.10	0.51
1:M:168:VAL:CG1	1:M:173:ILE:H	2.24	0.51
2:Q:52:ARG:NH1	2:Q:52:ARG:HG2	4.58	0.51
1:D:519:THR:HG23	1:E:39:VAL:HG23	1.92	0.51
1:C:348:ILE:CD1	1:C:367:ARG:HB3	3.03	0.51
1:J:39:VAL:C	1:J:40:LEU:HD12	2.37	0.51
1:N:342:GLU:HA	1:N:345:ILE:HD12	1.93	0.51
1:G:219:ILE:HG22	1:G:221:ILE:HG13	1.93	0.51
1:L:219:ILE:O	1:L:221:ILE:HG13	2.19	0.51
1:L:295:THR:HG22	1:L:317:GLY:HA3	1.93	0.51
1:E:149:THR:HG23	1:E:155:PRO:CA	2.37	0.51
1:N:84:VAL:HG12	1:N:84:VAL:O	2.10	0.51
1:J:194:PHE:CB	1:J:278:PRO:HB3	2.41	0.51
1:H:222:VAL:CG1	1:H:223:GLU:N	2.77	0.51
1:A:101:ARG:CG	1:A:102:GLU:N	2.76	0.51
1:C:74:LEU:HD21	1:C:93:THR:CG2	2.41	0.51
1:H:449:GLU:HB2	1:H:450:PRO:HD3	2.00	0.51
1:M:128:VAL:HA	1:M:131:ILE:HD12	1.97	0.51
1:E:249:ILE:HD11	1:E:331:ILE:HD11	1.93	0.51
2:S:21:GLU:H	2:S:21:GLU:CD	2.15	0.51
1:J:141:ARG:NH1	1:J:166:GLU:HG3	2.26	0.51
1:J:95:LEU:O	1:J:99:ILE:HG13	2.13	0.51
2:Q:41:GLN:HA	2:Q:74:LYS:HB3	2.52	0.51
1:C:209:THR:CG2	1:C:211:GLU:HG2	5.92	0.51
1:C:229:VAL:HG23	1:C:256:GLU:CD	2.31	0.51
1:C:281:GLY:O	1:C:284:ARG:HG2	2.51	0.51
1:F:352:LEU:C	1:F:354:THR:H	2.14	0.51
1:L:283:ARG:NH2	1:L:367:ARG:CD	2.89	0.51
2:S:79:GLU:O	2:S:80:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:ARG:HD2	1:G:67:GLU:OE2	2.12	0.51
1:M:340:ASP:O	1:M:343:ALA:HB3	2.19	0.51
1:H:24:ALA:O	1:H:28:LYS:HG2	2.10	0.51
1:F:300:ILE:O	1:F:300:ILE:HG22	2.15	0.51
1:M:123:ALA:HB2	1:M:440:ALA:HA	1.91	0.51
1:F:177:GLU:O	1:F:379:ARG:HA	2.11	0.51
1:C:289:LYS:CE	1:D:202:TYR:OH	2.59	0.51
2:R:62:LEU:C	2:R:64:VAL:H	2.15	0.50
2:T:54:LEU:HD21	2:U:57:GLY:H	1.76	0.50
1:F:477:ARG:HH11	1:F:477:ARG:HG3	1.75	0.50
1:J:359:TYR:O	1:J:363:LYS:HG2	2.58	0.50
1:C:219:ILE:HG22	1:C:221:ILE:HG13	1.93	0.50
1:G:294:VAL:HA	1:G:341:ILE:CD1	3.22	0.50
1:D:54:VAL:HG11	1:D:79:SER:HA	1.92	0.50
1:F:237:GLU:CB	2:T:28:GLY:HA3	2.41	0.50
1:H:168:VAL:HG11	1:H:173:ILE:N	2.25	0.50
1:J:352:LEU:HD21	1:J:365:GLN:HE22	1.78	0.50
1:H:344:ARG:HH11	1:H:344:ARG:HG3	1.90	0.50
2:O:33:PRO:C	2:O:35:THR:H	2.14	0.50
2:O:50:THR:CG2	2:O:59:ARG:HD3	3.09	0.50
1:H:141:ARG:HH11	1:H:166:GLU:HG3	1.75	0.50
1:D:356:ASP:O	1:D:357:SER:C	2.49	0.50
1:M:437:ALA:O	1:M:441:LYS:HG3	2.10	0.50
1:D:147:VAL:CG2	1:D:410:ILE:HD11	2.40	0.50
1:D:147:VAL:HG23	1:D:410:ILE:HD11	1.92	0.50
1:I:283:ARG:HD3	1:I:363:LYS:HZ1	1.77	0.50
2:Q:84:GLY:O	2:Q:85:GLU:HB2	2.11	0.50
2:U:42:LYS:HA	2:U:70:VAL:O	2.11	0.50
1:E:214:LEU:HB3	1:E:245:PRO:CB	2.41	0.50
1:C:343:ALA:HB2	1:D:207:PRO:CB	7.37	0.50
1:J:168:VAL:HG21	1:J:376:ALA:HB2	1.93	0.50
2:R:100:GLN:HG2	2:S:9:LYS:HE2	5.80	0.50
1:D:218:PHE:CE1	1:D:242:THR:HG21	2.45	0.50
1:K:232:LEU:O	1:K:232:LEU:HD23	2.15	0.50
1:N:114:LEU:O	1:N:118:ARG:HG3	2.12	0.50
1:C:147:VAL:HG23	1:C:410:ILE:HD11	1.94	0.50
1:B:189:VAL:CG1	1:B:193:GLN:HG2	3.66	0.50
1:M:455:ALA:HB1	1:M:465:ILE:HD12	1.98	0.50
1:H:102:GLU:HB3	5:H:601:DMS:H13	1.92	0.50
1:H:28:LYS:NZ	1:H:97:GLN:HE22	2.20	0.50
1:L:253:VAL:O	1:L:258:LEU:HD22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD13	1:D:26:ALA:HB2	2.21	0.50
1:K:65:HIS:O	1:K:69:ILE:HG13	2.14	0.50
2:Q:6:THR:HG21	2:Q:82:ILE:HG21	4.29	0.50
2:T:82:ILE:O	2:T:82:ILE:HG22	3.16	0.50
1:G:150:ILE:HD11	1:G:495:ILE:CA	2.23	0.50
1:I:217:ALA:HB2	1:I:245:PRO:CG	2.31	0.50
1:J:283:ARG:CG	1:J:363:LYS:HZ2	2.49	0.50
1:C:283:ARG:NH2	1:C:366:GLU:OE2	3.00	0.50
1:E:168:VAL:HG21	1:E:376:ALA:HB2	1.98	0.50
1:M:178:GLU:OE2	1:M:392:LYS:HE3	2.16	0.50
1:J:50:THR:CG2	1:J:51:LYS:H	2.24	0.50
1:I:337:LYS:HB2	1:I:340:ASP:OD2	2.15	0.50
1:M:518:THR:HG22	1:M:518:THR:O	2.12	0.50
1:B:10:GLU:N	1:B:13:ARG:HH12	2.10	0.50
1:K:449:GLU:HB2	1:K:450:PRO:HD3	1.94	0.50
1:A:161:ILE:HD12	1:A:399:LEU:CD2	2.51	0.50
1:C:425:VAL:O	1:C:429:ILE:HG13	2.11	0.50
2:P:21:GLU:O	2:P:22:GLU:C	2.50	0.50
2:Q:13:ASP:OD2	2:Q:92:GLU:HB3	2.47	0.50
2:U:19:ARG:HE	2:U:40:PRO:HG2	5.24	0.50
1:G:136:ILE:CD1	1:G:477:ARG:HH21	2.23	0.50
1:E:198:TYR:O	1:E:198:TYR:HD1	2.37	0.50
1:C:345:ILE:HG13	1:C:368:LEU:HD23	7.75	0.50
1:A:54:VAL:HG22	1:A:89:THR:HG21	1.94	0.50
1:J:168:VAL:CG1	1:J:173:ILE:H	2.24	0.50
2:R:97:ALA:HA	2:S:11:LEU:HD12	2.01	0.50
1:M:40:LEU:N	1:M:40:LEU:HD12	2.27	0.50
1:L:228:ASN:HB3	1:L:231:GLU:HG2	1.92	0.50
1:G:199:ILE:O	1:G:199:ILE:HG22	2.15	0.50
1:A:448:GLU:OE1	1:A:452:ARG:NH2	2.45	0.50
1:N:481:ASN:HD21	1:N:484:THR:HG23	1.77	0.50
2:T:50:THR:HG23	2:T:59:ARG:HD3	1.94	0.50
1:G:157:VAL:O	1:G:161:ILE:HG12	2.16	0.50
1:B:425:VAL:O	1:B:429:ILE:HG13	2.11	0.50
1:B:217:ALA:HB2	1:B:245:PRO:HB2	1.93	0.50
1:K:283:ARG:HH21	1:K:367:ARG:HD2	2.30	0.50
1:I:283:ARG:HG2	1:I:363:LYS:HZ2	1.76	0.50
1:B:264:ASN:OD1	2:P:30:ILE:HA	2.12	0.50
1:L:298:THR:N	1:L:315:MET:O	2.43	0.50
1:G:477:ARG:NH1	1:G:477:ARG:HG3	2.42	0.50
1:C:236:LEU:CB	2:Q:30:ILE:CD1	2.86	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:LYS:HA	1:C:270:LEU:O	2.19	0.50
1:F:515:LEU:HD12	1:G:49:ILE:HG21	1.92	0.50
1:E:351:GLU:CG	1:F:326:LYS:HZ1	2.24	0.50
2:O:52:ARG:HH21	2:P:53:VAL:CB	2.23	0.50
2:Q:43:GLY:O	2:Q:69:ILE:HA	2.77	0.50
1:K:219:ILE:O	1:K:221:ILE:HG13	2.16	0.50
2:S:50:THR:CG2	2:S:59:ARG:HD3	2.47	0.50
1:C:149:THR:HG23	1:C:155:PRO:CA	2.44	0.50
1:I:114:LEU:O	1:I:118:ARG:HG3	2.12	0.50
1:I:84:VAL:O	1:I:84:VAL:HG12	2.11	0.50
1:G:466:VAL:HG12	1:G:470:LEU:HD12	1.93	0.50
1:L:312:THR:O	1:L:314:SER:N	2.43	0.50
1:J:218:PHE:HB3	1:J:316:LEU:HG	1.93	0.50
1:M:131:ILE:HD13	1:M:502:THR:HG22	1.92	0.50
1:M:204:VAL:HG13	1:M:211:GLU:O	2.11	0.50
1:A:199:ILE:HG22	1:A:199:ILE:O	2.10	0.50
1:H:19:GLY:HA3	1:H:67:GLU:O	2.12	0.50
2:Q:90:LEU:N	2:Q:90:LEU:HD23	3.35	0.50
1:E:218:PHE:HA	1:E:317:GLY:O	2.54	0.50
2:T:85:GLU:OE1	2:T:85:GLU:HA	2.11	0.50
2:U:80:ILE:CG2	2:U:81:GLU:N	2.74	0.50
1:G:410:ILE:HD11	1:G:496:VAL:CG2	2.49	0.50
1:F:410:ILE:HG12	1:F:496:VAL:HB	2.07	0.50
2:T:33:PRO:C	2:T:35:THR:H	2.15	0.50
1:I:259:ALA:O	1:I:263:VAL:HG23	2.11	0.50
1:G:238:GLN:C	1:G:313:LEU:HD21	2.83	0.50
1:G:205:THR:HB	1:G:213:VAL:H	1.84	0.50
1:N:352:LEU:HD21	1:N:365:GLN:HE22	1.77	0.50
1:A:49:ILE:HG21	1:G:515:LEU:HD12	2.08	0.50
1:K:66:LEU:HD22	1:K:522:VAL:HG21	1.93	0.50
1:C:477:ARG:HH11	1:C:477:ARG:HG3	1.75	0.50
1:C:25:ASN:HA	1:C:28:LYS:HG2	1.93	0.50
1:D:520:GLU:HB3	1:E:29:VAL:HG11	2.01	0.50
2:S:71:VAL:HG23	2:S:99:LEU:HD13	1.93	0.50
1:H:416:VAL:HG21	1:H:479:GLY:HA3	1.98	0.50
1:M:25:ASN:HA	1:M:28:LYS:HE2	1.93	0.50
1:E:6:LEU:HD22	1:E:523:VAL:HG22	1.96	0.50
1:B:263:VAL:O	1:B:267:ARG:HB2	2.32	0.50
2:S:38:GLU:HG3	2:S:74:LYS:NZ	2.26	0.50
2:T:17:VAL:CG2	2:T:45:VAL:HA	3.81	0.50
2:U:18:LYS:HE3	2:U:86:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:283:ARG:NH2	1:M:367:ARG:CD	2.75	0.50
1:J:325:THR:CG2	1:J:326:LYS:N	2.74	0.50
1:D:168:VAL:CG1	1:D:172:GLY:HA3	2.29	0.50
2:O:79:GLU:O	2:O:80:ILE:HG13	2.11	0.50
1:M:197:GLY:HA3	1:M:325:THR:O	2.22	0.50
1:F:236:LEU:HB2	2:T:30:ILE:CD1	2.41	0.50
1:D:250:ALA:O	1:D:252:ASP:N	2.75	0.50
1:L:168:VAL:HG21	1:L:376:ALA:HB2	1.97	0.50
1:A:220:LEU:HD23	1:A:248:ILE:HG23	2.01	0.50
1:A:261:LEU:O	1:A:265:LYS:HB2	2.10	0.50
1:L:61:GLU:O	1:M:4:LYS:N	2.36	0.50
1:M:526:LYS:CD	1:M:527:PRO:HD2	2.42	0.50
1:K:300:ILE:O	1:K:300:ILE:HG22	2.11	0.50
1:F:498:PRO:HG2	1:F:501:VAL:CG2	2.42	0.50
1:L:408:GLU:OE1	1:L:500:LYS:HA	2.11	0.50
1:M:194:PHE:CB	1:M:278:PRO:HB3	2.42	0.50
1:J:455:ALA:HB1	1:J:465:ILE:HD12	1.98	0.50
1:E:23:VAL:CG1	1:E:74:LEU:HD23	2.40	0.50
1:I:146:GLU:O	1:I:150:ILE:HG13	2.12	0.50
1:H:204:VAL:HG13	1:H:211:GLU:O	2.12	0.50
1:G:194:PHE:CD1	1:G:196:LYS:HB2	2.72	0.50
1:C:356:ASP:O	1:C:357:SER:C	2.50	0.50
2:Q:17:VAL:CG2	2:Q:88:VAL:HB	4.88	0.50
2:U:48:VAL:CG1	2:U:62:LEU:CD1	2.85	0.50
1:E:136:ILE:CD1	1:E:477:ARG:HH21	2.31	0.50
1:B:279:GLY:O	1:B:284:ARG:HD3	2.85	0.50
1:F:347:GLY:O	1:F:351:GLU:HB2	2.29	0.50
1:G:198:TYR:O	1:G:198:TYR:HD1	1.95	0.50
1:M:385:GLU:HB2	1:N:280:PHE:CD2	2.46	0.50
1:I:168:VAL:HG11	1:I:173:ILE:N	2.25	0.50
2:U:32:LEU:O	2:U:37:LYS:NZ	4.44	0.50
1:F:498:PRO:HG2	1:F:501:VAL:HG22	1.94	0.50
1:I:194:PHE:CG	1:I:278:PRO:HB3	2.47	0.50
1:G:465:ILE:HD13	1:G:480:PHE:CD2	2.46	0.50
1:B:101:ARG:CG	1:B:102:GLU:N	2.80	0.50
1:M:114:LEU:O	1:M:118:ARG:HG3	2.12	0.50
1:J:141:ARG:HH11	1:J:166:GLU:HG3	1.77	0.50
1:E:95:LEU:O	1:E:99:ILE:HG13	2.24	0.50
1:K:462:GLY:O	1:K:466:VAL:HG23	2.14	0.50
2:T:48:VAL:HG13	2:T:62:LEU:CD1	4.90	0.50
1:A:168:VAL:CG1	1:A:172:GLY:HA3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG11	1:A:79:SER:HA	1.94	0.50
1:K:194:PHE:CB	1:K:278:PRO:HB3	2.49	0.50
1:A:526:LYS:HB3	1:A:529:LYS:HE3	1.93	0.50
1:K:455:ALA:HB1	1:K:465:ILE:HD12	1.96	0.50
1:M:43:LYS:HG2	1:N:525:GLU:HG3	1.94	0.50
1:I:239:VAL:HG22	1:I:313:LEU:CD1	2.46	0.50
1:E:73:LEU:CD2	1:F:47:PRO:HD2	2.42	0.50
2:Q:45:VAL:HG21	2:Q:64:VAL:CG1	2.41	0.49
2:O:10:PRO:HA	2:U:97:ALA:HB2	1.94	0.49
2:P:80:ILE:CG2	2:P:81:GLU:N	2.73	0.49
2:Q:54:LEU:HD11	2:R:57:GLY:HA2	1.94	0.49
2:O:84:GLY:HA3	2:U:27:LYS:HD3	1.93	0.49
1:M:175:THR:CG2	1:M:177:GLU:OE2	2.74	0.49
1:N:65:HIS:HD2	1:N:527:PRO:HG3	6.04	0.49
1:I:168:VAL:HG21	1:I:376:ALA:HB2	1.93	0.49
1:G:66:LEU:CD2	1:G:522:VAL:HG11	2.37	0.49
1:H:7:VAL:HG21	1:H:66:LEU:CD1	2.50	0.49
1:D:118:ARG:O	1:D:122:LYS:HG3	2.13	0.49
2:R:33:PRO:HG2	2:R:36:ALA:CB	2.81	0.49
1:F:466:VAL:HG12	1:F:470:LEU:HD12	1.94	0.49
1:E:348:ILE:HD13	1:E:367:ARG:HB3	1.93	0.49
1:M:218:PHE:HE1	1:M:242:THR:HG21	1.78	0.49
1:F:157:VAL:O	1:F:161:ILE:HG12	2.19	0.49
1:J:490:MET:HA	1:J:490:MET:HE2	1.92	0.49
1:E:194:PHE:CE1	1:E:329:THR:HB	3.08	0.49
1:L:481:ASN:HD21	1:L:484:THR:HG23	1.76	0.49
1:N:283:ARG:HD3	1:N:363:LYS:CE	2.41	0.49
2:T:14:ARG:HH11	2:T:14:ARG:HG3	1.77	0.49
1:I:322:VAL:HG22	1:I:331:ILE:HG12	2.10	0.49
1:B:168:VAL:HG21	1:B:376:ALA:HB2	1.93	0.49
1:M:526:LYS:HG3	1:M:527:PRO:HD2	1.94	0.49
1:I:39:VAL:C	1:I:40:LEU:HD12	2.35	0.49
1:K:222:VAL:CG1	1:K:223:GLU:N	2.78	0.49
1:L:290:ASP:N	1:L:344:ARG:NH1	2.60	0.49
1:L:127:ALA:O	1:L:131:ILE:HG13	2.21	0.49
1:H:18:ARG:HD2	1:H:67:GLU:OE1	2.12	0.49
2:S:89:ILE:O	2:S:89:ILE:HG22	2.33	0.49
1:B:418:LEU:H	1:B:418:LEU:HD12	1.77	0.49
1:G:10:GLU:N	1:G:13:ARG:NH1	2.68	0.49
1:E:229:VAL:HG23	1:E:256:GLU:CG	2.64	0.49
2:U:17:VAL:HG12	2:U:18:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ARG:HG3	1:B:477:ARG:HH11	1.80	0.49
1:C:150:ILE:CD1	1:C:496:VAL:H	2.26	0.49
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.77	0.49
1:J:283:ARG:HD3	1:J:363:LYS:HZ1	1.76	0.49
1:B:270:LEU:HG	1:B:272:VAL:HG13	1.92	0.49
1:G:364:LEU:O	1:G:368:LEU:HB2	3.32	0.49
1:C:51:LYS:HG2	1:C:51:LYS:O	2.19	0.49
1:B:54:VAL:HG11	1:B:79:SER:HA	1.98	0.49
1:F:233:LEU:HD23	2:T:30:ILE:CD1	2.42	0.49
1:K:168:VAL:CG1	1:K:173:ILE:H	2.24	0.49
1:I:307:LYS:HE3	1:I:310:ASN:HD21	1.80	0.49
1:H:228:ASN:HB3	1:H:231:GLU:HG2	1.96	0.49
2:Q:11:LEU:HB2	2:Q:14:ARG:NH1	5.40	0.49
1:A:4:LYS:HG3	1:B:59:GLU:O	2.12	0.49
1:D:193:GLN:HB3	1:D:330:THR:HG23	1.95	0.49
1:L:146:GLU:O	1:L:150:ILE:HG13	2.22	0.49
2:S:21:GLU:O	2:S:21:GLU:HG2	2.46	0.49
1:A:157:VAL:HG22	1:A:395:PHE:CZ	2.47	0.49
1:K:481:ASN:HD21	1:K:484:THR:HG23	1.81	0.49
1:B:225:LYS:HD3	1:B:254:GLU:OE1	2.64	0.49
1:G:179:SER:HB2	1:G:379:ARG:HB3	1.94	0.49
1:K:95:LEU:O	1:K:99:ILE:HG13	2.31	0.49
1:L:123:ALA:HB2	1:L:440:ALA:HA	1.94	0.49
1:K:283:ARG:NH1	1:K:363:LYS:HG3	2.49	0.49
2:P:100:GLN:CB	2:Q:9:LYS:HE2	2.42	0.49
2:Q:91:SER:OG	2:Q:93:ARG:NH1	4.81	0.49
1:M:283:ARG:HH21	1:M:367:ARG:CD	2.25	0.49
2:O:100:GLN:OE1	2:P:9:LYS:HE2	2.45	0.49
2:Q:52:ARG:HH21	2:R:53:VAL:CG1	2.25	0.49
1:C:284:ARG:O	1:C:288:LEU:HG	2.12	0.49
1:E:51:LYS:NZ	4:E:602:ADP:O1A	2.70	0.49
1:L:307:LYS:HE3	1:L:310:ASN:HD21	1.80	0.49
1:M:239:VAL:HG22	1:M:313:LEU:CD1	2.43	0.49
1:M:342:GLU:HA	1:M:345:ILE:HD12	2.01	0.49
1:J:292:ALA:HB1	1:J:297:GLY:O	2.23	0.49
1:H:194:PHE:CG	1:H:278:PRO:HB3	2.47	0.49
1:L:114:LEU:O	1:L:118:ARG:HG3	2.13	0.49
1:K:372:ALA:O	1:K:374:GLY:N	2.42	0.49
1:J:449:GLU:HB2	1:J:450:PRO:HD3	1.93	0.49
1:J:450:PRO:O	1:J:454:ILE:HG13	2.13	0.49
1:B:142:LYS:HE2	1:B:146:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ASP:O	1:B:357:SER:C	2.53	0.49
1:I:283:ARG:HH22	1:I:364:LEU:HA	1.88	0.49
2:P:30:ILE:O	2:P:30:ILE:HG22	2.12	0.49
2:U:45:VAL:CG2	2:U:70:VAL:HG13	5.57	0.49
1:C:222:VAL:HA	1:C:300:ILE:HB	2.19	0.49
1:M:178:GLU:O	1:M:321:ARG:CZ	2.60	0.49
1:F:54:VAL:HG11	1:F:79:SER:HA	1.94	0.49
2:P:50:THR:CG2	2:P:59:ARG:HD3	4.32	0.49
2:S:14:ARG:HH11	2:S:14:ARG:CG	2.23	0.49
1:N:7:VAL:HG21	1:N:66:LEU:CD1	2.42	0.49
1:G:230:ARG:O	1:G:234:PRO:HD2	2.13	0.49
1:L:269:THR:HA	1:M:256:GLU:HG3	1.92	0.49
1:E:498:PRO:HG2	1:E:501:VAL:HG22	1.94	0.49
1:M:84:VAL:HG12	1:M:84:VAL:O	2.13	0.49
1:F:179:SER:HB2	1:F:379:ARG:HB3	1.95	0.49
1:M:28:LYS:NZ	1:M:97:GLN:HE22	2.12	0.49
1:E:194:PHE:CD1	1:E:196:LYS:HB2	2.48	0.49
1:B:417:THR:HG23	1:B:418:LEU:HD12	1.94	0.49
1:A:417:THR:HG23	1:A:418:LEU:HD12	1.95	0.49
1:A:29:VAL:HG13	1:G:520:GLU:HG2	1.96	0.49
1:D:25:ASN:HA	1:D:28:LYS:HG2	1.93	0.49
1:B:6:LEU:HD22	1:B:523:VAL:HG22	1.94	0.49
1:D:150:ILE:HD12	1:D:496:VAL:H	1.76	0.49
2:P:100:GLN:OE1	2:Q:9:LYS:HE2	2.13	0.49
2:U:45:VAL:HG21	2:U:64:VAL:CG1	2.40	0.49
1:J:325:THR:CG2	1:J:327:ASP:H	2.04	0.49
1:A:142:LYS:O	1:A:146:GLU:HG3	2.33	0.49
1:F:218:PHE:CE1	1:F:242:THR:HG21	3.01	0.49
2:O:78:THR:HG22	2:O:79:GLU:N	2.26	0.49
1:M:297:GLY:HA3	1:M:317:GLY:N	2.34	0.49
1:E:224:LYS:CE	1:E:301:SER:HA	2.35	0.49
1:C:312:THR:HB	1:C:314:SER:OG	2.12	0.49
1:L:168:VAL:HG11	1:L:173:ILE:N	2.27	0.49
1:G:245:PRO:HA	1:G:271:SER:OG	2.50	0.49
1:B:304:LEU:HD11	1:C:262:VAL:HG11	1.94	0.49
2:S:81:GLU:HA	2:S:86:GLU:HA	1.93	0.49
1:G:72:GLN:NE2	1:G:75:LYS:NZ	2.60	0.49
1:C:72:GLN:NE2	1:C:75:LYS:NZ	2.59	0.49
1:F:460:TYR:HB3	1:F:465:ILE:HD11	2.01	0.49
1:I:232:LEU:HD23	1:I:236:LEU:HB2	1.98	0.49
1:N:218:PHE:HB3	1:N:316:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG11	1:G:520:GLU:HB3	1.93	0.49
2:S:22:GLU:OE1	2:S:22:GLU:N	2.39	0.49
1:F:425:VAL:O	1:F:429:ILE:HG13	2.13	0.49
1:N:210:MET:HE2	1:N:210:MET:HA	1.95	0.49
1:E:468:GLN:O	1:E:471:ALA:HB3	2.12	0.49
1:A:14:ARG:NH1	1:A:17:GLU:OE1	2.46	0.49
1:F:417:THR:HG23	1:F:418:LEU:HD12	2.01	0.49
1:C:157:VAL:HG22	1:C:395:PHE:CZ	2.60	0.49
2:T:22:GLU:OE2	2:T:40:PRO:HD3	4.14	0.49
2:U:82:ILE:N	2:U:85:GLU:O	2.58	0.49
1:E:477:ARG:HH11	1:E:477:ARG:HG3	1.79	0.49
1:M:283:ARG:HD3	1:M:363:LYS:HE3	2.17	0.49
1:B:363:LYS:C	1:B:365:GLN:N	2.64	0.49
1:C:294:VAL:O	1:C:336:GLY:N	2.84	0.49
1:D:218:PHE:O	1:D:246:LEU:HD12	2.19	0.49
1:K:77:VAL:O	1:K:80:LYS:HG2	2.13	0.49
1:I:7:VAL:HG21	1:I:66:LEU:CD1	2.41	0.49
1:F:465:ILE:HD13	1:F:480:PHE:CE2	2.49	0.49
1:E:369:ALA:O	1:E:375:VAL:HG21	3.21	0.49
1:N:455:ALA:HB1	1:N:465:ILE:HD12	1.99	0.49
1:N:6:LEU:CD2	1:N:523:VAL:HG22	2.44	0.49
1:D:14:ARG:NH1	1:D:17:GLU:OE1	2.47	0.49
1:F:472:GLU:HB3	1:F:478:TYR:CD2	2.54	0.49
1:A:383:ALA:O	1:G:80:LYS:HE2	2.13	0.49
2:Q:93:ARG:O	2:R:14:ARG:NH2	2.80	0.49
1:B:220:LEU:HG	1:B:222:VAL:HG23	1.94	0.49
1:C:294:VAL:HG23	1:C:295:THR:N	4.63	0.49
1:C:345:ILE:HD12	1:C:371:LEU:O	4.48	0.49
1:E:287:MET:O	1:E:291:ILE:HG13	2.46	0.49
1:N:179:SER:CB	1:N:379:ARG:HB3	2.40	0.49
1:H:194:PHE:CB	1:H:278:PRO:HB3	2.45	0.49
1:D:287:MET:O	1:D:290:ASP:HB2	2.17	0.49
1:K:161:ILE:O	1:K:165:MET:HG3	2.13	0.49
1:L:232:LEU:HD23	1:L:236:LEU:HB2	1.96	0.49
1:F:31:LEU:HB2	1:F:90:THR:HG21	1.95	0.49
1:A:77:VAL:HG23	1:A:512:ILE:HG13	2.01	0.49
1:I:123:ALA:HB2	1:I:440:ALA:HA	1.94	0.49
2:P:100:GLN:CG	2:Q:9:LYS:HE2	2.42	0.49
2:R:48:VAL:HG12	2:R:62:LEU:HD12	5.16	0.49
1:M:168:VAL:HG21	1:M:376:ALA:HB2	1.95	0.49
1:D:198:TYR:CE1	1:D:326:LYS:HA	2.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:385:GLU:O	1:M:389:LYS:HG3	2.13	0.49
1:A:242:THR:HG22	1:A:244:LYS:HG2	2.13	0.49
1:H:39:VAL:C	1:H:40:LEU:HD12	2.36	0.49
1:J:234:PRO:HG3	1:J:309:GLU:CA	2.38	0.49
1:A:359:TYR:CE2	1:A:363:LYS:CE	3.96	0.49
1:J:385:GLU:HB2	1:K:280:PHE:CE2	2.65	0.49
1:F:149:THR:HG23	1:F:155:PRO:CA	2.49	0.49
2:S:81:GLU:HA	2:S:85:GLU:O	2.13	0.49
1:L:161:ILE:O	1:L:165:MET:HG3	2.18	0.49
1:D:161:ILE:HD12	1:D:399:LEU:HD21	1.96	0.49
1:G:526:LYS:CG	1:G:527:PRO:HD2	2.43	0.49
1:E:10:GLU:N	1:E:13:ARG:HH12	2.11	0.49
1:C:468:GLN:O	1:C:471:ALA:HB3	2.20	0.49
2:O:71:VAL:HG23	2:O:99:LEU:HD13	1.94	0.49
1:A:425:VAL:O	1:A:429:ILE:HG13	2.13	0.49
1:D:225:LYS:O	1:D:226:VAL:HG23	2.13	0.49
1:K:363:LYS:O	1:K:366:GLU:HG2	2.20	0.49
2:Q:17:VAL:HG23	2:Q:88:VAL:HB	4.64	0.49
1:N:283:ARG:HH22	1:N:364:LEU:HA	1.77	0.49
2:P:81:GLU:HA	2:P:85:GLU:O	2.19	0.49
2:O:84:GLY:CA	2:U:27:LYS:HD2	3.56	0.49
1:H:4:LYS:HG3	1:N:59:GLU:O	2.13	0.49
1:G:227:SER:HB3	1:G:254:GLU:CG	2.98	0.49
1:N:259:ALA:O	1:N:263:VAL:HG23	2.14	0.49
1:L:526:LYS:HG3	1:L:527:PRO:CD	2.43	0.49
1:J:161:ILE:O	1:J:165:MET:HG3	2.13	0.49
1:B:465:ILE:HD13	1:B:480:PHE:CD2	2.48	0.49
1:E:74:LEU:HD21	1:E:93:THR:CG2	2.47	0.49
1:J:25:ASN:HA	1:J:28:LYS:HE2	1.95	0.49
1:G:6:LEU:CD2	1:G:523:VAL:HG22	2.43	0.49
1:A:205:THR:HB	1:A:213:VAL:H	1.82	0.49
1:A:144:ILE:CD1	1:A:165:MET:HG2	2.43	0.49
1:H:123:ALA:HB2	1:H:440:ALA:HA	1.97	0.49
1:D:361:ARG:O	1:D:365:GLN:HB2	2.13	0.48
1:I:219:ILE:O	1:I:221:ILE:HG13	2.12	0.48
1:M:295:THR:HG22	1:M:317:GLY:HA3	1.94	0.48
1:B:247:LEU:HD22	1:B:322:VAL:HG11	1.94	0.48
1:B:50:THR:HA	1:B:390:GLU:OE1	2.13	0.48
1:K:232:LEU:HD23	1:K:236:LEU:HB2	1.97	0.48
1:M:253:VAL:HG11	1:M:261:LEU:HD12	1.95	0.48
1:H:522:VAL:HA	1:N:39:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:THR:CG2	1:E:155:PRO:HA	2.40	0.48
1:I:228:ASN:HB3	1:I:231:GLU:HG2	1.95	0.48
1:L:84:VAL:HG12	1:L:84:VAL:O	2.15	0.48
1:M:408:GLU:OE1	1:M:500:LYS:HA	2.87	0.48
1:A:465:ILE:HD13	1:A:480:PHE:CE2	2.51	0.48
1:M:232:LEU:HD23	1:M:236:LEU:HB2	1.99	0.48
1:D:448:GLU:OE1	1:D:452:ARG:NH2	2.46	0.48
1:I:416:VAL:HG21	1:I:490:MET:HG3	1.94	0.48
1:E:194:PHE:HD1	1:E:196:LYS:HB2	1.78	0.48
1:L:375:VAL:HG12	1:L:375:VAL:O	2.13	0.48
1:D:425:VAL:O	1:D:429:ILE:HG13	2.18	0.48
1:B:264:ASN:HB3	1:B:269:THR:HB	1.95	0.48
2:Q:17:VAL:HG12	2:Q:18:LYS:N	2.29	0.48
2:Q:96:LEU:HD23	2:R:14:ARG:HE	1.78	0.48
1:F:359:TYR:CZ	1:F:363:LYS:HE2	2.49	0.48
1:B:239:VAL:HG11	1:B:246:LEU:HB2	2.04	0.48
1:K:217:ALA:HB2	1:K:245:PRO:CG	2.33	0.48
1:L:50:THR:CG2	1:L:52:ASP:H	2.13	0.48
1:E:227:SER:CB	1:E:254:GLU:HG3	2.31	0.48
1:E:352:LEU:HD21	1:E:365:GLN:CG	2.42	0.48
2:Q:56:ASN:N	2:Q:56:ASN:HD22	4.50	0.48
1:F:232:LEU:HD23	1:F:308:LEU:HD21	1.94	0.48
1:D:222:VAL:HB	1:D:250:ALA:HB2	1.94	0.48
1:N:168:VAL:HG11	1:N:173:ILE:N	2.29	0.48
1:K:295:THR:HG22	1:K:317:GLY:CA	2.44	0.48
1:C:408:GLU:OE1	1:C:503:ARG:NH2	2.46	0.48
1:L:194:PHE:CG	1:L:278:PRO:HB3	2.48	0.48
1:M:222:VAL:HG12	1:M:223:GLU:H	1.77	0.48
1:D:72:GLN:NE2	1:D:75:LYS:NZ	2.68	0.48
1:A:18:ARG:HD2	1:A:67:GLU:OE2	2.17	0.48
1:I:161:ILE:O	1:I:165:MET:HG3	2.14	0.48
1:N:452:ARG:HG2	1:N:452:ARG:NH1	2.37	0.48
1:I:218:PHE:HE1	1:I:242:THR:HG21	1.78	0.48
1:B:144:ILE:CD1	1:B:165:MET:HG2	2.44	0.48
1:A:431:LYS:HG3	1:A:431:LYS:O	2.12	0.48
1:F:356:ASP:O	1:F:357:SER:C	2.52	0.48
1:B:25:ASN:HA	1:B:28:LYS:HG2	1.94	0.48
1:D:490:MET:HE1	1:D:495:ILE:HG21	1.96	0.48
2:P:99:LEU:HD21	2:Q:82:ILE:HD13	3.08	0.48
2:Q:49:GLY:O	2:Q:62:LEU:HD11	2.14	0.48
2:T:79:GLU:HA	2:T:87:TYR:O	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:490:MET:HE1	1:G:495:ILE:HG21	2.07	0.48
1:A:142:LYS:HE2	1:A:146:GLU:OE2	2.13	0.48
1:K:325:THR:CG2	1:K:326:LYS:N	2.76	0.48
1:K:233:LEU:O	1:K:237:GLU:HB2	2.14	0.48
1:K:136:ILE:HB	1:K:410:ILE:CG1	3.03	0.48
2:S:18:LYS:HE3	2:S:86:GLU:O	2.54	0.48
1:N:81:THR:OG1	1:N:508:ASN:ND2	2.46	0.48
1:C:417:THR:HG23	1:C:418:LEU:HD12	1.95	0.48
1:D:10:GLU:N	1:D:13:ARG:NH1	2.61	0.48
1:A:95:LEU:O	1:A:99:ILE:HG13	2.15	0.48
1:J:390:GLU:OE1	1:J:394:ARG:NH1	2.46	0.48
1:N:462:GLY:O	1:N:466:VAL:HG23	2.14	0.48
1:D:359:TYR:OH	1:D:363:LYS:HE3	2.14	0.48
2:U:13:ASP:CA	2:U:62:LEU:HD21	2.43	0.48
2:U:79:GLU:HG2	2:U:88:VAL:HG12	3.82	0.48
1:E:147:VAL:HG23	1:E:410:ILE:HD11	1.95	0.48
2:R:53:VAL:HG22	2:R:59:ARG:CG	2.42	0.48
1:M:47:PRO:HB3	1:N:69:ILE:HG23	2.02	0.48
1:N:7:VAL:HG12	1:N:12:ALA:HB2	1.95	0.48
1:G:224:LYS:HD2	1:G:224:LYS:N	4.80	0.48
1:N:120:ILE:HG23	1:N:443:VAL:CG2	2.43	0.48
1:H:385:GLU:HB2	1:I:280:PHE:CD2	2.66	0.48
1:A:198:TYR:HD1	1:A:198:TYR:O	1.96	0.48
1:F:72:GLN:NE2	1:F:75:LYS:NZ	2.59	0.48
1:N:232:LEU:HD23	1:N:236:LEU:HB2	2.17	0.48
1:J:312:THR:C	1:J:314:SER:N	2.71	0.48
1:E:14:ARG:NH1	1:E:17:GLU:OE1	2.55	0.48
1:F:10:GLU:N	1:F:13:ARG:NH1	2.67	0.48
1:L:449:GLU:HB2	1:L:450:PRO:HD3	2.04	0.48
1:L:416:VAL:HG21	1:L:479:GLY:HA3	1.95	0.48
1:E:229:VAL:HG23	1:E:256:GLU:HG3	1.95	0.48
2:Q:15:VAL:HG22	2:Q:62:LEU:HD13	7.19	0.48
2:R:46:ILE:O	2:R:46:ILE:HG22	2.12	0.48
1:E:237:GLU:HG2	2:S:30:ILE:HD12	1.96	0.48
2:T:16:VAL:HB	2:T:47:ALA:HB3	2.27	0.48
2:P:11:LEU:O	2:P:13:ASP:N	2.94	0.48
1:C:235:ILE:CG1	1:C:311:ALA:HB3	2.43	0.48
2:O:17:VAL:HG12	2:O:18:LYS:N	2.29	0.48
1:G:363:LYS:HA	1:G:366:GLU:OE2	3.21	0.48
1:D:300:ILE:O	1:D:300:ILE:HG22	2.13	0.48
1:N:168:VAL:CG1	1:N:173:ILE:H	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:39:VAL:C	1:N:40:LEU:HD12	2.38	0.48
1:B:204:VAL:HG13	1:B:211:GLU:O	2.40	0.48
1:H:259:ALA:O	1:H:263:VAL:HG23	2.24	0.48
1:N:84:VAL:HG12	1:N:500:LYS:CE	2.42	0.48
1:D:284:ARG:HG3	1:D:284:ARG:HH11	1.79	0.48
1:F:288:LEU:HD23	1:F:291:ILE:HD12	1.95	0.48
1:H:69:ILE:O	1:H:73:LEU:HB2	2.16	0.48
1:G:417:THR:HG23	1:G:418:LEU:HD12	2.00	0.48
1:K:71:ALA:O	1:K:75:LYS:HG3	2.13	0.48
2:U:8:ILE:CG2	2:U:9:LYS:N	3.29	0.48
1:G:410:ILE:HD11	1:G:496:VAL:HG21	1.94	0.48
2:P:17:VAL:CG1	2:P:43:GLY:HA3	2.44	0.48
1:G:287:MET:O	1:G:291:ILE:HG13	2.13	0.48
1:E:50:THR:HA	1:E:390:GLU:OE1	2.26	0.48
1:F:519:THR:HG23	1:G:39:VAL:HG23	1.96	0.48
1:H:283:ARG:CZ	1:H:363:LYS:HG3	2.44	0.48
2:S:13:ASP:OD1	2:S:92:GLU:HB2	2.14	0.48
1:L:269:THR:HA	1:M:256:GLU:CD	2.34	0.48
1:J:295:THR:HG22	1:J:317:GLY:CA	2.53	0.48
1:K:123:ALA:HB2	1:K:440:ALA:HA	1.96	0.48
1:H:120:ILE:HG23	1:H:443:VAL:CG2	2.44	0.48
1:L:194:PHE:CB	1:L:278:PRO:HB3	2.44	0.48
1:I:300:ILE:O	1:I:300:ILE:HG22	2.22	0.48
1:G:498:PRO:HG2	1:G:501:VAL:CG2	2.46	0.48
1:F:503:ARG:O	1:F:507:GLN:HG3	2.19	0.48
1:F:69:ILE:HG23	1:G:47:PRO:HG3	2.04	0.48
1:A:465:ILE:HD13	1:A:480:PHE:CD2	2.53	0.48
1:G:460:TYR:HB3	1:G:465:ILE:HD11	2.02	0.48
1:D:345:ILE:HG23	1:D:368:LEU:CD1	2.56	0.48
1:A:23:VAL:CG1	1:A:74:LEU:HD23	2.43	0.48
1:G:101:ARG:CG	1:G:102:GLU:N	2.76	0.48
1:B:323:ARG:HG2	1:B:323:ARG:HH11	2.00	0.48
1:B:331:ILE:HG22	1:B:331:ILE:O	2.66	0.48
1:A:457:ASN:N	1:A:457:ASN:HD22	2.26	0.48
1:A:80:LYS:HE2	1:B:383:ALA:O	2.14	0.48
1:I:390:GLU:OE1	1:I:394:ARG:NH1	2.51	0.48
1:K:171:GLU:OE1	1:K:366:GLU:HB3	2.64	0.48
1:N:360:ALA:O	1:N:364:LEU:HD13	2.13	0.48
2:S:96:LEU:HA	2:T:14:ARG:NH1	4.96	0.48
1:B:150:ILE:O	1:B:153:ASN:N	2.71	0.48
1:H:197:GLY:HA3	1:H:325:THR:O	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:283:ARG:HH12	1:J:363:LYS:HB2	3.79	0.48
2:O:80:ILE:CG2	2:O:81:GLU:N	2.77	0.48
1:A:247:LEU:HD13	1:A:324:ILE:HD11	1.95	0.48
1:A:173:ILE:HD11	1:A:365:GLN:HG3	2.35	0.48
1:H:295:THR:HG22	1:H:317:GLY:HA3	1.95	0.48
1:G:503:ARG:O	1:G:507:GLN:HG3	2.14	0.48
1:N:194:PHE:CB	1:N:278:PRO:HB3	2.47	0.48
1:N:194:PHE:CG	1:N:278:PRO:HB3	2.52	0.48
1:E:118:ARG:O	1:E:122:LYS:HG3	2.14	0.48
1:I:175:THR:CG2	1:I:177:GLU:OE2	2.61	0.48
1:A:323:ARG:NH1	1:A:323:ARG:HG2	2.50	0.48
1:I:28:LYS:NZ	1:I:97:GLN:HE22	2.11	0.48
1:E:6:LEU:CD2	1:E:523:VAL:HG22	2.52	0.48
1:C:157:VAL:O	1:C:161:ILE:HG12	2.18	0.48
2:R:22:GLU:OE1	2:R:22:GLU:N	2.38	0.48
1:J:481:ASN:HD21	1:J:484:THR:HG23	1.79	0.48
1:J:71:ALA:O	1:J:75:LYS:HG3	2.14	0.48
1:K:117:LYS:O	1:K:121:GLU:HG3	2.16	0.48
1:F:392:LYS:O	1:F:396:GLU:HG3	2.18	0.48
1:I:437:ALA:O	1:I:441:LYS:HG3	2.14	0.48
1:K:239:VAL:HG22	1:K:313:LEU:CD1	2.44	0.48
1:B:229:VAL:HG23	1:B:256:GLU:OE2	2.13	0.48
2:Q:16:VAL:CG1	2:Q:46:ILE:HD12	6.74	0.48
2:U:19:ARG:NH2	2:U:39:LYS:HB3	4.02	0.48
2:U:81:GLU:CG	2:U:85:GLU:H	2.27	0.48
2:Q:56:ASN:N	2:Q:56:ASN:ND2	4.04	0.48
1:A:220:LEU:HD13	1:A:235:ILE:HD12	2.97	0.48
1:M:307:LYS:HB2	1:M:310:ASN:ND2	2.34	0.48
1:I:40:LEU:HD12	1:I:40:LEU:N	2.28	0.48
1:C:202:TYR:HD2	1:C:266:LEU:HD21	2.19	0.48
1:C:248:ILE:CD1	1:C:261:LEU:HD21	2.75	0.48
1:K:194:PHE:N	1:K:194:PHE:CD2	2.86	0.48
1:H:84:VAL:O	1:H:84:VAL:HG12	2.13	0.48
1:G:498:PRO:HG2	1:G:501:VAL:HG22	1.96	0.48
1:F:287:MET:O	1:F:290:ASP:HB2	2.13	0.48
1:E:307:LYS:HB2	1:E:310:ASN:HD22	2.90	0.48
1:H:161:ILE:O	1:H:165:MET:HG3	2.17	0.48
1:E:157:VAL:O	1:E:161:ILE:HG12	2.13	0.48
1:F:95:LEU:O	1:F:99:ILE:HG13	2.16	0.48
2:T:10:PRO:HB2	2:T:14:ARG:CB	3.28	0.48
1:E:490:MET:HE1	1:E:495:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ALA:O	1:C:278:PRO:O	2.32	0.48
2:O:18:LYS:NZ	2:O:85:GLU:OE1	2.95	0.48
1:G:360:ALA:O	1:G:364:LEU:HG	2.29	0.48
1:G:54:VAL:HG11	1:G:79:SER:HA	1.96	0.48
1:F:198:TYR:CE1	1:F:326:LYS:HA	2.49	0.48
1:D:247:LEU:HD13	1:D:324:ILE:HD11	1.95	0.48
1:F:232:LEU:HB3	1:F:236:LEU:HD11	1.95	0.48
1:A:246:LEU:CB	1:A:272:VAL:HG12	2.37	0.48
1:M:69:ILE:O	1:M:73:LEU:HB2	2.17	0.48
1:K:84:VAL:O	1:K:84:VAL:HG12	2.14	0.48
1:G:344:ARG:HD2	1:G:344:ARG:HA	1.60	0.48
1:E:199:ILE:HD12	1:E:274:ALA:HB1	2.38	0.48
1:L:175:THR:CG2	1:L:177:GLU:OE2	2.65	0.48
1:C:101:ARG:CG	1:C:102:GLU:N	2.78	0.48
1:A:25:ASN:HA	1:A:28:LYS:HG2	1.97	0.48
2:Q:62:LEU:C	2:Q:64:VAL:H	2.18	0.48
2:Q:90:LEU:H	2:Q:90:LEU:CD2	3.92	0.48
2:R:11:LEU:O	2:R:13:ASP:N	3.00	0.48
2:O:13:ASP:OD1	2:O:13:ASP:C	2.81	0.48
2:U:17:VAL:CG2	2:U:70:VAL:HG21	4.21	0.48
1:F:410:ILE:HD11	1:F:496:VAL:CG2	2.49	0.48
2:R:50:THR:HG22	2:R:51:GLY:O	2.63	0.48
1:F:218:PHE:HE1	1:F:244:LYS:HB2	2.12	0.48
1:C:265:LYS:HZ2	1:C:271:SER:HB2	2.85	0.48
1:C:265:LYS:HD2	1:C:271:SER:HA	2.76	0.48
1:G:281:GLY:O	1:G:284:ARG:HG2	2.60	0.48
1:C:54:VAL:HG11	1:C:79:SER:HA	1.95	0.48
1:K:30:THR:HB	1:K:51:LYS:O	2.30	0.48
1:A:250:ALA:O	1:A:252:ASP:N	2.55	0.48
1:N:168:VAL:HG21	1:N:376:ALA:HB2	1.94	0.48
1:B:303:GLU:O	1:C:259:ALA:HA	5.57	0.48
1:N:222:VAL:CG1	1:N:223:GLU:N	2.76	0.48
1:N:178:GLU:OE2	1:N:392:LYS:HE3	2.25	0.48
1:F:6:LEU:CD2	1:F:523:VAL:HG22	2.49	0.48
1:C:14:ARG:NH1	1:C:17:GLU:OE1	2.49	0.48
1:L:131:ILE:HD13	1:L:502:THR:HG22	1.95	0.48
2:T:80:ILE:HD12	2:T:80:ILE:N	2.66	0.47
1:M:168:VAL:HG12	1:M:172:GLY:CA	2.33	0.47
1:E:245:PRO:HA	1:E:271:SER:OG	2.14	0.47
1:B:218:PHE:O	1:B:246:LEU:HD12	2.49	0.47
2:O:80:ILE:CG1	2:U:41:GLN:OE1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:50:THR:CG2	1:I:52:ASP:H	2.10	0.47
1:A:217:ALA:HB2	1:A:245:PRO:HB2	1.95	0.47
1:A:261:LEU:HD22	1:A:272:VAL:HG21	1.96	0.47
1:J:297:GLY:HA3	1:J:317:GLY:N	2.35	0.47
1:L:7:VAL:HG21	1:L:66:LEU:CD1	2.51	0.47
1:K:79:SER:O	1:K:81:THR:N	2.47	0.47
1:G:190:GLU:OE2	1:G:190:GLU:HA	4.77	0.47
1:F:178:GLU:CG	1:F:388:LEU:HD21	2.45	0.47
1:D:344:ARG:HA	1:D:344:ARG:HD2	1.66	0.47
1:L:458:ALA:O	1:M:114:LEU:CD1	2.62	0.47
1:L:24:ALA:O	1:L:28:LYS:HG2	2.13	0.47
1:J:146:GLU:O	1:J:150:ILE:HG13	2.14	0.47
1:D:528:GLU:H	1:D:528:GLU:CD	2.17	0.47
1:K:283:ARG:HA	1:K:283:ARG:HD2	1.69	0.47
1:K:283:ARG:HD3	1:K:363:LYS:NZ	2.32	0.47
1:B:229:VAL:HG12	1:B:233:LEU:CD1	2.49	0.47
1:B:490:MET:HE1	1:B:495:ILE:HG21	2.09	0.47
1:I:297:GLY:HA3	1:I:317:GLY:N	2.28	0.47
1:I:295:THR:HG22	1:I:317:GLY:HA3	2.05	0.47
2:O:85:GLU:OE1	2:O:85:GLU:HA	2.15	0.47
1:N:526:LYS:HD2	1:N:527:PRO:HD2	1.93	0.47
2:S:46:ILE:O	2:S:46:ILE:HG22	2.14	0.47
1:A:173:ILE:HG13	1:A:365:GLN:HG3	2.49	0.47
1:L:81:THR:OG1	1:L:508:ASN:ND2	2.59	0.47
1:E:503:ARG:O	1:E:507:GLN:HG3	2.30	0.47
1:A:149:THR:CG2	1:A:155:PRO:HA	2.47	0.47
1:A:460:TYR:HB3	1:A:465:ILE:HD11	1.95	0.47
1:N:161:ILE:O	1:N:165:MET:HG3	2.17	0.47
1:C:23:VAL:CG1	1:C:74:LEU:HD23	2.51	0.47
1:J:416:VAL:HG21	1:J:479:GLY:HA3	2.02	0.47
1:A:349:LYS:C	1:A:351:GLU:H	2.16	0.47
2:T:80:ILE:O	2:T:86:GLU:HA	2.36	0.47
2:U:12:GLY:O	2:U:13:ASP:HB3	2.71	0.47
1:K:298:THR:N	1:K:315:MET:O	2.47	0.47
2:P:81:GLU:HA	2:P:86:GLU:HA	1.96	0.47
1:M:247:LEU:HD13	1:M:324:ILE:HD11	2.00	0.47
1:F:7:VAL:CG2	1:F:66:LEU:HD11	2.41	0.47
1:H:283:ARG:HD3	1:H:363:LYS:CE	2.51	0.47
1:E:251:GLU:O	1:E:252:ASP:HB2	2.14	0.47
1:K:50:THR:HG21	1:K:55:THR:HB	2.02	0.47
1:D:265:LYS:HA	1:D:270:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:206:ASN:HD21	1:M:389:LYS:HE2	1.80	0.47
1:B:289:LYS:HE2	1:C:202:TYR:HH	1.79	0.47
2:Q:10:PRO:HB2	2:Q:14:ARG:O	2.14	0.47
2:S:18:LYS:HZ1	2:S:85:GLU:CD	2.17	0.47
1:B:422:ILE:HD12	1:B:470:LEU:HD21	2.06	0.47
1:M:194:PHE:CG	1:M:278:PRO:HB3	2.50	0.47
2:O:56:ASN:HB2	2:O:58:GLN:HG3	1.96	0.47
1:J:28:LYS:HZ2	1:J:97:GLN:HE22	1.63	0.47
1:D:159:LYS:HE2	1:D:163:ASP:OD2	2.14	0.47
1:E:201:PRO:O	1:E:204:VAL:HG23	3.64	0.47
1:K:146:GLU:O	1:K:150:ILE:HG13	2.14	0.47
1:C:6:LEU:CD2	1:C:523:VAL:HG22	2.44	0.47
1:K:450:PRO:O	1:K:454:ILE:HG13	2.31	0.47
1:B:6:LEU:CD2	1:B:523:VAL:HG22	2.45	0.47
1:M:49:ILE:HG13	1:M:49:ILE:O	2.25	0.47
2:T:69:ILE:HB	2:T:99:LEU:CB	3.23	0.47
2:U:48:VAL:HG13	2:U:62:LEU:HD12	2.16	0.47
1:G:37:ASN:HB3	1:G:50:THR:O	2.14	0.47
1:E:345:ILE:HG23	1:E:368:LEU:HD13	6.94	0.47
1:N:69:ILE:O	1:N:73:LEU:HB2	2.14	0.47
1:K:168:VAL:CG2	1:K:376:ALA:HB2	2.44	0.47
1:K:226:VAL:CG1	1:K:232:LEU:HD12	2.48	0.47
1:G:248:ILE:HD12	1:G:261:LEU:CD2	2.82	0.47
1:I:228:ASN:ND2	1:I:230:ARG:HB3	2.24	0.47
1:E:210:MET:HE3	1:E:210:MET:HA	1.96	0.47
1:A:161:ILE:HD12	1:A:399:LEU:HD21	2.07	0.47
1:A:344:ARG:HA	1:A:344:ARG:HD2	1.67	0.47
2:Q:80:ILE:CG1	2:Q:81:GLU:H	4.24	0.47
2:Q:8:ILE:H	2:Q:8:ILE:HD12	1.78	0.47
2:O:13:ASP:HB2	2:O:62:LEU:CD2	2.44	0.47
1:J:363:LYS:O	1:J:366:GLU:HG2	2.14	0.47
1:J:375:VAL:HG12	1:J:375:VAL:O	2.20	0.47
1:H:81:THR:OG1	1:H:508:ASN:ND2	2.60	0.47
1:K:300:ILE:HG21	1:K:308:LEU:CD2	2.42	0.47
1:K:7:VAL:HG21	1:K:66:LEU:CD1	2.47	0.47
1:G:267:ARG:NH1	1:G:267:ARG:HG3	4.72	0.47
1:B:149:THR:HG23	1:B:155:PRO:CA	2.41	0.47
1:F:118:ARG:O	1:F:122:LYS:HG3	2.15	0.47
1:G:307:LYS:HB3	1:G:310:ASN:HD22	2.92	0.47
1:J:131:ILE:HD13	1:J:502:THR:HG22	2.01	0.47
2:T:50:THR:CG2	2:T:59:ARG:HD3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HD12	1:A:165:MET:HG2	1.96	0.47
1:F:526:LYS:O	1:F:527:PRO:C	2.52	0.47
1:D:518:THR:OG1	1:E:37:ASN:ND2	2.57	0.47
1:A:10:GLU:N	1:A:13:ARG:NH1	2.62	0.47
1:N:19:GLY:HA3	1:N:67:GLU:O	2.14	0.47
1:F:468:GLN:O	1:F:471:ALA:HB3	2.16	0.47
1:M:416:VAL:HG21	1:M:479:GLY:HA3	1.98	0.47
2:T:44:LYS:HA	2:T:68:ASP:O	2.13	0.47
1:D:150:ILE:HG22	1:D:151:SER:N	2.28	0.47
2:R:8:ILE:CG2	2:R:16:VAL:HG21	2.42	0.47
2:T:51:GLY:HA2	2:T:62:LEU:HD21	4.10	0.47
1:E:265:LYS:HD3	1:E:272:VAL:H	1.80	0.47
1:E:265:LYS:HA	1:E:270:LEU:O	2.14	0.47
2:R:54:LEU:HD21	2:S:55:GLU:CA	3.86	0.47
1:J:168:VAL:CG2	1:J:376:ALA:HB2	2.44	0.47
1:H:168:VAL:HG12	1:H:172:GLY:CA	2.34	0.47
1:G:7:VAL:HG12	1:G:12:ALA:HB2	2.08	0.47
1:L:120:ILE:HG23	1:L:443:VAL:CG2	2.53	0.47
1:I:290:ASP:N	1:I:344:ARG:NH1	2.66	0.47
2:S:100:GLN:CD	2:T:9:LYS:HE2	2.35	0.47
1:M:161:ILE:O	1:M:165:MET:HG3	2.16	0.47
1:H:178:GLU:OE2	1:H:392:LYS:HE3	2.15	0.47
1:M:316:LEU:H	1:M:316:LEU:HD23	1.81	0.47
1:H:372:ALA:O	1:H:374:GLY:N	2.59	0.47
1:F:520:GLU:HG2	1:G:29:VAL:HG13	1.96	0.47
1:M:425:VAL:O	1:M:429:ILE:HG13	2.29	0.47
1:F:289:LYS:O	1:F:292:ALA:HB3	2.15	0.47
1:A:201:PRO:O	1:A:204:VAL:HG23	2.48	0.47
2:R:45:VAL:HG21	2:R:64:VAL:CG1	2.48	0.47
1:A:360:ALA:O	1:A:364:LEU:HG	2.15	0.47
2:O:10:PRO:HG2	2:O:49:GLY:HA2	1.97	0.47
1:M:228:ASN:ND2	1:M:230:ARG:HB3	2.25	0.47
2:P:84:GLY:O	2:P:85:GLU:HB2	2.14	0.47
1:E:240:ALA:HB2	1:E:270:LEU:HD22	1.96	0.47
1:B:290:ASP:HB3	1:B:371:LEU:HD21	1.97	0.47
1:K:375:VAL:O	1:K:375:VAL:HG12	2.15	0.47
1:E:54:VAL:CG2	1:E:89:THR:HG21	2.44	0.47
1:E:293:ALA:HB1	1:E:340:ASP:HB3	3.39	0.47
1:B:52:ASP:OD1	1:B:54:VAL:HG23	2.14	0.47
1:B:54:VAL:HG13	1:B:89:THR:HG21	1.95	0.47
1:F:236:LEU:CB	2:T:30:ILE:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:13:ASP:OD1	2:S:13:ASP:C	2.56	0.47
1:D:250:ALA:C	1:D:252:ASP:N	2.85	0.47
1:C:224:LYS:N	1:C:224:LYS:HD2	4.81	0.47
1:A:203:PHE:HA	1:A:265:LYS:HE3	1.97	0.47
1:A:288:LEU:HA	1:A:291:ILE:HD12	2.75	0.47
1:A:359:TYR:OH	1:A:363:LYS:HE3	2.15	0.47
1:B:289:LYS:O	1:B:292:ALA:HB3	2.15	0.47
1:C:149:THR:CG2	1:C:155:PRO:HA	2.48	0.47
1:C:199:ILE:HG12	1:C:276:LYS:HZ2	6.03	0.47
1:D:503:ARG:O	1:D:507:GLN:HG3	2.19	0.47
1:E:128:VAL:HA	1:E:131:ILE:HD12	2.07	0.47
1:H:226:VAL:CG1	1:H:232:LEU:HD12	2.43	0.47
1:L:194:PHE:N	1:L:194:PHE:CD2	2.82	0.47
1:M:408:GLU:OE2	1:M:500:LYS:HG3	2.89	0.47
1:N:300:ILE:HG22	1:N:300:ILE:O	2.14	0.47
1:K:114:LEU:O	1:K:118:ARG:HG3	2.14	0.47
1:E:199:ILE:O	1:E:199:ILE:HG22	2.24	0.47
1:I:79:SER:O	1:I:81:THR:N	2.55	0.47
1:N:239:VAL:HG22	1:N:313:LEU:CD1	2.59	0.47
1:I:253:VAL:HG11	1:I:261:LEU:HD12	2.03	0.47
1:H:146:GLU:O	1:H:150:ILE:HG13	2.18	0.47
1:K:425:VAL:O	1:K:429:ILE:HG13	2.15	0.47
1:B:340:ASP:O	1:B:344:ARG:HB2	2.22	0.47
1:C:161:ILE:HD12	1:C:399:LEU:CD2	2.45	0.47
1:F:10:GLU:N	1:F:13:ARG:HH12	2.19	0.47
1:G:418:LEU:H	1:G:418:LEU:HD12	1.89	0.47
1:I:481:ASN:HD21	1:I:484:THR:HG23	1.84	0.47
1:A:253:VAL:HG21	1:A:274:ALA:HB1	2.19	0.47
1:B:179:SER:OG	1:B:180:LYS:N	2.51	0.47
1:H:49:ILE:HG13	1:H:49:ILE:O	2.16	0.47
1:H:390:GLU:OE1	1:H:394:ARG:NH1	2.48	0.47
2:T:80:ILE:CG2	2:T:81:GLU:N	2.78	0.47
1:M:168:VAL:CG2	1:M:376:ALA:HB2	2.45	0.47
1:C:260:THR:HG22	1:C:264:ASN:ND2	2.63	0.47
1:G:294:VAL:O	1:G:336:GLY:N	2.82	0.47
1:E:54:VAL:HG11	1:E:79:SER:HA	1.99	0.47
1:C:168:VAL:O	1:C:172:GLY:HA3	2.22	0.47
1:H:286:GLU:HG3	1:H:367:ARG:NH2	2.29	0.47
1:E:289:LYS:O	1:E:292:ALA:HB3	2.40	0.47
1:C:301:SER:HB2	1:C:304:LEU:CB	2.45	0.47
2:S:5:LYS:CG	2:S:6:THR:N	4.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:CD1	1:A:365:GLN:HG3	3.02	0.47
1:N:219:ILE:O	1:N:221:ILE:HG13	2.15	0.47
1:C:199:ILE:HG23	1:C:276:LYS:NZ	4.93	0.47
1:K:74:LEU:HA	1:K:512:ILE:HD13	1.96	0.47
1:K:224:LYS:CG	1:K:225:LYS:N	2.77	0.47
1:K:253:VAL:O	1:K:258:LEU:HD22	2.16	0.47
1:J:452:ARG:HG2	1:J:452:ARG:NH1	2.33	0.47
1:H:450:PRO:O	1:H:454:ILE:HG13	2.33	0.47
1:N:146:GLU:O	1:N:150:ILE:HG13	2.14	0.47
1:G:10:GLU:N	1:G:13:ARG:HH12	2.19	0.47
1:J:181:SER:HA	1:K:282:ASP:OD2	2.37	0.47
1:M:5:ILE:HG23	1:M:5:ILE:O	2.15	0.47
1:E:25:ASN:HA	1:E:28:LYS:HG2	1.96	0.47
1:G:77:VAL:HG23	1:G:512:ILE:HG13	1.96	0.47
1:N:449:GLU:HB2	1:N:450:PRO:HD3	1.97	0.47
1:D:232:LEU:HB3	1:D:236:LEU:CD1	2.45	0.47
1:A:351:GLU:OE2	1:B:326:LYS:NZ	2.38	0.47
2:P:91:SER:O	2:P:95:LEU:HG	2.25	0.47
1:G:352:LEU:HD21	1:G:365:GLN:CG	5.69	0.47
1:B:66:LEU:CD2	1:B:522:VAL:HG11	2.51	0.47
1:H:79:SER:O	1:H:81:THR:N	2.48	0.47
1:H:114:LEU:O	1:H:118:ARG:HG3	2.15	0.47
1:J:194:PHE:N	1:J:194:PHE:CD2	2.84	0.47
2:R:32:LEU:CD2	2:R:33:PRO:HD2	2.84	0.47
1:D:360:ALA:O	1:D:364:LEU:HG	2.15	0.47
1:F:465:ILE:HD13	1:F:480:PHE:CD2	2.53	0.47
1:L:312:THR:C	1:L:314:SER:N	2.67	0.47
2:O:38:GLU:OE1	2:O:74:LYS:NZ	4.18	0.47
1:D:167:LYS:HB2	1:D:188:PHE:CE2	2.49	0.47
1:C:194:PHE:CD1	1:C:196:LYS:HB2	2.74	0.47
1:H:282:ASP:OD2	1:N:181:SER:HA	2.51	0.47
1:B:152:ALA:HB2	1:B:398:ALA:HB2	1.97	0.47
2:Q:81:GLU:HA	2:Q:86:GLU:HA	1.96	0.47
1:A:350:LYS:C	1:B:208:GLU:HA	7.92	0.47
2:O:54:LEU:HG	2:O:55:GLU:H	1.80	0.47
1:M:173:ILE:HG13	1:M:370:LYS:HA	1.97	0.47
1:M:173:ILE:HD11	1:M:370:LYS:CG	2.45	0.47
1:N:325:THR:CG2	1:N:326:LYS:N	2.78	0.47
1:L:219:ILE:HD13	1:L:331:ILE:HD13	1.97	0.47
2:U:25:LYS:HG2	2:U:31:VAL:HG22	1.97	0.47
1:I:222:VAL:CG1	1:I:223:GLU:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:224:LYS:CG	1:L:225:LYS:N	2.76	0.47
1:K:316:LEU:HD23	1:K:316:LEU:O	2.14	0.47
1:E:417:THR:HG23	1:E:418:LEU:HD12	1.97	0.47
1:C:177:GLU:O	1:C:379:ARG:HA	2.15	0.47
1:B:478:TYR:CE1	1:B:487:PHE:HB3	2.56	0.47
1:E:179:SER:HB2	1:E:379:ARG:HB3	2.05	0.47
1:G:142:LYS:O	1:G:146:GLU:HG3	2.18	0.47
1:L:475:ASN:OD1	1:L:477:ARG:N	2.43	0.47
1:A:472:GLU:HB3	1:A:478:TYR:CD2	2.49	0.47
1:B:229:VAL:HG23	1:B:256:GLU:CG	2.52	0.46
2:U:79:GLU:O	2:U:80:ILE:HG13	2.15	0.46
1:B:410:ILE:HD11	1:B:496:VAL:HG21	2.22	0.46
1:C:264:ASN:HB3	1:C:269:THR:HB	1.95	0.46
1:C:348:ILE:HG23	1:C:368:LEU:HG	6.78	0.46
1:E:293:ALA:O	1:E:336:GLY:HA3	2.15	0.46
1:M:383:ALA:CB	1:N:359:TYR:OH	2.63	0.46
1:J:46:SER:HB2	1:J:47:PRO:CD	2.37	0.46
1:K:179:SER:CB	1:K:379:ARG:HB3	2.39	0.46
1:M:66:LEU:HD22	1:M:522:VAL:HG21	2.00	0.46
1:L:149:THR:HG23	1:L:155:PRO:CA	2.40	0.46
1:N:66:LEU:HD22	1:N:522:VAL:HG21	1.97	0.46
1:A:283:ARG:CZ	1:A:363:LYS:HB2	4.58	0.46
1:H:194:PHE:HB2	1:H:278:PRO:HB3	2.03	0.46
2:S:19:ARG:HB3	2:S:40:PRO:HG2	2.07	0.46
1:B:189:VAL:HG12	1:B:190:GLU:N	2.30	0.46
1:N:79:SER:O	1:N:81:THR:N	2.47	0.46
1:G:108:ALA:CB	1:N:109:ALA:CB	2.93	0.46
1:M:202:TYR:CD2	1:M:266:LEU:HD11	2.54	0.46
1:M:202:TYR:HD2	1:M:266:LEU:HD11	1.84	0.46
1:D:410:ILE:HG12	1:D:496:VAL:HB	2.06	0.46
2:R:48:VAL:CG1	2:R:62:LEU:HD23	2.46	0.46
2:R:84:GLY:O	2:R:85:GLU:HB2	2.16	0.46
2:T:72:PHE:CD2	2:T:90:LEU:CD2	5.28	0.46
2:T:91:SER:O	2:T:95:LEU:HG	2.14	0.46
1:C:296:GLY:CA	1:C:336:GLY:HA2	2.44	0.46
1:D:239:VAL:HG11	1:D:246:LEU:HB2	1.96	0.46
1:H:46:SER:HB2	1:H:47:PRO:CD	2.43	0.46
1:H:168:VAL:HG21	1:H:376:ALA:HB2	1.96	0.46
1:H:66:LEU:HD22	1:H:522:VAL:HG21	1.99	0.46
1:I:120:ILE:HG23	1:I:443:VAL:CG2	2.57	0.46
1:G:128:VAL:HG13	1:G:503:ARG:HG3	2.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:224:LYS:CG	1:N:225:LYS:N	2.78	0.46
1:I:224:LYS:CG	1:I:225:LYS:N	2.78	0.46
1:F:128:VAL:HA	1:F:131:ILE:HD12	1.97	0.46
1:F:72:GLN:HE22	1:F:75:LYS:HZ3	1.60	0.46
1:G:422:ILE:HD12	1:G:470:LEU:HD21	1.98	0.46
1:C:4:LYS:HG3	1:D:59:GLU:O	2.39	0.46
1:G:231:GLU:HB2	1:G:308:LEU:HD23	2.62	0.46
1:D:418:LEU:H	1:D:418:LEU:HD12	1.81	0.46
1:D:179:SER:OG	1:D:180:LYS:N	2.54	0.46
1:D:303:GLU:HA	1:E:259:ALA:HB2	3.46	0.46
2:Q:97:ALA:HA	2:R:11:LEU:HG	1.98	0.46
1:D:359:TYR:CZ	1:D:363:LYS:CE	2.98	0.46
1:E:218:PHE:HE1	1:E:244:LYS:HB2	1.95	0.46
1:E:235:ILE:HG12	1:E:311:ALA:CB	2.37	0.46
1:E:232:LEU:O	1:E:235:ILE:HG22	5.79	0.46
1:E:410:ILE:HD11	1:E:496:VAL:HG21	2.01	0.46
1:M:363:LYS:O	1:M:366:GLU:HG2	2.16	0.46
1:I:217:ALA:HB1	1:I:245:PRO:O	2.26	0.46
2:Q:54:LEU:CD1	2:R:57:GLY:N	2.79	0.46
1:D:301:SER:HB2	1:D:304:LEU:HB3	2.07	0.46
1:J:283:ARG:HD2	1:J:283:ARG:HA	1.70	0.46
1:J:311:ALA:HA	1:J:315:MET:SD	2.64	0.46
1:C:345:ILE:HG12	1:C:368:LEU:CD2	5.42	0.46
1:B:321:ARG:O	1:B:322:VAL:HG23	2.42	0.46
1:E:363:LYS:C	1:E:365:GLN:H	2.88	0.46
1:F:229:VAL:HG23	1:F:256:GLU:OE2	2.18	0.46
1:M:179:SER:CB	1:M:379:ARG:HB3	2.38	0.46
1:J:77:VAL:O	1:J:80:LYS:HG2	2.27	0.46
1:L:360:ALA:HA	1:L:363:LYS:CG	2.74	0.46
2:U:33:PRO:C	2:U:35:THR:H	2.19	0.46
2:S:17:VAL:HG12	2:S:18:LYS:N	2.31	0.46
1:J:465:ILE:HD13	1:J:480:PHE:CD1	2.51	0.46
1:K:253:VAL:HG11	1:K:261:LEU:HD12	2.03	0.46
1:B:199:ILE:O	1:B:199:ILE:HG22	2.19	0.46
1:C:286:GLU:OE1	1:C:344:ARG:NH2	2.48	0.46
1:C:289:LYS:NZ	1:D:202:TYR:CZ	2.66	0.46
1:F:396:GLU:O	1:F:400:ASN:ND2	2.48	0.46
1:C:179:SER:OG	1:C:180:LYS:N	2.49	0.46
2:Q:24:PRO:HG2	2:Q:25:LYS:H	2.07	0.46
1:G:103:GLY:O	1:G:107:VAL:HG23	2.15	0.46
2:O:13:ASP:OD1	2:O:13:ASP:O	3.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:62:LEU:C	2:P:64:VAL:H	2.23	0.46
2:P:52:ARG:NH2	2:Q:53:VAL:O	3.60	0.46
1:A:230:ARG:HA	1:A:233:LEU:HD12	1.98	0.46
1:C:238:GLN:C	1:C:313:LEU:HD21	2.79	0.46
1:C:279:GLY:C	1:C:284:ARG:HB3	2.36	0.46
2:O:84:GLY:O	2:O:85:GLU:HB2	2.15	0.46
1:N:526:LYS:O	1:N:527:PRO:C	2.54	0.46
1:D:54:VAL:CG2	1:D:89:THR:HG21	2.44	0.46
1:L:168:VAL:CG2	1:L:376:ALA:HB2	2.47	0.46
1:A:66:LEU:CD2	1:A:522:VAL:HG11	2.38	0.46
1:G:298:THR:HG23	1:G:304:LEU:CD1	7.64	0.46
1:I:375:VAL:HG12	1:I:375:VAL:O	2.17	0.46
1:A:498:PRO:HG2	1:A:501:VAL:HG22	1.96	0.46
1:K:408:GLU:HB2	1:K:500:LYS:HB2	2.60	0.46
1:J:290:ASP:N	1:J:344:ARG:NH1	2.72	0.46
1:D:149:THR:HG23	1:D:155:PRO:CA	2.43	0.46
1:E:231:GLU:O	1:E:309:GLU:HA	2.15	0.46
1:H:372:ALA:C	1:H:374:GLY:N	2.80	0.46
1:L:452:ARG:HG2	1:L:452:ARG:NH1	2.32	0.46
1:M:452:ARG:HG2	1:M:452:ARG:NH1	2.32	0.46
1:D:468:GLN:O	1:D:471:ALA:HB3	2.17	0.46
1:I:69:ILE:O	1:I:73:LEU:HB2	2.15	0.46
1:B:17:GLU:HB2	1:B:104:LEU:CD1	2.64	0.46
1:E:192:TYR:C	1:E:192:TYR:CD2	2.88	0.46
1:A:216:ASP:HA	1:A:319:ALA:O	2.28	0.46
1:G:141:ARG:NH2	1:G:163:ASP:OD1	2.38	0.46
1:K:19:GLY:HA3	1:K:67:GLU:O	2.15	0.46
1:C:231:GLU:HB3	1:C:308:LEU:HB3	2.44	0.46
2:R:79:GLU:C	2:R:80:ILE:HD12	2.36	0.46
2:O:100:GLN:OE1	2:P:9:LYS:CE	2.84	0.46
1:C:345:ILE:HG12	1:C:368:LEU:HD23	6.25	0.46
1:F:228:ASN:HD22	1:F:231:GLU:HG3	2.16	0.46
1:J:168:VAL:HG12	1:J:172:GLY:CA	2.35	0.46
1:I:168:VAL:CG2	1:I:376:ALA:HB2	2.44	0.46
1:I:385:GLU:O	1:I:389:LYS:HG3	2.15	0.46
1:J:307:LYS:HE3	1:J:310:ASN:HD21	1.83	0.46
1:H:297:GLY:HA3	1:H:317:GLY:N	2.30	0.46
1:N:117:LYS:O	1:N:120:ILE:N	2.48	0.46
1:G:229:VAL:HG11	2:U:32:LEU:CD2	2.45	0.46
1:J:222:VAL:CG1	1:J:223:GLU:N	2.81	0.46
2:P:73:ALA:O	2:P:75:TYR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:GLU:OE2	1:J:392:LYS:HE3	2.20	0.46
1:L:218:PHE:HE1	1:L:242:THR:HG21	1.82	0.46
1:J:425:VAL:O	1:J:429:ILE:HG13	2.16	0.46
1:D:232:LEU:HD23	1:D:308:LEU:HD21	2.06	0.46
1:C:528:GLU:OE1	1:C:528:GLU:N	2.48	0.46
1:E:123:ALA:HB3	1:E:443:VAL:HG21	1.98	0.46
1:F:227:SER:C	1:F:257:ALA:HB2	2.36	0.46
1:H:462:GLY:O	1:H:466:VAL:HG23	2.19	0.46
2:T:20:ILE:CD1	2:T:42:LYS:HG3	5.83	0.46
2:U:15:VAL:CG2	2:U:45:VAL:HG13	4.11	0.46
2:U:20:ILE:CD1	2:U:44:LYS:HG3	4.13	0.46
1:C:283:ARG:HH22	1:C:366:GLU:CG	3.07	0.46
1:G:363:LYS:C	1:G:365:GLN:H	2.18	0.46
1:G:345:ILE:HD11	1:G:368:LEU:HD23	7.90	0.46
1:E:31:LEU:HD12	4:E:602:ADP:H5'1	2.40	0.46
1:E:343:ALA:HB2	1:F:207:PRO:HB2	1.97	0.46
1:E:518:THR:OG1	1:F:37:ASN:ND2	2.48	0.46
1:F:54:VAL:CG2	1:F:89:THR:HG21	2.45	0.46
1:C:7:VAL:CG2	1:C:66:LEU:HD11	2.30	0.46
1:M:385:GLU:HB2	1:N:280:PHE:HE2	1.80	0.46
1:K:232:LEU:CD2	1:K:236:LEU:HD13	2.43	0.46
1:L:222:VAL:CG1	1:L:223:GLU:N	2.78	0.46
1:G:320:GLU:HB3	1:G:333:GLY:HA3	1.97	0.46
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.59	0.46
1:D:157:VAL:O	1:D:161:ILE:HG12	2.19	0.46
1:A:369:ALA:HB1	1:A:375:VAL:HG22	2.62	0.46
1:G:157:VAL:HG22	1:G:395:PHE:CZ	2.58	0.46
1:H:86:GLY:O	1:H:87:ASP:HB2	2.17	0.46
1:K:416:VAL:HG21	1:K:479:GLY:HA3	1.98	0.46
1:A:167:LYS:HB2	1:A:188:PHE:CE2	2.58	0.46
1:A:31:LEU:HB2	1:A:90:THR:HG21	1.97	0.46
2:U:56:ASN:ND2	2:U:58:GLN:CD	4.35	0.46
1:K:311:ALA:HA	1:K:315:MET:SD	2.55	0.46
1:B:361:ARG:O	1:B:365:GLN:HB2	2.33	0.46
1:D:7:VAL:HG12	1:D:12:ALA:HB2	1.98	0.46
1:E:292:ALA:O	1:E:293:ALA:C	2.54	0.46
2:R:70:VAL:HG11	2:R:95:LEU:CD2	2.34	0.46
1:N:46:SER:HB2	1:N:47:PRO:CD	2.36	0.46
1:C:299:VAL:O	1:C:304:LEU:HD12	7.62	0.46
1:C:299:VAL:N	1:C:304:LEU:HD12	9.72	0.46
1:N:168:VAL:CG2	1:N:376:ALA:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:THR:HG22	1:G:313:LEU:H	1.80	0.46
1:K:120:ILE:HG23	1:K:443:VAL:CG2	2.45	0.46
1:C:257:ALA:O	1:C:261:LEU:HD12	3.39	0.46
1:A:498:PRO:HG2	1:A:501:VAL:CG2	2.45	0.46
1:I:194:PHE:CB	1:I:278:PRO:HB3	2.46	0.46
1:K:316:LEU:HD23	1:K:316:LEU:H	1.91	0.46
1:G:310:ASN:HB3	2:O:34:ASP:OD2	2.15	0.46
1:L:316:LEU:O	1:L:316:LEU:HD23	2.16	0.46
1:D:10:GLU:N	1:D:13:ARG:HH12	2.19	0.46
1:D:421:ALA:O	1:D:425:VAL:HG23	2.30	0.46
1:D:457:ASN:N	1:D:457:ASN:HD22	2.14	0.46
1:M:433:GLU:HG2	1:M:434:GLY:N	2.35	0.46
1:F:372:ALA:C	1:F:374:GLY:N	2.76	0.46
1:H:437:ALA:O	1:H:441:LYS:HG3	2.27	0.46
1:E:289:LYS:HB3	1:E:344:ARG:NH2	3.62	0.46
1:F:236:LEU:HB3	2:T:30:ILE:HD13	2.74	0.46
1:M:206:ASN:HD21	1:M:389:LYS:CE	2.29	0.46
2:Q:22:GLU:OE2	2:Q:40:PRO:HD3	4.12	0.46
1:L:283:ARG:HA	1:L:283:ARG:HD2	1.70	0.46
1:C:503:ARG:O	1:C:507:GLN:HG3	2.23	0.46
1:N:228:ASN:HB3	1:N:231:GLU:HG2	1.97	0.46
1:D:178:GLU:CG	1:D:388:LEU:HD21	2.48	0.46
1:G:321:ARG:HG2	1:G:322:VAL:N	2.31	0.46
1:E:231:GLU:HB3	1:E:308:LEU:HB3	1.97	0.46
1:L:316:LEU:H	1:L:316:LEU:HD23	1.80	0.46
1:N:71:ALA:O	1:N:75:LYS:HG3	2.28	0.46
1:J:372:ALA:O	1:J:374:GLY:N	2.45	0.46
1:B:123:ALA:HB3	1:B:443:VAL:HG21	2.04	0.46
1:K:204:VAL:HG13	1:K:211:GLU:O	2.16	0.46
2:P:22:GLU:N	2:P:22:GLU:OE1	3.18	0.46
1:A:147:VAL:HG23	1:A:410:ILE:HD11	1.97	0.46
1:I:311:ALA:HA	1:I:315:MET:SD	2.56	0.46
1:L:325:THR:CG2	1:L:326:LYS:N	2.79	0.46
1:E:270:LEU:HG	1:E:272:VAL:HG13	2.51	0.46
1:F:246:LEU:CB	1:F:272:VAL:HG12	2.63	0.46
1:C:222:VAL:HG22	1:C:300:ILE:HD12	1.97	0.46
1:C:363:LYS:C	1:C:365:GLN:H	2.19	0.46
1:G:284:ARG:HH11	1:G:284:ARG:HG3	1.80	0.46
1:H:283:ARG:CD	1:H:363:LYS:NZ	3.14	0.46
2:S:13:ASP:CA	2:S:62:LEU:HD21	2.47	0.46
1:M:208:GLU:OE1	1:M:389:LYS:NZ	3.00	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:VAL:CG2	1:H:376:ALA:HB2	2.46	0.46
1:K:246:LEU:HB3	1:K:272:VAL:CG1	2.44	0.46
1:F:354:THR:O	1:F:354:THR:HG22	2.16	0.46
1:I:117:LYS:O	1:I:121:GLU:HG3	2.16	0.46
1:H:385:GLU:HB2	1:I:280:PHE:CE2	2.71	0.46
1:B:118:ARG:O	1:B:122:LYS:HG3	2.16	0.46
1:E:72:GLN:NE2	1:E:75:LYS:NZ	2.69	0.46
1:A:416:VAL:HG21	1:A:479:GLY:HA3	2.03	0.46
1:H:131:ILE:HD13	1:H:502:THR:HG22	1.97	0.46
2:Q:24:PRO:HG2	2:Q:25:LYS:HG3	2.54	0.46
1:N:363:LYS:O	1:N:366:GLU:HG2	2.22	0.46
2:T:17:VAL:O	2:T:87:TYR:HB3	2.16	0.46
2:T:82:ILE:HD12	2:T:87:TYR:CE1	4.10	0.46
2:U:42:LYS:HG3	2:U:43:GLY:N	4.84	0.46
2:U:13:ASP:HA	2:U:62:LEU:HD21	1.98	0.46
2:Q:58:GLN:OE1	2:R:57:GLY:HA3	5.26	0.46
1:J:283:ARG:NH2	1:J:367:ARG:CD	2.78	0.46
1:M:50:THR:CG2	1:M:51:LYS:H	2.20	0.46
2:S:62:LEU:C	2:S:64:VAL:H	2.21	0.46
1:H:490:MET:HA	1:H:490:MET:CE	2.51	0.46
1:I:342:GLU:HA	1:I:345:ILE:HD12	2.01	0.46
1:I:307:LYS:HB2	1:I:310:ASN:ND2	2.31	0.46
1:N:297:GLY:HA3	1:N:317:GLY:N	2.33	0.46
1:E:69:ILE:CD1	1:F:41:GLU:HB2	2.42	0.46
1:E:178:GLU:CG	1:E:388:LEU:HD21	2.43	0.46
1:A:529:LYS:HE2	1:B:63:GLU:OE2	2.16	0.46
1:G:189:VAL:HG13	1:G:190:GLU:H	1.79	0.46
1:E:422:ILE:HD12	1:E:470:LEU:HD21	2.08	0.46
1:B:332:VAL:HG12	1:B:333:GLY:N	2.33	0.46
1:M:81:THR:OG1	1:M:508:ASN:ND2	2.49	0.46
1:D:478:TYR:CE1	1:D:487:PHE:HB3	2.51	0.46
1:N:416:VAL:HG21	1:N:479:GLY:HA3	1.98	0.46
1:E:167:LYS:HB2	1:E:188:PHE:CE2	2.51	0.46
2:R:38:GLU:HG2	2:R:38:GLU:H	1.54	0.46
1:N:204:VAL:HG13	1:N:211:GLU:O	2.15	0.46
1:A:179:SER:OG	1:A:180:LYS:N	2.49	0.46
1:E:263:VAL:HG13	1:E:267:ARG:NH1	2.31	0.45
1:D:305:GLY:HA3	2:S:33:PRO:HB2	1.96	0.45
2:Q:73:ALA:O	2:Q:75:TYR:CD1	3.87	0.45
2:Q:77:GLY:O	2:Q:78:THR:O	2.92	0.45
1:N:283:ARG:HD2	1:N:283:ARG:HA	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:17:VAL:O	2:U:87:TYR:HB3	2.16	0.45
1:B:410:ILE:HG12	1:B:496:VAL:HB	2.42	0.45
1:I:219:ILE:HD13	1:I:331:ILE:HD13	2.02	0.45
1:N:197:GLY:HA3	1:N:325:THR:O	2.19	0.45
1:C:287:MET:O	1:C:290:ASP:HB2	2.34	0.45
1:G:295:THR:C	1:G:336:GLY:H	3.18	0.45
1:I:37:ASN:HD21	1:I:51:LYS:CE	2.39	0.45
1:E:283:ARG:O	1:E:287:MET:HG3	2.15	0.45
1:D:235:ILE:HG21	1:D:311:ALA:CB	4.80	0.45
1:A:250:ALA:O	1:A:251:GLU:C	2.53	0.45
1:K:309:GLU:OE1	1:K:309:GLU:N	2.40	0.45
1:G:262:VAL:O	1:G:265:LYS:HB3	2.75	0.45
1:N:253:VAL:HG11	1:N:261:LEU:HD12	1.99	0.45
1:J:179:SER:CB	1:J:379:ARG:HB3	2.41	0.45
1:H:307:LYS:HE3	1:H:310:ASN:HD21	1.80	0.45
1:L:84:VAL:HG12	1:L:500:LYS:CE	2.45	0.45
1:H:224:LYS:CG	1:H:225:LYS:N	2.79	0.45
1:M:120:ILE:HG23	1:M:443:VAL:CG2	2.46	0.45
1:L:352:LEU:HD21	1:L:365:GLN:HE22	1.84	0.45
1:D:74:LEU:HD21	1:D:93:THR:CG2	2.45	0.45
1:B:452:ARG:HH11	1:B:463:SER:HA	1.83	0.45
1:I:452:ARG:NH1	1:I:452:ARG:HG2	2.31	0.45
1:A:337:LYS:O	1:A:340:ASP:HB2	2.15	0.45
1:K:63:GLU:HG2	1:L:3:ALA:HB1	1.97	0.45
1:L:390:GLU:OE1	1:L:394:ARG:NH1	2.49	0.45
1:I:526:LYS:HG3	1:I:527:PRO:HD2	1.98	0.45
2:Q:85:GLU:HA	2:Q:85:GLU:OE1	2.15	0.45
1:A:345:ILE:C	1:A:347:GLY:H	2.19	0.45
1:A:351:GLU:HB2	1:B:207:PRO:O	8.57	0.45
2:T:71:VAL:HG23	2:T:99:LEU:HD13	1.98	0.45
2:Q:50:THR:HB	2:Q:59:ARG:CZ	5.31	0.45
2:U:73:ALA:O	2:U:75:TYR:N	2.49	0.45
1:G:292:ALA:O	1:G:293:ALA:C	2.78	0.45
1:E:31:LEU:HD13	1:E:90:THR:HG22	1.98	0.45
1:M:175:THR:OG1	1:M:330:THR:HG21	2.16	0.45
1:E:227:SER:HB3	1:E:254:GLU:CG	2.33	0.45
1:C:54:VAL:CG2	1:C:89:THR:HG21	2.47	0.45
1:D:219:ILE:N	1:D:317:GLY:O	2.40	0.45
1:J:309:GLU:OE1	1:J:309:GLU:N	2.42	0.45
1:L:79:SER:C	1:L:81:THR:N	2.68	0.45
1:A:503:ARG:O	1:A:507:GLN:HG3	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:117:LYS:O	1:N:118:ARG:C	2.55	0.45
1:M:268:GLY:HA3	1:N:227:SER:CB	2.43	0.45
1:B:189:VAL:HG13	1:B:190:GLU:H	1.81	0.45
1:E:460:TYR:HB3	1:E:465:ILE:HD11	2.07	0.45
1:D:422:ILE:HD12	1:D:470:LEU:HD21	2.01	0.45
1:G:207:PRO:O	1:G:210:MET:HE3	2.16	0.45
1:N:312:THR:HG22	1:N:313:LEU:N	2.31	0.45
1:A:418:LEU:HD12	1:A:418:LEU:H	1.82	0.45
1:C:472:GLU:HB3	1:C:478:TYR:CD2	2.51	0.45
1:E:113:PRO:HG3	1:F:36:ARG:NH1	2.47	0.45
1:D:173:ILE:HG22	1:D:173:ILE:O	2.16	0.45
1:E:242:THR:HG22	1:E:244:LYS:HG2	3.48	0.45
2:U:91:SER:O	2:U:95:LEU:HG	2.17	0.45
1:B:220:LEU:HD13	1:B:235:ILE:HD13	1.98	0.45
1:C:204:VAL:HG12	1:C:206:ASN:O	2.88	0.45
1:C:232:LEU:HB3	1:C:236:LEU:CD1	2.56	0.45
1:L:50:THR:HG21	1:L:55:THR:HB	1.97	0.45
2:Q:56:ASN:OD1	2:R:56:ASN:HA	3.71	0.45
1:D:51:LYS:O	1:D:51:LYS:HG2	2.20	0.45
1:K:46:SER:CB	1:K:47:PRO:HD2	2.38	0.45
1:M:59:GLU:OE1	1:N:4:LYS:NZ	2.74	0.45
1:G:265:LYS:HD3	1:G:272:VAL:H	4.36	0.45
1:H:295:THR:HG22	1:H:317:GLY:CA	2.47	0.45
1:B:506:LEU:HD12	1:B:506:LEU:O	2.16	0.45
1:J:194:PHE:CE1	1:J:278:PRO:HD3	2.52	0.45
2:S:100:GLN:CB	2:T:9:LYS:HE3	4.13	0.45
1:N:385:GLU:O	1:N:389:LYS:HG3	2.20	0.45
1:B:74:LEU:HD21	1:B:93:THR:CG2	2.50	0.45
1:D:455:ALA:O	1:D:458:ALA:HB3	2.17	0.45
1:I:372:ALA:C	1:I:374:GLY:N	2.83	0.45
1:E:101:ARG:CG	1:E:102:GLU:N	2.79	0.45
1:L:253:VAL:HG11	1:L:261:LEU:HD12	1.98	0.45
1:A:350:LYS:CG	1:B:208:GLU:CD	9.15	0.45
2:Q:60:VAL:HG21	2:R:53:VAL:HG11	2.38	0.45
1:J:283:ARG:HG2	1:J:363:LYS:NZ	2.31	0.45
2:O:79:GLU:C	2:O:80:ILE:HD12	2.36	0.45
1:M:178:GLU:H	1:M:321:ARG:HH11	1.64	0.45
1:L:47:PRO:CB	1:M:69:ILE:HG23	2.53	0.45
1:G:236:LEU:O	1:G:240:ALA:HB2	2.38	0.45
1:N:295:THR:HG22	1:N:317:GLY:HA3	1.99	0.45
1:H:84:VAL:HG12	1:H:500:LYS:CE	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLU:CG	1:A:388:LEU:HD21	2.55	0.45
1:I:232:LEU:CD2	1:I:236:LEU:HD13	2.47	0.45
1:N:425:VAL:O	1:N:429:ILE:HG13	2.27	0.45
1:H:71:ALA:O	1:H:75:LYS:HG3	2.42	0.45
1:D:396:GLU:O	1:D:400:ASN:ND2	2.49	0.45
1:D:205:THR:HB	1:D:213:VAL:H	1.87	0.45
1:K:286:GLU:HG3	1:K:367:ARG:NH2	2.36	0.45
2:P:41:GLN:HG2	2:P:74:LYS:CB	2.40	0.45
2:Q:16:VAL:O	2:Q:46:ILE:N	2.66	0.45
1:F:283:ARG:HB2	1:F:283:ARG:HH11	1.82	0.45
1:I:197:GLY:HA3	1:I:325:THR:O	2.16	0.45
1:J:283:ARG:HD3	1:J:363:LYS:HE3	1.99	0.45
1:E:66:LEU:HD22	1:E:522:VAL:CG1	2.42	0.45
1:G:198:TYR:CE1	1:G:326:LYS:HA	2.52	0.45
1:M:253:VAL:O	1:M:258:LEU:HD22	2.16	0.45
1:N:77:VAL:O	1:N:80:LYS:HG2	2.25	0.45
1:A:287:MET:O	1:A:290:ASP:HB2	2.17	0.45
1:A:359:TYR:CE1	1:A:363:LYS:HE2	2.52	0.45
1:B:304:LEU:O	1:C:263:VAL:CG2	4.34	0.45
1:L:66:LEU:HD22	1:L:522:VAL:HG21	2.01	0.45
1:D:124:VAL:HG13	1:D:506:LEU:HG	1.98	0.45
1:K:80:LYS:HE3	1:K:508:ASN:OD1	2.16	0.45
2:S:98:VAL:O	2:T:9:LYS:N	2.46	0.45
1:C:247:LEU:HD13	1:C:324:ILE:HD11	2.01	0.45
1:E:29:VAL:HG12	1:E:29:VAL:O	2.29	0.45
1:B:280:PHE:O	1:B:281:GLY:C	2.55	0.45
1:I:49:ILE:HG13	1:I:49:ILE:O	2.18	0.45
1:C:103:GLY:O	1:C:107:VAL:HG23	2.17	0.45
1:D:206:ASN:HB3	1:D:209:THR:OG1	2.29	0.45
1:E:230:ARG:O	1:E:234:PRO:HD2	2.35	0.45
1:E:264:ASN:ND2	2:S:30:ILE:HG23	2.31	0.45
2:U:64:VAL:HG22	2:U:98:VAL:HG21	2.64	0.45
1:F:235:ILE:CD1	1:F:311:ALA:CB	2.92	0.45
1:F:51:LYS:HG2	1:F:51:LYS:O	2.16	0.45
1:M:37:ASN:H	1:N:518:THR:HG22	1.81	0.45
1:L:86:GLY:O	1:L:87:ASP:HB2	2.20	0.45
1:I:187:LYS:HZ1	1:I:379:ARG:HG3	1.81	0.45
1:I:179:SER:CB	1:I:379:ARG:HB3	2.40	0.45
2:Q:19:ARG:HD3	2:Q:40:PRO:CG	3.43	0.45
1:E:72:GLN:HE22	1:E:75:LYS:HZ3	1.74	0.45
1:M:290:ASP:N	1:M:344:ARG:NH1	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:267:ARG:O	1:N:255:GLY:HA3	2.16	0.45
1:K:69:ILE:O	1:K:73:LEU:HB2	2.19	0.45
2:O:21:GLU:CD	2:O:21:GLU:H	2.20	0.45
1:A:321:ARG:O	1:A:322:VAL:HG23	2.50	0.45
1:J:18:ARG:HD2	1:J:67:GLU:OE1	2.16	0.45
1:M:19:GLY:HA3	1:M:67:GLU:O	2.16	0.45
1:K:8:PHE:N	1:K:8:PHE:CD1	2.90	0.45
2:Q:88:VAL:HG12	2:Q:90:LEU:HD22	3.86	0.45
1:A:348:ILE:HG21	1:A:364:LEU:O	2.16	0.45
1:D:283:ARG:HH12	1:D:363:LYS:HD3	4.74	0.45
1:E:238:GLN:O	1:E:313:LEU:HD11	2.16	0.45
2:U:65:LYS:O	2:U:68:ASP:OD2	3.27	0.45
1:E:150:ILE:HG22	1:E:151:SER:N	2.32	0.45
1:I:298:THR:N	1:I:315:MET:O	2.50	0.45
1:F:218:PHE:HA	1:F:317:GLY:O	2.19	0.45
1:G:368:LEU:O	1:G:368:LEU:HD23	4.90	0.45
1:I:50:THR:HG21	1:I:55:THR:HB	2.01	0.45
1:M:323:ARG:HH12	1:M:392:LYS:CE	2.28	0.45
1:E:277:ALA:HB1	1:E:278:PRO:HD2	2.73	0.45
1:E:220:LEU:HD11	1:E:300:ILE:HD11	2.28	0.45
2:S:45:VAL:O	2:S:46:ILE:HD13	2.45	0.45
1:A:263:VAL:O	1:A:267:ARG:HG2	2.17	0.45
1:L:283:ARG:HH22	1:L:364:LEU:HA	1.82	0.45
1:L:286:GLU:HG3	1:L:367:ARG:NH2	2.39	0.45
2:U:24:PRO:CB	2:U:37:LYS:NZ	5.29	0.45
1:G:247:LEU:HD13	1:G:324:ILE:HD11	2.03	0.45
1:F:69:ILE:CG2	1:G:47:PRO:HG3	2.53	0.45
1:E:231:GLU:HA	1:E:309:GLU:HB3	2.73	0.45
1:H:178:GLU:CD	1:H:392:LYS:HE3	2.36	0.45
1:I:178:GLU:OE2	1:I:392:LYS:HE3	2.17	0.45
1:F:14:ARG:NH1	1:F:17:GLU:OE1	2.50	0.45
1:B:14:ARG:NH1	1:B:17:GLU:OE1	2.49	0.45
1:J:95:LEU:HD21	1:J:450:PRO:HG2	1.99	0.45
1:K:8:PHE:O	1:K:11:ALA:HB3	2.20	0.45
2:O:89:ILE:O	2:O:89:ILE:HG22	2.16	0.45
2:U:22:GLU:N	2:U:22:GLU:OE1	2.39	0.45
1:G:215:GLU:O	1:G:216:ASP:C	2.53	0.45
1:E:103:GLY:HA2	1:E:442:ILE:HD13	1.99	0.45
1:J:92:ALA:HB2	1:J:505:ALA:HA	1.99	0.45
2:T:15:VAL:HG21	2:T:95:LEU:HD21	2.23	0.45
1:A:237:GLU:OE2	2:O:28:GLY:N	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:20:ILE:CG1	2:O:43:GLY:HA2	2.45	0.45
2:U:41:GLN:CD	2:U:41:GLN:H	4.18	0.45
1:G:294:VAL:HG23	1:G:295:THR:HG23	5.66	0.45
1:J:37:ASN:ND2	1:J:51:LYS:HE2	2.28	0.45
1:M:383:ALA:O	1:N:280:PHE:HD1	1.98	0.45
1:H:46:SER:CB	1:H:47:PRO:HD2	2.42	0.45
1:A:252:ASP:OD1	1:A:276:LYS:HE2	2.28	0.45
1:N:253:VAL:O	1:N:258:LEU:HD22	2.18	0.45
1:J:120:ILE:HG23	1:J:443:VAL:CG2	2.47	0.45
1:B:131:ILE:HD13	1:B:502:THR:HG22	1.99	0.45
1:N:194:PHE:N	1:N:194:PHE:CD2	2.84	0.45
1:E:231:GLU:HB2	1:E:308:LEU:HD23	1.97	0.45
1:E:348:ILE:HD11	1:E:367:ARG:CZ	2.46	0.45
2:Q:34:ASP:HA	2:Q:37:LYS:HE2	1.99	0.45
1:A:103:GLY:O	1:A:107:VAL:HG23	2.27	0.45
1:J:438:THR:O	1:J:441:LYS:HB2	2.16	0.45
1:H:117:LYS:O	1:H:121:GLU:HG3	2.17	0.45
2:Q:80:ILE:CG2	2:Q:81:GLU:N	2.79	0.45
2:T:84:GLY:O	2:T:85:GLU:HB2	2.17	0.45
2:U:81:GLU:HG3	2:U:85:GLU:O	2.29	0.45
1:H:325:THR:CG2	1:H:326:LYS:N	2.81	0.45
1:I:247:LEU:HD13	1:I:324:ILE:HD11	1.99	0.45
1:N:37:ASN:ND2	1:N:51:LYS:HE2	2.31	0.45
1:C:209:THR:CB	1:C:211:GLU:HG2	4.63	0.45
1:C:237:GLU:CG	2:Q:30:ILE:HD12	2.47	0.45
1:C:280:PHE:O	1:C:281:GLY:C	2.55	0.45
1:E:54:VAL:HG13	1:E:89:THR:HG21	1.98	0.45
1:D:220:LEU:HD11	1:D:300:ILE:CD1	2.72	0.45
1:M:522:VAL:CG2	1:M:522:VAL:O	2.64	0.45
1:H:194:PHE:CD2	1:H:194:PHE:N	2.90	0.45
1:C:253:VAL:HG11	1:C:261:LEU:CD1	2.96	0.45
1:H:114:LEU:HD12	1:N:459:GLY:CA	2.54	0.45
1:L:247:LEU:HD13	1:L:324:ILE:HD11	2.00	0.45
1:M:84:VAL:HG12	1:M:500:LYS:CE	2.49	0.45
1:E:348:ILE:HD11	1:E:367:ARG:NH2	2.32	0.45
1:H:239:VAL:HG22	1:H:313:LEU:CD1	2.47	0.45
1:N:128:VAL:HA	1:N:131:ILE:HD12	1.98	0.45
1:J:412:PRO:HB3	1:J:490:MET:HB2	2.00	0.45
1:F:478:TYR:CE1	1:F:487:PHE:HB3	2.59	0.45
1:J:437:ALA:O	1:J:441:LYS:HG3	2.21	0.45
1:F:199:ILE:HG22	1:F:199:ILE:O	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LYS:O	1:B:431:LYS:HG3	2.16	0.45
1:C:518:THR:OG1	1:D:37:ASN:ND2	2.50	0.45
1:L:19:GLY:HA3	1:L:67:GLU:O	2.20	0.45
1:I:283:ARG:HD2	1:I:283:ARG:HA	1.67	0.45
1:E:267:ARG:HG3	1:E:267:ARG:NH1	2.31	0.45
2:R:13:ASP:O	2:R:62:LEU:HD21	2.16	0.45
1:N:286:GLU:HG3	1:N:367:ARG:NH2	2.31	0.45
1:B:150:ILE:CD1	1:B:496:VAL:H	2.30	0.45
1:E:136:ILE:HB	1:E:410:ILE:HG22	2.22	0.45
1:M:283:ARG:HA	1:M:283:ARG:HD2	1.70	0.45
1:B:288:LEU:HD23	1:B:291:ILE:HD12	2.46	0.45
2:O:78:THR:HG22	2:O:80:ILE:CD1	2.46	0.45
1:G:352:LEU:HD13	1:G:364:LEU:CB	5.66	0.45
1:E:340:ASP:O	1:E:344:ARG:HB2	2.30	0.45
1:M:50:THR:HG21	1:M:55:THR:HB	1.99	0.45
1:F:229:VAL:HG23	1:F:256:GLU:CD	2.49	0.45
2:S:10:PRO:CB	2:S:14:ARG:O	2.62	0.45
1:K:187:LYS:HZ2	1:K:379:ARG:HG3	1.93	0.45
1:J:149:THR:HG23	1:J:155:PRO:CA	2.39	0.45
1:H:149:THR:HG23	1:H:155:PRO:CA	2.43	0.45
1:L:295:THR:HG22	1:L:317:GLY:CA	2.47	0.45
1:H:309:GLU:OE1	1:H:309:GLU:N	2.40	0.45
1:A:501:VAL:HG23	1:A:502:THR:H	1.92	0.45
1:J:300:ILE:HG21	1:J:308:LEU:CD2	2.48	0.45
1:J:66:LEU:HD22	1:J:522:VAL:HG21	2.01	0.45
1:B:23:VAL:CG1	1:B:74:LEU:HD23	2.51	0.45
1:F:23:VAL:CG1	1:F:74:LEU:HD23	2.48	0.45
1:B:72:GLN:NE2	1:B:75:LYS:NZ	2.69	0.45
1:B:159:LYS:HE2	1:B:163:ASP:OD2	2.16	0.45
1:B:526:LYS:CG	1:B:527:PRO:HD2	2.90	0.45
1:D:189:VAL:CG1	1:D:193:GLN:HG2	2.47	0.45
1:E:161:ILE:HD12	1:E:399:LEU:CD2	2.66	0.45
1:E:13:ARG:HB3	1:E:104:LEU:HD22	2.06	0.45
1:F:418:LEU:H	1:F:418:LEU:HD12	1.81	0.45
1:C:194:PHE:HD1	1:C:196:LYS:HB2	2.19	0.45
1:K:201:PRO:O	1:K:204:VAL:HG23	2.16	0.45
1:L:18:ARG:HD2	1:L:67:GLU:OE1	2.25	0.45
1:H:41:GLU:OE2	1:I:525:GLU:N	2.49	0.45
1:H:202:TYR:HD2	1:H:266:LEU:HD11	1.82	0.45
1:I:449:GLU:HB2	1:I:450:PRO:HD3	1.99	0.45
1:N:86:GLY:O	1:N:87:ASP:HB2	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:ASN:HB3	1:F:269:THR:HB	2.15	0.45
2:R:18:LYS:HZ1	2:R:85:GLU:CD	2.48	0.44
1:E:150:ILE:O	1:E:153:ASN:N	2.58	0.44
1:E:248:ILE:CD1	1:E:261:LEU:HD21	2.44	0.44
1:F:235:ILE:O	1:F:239:VAL:HG23	2.17	0.44
1:M:325:THR:HG22	1:M:327:ASP:N	2.09	0.44
1:H:283:ARG:O	1:H:287:MET:HG3	2.34	0.44
1:E:286:GLU:OE2	1:E:344:ARG:NH2	2.43	0.44
1:E:343:ALA:HB2	1:F:207:PRO:CB	2.47	0.44
1:A:518:THR:OG1	1:B:37:ASN:ND2	2.68	0.44
1:C:7:VAL:HG21	1:C:66:LEU:CD1	2.33	0.44
1:M:47:PRO:CG	1:N:73:LEU:HD13	2.47	0.44
1:C:349:LYS:C	1:C:351:GLU:N	2.69	0.44
1:F:229:VAL:HG23	1:F:256:GLU:CG	2.47	0.44
2:T:31:VAL:HG12	2:T:32:LEU:N	3.14	0.44
1:D:246:LEU:O	1:D:272:VAL:HA	2.16	0.44
1:H:412:PRO:HB3	1:H:490:MET:HB2	2.07	0.44
1:L:41:GLU:HG2	1:M:524:ALA:HA	2.55	0.44
1:K:46:SER:HB2	1:K:47:PRO:CD	2.38	0.44
1:N:149:THR:HG23	1:N:155:PRO:CA	2.41	0.44
2:S:8:ILE:HD12	2:S:8:ILE:H	1.82	0.44
1:H:232:LEU:HD23	1:H:236:LEU:HB2	2.00	0.44
1:H:280:PHE:CE2	1:N:385:GLU:HB2	3.10	0.44
1:J:224:LYS:CG	1:J:225:LYS:N	2.80	0.44
1:K:228:ASN:HB3	1:K:231:GLU:HG2	1.99	0.44
1:G:220:LEU:HG	1:G:222:VAL:HG23	1.97	0.44
1:G:207:PRO:O	1:G:210:MET:CE	2.66	0.44
1:K:372:ALA:C	1:K:374:GLY:N	2.69	0.44
1:A:6:LEU:CD2	1:A:523:VAL:HG22	2.51	0.44
1:A:520:GLU:HG2	1:B:29:VAL:HG13	2.04	0.44
1:B:10:GLU:HA	1:B:13:ARG:HH11	1.83	0.44
1:E:457:ASN:HD22	1:E:457:ASN:N	2.18	0.44
1:J:204:VAL:HG13	1:J:211:GLU:O	2.18	0.44
2:T:22:GLU:HG2	2:T:40:PRO:HB3	4.77	0.44
2:Q:45:VAL:HG12	2:Q:46:ILE:H	2.67	0.44
2:Q:84:GLY:O	2:Q:85:GLU:HG2	4.07	0.44
1:C:277:ALA:CB	1:C:284:ARG:HD2	3.09	0.44
1:C:168:VAL:CG1	1:C:168:VAL:O	2.65	0.44
1:E:222:VAL:O	1:E:250:ALA:HA	2.17	0.44
1:E:291:ILE:O	1:E:294:VAL:HG22	2.18	0.44
2:R:91:SER:O	2:R:95:LEU:HG	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:SER:HA	1:C:254:GLU:O	2.41	0.44
1:A:515:LEU:HD12	1:B:49:ILE:CG2	2.46	0.44
1:L:47:PRO:HG2	1:M:73:LEU:HD13	2.13	0.44
1:N:307:LYS:HB2	1:N:310:ASN:ND2	2.33	0.44
1:K:385:GLU:O	1:K:389:LYS:HG3	2.18	0.44
1:G:229:VAL:HG23	1:G:256:GLU:CG	2.47	0.44
1:H:300:ILE:HG21	1:H:308:LEU:CD2	2.45	0.44
1:B:349:LYS:O	1:B:351:GLU:N	2.51	0.44
1:C:422:ILE:HD12	1:C:470:LEU:HD21	2.01	0.44
1:F:287:MET:O	1:F:291:ILE:HG13	2.31	0.44
1:J:458:ALA:C	1:K:114:LEU:CD1	2.85	0.44
1:D:321:ARG:HB3	1:D:332:VAL:HB	2.00	0.44
1:H:375:VAL:O	1:H:375:VAL:HG12	2.18	0.44
1:J:65:HIS:CD2	1:J:527:PRO:HG3	3.60	0.44
1:H:253:VAL:HG11	1:H:261:LEU:HD12	1.99	0.44
1:A:369:ALA:HB1	1:A:375:VAL:HG23	2.46	0.44
1:C:421:ALA:O	1:C:425:VAL:HG23	2.18	0.44
1:A:478:TYR:CE1	1:A:487:PHE:HB3	2.52	0.44
1:D:392:LYS:O	1:D:396:GLU:HG3	2.17	0.44
1:I:19:GLY:HA3	1:I:67:GLU:O	2.23	0.44
1:B:77:VAL:HG23	1:B:512:ILE:HG13	2.15	0.44
1:K:202:TYR:HD2	1:K:266:LEU:HD11	1.82	0.44
1:A:33:PRO:HD3	4:A:602:ADP:C5	2.58	0.44
2:O:15:VAL:CG2	2:O:95:LEU:HD11	2.30	0.44
2:U:69:ILE:O	2:U:98:VAL:HG13	2.17	0.44
1:J:360:ALA:O	1:J:364:LEU:HD13	2.33	0.44
1:B:218:PHE:HA	1:B:317:GLY:O	2.17	0.44
2:O:78:THR:CG2	2:O:80:ILE:HD11	2.46	0.44
1:H:283:ARG:HH12	1:H:364:LEU:HD11	2.36	0.44
1:I:309:GLU:N	1:I:309:GLU:OE1	2.42	0.44
1:K:292:ALA:HB1	1:K:297:GLY:O	2.18	0.44
1:M:362:GLU:HA	1:M:365:GLN:CG	2.63	0.44
1:K:123:ALA:HB3	1:K:443:VAL:HG21	2.16	0.44
1:K:278:PRO:O	1:K:284:ARG:HD3	2.17	0.44
1:A:47:PRO:HD2	1:G:73:LEU:CD2	2.89	0.44
2:Q:89:ILE:O	2:Q:89:ILE:CG2	2.87	0.44
1:M:222:VAL:CG1	1:M:223:GLU:N	2.80	0.44
1:L:74:LEU:HA	1:L:512:ILE:HD13	1.98	0.44
1:M:408:GLU:HB2	1:M:500:LYS:HB2	2.23	0.44
1:M:268:GLY:C	1:N:227:SER:HG	2.14	0.44
1:D:101:ARG:CG	1:D:102:GLU:H	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:LEU:HB2	1:G:90:THR:HG21	2.01	0.44
2:R:78:THR:HG22	2:R:80:ILE:CD1	2.47	0.44
2:Q:100:GLN:OE1	2:R:9:LYS:HE2	2.35	0.44
2:T:51:GLY:HA3	2:T:60:VAL:O	2.17	0.44
2:T:72:PHE:CD2	2:T:90:LEU:HD22	5.06	0.44
1:C:283:ARG:HH12	1:C:363:LYS:CB	3.14	0.44
1:J:30:THR:HB	1:J:51:LYS:O	2.17	0.44
1:C:301:SER:HB2	1:C:304:LEU:HB3	1.99	0.44
1:J:307:LYS:HB2	1:J:310:ASN:ND2	2.32	0.44
1:H:80:LYS:HE3	1:H:508:ASN:OD1	2.18	0.44
1:L:283:ARG:HH21	1:L:367:ARG:HD3	1.92	0.44
1:I:66:LEU:HD22	1:I:522:VAL:HG21	1.98	0.44
2:S:75:TYR:CD1	2:S:76:GLY:N	2.93	0.44
1:J:84:VAL:HG12	1:J:500:LYS:CE	2.52	0.44
1:H:313:LEU:O	1:H:313:LEU:HG	2.24	0.44
1:H:455:ALA:HB1	1:H:465:ILE:HD12	2.00	0.44
1:F:179:SER:OG	1:F:180:LYS:N	2.51	0.44
1:M:24:ALA:O	1:M:28:LYS:HG2	2.26	0.44
1:D:13:ARG:HB3	1:D:104:LEU:HD22	2.05	0.44
2:T:65:LYS:O	2:T:68:ASP:HB2	3.78	0.44
1:J:433:GLU:HG2	1:J:434:GLY:N	2.33	0.44
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.98	0.44
1:D:103:GLY:O	1:D:107:VAL:HG23	2.24	0.44
1:I:352:LEU:HD21	1:I:365:GLN:NE2	2.33	0.44
2:Q:41:GLN:HE21	2:Q:73:ALA:HA	3.39	0.44
2:Q:79:GLU:HG2	2:Q:88:VAL:HG13	1.99	0.44
2:R:18:LYS:HG2	2:R:87:TYR:CE2	2.64	0.44
2:R:79:GLU:HG2	2:R:88:VAL:HG22	2.08	0.44
2:R:81:GLU:HG3	2:R:85:GLU:O	2.24	0.44
1:C:232:LEU:HB3	1:C:236:LEU:HD11	2.12	0.44
1:C:294:VAL:HA	1:C:341:ILE:HD11	2.73	0.44
2:O:18:LYS:NZ	2:O:85:GLU:CD	2.87	0.44
1:H:37:ASN:ND2	1:H:51:LYS:HE2	2.26	0.44
1:C:224:LYS:H	1:C:224:LYS:CD	3.81	0.44
1:M:352:LEU:HD21	1:M:365:GLN:HE22	1.83	0.44
1:L:228:ASN:ND2	1:L:230:ARG:HB3	2.29	0.44
2:S:20:ILE:O	2:S:40:PRO:HB3	2.45	0.44
1:D:23:VAL:CG1	1:D:74:LEU:HD23	2.47	0.44
1:E:526:LYS:HA	1:E:527:PRO:HD3	1.82	0.44
2:O:73:ALA:O	2:O:75:TYR:N	2.51	0.44
1:B:460:TYR:HB3	1:B:465:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:THR:OG1	1:I:508:ASN:ND2	2.50	0.44
1:G:237:GLU:OE2	2:U:28:GLY:N	3.70	0.44
1:G:463:SER:O	1:G:467:GLN:HG2	2.29	0.44
1:J:253:VAL:HG11	1:J:261:LEU:HD12	1.99	0.44
1:D:31:LEU:HB2	1:D:90:THR:HG21	2.10	0.44
1:I:181:SER:HA	1:J:282:ASP:OD2	2.42	0.44
1:E:256:GLU:OE1	2:S:35:THR:C	3.84	0.44
2:R:78:THR:CG2	2:R:80:ILE:HD11	2.48	0.44
2:T:84:GLY:O	2:T:85:GLU:HG2	4.06	0.44
2:U:53:VAL:HG22	2:U:59:ARG:CG	2.48	0.44
2:P:52:ARG:HD3	2:P:92:GLU:OE2	3.35	0.44
2:Q:54:LEU:HD11	2:R:57:GLY:N	2.31	0.44
1:E:227:SER:HA	1:E:254:GLU:O	2.17	0.44
1:D:250:ALA:O	1:D:251:GLU:C	2.65	0.44
1:B:39:VAL:HG22	1:B:49:ILE:HG12	1.99	0.44
1:J:187:LYS:HZ1	1:J:379:ARG:HG3	1.83	0.44
1:H:342:GLU:HA	1:H:345:ILE:HD12	2.00	0.44
1:D:501:VAL:HG23	1:D:502:THR:H	1.84	0.44
1:K:222:VAL:CG1	1:K:223:GLU:H	2.32	0.44
2:S:19:ARG:HA	2:S:42:LYS:O	2.17	0.44
2:S:78:THR:HG22	2:S:79:GLU:N	2.32	0.44
1:H:247:LEU:HD13	1:H:324:ILE:HD11	2.02	0.44
1:F:74:LEU:HD21	1:F:93:THR:CG2	2.47	0.44
1:L:178:GLU:OE2	1:L:392:LYS:HE3	2.18	0.44
1:N:175:THR:CG2	1:N:177:GLU:OE2	2.65	0.44
1:B:307:LYS:HG3	2:Q:34:ASP:O	4.46	0.44
1:J:175:THR:CG2	1:J:177:GLU:OE2	2.69	0.44
1:L:22:ALA:HB1	1:M:6:LEU:HD12	1.99	0.44
1:J:412:PRO:HD2	1:J:417:THR:OG1	2.17	0.44
1:A:27:VAL:O	1:A:29:VAL:N	2.77	0.44
1:B:88:GLY:HA2	4:B:602:ADP:O2B	2.34	0.44
1:D:410:ILE:HD11	1:D:496:VAL:HG21	2.05	0.44
2:Q:45:VAL:CG1	2:Q:46:ILE:N	3.25	0.44
1:E:233:LEU:N	1:E:234:PRO:HD2	2.49	0.44
2:U:81:GLU:HG3	2:U:85:GLU:C	2.38	0.44
1:B:490:MET:CE	1:B:495:ILE:HG21	2.62	0.44
1:A:519:THR:HG23	1:B:39:VAL:HG23	2.16	0.44
1:L:46:SER:HB2	1:L:47:PRO:CD	2.43	0.44
1:L:283:ARG:HD3	1:L:363:LYS:HE3	2.00	0.44
1:B:128:VAL:HA	1:B:131:ILE:HD12	2.04	0.44
2:S:34:ASP:HA	2:S:37:LYS:HE2	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:222:VAL:CG1	1:N:223:GLU:H	2.31	0.44
1:B:352:LEU:C	1:B:354:THR:H	2.30	0.44
2:O:33:PRO:O	2:O:35:THR:N	2.51	0.44
1:A:229:VAL:HG23	1:A:256:GLU:CG	2.47	0.44
1:A:101:ARG:CG	1:A:102:GLU:H	2.37	0.44
1:C:520:GLU:HB3	1:D:29:VAL:CG1	2.47	0.44
1:A:10:GLU:N	1:A:13:ARG:HH12	2.15	0.44
1:B:180:LYS:HD3	1:B:180:LYS:HA	1.81	0.44
1:K:49:ILE:HG13	1:K:49:ILE:O	2.18	0.44
1:C:323:ARG:HG2	1:C:323:ARG:HH11	1.82	0.44
1:G:457:ASN:N	1:G:457:ASN:HD22	2.25	0.44
1:I:478:TYR:CZ	1:I:487:PHE:HB3	2.53	0.44
1:N:160:LEU:HD22	1:N:186:LEU:HB2	2.00	0.44
1:M:285:LYS:HG2	1:M:289:LYS:HE3	2.00	0.44
1:E:410:ILE:HG12	1:E:496:VAL:HB	2.06	0.44
1:F:150:ILE:CD1	1:F:496:VAL:N	2.80	0.44
1:A:147:VAL:CG2	1:A:410:ILE:HD11	2.48	0.44
2:P:17:VAL:O	2:P:87:TYR:HB3	2.17	0.44
2:P:13:ASP:CA	2:P:62:LEU:HD21	2.48	0.44
1:K:37:ASN:ND2	1:K:51:LYS:HE2	2.29	0.44
1:G:238:GLN:HB3	1:G:313:LEU:CG	2.84	0.44
1:G:238:GLN:O	1:G:313:LEU:HD11	2.39	0.44
1:G:214:LEU:HB3	1:G:245:PRO:HB3	2.70	0.44
1:G:270:LEU:HG	1:G:272:VAL:HG13	1.98	0.44
1:N:253:VAL:HG21	1:N:274:ALA:HB1	2.00	0.44
1:E:501:VAL:CG2	1:E:502:THR:N	2.87	0.44
1:H:385:GLU:O	1:H:389:LYS:HG3	2.18	0.44
1:L:526:LYS:O	1:L:527:PRO:C	2.56	0.44
2:P:8:ILE:CD1	2:P:8:ILE:N	2.80	0.44
1:J:460:TYR:CE2	1:J:480:PHE:HZ	2.50	0.44
1:H:312:THR:C	1:H:314:SER:N	2.71	0.44
1:N:316:LEU:HD23	1:N:316:LEU:H	1.87	0.44
1:G:233:LEU:CD2	2:U:30:ILE:HG21	2.48	0.44
2:O:53:VAL:HG22	2:O:59:ARG:HE	1.82	0.44
1:D:337:LYS:O	1:D:340:ASP:HB2	2.39	0.44
1:F:250:ALA:O	1:F:252:ASP:N	2.55	0.44
1:B:398:ALA:O	1:B:401:ALA:HB3	2.37	0.44
1:M:18:ARG:HD2	1:M:67:GLU:OE1	2.20	0.44
1:N:298:THR:N	1:N:315:MET:O	2.51	0.44
1:E:152:ALA:HB2	1:E:398:ALA:HB2	2.00	0.44
1:D:264:ASN:HB3	1:D:269:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PRO:HG3	1:D:36:ARG:NH1	2.32	0.44
1:E:478:TYR:CE1	1:E:487:PHE:HB3	2.53	0.44
2:O:54:LEU:HD13	2:P:55:GLU:C	4.09	0.44
1:A:410:ILE:HG12	1:A:496:VAL:HB	2.01	0.44
2:P:48:VAL:CG1	2:P:62:LEU:CD1	2.93	0.44
2:P:48:VAL:HG12	2:P:62:LEU:CD1	2.29	0.44
1:C:218:PHE:HE1	1:C:244:LYS:HB2	1.95	0.44
1:C:235:ILE:CD1	1:C:311:ALA:HB1	3.07	0.44
1:C:217:ALA:CB	1:C:245:PRO:HB2	2.44	0.44
1:C:348:ILE:HD12	1:C:367:ARG:HE	4.12	0.44
1:G:277:ALA:CB	1:G:284:ARG:HD2	2.78	0.44
1:M:295:THR:HG22	1:M:317:GLY:CA	2.48	0.44
1:J:37:ASN:OD1	1:K:515:LEU:HD12	2.18	0.44
2:R:97:ALA:CA	2:S:11:LEU:HD13	2.65	0.44
1:D:218:PHE:CE1	1:D:244:LYS:HB2	2.52	0.44
1:D:218:PHE:HA	1:D:317:GLY:O	2.18	0.44
1:J:46:SER:CB	1:J:47:PRO:HD2	2.37	0.44
1:L:39:VAL:HG11	1:M:69:ILE:HG21	1.98	0.44
1:M:526:LYS:CG	1:M:527:PRO:HD2	2.48	0.44
1:E:515:LEU:HD12	1:F:49:ILE:CG2	2.44	0.44
1:F:348:ILE:HG21	1:F:364:LEU:O	2.18	0.44
1:K:384:THR:HG22	1:K:385:GLU:N	2.33	0.44
1:J:194:PHE:HB2	1:J:278:PRO:HB3	1.99	0.44
1:A:34:ARG:NH1	1:G:112:ASN:HD21	2.16	0.44
1:A:422:ILE:HD12	1:A:470:LEU:HD21	2.00	0.44
1:J:232:LEU:CD2	1:J:236:LEU:HD13	2.51	0.44
1:D:229:VAL:HG23	1:D:256:GLU:OE2	2.24	0.44
1:G:247:LEU:HD22	1:G:322:VAL:CG1	2.99	0.44
1:B:455:ALA:O	1:B:458:ALA:HB3	2.31	0.44
1:J:312:THR:O	1:J:314:SER:N	2.48	0.44
1:K:178:GLU:CD	1:K:392:LYS:HE3	2.38	0.44
1:J:69:ILE:O	1:J:73:LEU:HB2	2.24	0.44
2:O:59:ARG:O	2:O:61:PRO:HD3	2.42	0.44
1:C:289:LYS:HE2	1:D:202:TYR:OH	2.18	0.44
1:F:123:ALA:HA	1:F:428:LEU:HD23	2.05	0.44
1:K:478:TYR:CZ	1:K:487:PHE:HB3	2.57	0.44
1:K:290:ASP:N	1:K:344:ARG:NH1	2.66	0.43
2:P:21:GLU:C	2:P:22:GLU:O	2.54	0.43
2:Q:48:VAL:HG13	2:Q:62:LEU:HD12	5.42	0.43
2:Q:81:GLU:HA	2:Q:85:GLU:O	2.18	0.43
2:R:18:LYS:HE3	2:R:86:GLU:O	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:17:VAL:CG1	2:R:18:LYS:N	2.81	0.43
2:U:50:THR:CG2	2:U:59:ARG:HD3	2.48	0.43
2:U:45:VAL:HG22	2:U:70:VAL:CG1	4.93	0.43
1:G:150:ILE:HD12	1:G:496:VAL:H	1.98	0.43
1:N:30:THR:HB	1:N:51:LYS:O	2.22	0.43
1:B:265:LYS:HA	1:B:270:LEU:O	2.17	0.43
1:B:284:ARG:HG3	1:B:284:ARG:NH1	4.35	0.43
1:C:345:ILE:HG22	1:C:346:ASN:N	2.33	0.43
1:C:348:ILE:HD11	1:C:367:ARG:HB3	2.73	0.43
1:G:349:LYS:C	1:G:351:GLU:N	2.71	0.43
1:E:31:LEU:CD1	4:E:602:ADP:H5'1	2.78	0.43
1:H:283:ARG:HD2	1:H:283:ARG:HA	1.74	0.43
1:E:355:THR:CG2	1:E:360:ALA:HB3	2.48	0.43
1:M:46:SER:CB	1:M:47:PRO:HD2	2.41	0.43
1:F:229:VAL:HG12	1:F:233:LEU:CD1	2.44	0.43
2:R:98:VAL:O	2:S:9:LYS:HB2	2.18	0.43
1:L:307:LYS:HB2	1:L:310:ASN:ND2	2.35	0.43
1:N:292:ALA:HB1	1:N:297:GLY:O	2.28	0.43
1:L:194:PHE:CE2	1:L:329:THR:HB	2.53	0.43
1:L:247:LEU:HD22	1:L:322:VAL:CG1	2.53	0.43
1:J:286:GLU:OE2	1:J:344:ARG:NH2	2.50	0.43
1:E:455:ALA:O	1:E:458:ALA:HB3	2.30	0.43
1:L:465:ILE:HD13	1:L:480:PHE:CD1	2.59	0.43
1:M:316:LEU:HD23	1:M:316:LEU:O	2.18	0.43
1:J:526:LYS:HG3	1:J:527:PRO:HD2	1.99	0.43
1:J:316:LEU:H	1:J:316:LEU:HD23	1.85	0.43
1:I:130:LYS:O	1:I:134:LEU:HB2	2.25	0.43
1:K:452:ARG:NH1	1:K:452:ARG:HG2	2.33	0.43
1:B:344:ARG:HA	1:B:344:ARG:HD2	1.80	0.43
1:M:285:LYS:O	1:M:289:LYS:HG3	2.19	0.43
1:C:80:LYS:HE2	1:D:383:ALA:O	2.18	0.43
1:K:412:PRO:HB3	1:K:490:MET:HB2	2.07	0.43
2:T:22:GLU:N	2:T:22:GLU:OE1	2.46	0.43
1:B:256:GLU:HB3	2:P:35:THR:HB	2.00	0.43
2:T:17:VAL:HG12	2:T:18:LYS:N	2.33	0.43
1:G:410:ILE:HG12	1:G:496:VAL:HB	2.00	0.43
1:A:150:ILE:CD1	1:A:496:VAL:N	2.82	0.43
1:K:197:GLY:HA3	1:K:325:THR:O	2.20	0.43
2:P:20:ILE:O	2:P:40:PRO:HB3	2.18	0.43
1:F:235:ILE:HD13	1:F:235:ILE:HG21	1.82	0.43
1:F:265:LYS:HA	1:F:270:LEU:O	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:TYR:CE1	1:G:363:LYS:HE2	2.52	0.43
1:M:342:GLU:O	1:M:346:ASN:ND2	2.57	0.43
1:A:283:ARG:O	1:A:287:MET:HG3	2.53	0.43
1:L:117:LYS:O	1:L:121:GLU:HG3	2.18	0.43
1:I:300:ILE:HG21	1:I:308:LEU:CD2	2.46	0.43
1:L:385:GLU:O	1:L:389:LYS:HG3	2.16	0.43
1:J:7:VAL:HG21	1:J:66:LEU:CD1	2.47	0.43
2:S:17:VAL:CG1	2:S:43:GLY:HA3	2.52	0.43
1:E:231:GLU:CB	1:E:308:LEU:HD23	2.49	0.43
1:M:194:PHE:HB2	1:M:278:PRO:HB3	1.99	0.43
1:K:465:ILE:HD13	1:K:480:PHE:CD1	2.56	0.43
1:G:452:ARG:HH11	1:G:463:SER:HA	1.81	0.43
1:I:316:LEU:HD23	1:I:316:LEU:O	2.18	0.43
1:I:253:VAL:O	1:I:258:LEU:HD22	2.18	0.43
1:I:425:VAL:O	1:I:429:ILE:HG13	2.19	0.43
1:A:157:VAL:O	1:A:161:ILE:HG12	2.17	0.43
1:M:412:PRO:HB3	1:M:490:MET:HB2	2.00	0.43
1:F:221:ILE:HG22	1:F:299:VAL:HG13	2.00	0.43
2:Q:38:GLU:HG2	2:Q:38:GLU:H	1.58	0.43
1:L:342:GLU:O	1:L:346:ASN:ND2	2.51	0.43
2:T:38:GLU:O	2:T:39:LYS:C	2.89	0.43
1:A:354:THR:HG22	1:A:354:THR:O	2.20	0.43
2:T:60:VAL:HG13	2:T:61:PRO:CD	3.78	0.43
2:U:17:VAL:CG1	2:U:43:GLY:HA3	2.48	0.43
1:B:147:VAL:HG23	1:B:410:ILE:HD11	2.00	0.43
1:C:297:GLY:H	1:C:317:GLY:HA2	1.83	0.43
1:G:341:ILE:C	1:G:343:ALA:N	3.34	0.43
1:E:33:PRO:HG3	4:E:602:ADP:C6	2.53	0.43
1:H:50:THR:HG21	1:H:55:THR:HB	2.02	0.43
1:M:46:SER:HB2	1:M:47:PRO:CD	2.42	0.43
1:D:220:LEU:HD13	1:D:235:ILE:HD12	2.98	0.43
1:C:312:THR:HG22	1:C:314:SER:N	3.19	0.43
1:L:39:VAL:HG11	1:M:69:ILE:CG2	2.48	0.43
1:J:342:GLU:HA	1:J:345:ILE:HD12	1.99	0.43
1:A:307:LYS:HG3	2:P:34:ASP:HB3	2.51	0.43
1:C:501:VAL:HG23	1:C:502:THR:H	1.81	0.43
1:B:503:ARG:O	1:B:507:GLN:HG3	2.18	0.43
1:A:72:GLN:HE22	1:A:75:LYS:HZ3	1.69	0.43
1:N:277:ALA:HB1	1:N:284:ARG:HD2	2.06	0.43
1:C:321:ARG:O	1:C:322:VAL:HG23	2.50	0.43
1:D:23:VAL:HB	1:D:74:LEU:HD23	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:PRO:O	1:E:210:MET:HE3	2.18	0.43
1:B:307:LYS:HB2	1:B:310:ASN:HD22	1.83	0.43
1:D:452:ARG:HH11	1:D:463:SER:HA	1.84	0.43
1:L:425:VAL:O	1:L:429:ILE:HG13	2.17	0.43
1:A:421:ALA:O	1:A:425:VAL:HG23	2.28	0.43
1:L:332:VAL:HG22	1:L:375:VAL:HG11	2.02	0.43
1:L:132:LYS:C	1:L:134:LEU:H	2.24	0.43
1:M:132:LYS:C	1:M:134:LEU:H	2.22	0.43
1:B:80:LYS:HG2	1:C:383:ALA:O	2.51	0.43
1:N:433:GLU:HG2	1:N:434:GLY:N	2.33	0.43
1:K:433:GLU:HG2	1:K:434:GLY:N	2.36	0.43
1:L:478:TYR:CZ	1:L:487:PHE:HB3	2.54	0.43
1:B:267:ARG:HB3	1:B:269:THR:OG1	2.60	0.43
2:P:41:GLN:HB3	2:P:72:PHE:O	2.18	0.43
2:Q:98:VAL:HB	2:R:9:LYS:HB2	2.53	0.43
2:Q:96:LEU:O	2:R:10:PRO:HA	3.00	0.43
1:L:311:ALA:HA	1:L:315:MET:SD	2.58	0.43
2:O:9:LYS:HE3	2:U:100:GLN:HB2	3.32	0.43
2:U:70:VAL:O	2:U:71:VAL:HG23	3.49	0.43
1:G:150:ILE:CD1	1:G:496:VAL:N	2.95	0.43
2:P:80:ILE:CG2	2:P:81:GLU:H	2.31	0.43
1:C:341:ILE:O	1:C:345:ILE:HG22	5.27	0.43
1:E:7:VAL:CG2	1:E:66:LEU:HD11	2.47	0.43
1:M:178:GLU:CA	1:M:321:ARG:NH1	2.79	0.43
1:B:289:LYS:CE	1:C:202:TYR:OH	2.60	0.43
1:N:444:ARG:HG2	1:N:444:ARG:O	2.18	0.43
2:S:78:THR:HG22	2:S:80:ILE:HD11	2.06	0.43
1:F:72:GLN:HE22	1:F:75:LYS:HZ1	1.66	0.43
1:G:340:ASP:O	1:G:344:ARG:HB2	2.19	0.43
1:F:422:ILE:HD12	1:F:470:LEU:HD21	2.04	0.43
1:K:312:THR:C	1:K:314:SER:N	2.72	0.43
2:T:66:GLU:HG2	2:T:67:GLY:H	4.42	0.43
1:I:316:LEU:HD23	1:I:316:LEU:H	1.82	0.43
1:F:448:GLU:OE1	1:F:452:ARG:NH2	2.51	0.43
1:F:520:GLU:HB3	1:G:29:VAL:CG1	2.48	0.43
1:D:179:SER:HB2	1:D:379:ARG:HB3	2.00	0.43
1:M:71:ALA:O	1:M:75:LYS:HG3	2.18	0.43
1:A:209:THR:O	1:A:211:GLU:HG3	2.18	0.43
1:A:506:LEU:O	1:A:506:LEU:HD12	2.35	0.43
1:B:296:GLY:CA	1:B:336:GLY:HA2	2.48	0.43
1:D:77:VAL:HG23	1:D:512:ILE:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:20:ILE:O	2:T:20:ILE:HG22	3.30	0.43
1:B:325:THR:CG2	1:B:326:LYS:H	2.25	0.43
1:E:242:THR:HG22	1:E:242:THR:O	2.18	0.43
2:P:19:ARG:HA	2:P:42:LYS:O	2.28	0.43
2:P:15:VAL:CG1	2:P:45:VAL:HG13	2.42	0.43
2:P:13:ASP:HB2	2:P:52:ARG:HB3	3.76	0.43
1:J:360:ALA:O	1:J:364:LEU:CD1	2.78	0.43
1:K:332:VAL:HG22	1:K:375:VAL:CG1	2.74	0.43
2:Q:31:VAL:O	2:Q:32:LEU:O	3.73	0.43
1:K:217:ALA:HB1	1:K:245:PRO:O	2.19	0.43
1:F:168:VAL:CG1	1:F:168:VAL:O	2.66	0.43
1:E:341:ILE:O	1:E:345:ILE:HG22	2.19	0.43
1:A:51:LYS:O	1:A:51:LYS:HG2	2.18	0.43
1:L:39:VAL:HB	1:M:522:VAL:HG12	2.32	0.43
1:L:179:SER:HB2	1:L:379:ARG:CB	2.41	0.43
1:I:270:LEU:CD2	1:I:272:VAL:HG13	2.38	0.43
1:H:79:SER:C	1:H:81:THR:N	2.72	0.43
1:C:199:ILE:O	1:C:199:ILE:HG22	2.19	0.43
1:K:267:ARG:O	1:L:256:GLU:HG3	2.27	0.43
2:U:33:PRO:O	2:U:36:ALA:N	2.80	0.43
1:K:84:VAL:HG12	1:K:500:LYS:CE	2.44	0.43
1:D:288:LEU:HD23	1:D:291:ILE:HD12	2.01	0.43
1:F:345:ILE:HG23	1:F:368:LEU:CD1	2.53	0.43
1:G:320:GLU:O	1:G:321:ARG:HB2	2.19	0.43
1:F:73:LEU:CD2	1:G:47:PRO:HD2	2.49	0.43
1:L:300:ILE:O	1:L:300:ILE:HG22	2.29	0.43
1:J:313:LEU:HG	1:J:313:LEU:O	2.19	0.43
1:D:332:VAL:HG12	1:D:333:GLY:N	2.35	0.43
1:K:28:LYS:HZ2	1:K:97:GLN:HE22	1.79	0.43
1:G:23:VAL:CG1	1:G:74:LEU:HD23	2.49	0.43
1:H:253:VAL:O	1:H:258:LEU:HD22	2.17	0.43
1:C:101:ARG:CG	1:C:102:GLU:H	2.35	0.43
1:B:396:GLU:O	1:B:400:ASN:ND2	2.66	0.43
1:L:313:LEU:O	1:L:313:LEU:HG	2.17	0.43
1:A:478:TYR:CZ	1:A:487:PHE:HB3	2.54	0.43
1:J:49:ILE:O	1:J:49:ILE:HG13	2.19	0.43
1:B:198:TYR:O	1:B:198:TYR:HD1	2.01	0.43
1:N:132:LYS:C	1:N:134:LEU:H	2.21	0.43
1:L:71:ALA:O	1:L:75:LYS:HG3	2.43	0.43
1:K:360:ALA:O	1:K:364:LEU:CD1	2.70	0.43
2:P:71:VAL:HG13	2:Q:80:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:78:THR:CG2	2:R:79:GLU:N	2.81	0.43
2:O:13:ASP:CA	2:O:62:LEU:HD21	2.49	0.43
2:T:11:LEU:O	2:T:13:ASP:N	2.52	0.43
1:M:190:GLU:HG3	1:M:341:ILE:HD13	1.99	0.43
1:E:262:VAL:O	1:E:265:LYS:HB3	2.19	0.43
1:F:218:PHE:CZ	1:F:242:THR:HG21	3.00	0.43
1:F:218:PHE:CE1	1:F:244:LYS:HB2	2.80	0.43
1:J:360:ALA:O	1:J:363:LYS:HG2	2.17	0.43
1:A:228:ASN:ND2	1:A:230:ARG:HB2	2.52	0.43
1:E:198:TYR:CD1	1:E:198:TYR:O	3.08	0.43
1:E:31:LEU:HB2	1:E:90:THR:CG2	2.47	0.43
1:E:345:ILE:HG22	1:E:346:ASN:N	2.90	0.43
1:D:54:VAL:HG13	1:D:89:THR:HG21	2.00	0.43
1:A:218:PHE:CE1	1:A:242:THR:HG21	2.63	0.43
1:A:218:PHE:HA	1:A:317:GLY:O	2.18	0.43
1:K:307:LYS:HB2	1:K:310:ASN:ND2	2.38	0.43
1:L:40:LEU:CD1	1:L:40:LEU:N	2.81	0.43
1:K:342:GLU:O	1:K:346:ASN:ND2	2.51	0.43
1:C:267:ARG:NH1	1:C:267:ARG:HG3	4.70	0.43
1:N:117:LYS:O	1:N:121:GLU:HG3	2.24	0.43
1:M:277:ALA:HB1	1:M:284:ARG:HD2	2.07	0.43
1:B:193:GLN:HB2	1:B:329:THR:O	2.40	0.43
1:D:253:VAL:HG21	1:D:274:ALA:HB1	2.01	0.43
1:A:452:ARG:HH11	1:A:463:SER:HA	1.83	0.43
1:C:144:ILE:HD13	1:C:402:THR:CG2	2.66	0.43
1:L:95:LEU:O	1:L:99:ILE:HG13	2.18	0.43
1:E:103:GLY:O	1:E:107:VAL:HG23	2.31	0.43
1:H:193:GLN:HE21	1:H:330:THR:CG2	2.31	0.43
1:A:84:VAL:HG12	1:A:84:VAL:O	2.18	0.43
1:N:49:ILE:HG13	1:N:49:ILE:O	2.21	0.43
1:M:8:PHE:CD1	1:M:8:PHE:N	2.87	0.43
1:I:86:GLY:O	1:I:87:ASP:HB2	2.23	0.43
1:E:475:ASN:HA	1:E:476:PRO:HD2	1.92	0.43
1:G:264:ASN:OD1	1:G:269:THR:HG21	2.62	0.43
1:H:433:GLU:HG2	1:H:434:GLY:N	2.34	0.43
1:F:152:ALA:HB2	1:F:398:ALA:HB2	2.00	0.43
1:K:86:GLY:O	1:K:87:ASP:HB2	2.19	0.43
1:G:297:GLY:N	1:G:317:GLY:HA2	2.34	0.43
2:Q:71:VAL:HG23	2:Q:99:LEU:HD13	2.01	0.43
1:D:359:TYR:CE1	1:D:363:LYS:HE3	3.18	0.43
1:E:237:GLU:O	1:E:238:GLN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:13:ASP:O	2:U:13:ASP:OD1	2.44	0.43
2:P:78:THR:HG22	2:P:79:GLU:N	2.36	0.43
1:B:242:THR:HG22	1:B:244:LYS:HG2	2.35	0.43
1:C:229:VAL:O	1:C:233:LEU:HG	2.18	0.43
1:C:219:ILE:N	1:C:317:GLY:O	2.47	0.43
1:C:237:GLU:HG2	2:Q:30:ILE:HD12	2.00	0.43
2:Q:33:PRO:HG2	2:Q:33:PRO:O	2.42	0.43
1:G:51:LYS:HG2	1:G:51:LYS:O	2.19	0.43
1:C:54:VAL:HG13	1:C:89:THR:HG21	2.07	0.43
1:B:51:LYS:O	1:B:51:LYS:HG2	2.18	0.43
1:H:412:PRO:HD2	1:H:417:THR:OG1	2.32	0.43
1:A:66:LEU:HD22	1:A:522:VAL:CG1	2.42	0.43
1:A:261:LEU:CD2	1:A:272:VAL:HG21	2.48	0.43
1:N:261:LEU:HD22	1:N:272:VAL:HG21	1.99	0.43
1:J:411:VAL:O	1:J:496:VAL:CG1	2.68	0.43
1:C:506:LEU:HD12	1:C:506:LEU:O	2.18	0.43
1:H:352:LEU:HD21	1:H:365:GLN:HE22	1.84	0.43
1:J:385:GLU:O	1:J:389:LYS:HG3	2.19	0.43
1:H:222:VAL:CG1	1:H:223:GLU:H	2.32	0.43
1:F:288:LEU:HD23	1:F:288:LEU:HA	1.88	0.43
1:E:210:MET:CE	1:E:210:MET:HA	2.49	0.43
1:B:72:GLN:HE22	1:B:75:LYS:HZ1	1.74	0.43
1:G:74:LEU:HD21	1:G:93:THR:CG2	2.50	0.43
1:E:421:ALA:O	1:E:425:VAL:HG23	2.28	0.43
1:F:452:ARG:HH11	1:F:463:SER:HA	1.85	0.43
1:F:344:ARG:HA	1:F:344:ARG:HD2	1.63	0.43
1:B:323:ARG:HG2	1:B:323:ARG:NH1	2.53	0.43
1:K:18:ARG:HD2	1:K:67:GLU:OE1	2.25	0.43
1:J:372:ALA:C	1:J:374:GLY:H	2.20	0.43
1:H:5:ILE:O	1:H:5:ILE:HG23	2.23	0.43
1:L:433:GLU:HG2	1:L:434:GLY:N	2.36	0.43
1:B:518:THR:OG1	1:C:37:ASN:ND2	2.64	0.43
2:Q:15:VAL:CG2	2:Q:62:LEU:HD13	7.35	0.43
1:E:232:LEU:HB3	1:E:236:LEU:CD1	2.48	0.43
2:U:71:VAL:CG2	2:U:99:LEU:HG	5.26	0.43
1:L:37:ASN:ND2	1:L:51:LYS:HE2	2.26	0.43
1:H:286:GLU:HG3	1:H:367:ARG:HH22	1.84	0.43
1:H:283:ARG:CG	1:H:363:LYS:HZ1	2.64	0.43
1:A:297:GLY:H	1:A:317:GLY:HA2	1.84	0.43
1:L:41:GLU:OE2	1:M:524:ALA:HB1	2.54	0.43
1:B:303:GLU:HA	1:C:259:ALA:HB2	6.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:VAL:CG2	1:C:502:THR:N	2.82	0.43
1:L:283:ARG:HD3	1:L:363:LYS:HZ1	1.83	0.43
1:M:224:LYS:CG	1:M:225:LYS:N	2.78	0.43
1:D:72:GLN:HE22	1:D:75:LYS:HZ1	1.67	0.43
1:M:194:PHE:CD2	1:M:194:PHE:N	2.87	0.43
1:N:438:THR:O	1:N:441:LYS:HB2	2.19	0.43
1:B:472:GLU:HB3	1:B:478:TYR:CD2	2.61	0.43
1:H:285:LYS:O	1:H:289:LYS:HG3	2.22	0.43
1:F:457:ASN:N	1:F:457:ASN:HD22	2.17	0.43
1:G:475:ASN:HA	1:G:476:PRO:HD2	1.95	0.43
1:E:260:THR:OG1	2:S:33:PRO:CG	3.22	0.43
1:A:350:LYS:O	1:B:208:GLU:O	5.99	0.43
2:T:10:PRO:O	2:T:49:GLY:HA2	3.47	0.43
1:C:335:LYS:O	1:C:336:GLY:O	2.52	0.43
1:E:519:THR:HG23	1:F:39:VAL:HG23	2.00	0.43
1:E:345:ILE:HG23	1:E:368:LEU:CD1	6.22	0.43
1:B:37:ASN:HB3	1:B:50:THR:O	2.30	0.43
2:S:11:LEU:HB3	2:S:12:GLY:H	1.74	0.43
1:A:250:ALA:C	1:A:252:ASP:N	2.73	0.43
1:A:235:ILE:HD12	1:A:311:ALA:HB3	1.99	0.43
1:N:412:PRO:HB3	1:N:490:MET:HB2	2.03	0.43
1:K:307:LYS:HE3	1:K:310:ASN:HD21	1.82	0.43
1:H:179:SER:CB	1:H:379:ARG:HB3	2.38	0.43
1:G:209:THR:CG2	1:G:211:GLU:HG3	4.46	0.43
1:N:77:VAL:HG11	1:N:512:ILE:HG13	2.00	0.43
1:C:124:VAL:HG13	1:C:506:LEU:HG	2.00	0.43
2:S:80:ILE:HG22	2:S:81:GLU:H	1.83	0.43
1:A:198:TYR:CZ	1:A:326:LYS:HA	2.82	0.43
1:C:118:ARG:O	1:C:122:LYS:HG3	2.28	0.43
1:E:396:GLU:O	1:E:400:ASN:ND2	2.58	0.43
2:Q:21:GLU:CD	2:Q:21:GLU:H	2.22	0.43
1:D:84:VAL:HG12	1:D:84:VAL:O	2.28	0.43
1:C:392:LYS:O	1:C:396:GLU:HG3	2.19	0.43
1:B:103:GLY:HA2	1:B:442:ILE:HD13	2.00	0.43
1:I:92:ALA:HB2	1:I:505:ALA:HA	2.00	0.43
1:K:390:GLU:OE1	1:K:394:ARG:NH1	2.51	0.43
1:A:264:ASN:HB3	1:A:269:THR:HB	2.01	0.43
1:B:437:ALA:O	1:B:441:LYS:HG3	2.26	0.43
2:T:20:ILE:O	2:T:21:GLU:C	3.03	0.43
2:Q:98:VAL:HG12	2:Q:99:LEU:N	2.61	0.43
1:A:352:LEU:C	1:A:354:THR:H	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:286:GLU:HG3	1:N:367:ARG:HH22	1.84	0.43
2:T:78:THR:HG22	2:T:80:ILE:CD1	2.52	0.43
2:P:20:ILE:CG1	2:P:43:GLY:HA2	2.46	0.43
1:E:214:LEU:HB3	1:E:245:PRO:HB3	2.01	0.43
1:J:298:THR:N	1:J:315:MET:O	2.52	0.43
2:O:80:ILE:HG12	2:U:41:GLN:OE1	2.18	0.43
1:E:349:LYS:C	1:E:351:GLU:N	3.23	0.43
1:H:50:THR:CG2	1:H:51:LYS:H	2.28	0.43
1:E:224:LYS:N	1:E:224:LYS:HD2	2.33	0.43
1:L:47:PRO:HD2	1:M:72:GLN:HB3	2.01	0.43
1:L:47:PRO:CD	1:M:72:GLN:HB2	2.49	0.43
2:P:93:ARG:O	2:Q:14:ARG:NH2	2.87	0.43
1:J:384:THR:HG22	1:J:385:GLU:N	2.33	0.43
2:S:85:GLU:HA	2:S:85:GLU:OE1	2.19	0.43
2:S:18:LYS:HG2	2:S:87:TYR:CD2	3.89	0.43
1:F:288:LEU:HA	1:F:291:ILE:HD12	2.00	0.43
1:E:15:ALA:HA	1:E:18:ARG:CZ	2.53	0.43
1:A:74:LEU:HD21	1:A:93:THR:CG2	2.50	0.43
1:H:175:THR:CG2	1:H:177:GLU:OE2	2.71	0.43
1:K:175:THR:CG2	1:K:177:GLU:OE2	2.66	0.43
1:G:192:TYR:CD2	1:G:192:TYR:C	3.42	0.43
1:D:215:GLU:O	1:D:216:ASP:C	2.57	0.43
1:B:229:VAL:HG23	1:B:256:GLU:CD	2.51	0.42
2:R:62:LEU:HA	2:R:62:LEU:HD12	1.78	0.42
2:S:96:LEU:HD23	2:T:14:ARG:CZ	3.97	0.42
2:T:17:VAL:HG22	2:T:45:VAL:CA	3.79	0.42
2:T:49:GLY:O	2:T:62:LEU:CD1	2.65	0.42
2:T:62:LEU:HA	2:T:62:LEU:HD23	3.75	0.42
2:T:62:LEU:C	2:T:64:VAL:H	2.21	0.42
2:P:10:PRO:CB	2:P:14:ARG:O	2.96	0.42
1:C:245:PRO:HA	1:C:271:SER:OG	2.65	0.42
1:E:284:ARG:HH11	1:E:284:ARG:HG3	4.44	0.42
1:F:267:ARG:HG2	2:T:31:VAL:HG21	2.36	0.42
1:G:205:THR:N	1:G:211:GLU:O	2.65	0.42
1:L:297:GLY:CA	1:L:317:GLY:N	2.81	0.42
1:H:290:ASP:N	1:H:344:ARG:NH1	2.65	0.42
1:I:84:VAL:HG12	1:I:500:LYS:CE	2.47	0.42
1:C:426:GLU:OE2	1:C:444:ARG:NH1	2.66	0.42
1:F:279:GLY:O	1:F:284:ARG:HD3	2.19	0.42
1:D:441:LYS:O	1:D:444:ARG:HB3	2.25	0.42
1:K:458:ALA:O	1:L:114:LEU:CD1	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ILE:HD12	1:F:399:LEU:CD2	2.49	0.42
2:O:41:GLN:HB3	2:O:72:PHE:O	2.36	0.42
1:A:10:GLU:HA	1:A:13:ARG:HH11	1.84	0.42
1:A:179:SER:HB2	1:A:379:ARG:HB3	2.06	0.42
2:P:89:ILE:HG22	2:P:89:ILE:O	2.18	0.42
1:G:435:ASP:O	1:G:438:THR:HB	2.19	0.42
1:M:449:GLU:HB2	1:M:450:PRO:HD3	2.03	0.42
1:B:31:LEU:HD13	1:B:90:THR:HG22	2.14	0.42
2:Q:15:VAL:CG1	2:Q:16:VAL:N	4.32	0.42
2:T:78:THR:HG22	2:T:79:GLU:N	2.33	0.42
2:U:20:ILE:HD11	2:U:44:LYS:CG	4.26	0.42
1:M:411:VAL:HB	1:M:417:THR:OG1	2.19	0.42
2:O:97:ALA:HB2	2:P:10:PRO:HA	2.00	0.42
2:O:100:GLN:HG2	2:P:9:LYS:HE2	2.30	0.42
1:E:33:PRO:HD3	4:E:602:ADP:C5	2.54	0.42
1:C:167:LYS:O	1:C:168:VAL:HG23	2.26	0.42
1:E:294:VAL:O	1:E:336:GLY:N	2.52	0.42
1:D:219:ILE:HG22	1:D:221:ILE:HG13	2.00	0.42
1:A:246:LEU:O	1:A:272:VAL:HA	2.19	0.42
1:H:246:LEU:HB3	1:H:272:VAL:CG1	2.46	0.42
1:M:313:LEU:O	1:M:313:LEU:HG	2.19	0.42
1:N:40:LEU:HD21	1:N:56:VAL:HA	2.05	0.42
1:G:298:THR:HG23	1:G:304:LEU:HD13	7.77	0.42
2:Q:22:GLU:OE1	2:Q:22:GLU:N	2.42	0.42
1:A:128:VAL:HA	1:A:131:ILE:HD12	2.09	0.42
1:H:344:ARG:HG3	1:H:344:ARG:NH1	2.48	0.42
1:L:384:THR:HG22	1:L:385:GLU:N	2.34	0.42
1:F:217:ALA:CB	1:F:245:PRO:HB2	2.46	0.42
1:L:408:GLU:O	1:L:499:ALA:HB3	2.19	0.42
1:D:23:VAL:HG22	1:D:60:VAL:CG1	2.44	0.42
1:J:247:LEU:HD21	1:J:249:ILE:HD11	2.18	0.42
1:H:53:GLY:HA3	1:H:90:THR:OG1	2.20	0.42
1:K:460:TYR:CE2	1:K:480:PHE:HZ	2.37	0.42
1:H:316:LEU:H	1:H:316:LEU:HD23	1.83	0.42
1:G:23:VAL:HB	1:G:74:LEU:HD23	2.03	0.42
1:A:372:ALA:C	1:A:374:GLY:H	2.47	0.42
1:L:475:ASN:OD1	1:L:475:ASN:C	2.57	0.42
1:H:478:TYR:CZ	1:H:487:PHE:HB3	2.54	0.42
1:B:475:ASN:HA	1:B:476:PRO:HD2	1.93	0.42
1:H:8:PHE:O	1:H:11:ALA:HB3	2.25	0.42
1:K:285:LYS:HG2	1:K:289:LYS:HE3	2.05	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:HB3	1:A:443:VAL:HG21	2.03	0.42
2:P:33:PRO:C	2:P:35:THR:H	2.42	0.42
1:E:239:VAL:HG22	1:E:313:LEU:CD2	2.49	0.42
1:C:292:ALA:O	1:C:294:VAL:N	2.75	0.42
1:B:168:VAL:O	1:B:172:GLY:HA3	2.26	0.42
1:M:325:THR:CG2	1:M:326:LYS:N	2.82	0.42
1:E:352:LEU:C	1:E:354:THR:H	2.44	0.42
1:M:37:ASN:ND2	1:M:51:LYS:HE2	2.26	0.42
1:C:519:THR:HG23	1:D:39:VAL:HG23	2.01	0.42
1:G:235:ILE:HD11	1:G:311:ALA:HB2	2.26	0.42
2:S:49:GLY:O	2:S:62:LEU:CD1	3.00	0.42
1:D:218:PHE:CZ	1:D:242:THR:HG21	2.55	0.42
1:D:220:LEU:HD22	1:D:235:ILE:HD11	4.27	0.42
1:G:219:ILE:O	1:G:316:LEU:HB2	4.88	0.42
2:Q:19:ARG:HA	2:Q:42:LYS:O	2.19	0.42
1:J:222:VAL:CG1	1:J:223:GLU:H	2.39	0.42
1:I:194:PHE:HB2	1:I:278:PRO:HB3	2.02	0.42
1:J:249:ILE:O	1:J:249:ILE:CG2	2.70	0.42
1:E:159:LYS:HE2	1:E:163:ASP:OD2	2.19	0.42
1:A:23:VAL:HB	1:A:74:LEU:HD23	2.03	0.42
1:I:24:ALA:O	1:I:28:LYS:HG2	2.32	0.42
1:N:375:VAL:O	1:N:375:VAL:HG12	2.19	0.42
1:H:95:LEU:O	1:H:99:ILE:HG13	2.18	0.42
1:F:251:GLU:O	1:F:252:ASP:HB2	2.19	0.42
1:C:10:GLU:HA	1:C:13:ARG:HH11	1.89	0.42
1:L:95:LEU:HD21	1:L:450:PRO:HG2	2.10	0.42
1:F:206:ASN:HB3	1:F:209:THR:OG1	2.19	0.42
1:D:490:MET:CE	1:D:495:ILE:HG21	2.49	0.42
1:I:283:ARG:NH2	1:I:367:ARG:CD	2.82	0.42
2:T:10:PRO:CD	2:T:47:ALA:HB1	3.02	0.42
2:T:48:VAL:HG11	2:T:64:VAL:O	2.19	0.42
2:T:88:VAL:O	2:T:90:LEU:HD12	4.08	0.42
2:U:6:THR:HB	2:U:82:ILE:CG2	2.49	0.42
1:E:246:LEU:CB	1:E:272:VAL:HG12	2.56	0.42
1:A:236:LEU:CB	2:O:30:ILE:CD1	3.23	0.42
1:G:294:VAL:HG23	1:G:295:THR:N	4.68	0.42
1:M:178:GLU:O	1:M:321:ARG:NH1	2.53	0.42
2:R:42:LYS:HA	2:R:70:VAL:O	2.20	0.42
2:S:91:SER:O	2:S:95:LEU:HG	2.24	0.42
1:A:297:GLY:N	1:A:317:GLY:HA2	2.34	0.42
1:M:7:VAL:HG21	1:M:66:LEU:CD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:O	1:C:262:VAL:HG23	2.29	0.42
1:D:131:ILE:HD13	1:D:502:THR:HG22	2.01	0.42
1:I:294:VAL:HA	1:I:341:ILE:HD11	2.22	0.42
1:G:149:THR:HG23	1:G:155:PRO:CA	2.44	0.42
1:N:194:PHE:HB2	1:N:278:PRO:HB3	2.06	0.42
1:J:458:ALA:C	1:K:114:LEU:HD12	2.39	0.42
1:L:178:GLU:CD	1:L:392:LYS:HE3	2.40	0.42
1:J:488:VAL:HG23	1:J:490:MET:CE	2.50	0.42
1:F:341:ILE:O	1:F:344:ARG:N	2.51	0.42
1:E:123:ALA:HB2	1:E:440:ALA:HA	2.03	0.42
1:B:80:LYS:HE2	1:C:383:ALA:O	2.18	0.42
1:N:102:GLU:HB2	1:N:442:ILE:HG23	2.10	0.42
1:G:404:ALA:HB1	1:G:500:LYS:HB3	2.01	0.42
1:F:404:ALA:HB1	1:F:500:LYS:HB3	2.02	0.42
1:I:286:GLU:HG3	1:I:367:ARG:NH2	2.34	0.42
2:R:16:VAL:HG12	2:R:16:VAL:O	2.18	0.42
2:O:11:LEU:O	2:O:13:ASP:N	3.07	0.42
2:U:20:ILE:HG13	2:U:43:GLY:CA	2.65	0.42
2:P:17:VAL:HG12	2:P:43:GLY:HA3	2.11	0.42
1:A:233:LEU:HA	2:O:30:ILE:HD13	2.32	0.42
1:C:237:GLU:OE2	2:Q:28:GLY:HA3	3.05	0.42
2:Q:32:LEU:HG	2:Q:36:ALA:HB3	2.00	0.42
1:B:167:LYS:O	1:B:168:VAL:HG23	2.19	0.42
1:E:345:ILE:HD12	1:E:371:LEU:O	2.20	0.42
1:F:207:PRO:HA	1:F:210:MET:HE1	2.17	0.42
1:M:36:ARG:HD2	1:N:518:THR:HG23	2.02	0.42
1:A:7:VAL:HG12	1:A:12:ALA:HB2	2.02	0.42
1:I:40:LEU:HD21	1:I:56:VAL:HA	2.05	0.42
1:J:228:ASN:ND2	1:J:230:ARG:HB3	2.25	0.42
1:E:124:VAL:HG13	1:E:506:LEU:HG	2.01	0.42
2:U:32:LEU:HD12	2:U:36:ALA:CB	5.49	0.42
1:N:384:THR:HG22	1:N:385:GLU:N	2.35	0.42
1:H:177:GLU:HB3	1:H:321:ARG:NH1	2.34	0.42
1:B:307:LYS:HE3	2:Q:34:ASP:O	5.05	0.42
1:I:312:THR:C	1:I:314:SER:N	2.73	0.42
1:J:32:GLY:HA3	1:J:454:ILE:HG23	2.01	0.42
1:H:202:TYR:CD2	1:H:266:LEU:HD11	2.55	0.42
1:C:33:PRO:HD3	4:C:602:ADP:C5	2.85	0.42
1:A:76:GLU:CD	1:B:386:THR:HG1	2.45	0.42
1:H:477:ARG:HD3	1:H:491:VAL:HG21	2.01	0.42
1:L:8:PHE:O	1:L:11:ALA:HB3	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:ASP:HA	1:E:319:ALA:O	2.67	0.42
2:Q:81:GLU:C	2:Q:82:ILE:HG13	2.39	0.42
2:Q:77:GLY:HA3	2:Q:90:LEU:HD23	1.99	0.42
1:A:351:GLU:HG3	1:B:210:MET:CE	7.65	0.42
1:E:242:THR:HG22	1:E:244:LYS:HG3	2.01	0.42
1:F:150:ILE:HD12	1:F:496:VAL:H	1.83	0.42
1:I:295:THR:HG22	1:I:317:GLY:CA	2.55	0.42
2:P:10:PRO:HG2	2:P:49:GLY:CA	2.71	0.42
2:Q:50:THR:CG2	2:Q:59:ARG:HD3	2.49	0.42
1:J:283:ARG:HD3	1:J:363:LYS:CE	2.49	0.42
1:C:237:GLU:O	1:C:238:GLN:C	2.69	0.42
1:C:221:ILE:HG23	1:C:288:LEU:HD22	2.01	0.42
1:E:50:THR:CG2	1:E:52:ASP:HB3	2.48	0.42
1:L:49:ILE:HG13	1:L:49:ILE:O	2.19	0.42
1:D:235:ILE:HD13	1:D:235:ILE:HG21	1.77	0.42
1:F:247:LEU:HD13	1:F:324:ILE:HD11	2.01	0.42
1:M:65:HIS:HD2	1:M:527:PRO:HG3	2.68	0.42
1:G:224:LYS:H	1:G:224:LYS:CD	3.76	0.42
1:G:227:SER:CB	1:G:254:GLU:HG3	3.04	0.42
1:E:506:LEU:O	1:E:506:LEU:HD12	2.28	0.42
1:D:233:LEU:HD23	2:R:30:ILE:HD13	2.01	0.42
1:B:373:GLY:O	1:B:375:VAL:HG23	2.20	0.42
1:A:463:SER:O	1:A:467:GLN:HG2	2.21	0.42
1:L:449:GLU:O	1:L:450:PRO:C	2.58	0.42
1:E:188:PHE:N	1:E:188:PHE:CD1	2.88	0.42
1:E:472:GLU:HB3	1:E:478:TYR:CD2	2.54	0.42
1:B:31:LEU:HB2	1:B:90:THR:HG21	2.00	0.42
2:U:21:GLU:H	2:U:21:GLU:CD	2.22	0.42
1:B:312:THR:HB	1:B:314:SER:OG	2.31	0.42
2:S:51:GLY:HA3	2:S:60:VAL:O	2.49	0.42
1:D:150:ILE:O	1:D:153:ASN:N	2.51	0.42
2:T:20:ILE:N	2:T:42:LYS:O	3.25	0.42
2:Q:17:VAL:HG22	2:Q:90:LEU:HD21	6.90	0.42
2:O:11:LEU:O	2:O:12:GLY:O	2.38	0.42
1:A:150:ILE:O	1:A:153:ASN:N	2.54	0.42
2:P:42:LYS:HA	2:P:70:VAL:O	2.20	0.42
1:C:217:ALA:HB1	1:C:245:PRO:O	2.20	0.42
1:A:50:THR:HA	1:A:390:GLU:OE1	2.34	0.42
1:D:79:SER:O	1:D:82:ASN:N	2.61	0.42
2:O:52:ARG:NH2	2:P:53:VAL:O	2.53	0.42
1:K:149:THR:HG23	1:K:155:PRO:CA	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:40:LEU:HD21	1:M:56:VAL:HA	2.06	0.42
1:K:411:VAL:O	1:K:496:VAL:CG1	2.72	0.42
1:K:277:ALA:HB1	1:K:284:ARG:HD2	2.05	0.42
1:L:360:ALA:CA	1:L:363:LYS:HG3	3.61	0.42
1:K:79:SER:C	1:K:81:THR:N	2.72	0.42
1:B:149:THR:CG2	1:B:155:PRO:HA	2.44	0.42
1:C:146:GLU:O	1:C:147:VAL:C	2.60	0.42
1:N:290:ASP:N	1:N:344:ARG:NH1	2.66	0.42
1:G:189:VAL:HG12	1:G:190:GLU:N	2.33	0.42
1:N:130:LYS:O	1:N:134:LEU:HB2	2.20	0.42
1:M:8:PHE:O	1:M:11:ALA:HB3	2.21	0.42
1:E:180:LYS:HA	1:E:180:LYS:HD3	1.85	0.42
1:I:358:GLU:HG2	1:I:473:THR:HG21	42.14	0.42
1:C:95:LEU:O	1:C:99:ILE:HG13	2.20	0.42
1:I:433:GLU:HG2	1:I:434:GLY:N	2.36	0.42
1:L:202:TYR:HD2	1:L:266:LEU:HD11	1.84	0.42
1:F:205:THR:HB	1:F:213:VAL:H	1.87	0.42
1:K:286:GLU:OE2	1:K:344:ARG:NH2	2.63	0.42
1:I:283:ARG:NH1	1:I:364:LEU:HD12	2.49	0.42
2:T:42:LYS:HE2	2:T:42:LYS:HB3	2.36	0.42
2:P:27:LYS:HD3	2:Q:84:GLY:CA	2.49	0.42
2:P:71:VAL:HG23	2:P:99:LEU:HD13	2.01	0.42
2:Q:71:VAL:C	2:Q:72:PHE:HD2	3.25	0.42
2:U:81:GLU:HG3	2:U:85:GLU:N	2.28	0.42
1:C:150:ILE:O	1:C:153:ASN:N	2.58	0.42
1:F:239:VAL:HG11	1:F:246:LEU:HB2	2.01	0.42
1:L:217:ALA:HB1	1:L:245:PRO:O	2.20	0.42
1:A:233:LEU:HD23	2:O:30:ILE:CD1	2.48	0.42
1:E:198:TYR:HB3	1:E:324:ILE:HG21	2.90	0.42
1:C:206:ASN:HA	1:C:207:PRO:HD3	1.81	0.42
1:C:348:ILE:HD11	1:C:367:ARG:CD	4.27	0.42
1:C:345:ILE:HG23	1:C:368:LEU:HD13	2.02	0.42
1:C:343:ALA:HB2	1:D:207:PRO:HB2	6.61	0.42
1:E:31:LEU:HD23	1:E:453:GLN:HB3	2.18	0.42
1:E:225:LYS:HD3	1:E:254:GLU:OE1	2.19	0.42
1:C:79:SER:O	1:C:82:ASN:N	2.53	0.42
2:R:100:GLN:HB2	2:S:7:VAL:HB	2.01	0.42
1:L:40:LEU:HD21	1:L:56:VAL:HA	2.03	0.42
1:L:187:LYS:HZ2	1:L:379:ARG:HG3	1.82	0.42
1:G:253:VAL:HG11	1:G:261:LEU:CD1	2.86	0.42
1:M:149:THR:HG23	1:M:155:PRO:CA	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LYS:CE	2:S:34:ASP:HB3	4.65	0.42
1:B:65:HIS:O	1:B:69:ILE:HG13	2.34	0.42
1:I:222:VAL:CG1	1:I:223:GLU:H	2.32	0.42
2:S:19:ARG:HB3	2:S:40:PRO:CG	2.59	0.42
1:G:332:VAL:HG12	1:G:333:GLY:N	2.34	0.42
1:I:178:GLU:CD	1:I:392:LYS:HE3	2.45	0.42
1:N:465:ILE:HD13	1:N:480:PHE:CD1	2.55	0.42
1:D:468:GLN:HB3	1:D:487:PHE:CE2	2.55	0.42
1:K:202:TYR:CD2	1:K:266:LEU:HD11	2.54	0.42
1:M:475:ASN:HA	1:M:476:PRO:HD2	1.98	0.42
1:K:283:ARG:HH12	1:K:364:LEU:CD1	2.31	0.42
2:Q:8:ILE:CD1	2:Q:8:ILE:N	2.77	0.42
1:A:345:ILE:HG23	1:A:368:LEU:CD1	2.62	0.42
2:T:82:ILE:C	2:T:84:GLY:N	3.14	0.42
1:G:147:VAL:CG2	1:G:410:ILE:HD11	2.63	0.42
2:R:53:VAL:HG22	2:R:59:ARG:HE	1.83	0.42
1:C:209:THR:HG21	1:C:211:GLU:CD	4.45	0.42
1:N:217:ALA:HB2	1:N:245:PRO:CG	2.31	0.42
1:M:178:GLU:CD	1:M:392:LYS:HE3	2.48	0.42
1:E:359:TYR:O	1:E:363:LYS:HG2	2.19	0.42
1:C:50:THR:HG23	1:C:390:GLU:OE1	2.22	0.42
1:C:349:LYS:O	1:C:351:GLU:N	2.53	0.42
1:D:244:LYS:HA	1:D:245:PRO:HD3	1.93	0.42
1:H:411:VAL:HB	1:H:417:THR:OG1	2.19	0.42
1:N:342:GLU:O	1:N:346:ASN:ND2	2.59	0.42
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.85	0.42
1:D:233:LEU:CD2	2:R:30:ILE:HG21	2.49	0.42
1:F:124:VAL:HG13	1:F:506:LEU:HG	2.02	0.42
1:B:373:GLY:O	1:B:374:GLY:C	2.57	0.42
1:D:345:ILE:HG22	1:D:346:ASN:N	2.49	0.42
1:J:303:GLU:C	1:J:305:GLY:N	2.73	0.42
1:D:463:SER:O	1:D:467:GLN:HG2	2.19	0.42
1:B:520:GLU:HG2	1:C:29:VAL:HG13	2.07	0.42
1:F:332:VAL:HG12	1:F:333:GLY:N	2.34	0.42
1:I:253:VAL:HG12	1:I:258:LEU:HB2	2.01	0.42
1:E:190:GLU:HA	1:E:190:GLU:OE2	2.20	0.42
1:J:253:VAL:O	1:J:258:LEU:HD22	2.19	0.42
1:B:9:ASP:C	1:B:13:ARG:NH1	2.73	0.42
1:N:207:PRO:O	1:N:210:MET:HE2	2.19	0.42
1:D:177:GLU:O	1:D:379:ARG:HA	2.38	0.42
1:C:478:TYR:CE1	1:C:487:PHE:HB3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:528:GLU:H	1:L:528:GLU:HG3	1.63	0.42
1:E:84:VAL:O	1:E:84:VAL:HG12	2.19	0.42
1:H:130:LYS:O	1:H:134:LEU:HB2	2.20	0.42
1:G:282:ASP:O	1:G:286:GLU:HG2	2.85	0.42
2:Q:18:LYS:HG2	2:Q:87:TYR:HD2	1.80	0.42
2:Q:70:VAL:O	2:Q:71:VAL:HG23	3.70	0.42
2:R:7:VAL:HG12	2:R:8:ILE:N	2.35	0.42
2:T:77:GLY:HA3	2:T:89:ILE:O	3.44	0.42
2:U:46:ILE:O	2:U:46:ILE:CG2	2.94	0.42
1:E:136:ILE:HD12	1:E:477:ARG:HH21	1.85	0.42
1:E:150:ILE:CD1	1:E:496:VAL:H	2.33	0.42
1:A:410:ILE:HD11	1:A:496:VAL:HG21	2.06	0.42
1:B:250:ALA:O	1:B:251:GLU:C	2.57	0.42
1:C:238:GLN:HB3	1:C:313:LEU:CG	2.80	0.42
1:C:291:ILE:O	1:C:294:VAL:HG22	4.89	0.42
1:G:278:PRO:HD2	1:G:288:LEU:HD21	2.53	0.42
1:G:368:LEU:HD12	1:G:368:LEU:O	2.19	0.42
1:G:235:ILE:CD1	1:G:311:ALA:CB	2.88	0.42
1:M:206:ASN:ND2	1:M:389:LYS:CE	2.79	0.42
1:B:66:LEU:HD22	1:B:522:VAL:CG1	2.46	0.42
1:G:225:LYS:HD3	1:G:254:GLU:OE1	2.45	0.42
1:J:74:LEU:HA	1:J:512:ILE:HD13	2.05	0.42
1:A:501:VAL:CG2	1:A:502:THR:N	2.83	0.42
1:L:360:ALA:C	1:L:363:LYS:HG3	3.42	0.42
1:H:300:ILE:HG22	1:H:300:ILE:O	2.20	0.42
2:S:80:ILE:CG2	2:S:81:GLU:H	2.32	0.42
2:O:8:ILE:CD1	2:O:8:ILE:N	2.79	0.42
1:J:178:GLU:CD	1:J:392:LYS:HE3	2.40	0.42
1:N:303:GLU:C	1:N:305:GLY:N	2.76	0.42
1:D:157:VAL:HG13	1:D:395:PHE:CD2	2.64	0.42
1:F:6:LEU:HD13	1:G:26:ALA:HB2	2.07	0.42
1:C:286:GLU:OE2	1:C:344:ARG:NH2	3.65	0.42
1:F:250:ALA:C	1:F:252:ASP:N	2.73	0.42
1:B:144:ILE:HD13	1:B:402:THR:CG2	2.50	0.42
1:C:13:ARG:HB3	1:C:104:LEU:HD22	2.01	0.42
1:G:9:ASP:HB3	1:G:10:GLU:H	1.61	0.42
1:C:179:SER:HB2	1:C:379:ARG:HB3	2.05	0.42
1:D:146:GLU:O	1:D:147:VAL:C	2.59	0.41
2:P:100:GLN:OXT	2:Q:7:VAL:HG23	3.35	0.41
2:Q:6:THR:HG22	2:Q:7:VAL:N	4.53	0.41
1:A:350:LYS:HB3	1:B:208:GLU:CB	7.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:78:THR:CG2	2:U:80:ILE:HD11	2.50	0.41
2:U:7:VAL:HG12	2:U:8:ILE:N	2.34	0.41
2:P:13:ASP:C	2:P:13:ASP:OD1	2.71	0.41
2:P:46:ILE:HG22	2:P:46:ILE:O	2.22	0.41
1:C:229:VAL:HG12	1:C:233:LEU:CG	2.81	0.41
2:O:78:THR:CG2	2:O:79:GLU:N	2.83	0.41
1:G:278:PRO:HG3	1:G:291:ILE:HD11	2.92	0.41
1:G:345:ILE:HD12	1:G:371:LEU:O	4.95	0.41
1:E:50:THR:CG2	1:E:51:LYS:N	2.71	0.41
1:K:50:THR:CG2	1:K:52:ASP:H	2.22	0.41
1:H:40:LEU:HD21	1:H:56:VAL:HA	2.05	0.41
1:H:194:PHE:CE1	1:H:278:PRO:HD3	2.67	0.41
1:H:277:ALA:HB1	1:H:284:ARG:HD2	2.05	0.41
1:N:464:VAL:HG12	1:N:468:GLN:NE2	2.26	0.41
1:G:256:GLU:HA	1:G:259:ALA:HB3	2.35	0.41
1:C:136:ILE:CD1	1:C:477:ARG:NH2	2.76	0.41
1:I:194:PHE:N	1:I:194:PHE:CD2	2.91	0.41
1:M:218:PHE:CZ	1:M:242:THR:HG21	2.57	0.41
1:M:53:GLY:HA3	1:M:90:THR:OG1	2.19	0.41
1:C:463:SER:O	1:C:467:GLN:HG2	2.20	0.41
1:E:463:SER:O	1:E:467:GLN:HG2	2.20	0.41
1:I:438:THR:O	1:I:441:LYS:HB2	2.27	0.41
1:B:478:TYR:CZ	1:B:487:PHE:HB3	2.58	0.41
1:N:201:PRO:O	1:N:204:VAL:HG23	2.20	0.41
1:K:412:PRO:HD2	1:K:417:THR:OG1	2.21	0.41
1:K:5:ILE:HG23	1:K:5:ILE:O	2.26	0.41
1:C:475:ASN:HA	1:C:476:PRO:HD2	1.94	0.41
1:I:283:ARG:HH12	1:I:364:LEU:CD1	2.30	0.41
1:A:346:ASN:O	1:A:350:LYS:HB2	2.54	0.41
2:T:62:LEU:HD23	2:T:92:GLU:OE1	4.92	0.41
2:T:71:VAL:HB	2:T:97:ALA:HB3	2.67	0.41
1:C:150:ILE:CD1	1:C:496:VAL:N	2.83	0.41
1:L:325:THR:HG22	1:L:327:ASP:N	2.08	0.41
1:J:360:ALA:HA	1:J:363:LYS:CG	2.74	0.41
1:A:232:LEU:C	1:A:234:PRO:HD2	2.66	0.41
1:G:349:LYS:HB2	1:G:368:LEU:HD11	5.93	0.41
1:C:167:LYS:HB2	1:C:188:PHE:CE2	2.68	0.41
1:H:30:THR:HB	1:H:51:LYS:O	2.30	0.41
1:N:412:PRO:HD2	1:N:417:THR:OG1	2.20	0.41
1:N:411:VAL:HB	1:N:417:THR:OG1	2.24	0.41
1:A:284:ARG:HA	1:A:287:MET:HB2	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:ARG:C	1:G:369:ALA:H	2.23	0.41
1:H:307:LYS:HB2	1:H:310:ASN:ND2	2.35	0.41
1:B:124:VAL:HG13	1:B:506:LEU:HG	2.01	0.41
1:D:307:LYS:HE3	2:S:34:ASP:CB	4.77	0.41
1:G:128:VAL:HA	1:G:131:ILE:HD12	2.04	0.41
1:A:426:GLU:OE2	1:A:444:ARG:NH1	2.69	0.41
1:N:236:LEU:HD12	1:N:236:LEU:HA	1.92	0.41
1:F:23:VAL:HB	1:F:74:LEU:HD23	2.07	0.41
1:M:79:SER:C	1:M:81:THR:N	2.73	0.41
1:I:132:LYS:C	1:I:134:LEU:H	2.23	0.41
1:G:161:ILE:HD12	1:G:399:LEU:CD2	2.50	0.41
1:E:77:VAL:HG23	1:E:512:ILE:HG13	2.05	0.41
1:E:173:ILE:O	1:E:173:ILE:HG22	2.18	0.41
1:G:180:LYS:HD3	1:G:180:LYS:HA	1.86	0.41
1:L:285:LYS:O	1:L:289:LYS:HG3	2.37	0.41
1:K:132:LYS:C	1:K:134:LEU:H	2.29	0.41
1:E:256:GLU:HA	1:E:259:ALA:HB3	2.02	0.41
2:S:33:PRO:C	2:S:35:THR:H	2.24	0.41
2:Q:80:ILE:CG1	2:Q:81:GLU:N	4.43	0.41
1:F:150:ILE:HG22	1:F:151:SER:N	2.38	0.41
1:C:250:ALA:O	1:C:251:GLU:C	2.57	0.41
1:C:269:THR:HG21	2:Q:31:VAL:H	1.85	0.41
1:M:47:PRO:HG2	1:N:73:LEU:CD1	2.51	0.41
1:J:270:LEU:CD2	1:J:272:VAL:HG13	2.51	0.41
1:A:239:VAL:HG11	1:A:246:LEU:HB2	2.02	0.41
1:K:40:LEU:HD21	1:K:56:VAL:HA	2.04	0.41
1:G:214:LEU:HB3	1:G:245:PRO:HB2	2.44	0.41
1:L:77:VAL:O	1:L:80:LYS:HG2	2.24	0.41
1:J:228:ASN:HB3	1:J:231:GLU:HG2	2.03	0.41
1:H:384:THR:HG22	1:H:385:GLU:N	2.36	0.41
2:S:79:GLU:HG2	2:S:88:VAL:HG22	2.20	0.41
1:D:348:ILE:CG2	1:D:364:LEU:O	2.71	0.41
1:D:352:LEU:C	1:D:354:THR:H	2.24	0.41
1:J:526:LYS:CG	1:J:527:PRO:HD2	2.50	0.41
1:H:303:GLU:C	1:H:305:GLY:N	2.75	0.41
1:F:101:ARG:CG	1:F:102:GLU:H	2.32	0.41
1:D:340:ASP:O	1:D:344:ARG:HB2	2.19	0.41
1:B:463:SER:O	1:B:467:GLN:HG2	2.23	0.41
1:C:159:LYS:HE2	1:C:163:ASP:OD2	2.21	0.41
1:B:13:ARG:HB3	1:B:104:LEU:HD22	2.01	0.41
1:G:10:GLU:HA	1:G:13:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LYS:HD3	1:D:180:LYS:HA	1.82	0.41
1:L:202:TYR:CD2	1:L:266:LEU:HD11	2.55	0.41
1:J:275:VAL:HG12	1:J:276:LYS:O	2.20	0.41
1:L:92:ALA:HB2	1:L:505:ALA:HA	2.02	0.41
1:F:193:GLN:HB2	1:F:329:THR:O	2.21	0.41
1:M:86:GLY:O	1:M:87:ASP:HB2	2.20	0.41
1:A:113:PRO:HG3	1:B:36:ARG:NH1	2.36	0.41
2:T:19:ARG:HA	2:T:42:LYS:O	2.21	0.41
1:E:264:ASN:OD1	1:E:269:THR:HG21	2.20	0.41
2:S:38:GLU:HG3	2:S:74:LYS:HZ3	1.84	0.41
1:E:136:ILE:CD1	1:E:477:ARG:NH2	2.84	0.41
1:M:173:ILE:HD11	1:M:370:LYS:HG2	2.01	0.41
2:P:45:VAL:O	2:P:46:ILE:HD13	2.21	0.41
1:A:228:ASN:ND2	1:A:231:GLU:HG3	2.34	0.41
1:C:235:ILE:HG12	1:C:311:ALA:HB3	2.02	0.41
1:B:54:VAL:HG13	1:B:89:THR:CG2	2.50	0.41
1:M:384:THR:HA	1:N:280:PHE:CD1	2.54	0.41
1:L:187:LYS:HZ1	1:L:379:ARG:HG3	2.00	0.41
1:L:283:ARG:HG2	1:L:363:LYS:NZ	2.34	0.41
1:L:225:LYS:HD3	1:L:254:GLU:OE2	2.25	0.41
1:H:384:THR:HB	1:H:387:GLU:H	1.86	0.41
1:A:198:TYR:CE1	1:A:326:LYS:HA	2.84	0.41
1:J:526:LYS:HD2	1:J:527:PRO:HD2	2.00	0.41
1:J:79:SER:O	1:J:81:THR:N	2.53	0.41
1:A:29:VAL:CG1	1:G:520:GLU:HB3	2.49	0.41
1:L:475:ASN:HA	1:L:476:PRO:HD2	1.94	0.41
1:I:487:PHE:C	1:I:488:VAL:HG13	2.41	0.41
1:L:285:LYS:HG2	1:L:289:LYS:HE3	2.06	0.41
1:A:489:ASP:HB3	1:A:492:GLU:HB3	2.07	0.41
1:J:8:PHE:O	1:J:11:ALA:HB3	2.20	0.41
1:I:210:MET:HE2	1:I:210:MET:HA	2.02	0.41
1:L:412:PRO:HB3	1:L:490:MET:HB2	2.09	0.41
1:F:142:LYS:O	1:F:146:GLU:HG3	2.20	0.41
1:K:360:ALA:HA	1:K:363:LYS:HG2	2.03	0.41
2:Q:82:ILE:O	2:Q:83:ASP:HB2	2.58	0.41
1:D:359:TYR:OH	1:D:363:LYS:NZ	3.08	0.41
2:U:20:ILE:HG13	2:U:43:GLY:C	3.81	0.41
1:E:490:MET:CE	1:E:495:ILE:HG21	2.50	0.41
1:G:150:ILE:O	1:G:153:ASN:N	2.54	0.41
1:I:217:ALA:O	1:I:318:ARG:HB2	2.23	0.41
1:F:239:VAL:O	1:F:242:THR:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:283:ARG:O	1:J:287:MET:HG3	2.21	0.41
1:C:203:PHE:CG	1:C:273:ALA:HA	2.75	0.41
1:C:287:MET:O	1:C:291:ILE:HG13	2.22	0.41
1:M:322:VAL:HG22	1:M:331:ILE:HG12	2.03	0.41
1:G:54:VAL:HG13	1:G:89:THR:HG21	2.07	0.41
1:H:283:ARG:CD	1:H:363:LYS:HZ1	2.76	0.41
1:F:33:PRO:HD3	4:F:602:ADP:C5	2.68	0.41
1:F:37:ASN:HB3	1:F:50:THR:O	2.20	0.41
1:H:37:ASN:HD21	1:H:51:LYS:CE	2.27	0.41
1:C:66:LEU:HD22	1:C:522:VAL:CG1	2.55	0.41
1:D:246:LEU:CB	1:D:272:VAL:HG12	2.42	0.41
1:L:309:GLU:N	1:L:309:GLU:OE1	2.41	0.41
1:I:46:SER:CB	1:I:47:PRO:HD2	2.39	0.41
1:L:117:LYS:O	1:L:120:ILE:N	2.63	0.41
1:G:267:ARG:HD2	2:U:31:VAL:HG21	3.83	0.41
1:D:228:ASN:HD21	1:D:230:ARG:HB2	1.85	0.41
1:D:20:VAL:HG13	1:D:74:LEU:HD13	2.02	0.41
1:I:278:PRO:O	1:I:284:ARG:HD3	2.20	0.41
1:F:345:ILE:HG22	1:F:346:ASN:N	2.36	0.41
1:J:117:LYS:O	1:J:118:ARG:C	2.61	0.41
1:D:101:ARG:HG3	1:D:102:GLU:H	1.89	0.41
1:G:478:TYR:CE1	1:G:487:PHE:HB3	2.59	0.41
1:C:319:ALA:HB1	1:C:332:VAL:O	2.31	0.41
1:B:157:VAL:O	1:B:161:ILE:HG12	2.20	0.41
2:Q:24:PRO:HG2	2:Q:25:LYS:N	2.63	0.41
1:F:260:THR:HG22	1:F:264:ASN:ND2	2.36	0.41
1:J:132:LYS:C	1:J:134:LEU:H	2.26	0.41
2:T:91:SER:O	2:T:92:GLU:C	3.16	0.41
2:U:12:GLY:HA2	2:U:51:GLY:H	5.74	0.41
1:G:168:VAL:HG12	1:G:172:GLY:CA	2.30	0.41
1:C:218:PHE:CE1	1:C:244:LYS:HB2	2.65	0.41
2:O:81:GLU:CG	2:O:85:GLU:H	2.31	0.41
2:O:80:ILE:HG13	2:U:41:GLN:OE1	2.21	0.41
1:B:167:LYS:HB2	1:B:188:PHE:CE2	2.54	0.41
1:M:219:ILE:HD13	1:M:331:ILE:HD13	2.03	0.41
1:B:212:ALA:HB3	1:B:324:ILE:CB	2.58	0.41
1:B:79:SER:O	1:B:82:ASN:N	2.53	0.41
1:D:235:ILE:HG12	1:D:311:ALA:HB3	2.01	0.41
1:L:87:ASP:O	1:L:501:VAL:HG13	2.21	0.41
1:I:411:VAL:HB	1:I:417:THR:OG1	2.24	0.41
1:M:239:VAL:HG11	1:M:246:LEU:HB2	2.06	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:261:LEU:HD22	1:M:272:VAL:HG21	2.02	0.41
1:G:312:THR:HG22	1:G:313:LEU:N	2.36	0.41
1:G:367:ARG:C	1:G:369:ALA:N	2.73	0.41
1:J:295:THR:CG2	1:J:318:ARG:N	2.84	0.41
1:H:219:ILE:O	1:H:221:ILE:HG13	2.21	0.41
2:P:97:ALA:HA	2:Q:11:LEU:HG	2.25	0.41
1:D:501:VAL:CG2	1:D:502:THR:N	2.84	0.41
1:E:408:GLU:OE1	1:E:503:ARG:NH2	2.76	0.41
1:L:384:THR:HB	1:L:387:GLU:H	1.89	0.41
1:A:529:LYS:HZ1	1:B:63:GLU:HB2	1.85	0.41
1:D:149:THR:CG2	1:D:155:PRO:HA	2.46	0.41
1:I:79:SER:C	1:I:81:THR:N	2.74	0.41
1:I:372:ALA:O	1:I:374:GLY:N	2.60	0.41
1:M:79:SER:O	1:M:81:THR:N	2.53	0.41
2:O:34:ASP:HA	2:O:37:LYS:HE2	2.02	0.41
1:E:157:VAL:HG13	1:E:395:PHE:CD2	2.55	0.41
1:N:313:LEU:HG	1:N:313:LEU:O	2.21	0.41
1:D:17:GLU:HB2	1:D:104:LEU:CD1	2.51	0.41
1:F:31:LEU:HD23	1:F:453:GLN:HB3	2.02	0.41
1:A:286:GLU:OE1	1:A:344:ARG:NH2	2.53	0.41
1:J:19:GLY:HA3	1:J:67:GLU:O	2.23	0.41
1:I:18:ARG:HD2	1:I:67:GLU:OE1	2.26	0.41
1:B:103:GLY:O	1:B:107:VAL:HG23	2.31	0.41
1:L:8:PHE:N	1:L:8:PHE:CD1	2.95	0.41
1:A:481:ASN:O	1:A:483:ALA:N	2.54	0.41
1:G:428:LEU:HD12	1:G:428:LEU:O	2.41	0.41
1:K:112:ASN:HA	1:K:113:PRO:HD3	1.96	0.41
1:C:428:LEU:O	1:C:428:LEU:HD12	2.19	0.41
1:A:280:PHE:O	1:A:281:GLY:C	2.59	0.41
1:M:298:THR:N	1:M:315:MET:O	2.55	0.41
1:K:283:ARG:HD3	1:K:363:LYS:HE3	2.03	0.41
1:A:345:ILE:HG22	1:A:346:ASN:N	2.36	0.41
2:T:63:GLU:HB3	2:U:11:LEU:HD11	5.14	0.41
2:U:10:PRO:O	2:U:11:LEU:HD22	4.23	0.41
2:O:97:ALA:HB1	2:P:9:LYS:O	2.21	0.41
1:E:214:LEU:HB3	1:E:245:PRO:HB2	2.02	0.41
1:C:241:GLN:HE21	2:Q:28:GLY:HA2	1.85	0.41
1:G:359:TYR:O	1:G:363:LYS:HG2	2.57	0.41
1:E:220:LEU:HD11	1:E:300:ILE:CD1	2.67	0.41
1:E:250:ALA:C	1:E:252:ASP:N	2.75	0.41
1:E:277:ALA:HA	1:E:278:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:ARG:HD2	1:E:344:ARG:HA	1.98	0.41
1:D:50:THR:CG2	1:D:52:ASP:HB3	2.48	0.41
2:P:53:VAL:HG22	2:P:59:ARG:HG2	2.02	0.41
1:H:411:VAL:O	1:H:496:VAL:CG1	2.76	0.41
1:I:46:SER:HB2	1:I:47:PRO:CD	2.39	0.41
1:G:232:LEU:HB3	1:G:236:LEU:CD1	2.51	0.41
1:K:342:GLU:HA	1:K:345:ILE:HD12	2.02	0.41
1:H:408:GLU:OE2	1:H:500:LYS:HG3	2.20	0.41
1:J:232:LEU:CD2	1:J:236:LEU:HB2	2.50	0.41
1:D:72:GLN:HE22	1:D:75:LYS:HZ3	1.80	0.41
1:M:465:ILE:HD13	1:M:480:PHE:CD1	2.64	0.41
1:E:348:ILE:CD1	1:E:367:ARG:NE	2.84	0.41
1:E:23:VAL:HB	1:E:74:LEU:HD23	2.06	0.41
1:M:303:GLU:C	1:M:305:GLY:N	2.77	0.41
1:J:53:GLY:HA3	1:J:90:THR:OG1	2.27	0.41
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.55	0.41
1:F:220:LEU:HG	1:F:222:VAL:HG23	2.12	0.41
1:D:14:ARG:HD3	1:D:14:ARG:HA	2.00	0.41
1:F:402:THR:O	1:F:405:ALA:HB3	2.53	0.41
1:F:216:ASP:HA	1:F:319:ALA:O	2.28	0.41
1:J:473:THR:O	1:J:473:THR:HG22	2.21	0.41
1:I:475:ASN:HA	1:I:476:PRO:HD2	1.95	0.41
1:N:8:PHE:O	1:N:11:ALA:HB3	2.21	0.41
1:D:123:ALA:HA	1:D:428:LEU:HD23	2.02	0.41
2:T:69:ILE:HB	2:T:99:LEU:CD1	4.84	0.41
1:H:217:ALA:HB1	1:H:245:PRO:O	2.20	0.41
1:I:325:THR:CG2	1:I:326:LYS:N	2.87	0.41
1:C:204:VAL:HG13	1:C:210:MET:C	3.40	0.41
1:C:235:ILE:HD13	1:C:235:ILE:HG21	1.80	0.41
1:C:239:VAL:HG11	1:C:246:LEU:HB2	2.03	0.41
1:C:283:ARG:HH11	1:C:363:LYS:HB3	2.80	0.41
2:O:17:VAL:CG1	2:O:43:GLY:HA3	2.54	0.41
2:O:20:ILE:O	2:O:40:PRO:HB3	2.27	0.41
1:G:352:LEU:C	1:G:354:THR:H	2.24	0.41
1:L:30:THR:HB	1:L:51:LYS:O	2.33	0.41
1:F:198:TYR:HD1	1:F:198:TYR:O	2.03	0.41
1:C:351:GLU:HG2	1:D:326:LYS:NZ	5.13	0.41
1:G:265:LYS:NZ	1:G:271:SER:HB2	5.26	0.41
1:L:283:ARG:HD3	1:L:363:LYS:CE	2.51	0.41
1:I:117:LYS:O	1:I:118:ARG:C	2.58	0.41
2:S:69:ILE:O	2:S:98:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.67	0.41
1:J:312:THR:HG22	1:J:313:LEU:N	2.39	0.41
1:H:312:THR:HG22	1:H:313:LEU:N	2.39	0.41
1:G:40:LEU:HD13	1:G:59:GLU:CG	2.50	0.41
1:B:101:ARG:CG	1:B:102:GLU:H	2.42	0.41
1:G:144:ILE:HD13	1:G:402:THR:CG2	2.55	0.41
1:E:123:ALA:HA	1:E:428:LEU:HD23	2.02	0.41
1:A:31:LEU:HD23	1:A:453:GLN:HB3	2.15	0.41
1:E:113:PRO:HD3	1:F:36:ARG:NH2	2.49	0.41
1:N:478:TYR:CZ	1:N:487:PHE:HB3	2.55	0.41
1:I:285:LYS:O	1:I:289:LYS:HG3	2.25	0.41
1:F:188:PHE:CD1	1:F:188:PHE:N	2.89	0.41
1:G:356:ASP:O	1:G:357:SER:C	2.59	0.41
1:D:194:PHE:CE1	1:D:329:THR:HB	2.56	0.41
1:D:136:ILE:CD1	1:D:477:ARG:NH2	2.79	0.41
2:S:33:PRO:HD2	2:S:36:ALA:CB	3.03	0.41
1:B:238:GLN:HB3	1:B:313:LEU:HG	2.26	0.41
2:R:9:LYS:HA	2:R:10:PRO:HD2	1.94	0.41
2:R:10:PRO:HB2	2:R:14:ARG:O	2.28	0.41
2:R:62:LEU:O	2:R:64:VAL:N	2.54	0.41
1:A:345:ILE:C	1:A:347:GLY:N	2.74	0.41
1:A:351:GLU:OE1	1:A:364:LEU:HD13	2.43	0.41
2:T:52:ARG:HG3	2:T:52:ARG:O	2.20	0.41
2:O:6:THR:HG22	2:O:7:VAL:N	4.46	0.41
2:O:9:LYS:HE2	2:U:100:GLN:OE1	2.21	0.41
2:U:13:ASP:HB2	2:U:62:LEU:CD2	2.39	0.41
2:U:62:LEU:O	2:U:64:VAL:N	2.55	0.41
2:O:54:LEU:CG	2:P:55:GLU:O	2.66	0.41
1:B:150:ILE:HD11	1:B:494:GLY:O	2.21	0.41
1:E:136:ILE:O	1:E:410:ILE:HG22	2.30	0.41
1:E:258:LEU:O	1:E:262:VAL:HG23	2.45	0.41
1:C:203:PHE:CE2	1:C:272:VAL:HG23	4.12	0.41
1:C:363:LYS:HD3	1:C:366:GLU:OE2	3.00	0.41
1:C:239:VAL:HG22	1:C:313:LEU:CD2	2.87	0.41
1:M:219:ILE:O	1:M:221:ILE:HG13	2.22	0.41
1:F:168:VAL:O	1:F:172:GLY:HA3	2.21	0.41
1:F:66:LEU:CD2	1:F:522:VAL:HG11	2.43	0.41
1:B:50:THR:CG2	1:B:52:ASP:HB3	2.50	0.41
1:B:54:VAL:CG2	1:B:89:THR:HG21	2.50	0.41
1:D:198:TYR:HB3	1:D:324:ILE:HG21	2.02	0.41
1:D:198:TYR:O	1:D:198:TYR:CD1	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:LEU:O	1:F:263:VAL:HG22	2.21	0.41
2:S:48:VAL:HG11	2:S:64:VAL:O	2.19	0.41
2:S:14:ARG:CG	2:S:14:ARG:NH1	2.83	0.41
1:L:246:LEU:HB3	1:L:272:VAL:CG1	2.47	0.41
1:H:490:MET:HA	1:H:490:MET:HE2	2.14	0.41
2:Q:20:ILE:CG1	2:Q:43:GLY:HA2	2.46	0.41
1:N:179:SER:HB2	1:N:379:ARG:CB	2.43	0.41
1:I:246:LEU:HB3	1:I:272:VAL:CG1	2.49	0.41
1:I:149:THR:HG23	1:I:155:PRO:CA	2.40	0.41
1:A:173:ILE:HD12	1:A:366:GLU:CA	2.45	0.41
1:I:74:LEU:HA	1:I:512:ILE:HD13	2.06	0.41
1:H:278:PRO:O	1:H:284:ARG:HD3	2.21	0.41
1:K:194:PHE:HB2	1:K:278:PRO:HB3	2.07	0.41
1:L:360:ALA:O	1:L:363:LYS:HG2	2.21	0.41
1:D:128:VAL:HA	1:D:131:ILE:HD12	2.01	0.41
1:A:68:ASN:O	1:A:72:GLN:HG2	2.20	0.41
1:G:229:VAL:HG11	2:U:32:LEU:HD11	4.52	0.41
1:N:228:ASN:ND2	1:N:230:ARG:HB3	2.32	0.41
1:L:277:ALA:HB1	1:L:284:ARG:HD2	2.08	0.41
1:K:228:ASN:ND2	1:K:230:ARG:HB3	2.29	0.41
1:J:344:ARG:HH11	1:J:344:ARG:HG3	1.84	0.41
1:N:247:LEU:HD22	1:N:322:VAL:CG1	2.49	0.41
1:C:72:GLN:O	1:C:75:LYS:N	2.54	0.41
1:F:455:ALA:O	1:F:458:ALA:HB3	2.41	0.41
1:E:231:GLU:HA	1:E:309:GLU:HG2	2.03	0.41
1:J:239:VAL:HG22	1:J:313:LEU:CD1	2.56	0.41
1:E:332:VAL:HG12	1:E:333:GLY:N	2.53	0.41
1:K:178:GLU:OE2	1:K:392:LYS:HE3	2.20	0.41
1:D:437:ALA:O	1:D:441:LYS:HG3	2.21	0.41
1:B:199:ILE:HD12	1:B:274:ALA:HB1	2.03	0.41
1:D:144:ILE:HD13	1:D:402:THR:CG2	2.70	0.41
1:F:250:ALA:O	1:F:251:GLU:C	2.60	0.41
1:C:332:VAL:HG12	1:C:333:GLY:N	2.36	0.41
1:F:289:LYS:HB3	1:F:344:ARG:NH2	3.43	0.41
1:F:24:ALA:O	1:F:28:LYS:HG2	2.20	0.41
1:A:29:VAL:CG1	1:G:520:GLU:CG	3.01	0.41
1:A:215:GLU:O	1:A:216:ASP:C	2.67	0.41
1:A:123:ALA:HB2	1:A:440:ALA:HA	2.03	0.41
1:C:123:ALA:HA	1:C:428:LEU:HD23	2.07	0.41
1:C:205:THR:HB	1:C:213:VAL:H	1.92	0.41
1:A:296:GLY:CA	1:A:336:GLY:HA2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:202:TYR:HD2	1:N:266:LEU:HD11	1.85	0.41
1:D:296:GLY:CA	1:D:336:GLY:HA2	2.59	0.41
1:A:475:ASN:HA	1:A:476:PRO:HD2	1.93	0.41
2:R:62:LEU:C	2:R:64:VAL:N	2.75	0.41
1:D:355:THR:CG2	1:D:361:ARG:HG2	2.50	0.41
1:E:238:GLN:C	1:E:313:LEU:HD21	2.41	0.41
2:O:45:VAL:O	2:O:46:ILE:HD13	2.24	0.41
2:T:54:LEU:HD13	2:U:57:GLY:CA	5.78	0.41
1:M:413:GLY:HA2	1:M:497:ASP:OD2	2.26	0.41
1:N:50:THR:HG21	1:N:55:THR:HB	2.02	0.41
1:B:222:VAL:HG22	1:B:300:ILE:HD12	2.25	0.41
1:E:79:SER:O	1:E:82:ASN:N	2.54	0.41
1:K:297:GLY:CA	1:K:317:GLY:N	2.84	0.41
1:N:362:GLU:HA	1:N:365:GLN:CG	2.51	0.41
1:M:77:VAL:HB	1:M:512:ILE:HD11	2.03	0.41
1:D:503:ARG:HG2	1:D:507:GLN:OE1	2.40	0.41
1:D:74:LEU:HD21	1:D:93:THR:HG23	2.03	0.41
1:F:220:LEU:HD23	1:F:248:ILE:HG23	2.13	0.41
1:F:421:ALA:O	1:F:425:VAL:HG23	2.20	0.41
1:G:152:ALA:HB2	1:G:398:ALA:HB2	2.08	0.41
2:T:46:ILE:O	2:T:46:ILE:HG22	2.24	0.41
1:M:478:TYR:CZ	1:M:487:PHE:HB3	2.56	0.41
1:K:283:ARG:HH12	1:K:363:LYS:HG3	2.25	0.40
1:D:359:TYR:CZ	1:D:363:LYS:HE2	2.56	0.40
2:S:97:ALA:HB2	2:T:10:PRO:HA	2.19	0.40
2:U:50:THR:HG22	2:U:51:GLY:O	2.21	0.40
2:P:81:GLU:HG3	2:P:85:GLU:O	2.21	0.40
2:R:50:THR:HG23	2:R:59:ARG:HD3	2.26	0.40
1:N:217:ALA:HB1	1:N:245:PRO:O	2.21	0.40
1:F:515:LEU:O	1:F:518:THR:OG1	2.45	0.40
1:E:278:PRO:HG3	1:E:291:ILE:CD1	2.50	0.40
1:E:296:GLY:CA	1:E:336:GLY:HA2	2.58	0.40
2:R:19:ARG:HA	2:R:42:LYS:O	2.20	0.40
1:F:237:GLU:OE2	2:T:28:GLY:N	2.54	0.40
2:S:9:LYS:HA	2:S:10:PRO:HD2	1.94	0.40
1:N:187:LYS:HZ2	1:N:379:ARG:HG3	1.98	0.40
1:L:221:ILE:HD11	1:L:291:ILE:HG22	2.04	0.40
2:S:53:VAL:HG22	2:S:59:ARG:HE	2.18	0.40
1:N:295:THR:HG22	1:N:317:GLY:CA	2.51	0.40
2:P:25:LYS:HG2	2:P:31:VAL:CG2	2.77	0.40
1:C:247:LEU:HD22	1:C:322:VAL:CG1	3.11	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:VAL:CG1	1:M:223:GLU:H	2.35	0.40
2:U:72:PHE:CZ	2:U:90:LEU:HD21	4.24	0.40
1:L:303:GLU:C	1:L:305:GLY:N	2.75	0.40
1:A:159:LYS:HE2	1:A:163:ASP:OD2	2.21	0.40
1:B:29:VAL:O	1:B:29:VAL:HG12	2.28	0.40
1:F:13:ARG:HB3	1:F:104:LEU:HD22	2.04	0.40
1:E:478:TYR:CZ	1:E:487:PHE:HB3	2.57	0.40
1:F:167:LYS:HB2	1:F:188:PHE:CE2	2.57	0.40
1:E:404:ALA:HB1	1:E:500:LYS:HB3	2.02	0.40
1:M:375:VAL:O	1:M:375:VAL:HG12	2.20	0.40
1:J:478:TYR:CZ	1:J:487:PHE:HB3	2.56	0.40
1:C:435:ASP:O	1:C:438:THR:HB	2.26	0.40
2:Q:13:ASP:O	2:Q:62:LEU:CD2	2.69	0.40
2:Q:41:GLN:OE1	2:R:80:ILE:HG12	3.93	0.40
1:A:351:GLU:HG3	1:B:210:MET:HE1	8.32	0.40
1:L:189:VAL:CG1	1:L:190:GLU:N	2.61	0.40
2:O:14:ARG:NE	2:U:96:LEU:HD23	2.33	0.40
2:O:92:GLU:HA	2:O:95:LEU:HD12	2.38	0.40
2:T:18:LYS:NZ	2:T:85:GLU:CD	2.80	0.40
2:U:45:VAL:O	2:U:46:ILE:HD13	2.20	0.40
1:C:150:ILE:HD12	1:C:496:VAL:H	1.86	0.40
2:P:19:ARG:HB3	2:P:40:PRO:HG2	2.05	0.40
1:B:251:GLU:CG	1:B:284:ARG:HH12	2.10	0.40
1:C:238:GLN:O	1:C:313:LEU:HD11	2.61	0.40
1:E:54:VAL:HG13	1:E:89:THR:CG2	2.52	0.40
1:I:37:ASN:ND2	1:I:51:LYS:HE2	2.34	0.40
2:S:12:GLY:O	2:S:13:ASP:CG	3.60	0.40
1:L:80:LYS:HE3	1:L:508:ASN:OD1	2.21	0.40
1:A:47:PRO:HG3	1:G:69:ILE:HG23	2.03	0.40
2:S:98:VAL:HB	2:T:9:LYS:HB2	2.03	0.40
1:K:268:GLY:O	1:L:228:ASN:HB2	2.21	0.40
1:D:229:VAL:HG11	2:R:32:LEU:HD21	2.02	0.40
1:G:206:ASN:OD1	1:G:207:PRO:HD2	2.51	0.40
1:C:17:GLU:HB2	1:C:104:LEU:CD1	2.62	0.40
1:F:180:LYS:HA	1:F:180:LYS:HD3	1.81	0.40
1:C:161:ILE:HD12	1:C:399:LEU:HD21	2.03	0.40
1:C:180:LYS:HA	1:C:180:LYS:HD3	1.87	0.40
1:C:478:TYR:CZ	1:C:487:PHE:HB3	2.61	0.40
1:C:123:ALA:HB2	1:C:440:ALA:HA	2.07	0.40
1:E:218:PHE:CE1	1:E:244:LYS:HB2	2.64	0.40
2:O:14:ARG:HG3	2:O:14:ARG:NH1	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:62:LEU:C	2:O:64:VAL:N	2.76	0.40
2:O:9:LYS:O	2:U:97:ALA:CA	2.68	0.40
2:T:69:ILE:CB	2:T:99:LEU:HD12	5.79	0.40
1:C:490:MET:HE1	1:C:495:ILE:HG21	2.10	0.40
1:A:146:GLU:O	1:A:147:VAL:C	2.59	0.40
1:L:197:GLY:HA3	1:L:325:THR:O	2.21	0.40
1:C:218:PHE:O	1:C:246:LEU:HD12	2.20	0.40
1:C:281:GLY:C	1:C:283:ARG:N	3.13	0.40
1:G:281:GLY:C	1:G:283:ARG:N	3.18	0.40
1:E:341:ILE:C	1:E:343:ALA:N	2.73	0.40
1:J:50:THR:HG21	1:J:55:THR:HB	2.03	0.40
1:L:270:LEU:CD2	1:L:272:VAL:HG13	2.45	0.40
1:C:304:LEU:HD23	1:C:304:LEU:HA	4.50	0.40
1:F:360:ALA:O	1:F:364:LEU:HG	2.22	0.40
1:K:194:PHE:CE1	1:K:278:PRO:HD3	2.73	0.40
1:G:503:ARG:HG2	1:G:507:GLN:OE1	2.21	0.40
1:K:337:LYS:C	1:K:339:GLU:N	2.74	0.40
1:A:40:LEU:HD13	1:A:59:GLU:CG	2.62	0.40
1:H:465:ILE:HD13	1:H:480:PHE:CD1	2.63	0.40
1:L:26:ALA:HB2	1:M:6:LEU:HD22	2.03	0.40
1:E:10:GLU:HA	1:E:13:ARG:HH11	1.86	0.40
1:G:506:LEU:HD12	1:G:506:LEU:O	2.22	0.40
1:N:390:GLU:OE1	1:N:394:ARG:NH1	2.62	0.40
1:D:88:GLY:HA2	4:D:602:ADP:O2B	2.22	0.40
1:C:249:ILE:HD11	1:C:331:ILE:HD11	2.68	0.40
2:Q:18:LYS:HZ1	2:Q:85:GLU:CD	2.24	0.40
2:R:78:THR:HG22	2:R:80:ILE:HD11	2.02	0.40
1:E:312:THR:HG22	1:E:313:LEU:N	2.37	0.40
1:C:218:PHE:CE1	1:C:242:THR:HG21	2.57	0.40
2:Q:30:ILE:HG22	2:Q:31:VAL:N	2.93	0.40
2:S:11:LEU:HD12	2:S:11:LEU:N	2.36	0.40
1:M:206:ASN:HD21	1:M:389:LYS:CG	2.35	0.40
1:A:244:LYS:HA	1:A:245:PRO:HD3	1.95	0.40
1:A:265:LYS:HA	1:A:270:LEU:O	2.21	0.40
1:K:232:LEU:C	1:K:234:PRO:HD2	2.44	0.40
1:I:342:GLU:O	1:I:346:ASN:ND2	2.56	0.40
1:I:267:ARG:HG2	1:J:256:GLU:CD	2.42	0.40
1:M:179:SER:HB2	1:M:379:ARG:CB	2.41	0.40
1:G:218:PHE:HE1	1:G:244:LYS:HD2	4.23	0.40
1:I:225:LYS:HD3	1:I:254:GLU:OE2	2.21	0.40
1:B:349:LYS:C	1:B:351:GLU:N	2.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLU:CD	1:B:364:LEU:HD13	2.66	0.40
1:N:178:GLU:CD	1:N:392:LYS:HE3	2.42	0.40
1:B:367:ARG:C	1:B:369:ALA:N	2.75	0.40
1:A:101:ARG:HG3	1:A:102:GLU:H	2.02	0.40
1:E:520:GLU:HG2	1:F:29:VAL:HG13	2.02	0.40
1:F:10:GLU:HA	1:F:13:ARG:HH11	1.90	0.40
1:D:123:ALA:HB3	1:D:443:VAL:HG21	2.03	0.40
1:I:285:LYS:HG2	1:I:289:LYS:HE3	2.07	0.40
1:B:403:ARG:HD3	1:B:403:ARG:HA	2.02	0.40
2:R:89:ILE:HG22	2:R:89:ILE:O	2.20	0.40
1:M:160:LEU:HD22	1:M:186:LEU:HB2	2.05	0.40
1:G:167:LYS:HB2	1:G:188:PHE:CE2	2.56	0.40
1:K:360:ALA:HA	1:K:363:LYS:CG	2.70	0.40
2:O:48:VAL:HG13	2:O:62:LEU:CD1	2.61	0.40
2:O:96:LEU:HD23	2:P:14:ARG:HE	1.85	0.40
2:O:17:VAL:HG21	2:O:90:LEU:HD12	2.19	0.40
1:G:283:ARG:HH12	1:G:363:LYS:CD	4.44	0.40
1:M:217:ALA:O	1:M:318:ARG:HB2	2.31	0.40
1:M:197:GLY:CA	1:M:325:THR:O	2.82	0.40
1:M:178:GLU:CD	1:M:323:ARG:NH2	2.74	0.40
1:E:343:ALA:HB2	1:F:207:PRO:HB3	2.40	0.40
1:A:37:ASN:HB3	1:A:50:THR:O	2.33	0.40
2:S:92:GLU:HA	2:S:95:LEU:HD12	2.04	0.40
1:C:306:PHE:CE2	1:C:315:MET:SD	4.01	0.40
1:L:66:LEU:O	1:L:69:ILE:HB	2.33	0.40
1:D:506:LEU:HD12	1:D:506:LEU:O	2.23	0.40
1:F:284:ARG:HG3	1:F:284:ARG:NH1	2.37	0.40
1:C:4:LYS:HE3	1:D:59:GLU:O	2.30	0.40
1:C:460:TYR:HB3	1:C:465:ILE:HD11	2.10	0.40
1:I:53:GLY:HA3	1:I:90:THR:OG1	2.22	0.40
1:F:222:VAL:HA	1:F:300:ILE:HB	2.03	0.40
1:C:192:TYR:HD2	1:C:192:TYR:C	3.06	0.40
1:C:9:ASP:HB3	1:C:10:GLU:H	1.55	0.40
1:C:457:ASN:N	1:C:457:ASN:ND2	2.70	0.40
1:C:157:VAL:HG13	1:C:395:PHE:CD2	2.57	0.40
1:D:232:LEU:HB3	1:D:236:LEU:HD11	2.03	0.40
1:I:338:LYS:HG2	1:I:338:LYS:O	2.29	0.40
1:L:437:ALA:O	1:L:441:LYS:HG3	2.27	0.40
2:P:54:LEU:HB3	2:P:58:GLN:HB3	2.04	0.40
1:A:194:PHE:CE1	1:A:329:THR:HB	2.56	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:474:LYS:CE	1:N:472:GLU:OE1[1_455]	1.85	0.35
1:d:474:LYS:CE	1:g:133:ALA:CB[1_455]	1.93	0.27
1:K:474:LYS:NZ	1:N:493:ALA:O[1_455]	1.93	0.27
1:d:474:LYS:NZ	1:g:133:ALA:CB[1_455]	1.95	0.25
1:C:141:ARG:NH2	1:L:353:GLU:OE1[1_565]	2.11	0.09
1:E:473:THR:OG1	1:N:474:LYS:CE[1_455]	2.17	0.03
1:E:474:LYS:NZ	1:N:472:GLU:OE1[1_455]	2.18	0.02
1:d:474:LYS:NZ	1:g:129:GLU:O[1_455]	2.19	0.01
1:d:474:LYS:CD	1:g:133:ALA:CB[1_455]	2.19	0.01

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	525/543 (97%)	456 (87%)	56 (11%)	13 (2%)	7 24
1	B	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	8 26
1	C	524/543 (96%)	451 (86%)	58 (11%)	15 (3%)	6 19
1	D	524/543 (96%)	441 (84%)	67 (13%)	16 (3%)	5 17
1	E	524/543 (96%)	440 (84%)	65 (12%)	19 (4%)	4 14
1	F	527/543 (97%)	453 (86%)	60 (11%)	14 (3%)	6 21
1	G	523/543 (96%)	447 (86%)	65 (12%)	11 (2%)	9 29
1	H	524/543 (96%)	457 (87%)	60 (12%)	7 (1%)	15 44
1	I	523/543 (96%)	457 (87%)	61 (12%)	5 (1%)	19 52
1	J	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	11 36
1	K	523/543 (96%)	458 (88%)	57 (11%)	8 (2%)	13 40
1	L	524/543 (96%)	454 (87%)	63 (12%)	7 (1%)	15 44
1	M	523/543 (96%)	455 (87%)	61 (12%)	7 (1%)	15 44
1	N	524/543 (96%)	457 (87%)	61 (12%)	6 (1%)	17 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	525/543 (97%)	453 (86%)	57 (11%)	15 (3%)	6	19
1	b	524/543 (96%)	452 (86%)	61 (12%)	11 (2%)	9	29
1	c	525/543 (97%)	446 (85%)	61 (12%)	18 (3%)	5	16
1	d	525/543 (97%)	451 (86%)	56 (11%)	18 (3%)	5	16
1	e	524/543 (96%)	455 (87%)	57 (11%)	12 (2%)	8	26
1	f	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	8	26
1	g	524/543 (96%)	450 (86%)	60 (12%)	14 (3%)	6	21
1	h	523/543 (96%)	459 (88%)	57 (11%)	7 (1%)	15	44
1	i	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	11	36
1	j	523/543 (96%)	454 (87%)	60 (12%)	9 (2%)	11	36
1	k	523/543 (96%)	456 (87%)	61 (12%)	6 (1%)	17	50
1	l	523/543 (96%)	457 (87%)	59 (11%)	7 (1%)	15	44
1	m	523/543 (96%)	465 (89%)	51 (10%)	7 (1%)	15	44
1	n	523/543 (96%)	459 (88%)	58 (11%)	6 (1%)	17	50
2	O	94/100 (94%)	74 (79%)	13 (14%)	7 (7%)	1	3
2	P	92/100 (92%)	72 (78%)	13 (14%)	7 (8%)	1	2
2	Q	94/100 (94%)	75 (80%)	12 (13%)	7 (7%)	1	3
2	R	94/100 (94%)	75 (80%)	11 (12%)	8 (8%)	1	2
2	S	94/100 (94%)	72 (77%)	17 (18%)	5 (5%)	2	7
2	T	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	1	3
2	U	94/100 (94%)	77 (82%)	10 (11%)	7 (7%)	1	3
2	o	94/100 (94%)	75 (80%)	13 (14%)	6 (6%)	2	4
2	p	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	1	3
2	q	94/100 (94%)	58 (62%)	21 (22%)	15 (16%)	0	0
2	r	94/100 (94%)	71 (76%)	17 (18%)	6 (6%)	2	4
2	s	94/100 (94%)	76 (81%)	13 (14%)	5 (5%)	2	7
2	t	94/100 (94%)	69 (73%)	17 (18%)	8 (8%)	1	2
2	u	94/100 (94%)	66 (70%)	18 (19%)	10 (11%)	0	1
All	All	15983/16604 (96%)	13715 (86%)	1863 (12%)	405 (2%)	7	24

All (405) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	278	PRO
1	B	9	ASP
1	B	278	PRO
1	C	9	ASP
1	C	278	PRO
1	C	279	GLY
1	D	9	ASP
1	D	190	GLU
1	D	278	PRO
1	E	9	ASP
1	E	292	ALA
1	E	293	ALA
1	F	9	ASP
1	F	278	PRO
1	G	9	ASP
1	G	278	PRO
1	H	9	ASP
1	I	9	ASP
1	J	9	ASP
1	K	9	ASP
1	L	9	ASP
1	M	9	ASP
1	N	9	ASP
2	O	74	LYS
2	P	22	GLU
2	P	74	LYS
2	Q	19	ARG
2	Q	54	LEU
2	Q	74	LYS
2	R	74	LYS
2	S	12	GLY
2	S	74	LYS
2	T	12	GLY
2	T	19	ARG
2	T	74	LYS
2	U	74	LYS
1	a	9	ASP
1	a	278	PRO
1	b	9	ASP
1	b	278	PRO
1	c	9	ASP
1	c	202	TYR

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Mol	Chain	Res	Type
1	c	292	ALA
1	c	293	ALA
1	c	338	LYS
1	d	9	ASP
1	d	278	PRO
1	e	9	ASP
1	e	278	PRO
1	e	373	GLY
1	f	9	ASP
1	f	278	PRO
1	f	279	GLY
1	g	9	ASP
1	h	9	ASP
1	i	9	ASP
1	j	9	ASP
1	k	9	ASP
1	l	9	ASP
1	m	9	ASP
1	n	9	ASP
2	o	12	GLY
2	o	19	ARG
2	o	74	LYS
2	p	12	GLY
2	p	74	LYS
2	q	22	GLU
2	q	51	GLY
2	q	54	LEU
2	q	63	GLU
2	r	12	GLY
2	r	19	ARG
2	r	54	LEU
2	r	74	LYS
2	s	12	GLY
2	s	74	LYS
2	t	63	GLU
2	u	50	THR
2	u	66	GLU
2	u	96	LEU
1	A	168	VAL
1	A	279	GLY
1	A	336	GLY
1	A	528	GLU

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Mol	Chain	Res	Type
1	B	168	VAL
1	B	216	ASP
1	B	279	GLY
1	B	350	LYS
1	B	374	GLY
1	B	434	GLY
1	C	168	VAL
1	C	169	GLY
1	C	281	GLY
1	C	336	GLY
1	C	434	GLY
1	D	168	VAL
1	D	336	GLY
1	E	28	LYS
1	E	179	SER
1	E	336	GLY
1	G	373	GLY
1	G	374	GLY
1	H	305	GLY
1	I	305	GLY
1	J	305	GLY
1	K	305	GLY
1	L	305	GLY
1	M	305	GLY
1	N	305	GLY
2	O	54	LEU
2	Q	12	GLY
2	Q	34	ASP
2	R	19	ARG
2	S	19	ARG
2	S	54	LEU
2	T	57	GLY
2	U	12	GLY
2	U	34	ASP
2	U	63	GLU
1	a	28	LYS
1	a	168	VAL
1	a	434	GLY
1	b	168	VAL
1	b	179	SER
1	c	168	VAL
1	c	276	LYS

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Mol	Chain	Res	Type
1	c	336	GLY
1	c	527	PRO
1	d	279	GLY
1	d	434	GLY
1	e	168	VAL
1	e	374	GLY
1	f	168	VAL
1	g	168	VAL
1	h	305	GLY
1	i	305	GLY
1	j	305	GLY
1	k	305	GLY
1	l	305	GLY
1	m	305	GLY
1	n	305	GLY
2	o	54	LEU
2	o	66	GLU
2	q	12	GLY
2	q	34	ASP
2	q	78	THR
2	s	54	LEU
2	u	19	ARG
2	u	63	GLU
1	A	482	ALA
1	C	216	ASP
1	C	350	LYS
1	D	199	ILE
1	D	216	ASP
1	E	168	VAL
1	E	276	LYS
1	E	342	GLU
1	F	169	GLY
1	F	190	GLU
1	F	216	ASP
1	F	350	LYS
1	G	168	VAL
1	G	216	ASP
1	G	434	GLY
1	H	80	LYS
1	J	313	LEU
1	K	80	LYS
1	L	80	LYS

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Mol	Chain	Res	Type
1	L	313	LEU
1	L	447	LEU
1	N	80	LYS
1	N	527	PRO
2	O	12	GLY
2	O	19	ARG
2	O	34	ASP
2	P	12	GLY
2	P	19	ARG
2	P	21	GLU
2	R	34	ASP
2	R	54	LEU
2	S	66	GLU
2	T	34	ASP
2	U	19	ARG
1	a	53	GLY
1	a	179	SER
1	b	53	GLY
1	b	434	GLY
1	c	53	GLY
1	c	169	GLY
1	c	434	GLY
1	d	168	VAL
1	d	251	GLU
1	d	281	GLY
1	e	350	LYS
1	f	216	ASP
1	f	336	GLY
1	f	434	GLY
1	g	292	ALA
1	g	434	GLY
1	h	80	LYS
1	h	447	LEU
1	i	80	LYS
1	j	80	LYS
1	j	313	LEU
1	l	474	LYS
1	m	474	LYS
1	n	80	LYS
2	q	32	LEU
2	q	33	PRO
2	q	73	ALA

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Mol	Chain	Res	Type
2	r	34	ASP
2	s	63	GLU
2	t	12	GLY
2	t	59	ARG
2	u	75	TYR
2	u	99	LEU
1	A	216	ASP
1	A	297	GLY
1	A	434	GLY
1	B	281	GLY
1	B	357	SER
1	B	373	GLY
1	C	357	SER
1	C	482	ALA
1	D	53	GLY
1	D	179	SER
1	D	224	LYS
1	E	207	PRO
1	E	482	ALA
1	E	527	PRO
1	F	230	ARG
1	F	279	GLY
1	G	224	LYS
1	H	313	LEU
1	H	474	LYS
1	I	313	LEU
1	J	80	LYS
1	J	447	LEU
1	J	474	LYS
1	K	313	LEU
1	K	447	LEU
1	K	474	LYS
1	M	80	LYS
1	M	189	VAL
1	N	313	LEU
1	N	474	LYS
2	P	85	GLU
2	Q	85	GLU
2	R	12	GLY
2	R	63	GLU
1	a	216	ASP
1	a	251	GLU

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Mol	Chain	Res	Type
1	a	357	SER
1	b	169	GLY
1	b	357	SER
1	c	482	ALA
1	d	179	SER
1	d	216	ASP
1	e	293	ALA
1	e	336	GLY
1	e	434	GLY
1	f	225	LYS
1	f	226	VAL
1	g	28	LYS
1	g	207	PRO
1	g	336	GLY
1	g	371	LEU
1	h	474	LYS
1	i	76	GLU
1	i	447	LEU
1	i	474	LYS
1	j	474	LYS
1	k	80	LYS
1	k	313	LEU
1	k	474	LYS
1	l	80	LYS
1	m	80	LYS
1	n	313	LEU
1	n	447	LEU
1	n	474	LYS
2	o	85	GLU
2	p	19	ARG
2	p	54	LEU
2	q	19	ARG
2	q	28	GLY
2	s	19	ARG
2	u	24	PRO
1	A	179	SER
1	C	224	LYS
1	D	28	LYS
1	D	279	GLY
1	D	354	THR
1	D	434	GLY
1	E	195	ASP

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Mol	Chain	Res	Type
1	E	202	TYR
1	E	371	LEU
1	E	374	GLY
1	F	168	VAL
1	F	353	GLU
1	G	292	ALA
1	G	350	LYS
1	H	300	ILE
1	I	80	LYS
1	I	474	LYS
1	J	101	ARG
1	L	474	LYS
1	M	474	LYS
2	O	50	THR
2	O	85	GLU
2	Q	63	GLU
2	R	85	GLU
2	T	85	GLU
1	a	230	ARG
1	a	482	ALA
1	b	28	LYS
1	c	179	SER
1	c	207	PRO
1	c	308	LEU
1	c	342	GLU
1	c	371	LEU
1	d	354	THR
1	d	357	SER
1	d	364	LEU
1	d	482	ALA
1	f	251	GLU
1	f	357	SER
1	g	179	SER
1	g	267	ARG
1	g	293	ALA
1	i	313	LEU
1	j	76	GLU
1	k	76	GLU
1	l	313	LEU
1	m	313	LEU
2	p	34	ASP
2	q	76	GLY

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Mol	Chain	Res	Type
2	r	85	GLU
2	t	22	GLU
1	B	482	ALA
1	D	169	GLY
1	E	53	GLY
1	F	346	ASN
1	F	357	SER
1	F	434	GLY
1	J	304	LEU
1	M	447	LEU
2	U	85	GLU
1	a	354	THR
1	b	281	GLY
1	d	169	GLY
1	d	292	ALA
1	d	336	GLY
1	e	357	SER
1	f	53	GLY
1	g	53	GLY
1	g	190	GLU
1	j	220	LEU
2	q	24	PRO
2	t	39	LYS
2	t	68	ASP
2	t	84	GLY
1	a	279	GLY
1	b	336	GLY
1	e	279	GLY
2	u	46	ILE
2	u	70	VAL
1	A	281	GLY
1	C	53	GLY
1	E	322	VAL
1	F	527	PRO
1	K	300	ILE
1	M	5	ILE
2	P	30	ILE
1	d	297	GLY
1	e	53	GLY
1	m	189	VAL
2	p	57	GLY
2	t	16	VAL

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Mol	Chain	Res	Type
1	A	53	GLY
1	E	434	GLY
1	G	53	GLY
2	T	53	VAL
1	d	53	GLY
1	g	169	GLY
1	h	300	ILE
1	i	189	VAL
1	C	297	GLY
1	D	226	VAL
1	J	488	VAL
1	L	189	VAL
2	R	67	GLY
1	h	488	VAL
1	i	488	VAL
1	l	189	VAL
1	l	300	ILE
1	m	300	ILE
2	q	70	VAL
1	H	488	VAL
1	K	189	VAL
2	U	67	GLY
1	a	281	GLY
1	j	300	ILE
1	j	488	VAL
2	p	30	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	412/423 (97%)	402 (98%)	10 (2%)	57 87
1	B	412/423 (97%)	399 (97%)	13 (3%)	46 80
1	C	411/423 (97%)	399 (97%)	12 (3%)	50 83
1	D	411/423 (97%)	401 (98%)	10 (2%)	57 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	411/423 (97%)	395 (96%)	16 (4%)	39	74
1	F	414/423 (98%)	405 (98%)	9 (2%)	60	89
1	G	410/423 (97%)	400 (98%)	10 (2%)	57	87
1	H	411/423 (97%)	403 (98%)	8 (2%)	65	91
1	I	410/423 (97%)	400 (98%)	10 (2%)	57	87
1	J	410/423 (97%)	400 (98%)	10 (2%)	57	87
1	K	410/423 (97%)	401 (98%)	9 (2%)	60	89
1	L	411/423 (97%)	401 (98%)	10 (2%)	57	87
1	M	410/423 (97%)	399 (97%)	11 (3%)	52	85
1	N	411/423 (97%)	401 (98%)	10 (2%)	57	87
1	a	412/423 (97%)	404 (98%)	8 (2%)	65	91
1	b	411/423 (97%)	401 (98%)	10 (2%)	57	87
1	c	412/423 (97%)	400 (97%)	12 (3%)	50	83
1	d	412/423 (97%)	401 (97%)	11 (3%)	52	85
1	e	411/423 (97%)	403 (98%)	8 (2%)	65	91
1	f	412/423 (97%)	404 (98%)	8 (2%)	65	91
1	g	411/423 (97%)	401 (98%)	10 (2%)	57	87
1	h	410/423 (97%)	400 (98%)	10 (2%)	57	87
1	i	410/423 (97%)	399 (97%)	11 (3%)	52	85
1	j	410/423 (97%)	398 (97%)	12 (3%)	50	83
1	k	410/423 (97%)	399 (97%)	11 (3%)	52	85
1	l	410/423 (97%)	400 (98%)	10 (2%)	57	87
1	m	410/423 (97%)	400 (98%)	10 (2%)	57	87
1	n	410/423 (97%)	401 (98%)	9 (2%)	60	89
2	O	81/83 (98%)	76 (94%)	5 (6%)	23	54
2	P	79/83 (95%)	76 (96%)	3 (4%)	40	74
2	Q	81/83 (98%)	78 (96%)	3 (4%)	41	76
2	R	81/83 (98%)	78 (96%)	3 (4%)	41	76
2	S	81/83 (98%)	78 (96%)	3 (4%)	41	76
2	T	81/83 (98%)	77 (95%)	4 (5%)	31	65
2	U	81/83 (98%)	78 (96%)	3 (4%)	41	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	o	81/83 (98%)	79 (98%)	2 (2%)	55 86
2	p	81/83 (98%)	78 (96%)	3 (4%)	41 76
2	q	81/83 (98%)	78 (96%)	3 (4%)	41 76
2	r	81/83 (98%)	78 (96%)	3 (4%)	41 76
2	s	81/83 (98%)	78 (96%)	3 (4%)	41 76
2	t	81/83 (98%)	78 (96%)	3 (4%)	41 76
2	u	81/83 (98%)	78 (96%)	3 (4%)	41 76
All	All	12637/13006 (97%)	12305 (97%)	332 (3%)	54 86

All (332) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	9	ASP
1	A	36	ARG
1	A	54	VAL
1	A	173	ILE
1	A	283	ARG
1	A	303	GLU
1	A	312	THR
1	A	340	ASP
1	A	351	GLU
1	B	5	ILE
1	B	9	ASP
1	B	36	ARG
1	B	54	VAL
1	B	173	ILE
1	B	234	PRO
1	B	280	PHE
1	B	283	ARG
1	B	290	ASP
1	B	303	GLU
1	B	340	ASP
1	B	351	GLU
1	B	410	ILE
1	C	5	ILE
1	C	9	ASP
1	C	36	ARG
1	C	54	VAL
1	C	89	THR

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Mol	Chain	Res	Type
1	C	173	ILE
1	C	283	ARG
1	C	303	GLU
1	C	312	THR
1	C	340	ASP
1	C	351	GLU
1	C	410	ILE
1	D	5	ILE
1	D	9	ASP
1	D	36	ARG
1	D	54	VAL
1	D	173	ILE
1	D	283	ARG
1	D	303	GLU
1	D	309	GLU
1	D	340	ASP
1	D	351	GLU
1	E	5	ILE
1	E	9	ASP
1	E	36	ARG
1	E	54	VAL
1	E	136	ILE
1	E	144	ILE
1	E	173	ILE
1	E	210	MET
1	E	235	ILE
1	E	251	GLU
1	E	298	THR
1	E	309	GLU
1	E	316	LEU
1	E	342	GLU
1	E	349	LYS
1	E	368	LEU
1	F	5	ILE
1	F	9	ASP
1	F	36	ARG
1	F	54	VAL
1	F	173	ILE
1	F	198	TYR
1	F	283	ARG
1	F	340	ASP
1	F	351	GLU

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Mol	Chain	Res	Type
1	G	5	ILE
1	G	9	ASP
1	G	36	ARG
1	G	54	VAL
1	G	198	TYR
1	G	283	ARG
1	G	303	GLU
1	G	312	THR
1	G	340	ASP
1	G	351	GLU
1	H	151	SER
1	H	153	ASN
1	H	190	GLU
1	H	270	LEU
1	H	316	LEU
1	H	325	THR
1	H	423	SER
1	H	456	GLU
1	I	151	SER
1	I	153	ASN
1	I	190	GLU
1	I	216	ASP
1	I	270	LEU
1	I	316	LEU
1	I	325	THR
1	I	363	LYS
1	I	423	SER
1	I	456	GLU
1	J	151	SER
1	J	153	ASN
1	J	194	PHE
1	J	216	ASP
1	J	270	LEU
1	J	316	LEU
1	J	325	THR
1	J	423	SER
1	J	456	GLU
1	J	527	PRO
1	K	151	SER
1	K	153	ASN
1	K	194	PHE
1	K	237	GLU

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Mol	Chain	Res	Type
1	K	270	LEU
1	K	316	LEU
1	K	363	LYS
1	K	423	SER
1	K	456	GLU
1	L	151	SER
1	L	153	ASN
1	L	194	PHE
1	L	270	LEU
1	L	316	LEU
1	L	325	THR
1	L	363	LYS
1	L	423	SER
1	L	456	GLU
1	L	522	VAL
1	M	151	SER
1	M	153	ASN
1	M	190	GLU
1	M	194	PHE
1	M	196	LYS
1	M	270	LEU
1	M	316	LEU
1	M	363	LYS
1	M	423	SER
1	M	456	GLU
1	M	522	VAL
1	N	151	SER
1	N	153	ASN
1	N	194	PHE
1	N	270	LEU
1	N	316	LEU
1	N	325	THR
1	N	363	LYS
1	N	423	SER
1	N	456	GLU
1	N	522	VAL
2	O	15	VAL
2	O	21	GLU
2	O	34	ASP
2	O	50	THR
2	O	55	GLU
2	P	15	VAL

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Mol	Chain	Res	Type
2	P	21	GLU
2	P	56	ASN
2	Q	21	GLU
2	Q	34	ASP
2	Q	48	VAL
2	R	21	GLU
2	R	55	GLU
2	R	62	LEU
2	S	21	GLU
2	S	48	VAL
2	S	56	ASN
2	T	13	ASP
2	T	21	GLU
2	T	34	ASP
2	T	48	VAL
2	U	13	ASP
2	U	21	GLU
2	U	92	GLU
1	a	5	ILE
1	a	9	ASP
1	a	36	ARG
1	a	54	VAL
1	a	173	ILE
1	a	303	GLU
1	a	340	ASP
1	a	351	GLU
1	b	5	ILE
1	b	9	ASP
1	b	36	ARG
1	b	54	VAL
1	b	173	ILE
1	b	216	ASP
1	b	303	GLU
1	b	312	THR
1	b	340	ASP
1	b	351	GLU
1	c	5	ILE
1	c	9	ASP
1	c	54	VAL
1	c	173	ILE
1	c	192	TYR
1	c	224	LYS

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Mol	Chain	Res	Type
1	c	251	GLU
1	c	298	THR
1	c	316	LEU
1	c	342	GLU
1	c	368	LEU
1	c	410	ILE
1	d	5	ILE
1	d	9	ASP
1	d	36	ARG
1	d	54	VAL
1	d	89	THR
1	d	173	ILE
1	d	198	TYR
1	d	303	GLU
1	d	340	ASP
1	d	351	GLU
1	d	365	GLN
1	e	5	ILE
1	e	9	ASP
1	e	36	ARG
1	e	54	VAL
1	e	173	ILE
1	e	303	GLU
1	e	340	ASP
1	e	351	GLU
1	f	5	ILE
1	f	9	ASP
1	f	36	ARG
1	f	54	VAL
1	f	173	ILE
1	f	303	GLU
1	f	340	ASP
1	f	351	GLU
1	g	5	ILE
1	g	9	ASP
1	g	36	ARG
1	g	54	VAL
1	g	173	ILE
1	g	204	VAL
1	g	251	GLU
1	g	298	THR
1	g	316	LEU

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Mol	Chain	Res	Type
1	g	342	GLU
1	h	151	SER
1	h	153	ASN
1	h	194	PHE
1	h	216	ASP
1	h	270	LEU
1	h	316	LEU
1	h	325	THR
1	h	363	LYS
1	h	423	SER
1	h	456	GLU
1	i	151	SER
1	i	153	ASN
1	i	194	PHE
1	i	270	LEU
1	i	283	ARG
1	i	316	LEU
1	i	325	THR
1	i	352	LEU
1	i	363	LYS
1	i	423	SER
1	i	456	GLU
1	j	151	SER
1	j	153	ASN
1	j	190	GLU
1	j	194	PHE
1	j	216	ASP
1	j	270	LEU
1	j	283	ARG
1	j	316	LEU
1	j	325	THR
1	j	363	LYS
1	j	423	SER
1	j	456	GLU
1	k	151	SER
1	k	190	GLU
1	k	194	PHE
1	k	216	ASP
1	k	270	LEU
1	k	283	ARG
1	k	316	LEU
1	k	325	THR

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Mol	Chain	Res	Type
1	k	363	LYS
1	k	423	SER
1	k	456	GLU
1	l	151	SER
1	l	153	ASN
1	l	190	GLU
1	l	194	PHE
1	l	196	LYS
1	l	270	LEU
1	l	316	LEU
1	l	363	LYS
1	l	423	SER
1	l	456	GLU
1	m	151	SER
1	m	153	ASN
1	m	194	PHE
1	m	270	LEU
1	m	302	GLU
1	m	316	LEU
1	m	325	THR
1	m	363	LYS
1	m	423	SER
1	m	456	GLU
1	n	151	SER
1	n	194	PHE
1	n	216	ASP
1	n	270	LEU
1	n	316	LEU
1	n	325	THR
1	n	363	LYS
1	n	423	SER
1	n	456	GLU
2	o	13	ASP
2	o	21	GLU
2	p	21	GLU
2	p	48	VAL
2	p	56	ASN
2	q	33	PRO
2	q	72	PHE
2	q	93	ARG
2	r	13	ASP
2	r	21	GLU

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Mol	Chain	Res	Type
2	r	48	VAL
2	s	13	ASP
2	s	21	GLU
2	s	22	GLU
2	t	14	ARG
2	t	69	ILE
2	t	72	PHE
2	u	31	VAL
2	u	70	VAL
2	u	74	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (271) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	106	ASN
1	A	228	ASN
1	A	310	ASN
1	A	400	ASN
1	A	457	ASN
1	B	72	GLN
1	B	228	ASN
1	B	310	ASN
1	B	400	ASN
1	B	457	ASN
1	C	72	GLN
1	C	106	ASN
1	C	241	GLN
1	C	310	ASN
1	C	400	ASN
1	C	457	ASN
1	D	72	GLN
1	D	106	ASN
1	D	310	ASN
1	D	400	ASN
1	D	457	ASN
1	E	72	GLN
1	E	193	GLN
1	E	310	ASN
1	E	346	ASN
1	E	400	ASN
1	E	457	ASN

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Mol	Chain	Res	Type
1	F	72	GLN
1	F	310	ASN
1	F	400	ASN
1	F	457	ASN
1	G	72	GLN
1	G	310	ASN
1	G	400	ASN
1	G	457	ASN
1	H	37	ASN
1	H	97	GLN
1	H	106	ASN
1	H	153	ASN
1	H	193	GLN
1	H	228	ASN
1	H	310	ASN
1	H	346	ASN
1	H	365	GLN
1	H	400	ASN
1	H	468	GLN
1	H	481	ASN
1	H	507	GLN
1	H	508	ASN
1	I	37	ASN
1	I	97	GLN
1	I	153	ASN
1	I	193	GLN
1	I	228	ASN
1	I	264	ASN
1	I	310	ASN
1	I	346	ASN
1	I	365	GLN
1	I	400	ASN
1	I	468	GLN
1	I	481	ASN
1	I	507	GLN
1	I	508	ASN
1	J	37	ASN
1	J	97	GLN
1	J	153	ASN
1	J	193	GLN
1	J	228	ASN
1	J	310	ASN

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Mol	Chain	Res	Type
1	J	346	ASN
1	J	365	GLN
1	J	400	ASN
1	J	468	GLN
1	J	481	ASN
1	J	507	GLN
1	J	508	ASN
1	K	37	ASN
1	K	97	GLN
1	K	106	ASN
1	K	112	ASN
1	K	153	ASN
1	K	193	GLN
1	K	228	ASN
1	K	264	ASN
1	K	310	ASN
1	K	346	ASN
1	K	365	GLN
1	K	400	ASN
1	K	468	GLN
1	K	481	ASN
1	K	507	GLN
1	K	508	ASN
1	L	37	ASN
1	L	97	GLN
1	L	153	ASN
1	L	193	GLN
1	L	228	ASN
1	L	310	ASN
1	L	365	GLN
1	L	400	ASN
1	L	468	GLN
1	L	481	ASN
1	L	507	GLN
1	L	508	ASN
1	M	37	ASN
1	M	97	GLN
1	M	153	ASN
1	M	193	GLN
1	M	228	ASN
1	M	310	ASN
1	M	346	ASN

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Mol	Chain	Res	Type
1	M	365	GLN
1	M	400	ASN
1	M	468	GLN
1	M	481	ASN
1	M	507	GLN
1	M	508	ASN
1	N	37	ASN
1	N	97	GLN
1	N	153	ASN
1	N	228	ASN
1	N	310	ASN
1	N	346	ASN
1	N	365	GLN
1	N	400	ASN
1	N	468	GLN
1	N	481	ASN
1	N	507	GLN
1	N	508	ASN
2	O	56	ASN
2	Q	41	GLN
1	a	72	GLN
1	a	106	ASN
1	a	228	ASN
1	a	310	ASN
1	a	400	ASN
1	a	457	ASN
1	b	72	GLN
1	b	106	ASN
1	b	228	ASN
1	b	310	ASN
1	b	400	ASN
1	b	457	ASN
1	c	72	GLN
1	c	106	ASN
1	c	310	ASN
1	c	346	ASN
1	c	400	ASN
1	c	457	ASN
1	d	72	GLN
1	d	310	ASN
1	d	400	ASN
1	d	457	ASN

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Mol	Chain	Res	Type
1	e	72	GLN
1	e	106	ASN
1	e	228	ASN
1	e	310	ASN
1	e	400	ASN
1	e	457	ASN
1	f	72	GLN
1	f	106	ASN
1	f	228	ASN
1	f	310	ASN
1	f	400	ASN
1	f	457	ASN
1	g	72	GLN
1	g	106	ASN
1	g	310	ASN
1	g	346	ASN
1	g	365	GLN
1	g	400	ASN
1	g	457	ASN
1	h	37	ASN
1	h	65	HIS
1	h	97	GLN
1	h	153	ASN
1	h	193	GLN
1	h	228	ASN
1	h	310	ASN
1	h	346	ASN
1	h	365	GLN
1	h	400	ASN
1	h	468	GLN
1	h	481	ASN
1	h	507	GLN
1	h	508	ASN
1	i	37	ASN
1	i	97	GLN
1	i	153	ASN
1	i	228	ASN
1	i	310	ASN
1	i	346	ASN
1	i	365	GLN
1	i	400	ASN
1	i	468	GLN

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Mol	Chain	Res	Type
1	i	481	ASN
1	i	507	GLN
1	i	508	ASN
1	j	37	ASN
1	j	65	HIS
1	j	97	GLN
1	j	153	ASN
1	j	193	GLN
1	j	228	ASN
1	j	264	ASN
1	j	310	ASN
1	j	365	GLN
1	j	400	ASN
1	j	468	GLN
1	j	481	ASN
1	j	507	GLN
1	j	508	ASN
1	k	37	ASN
1	k	97	GLN
1	k	153	ASN
1	k	193	GLN
1	k	228	ASN
1	k	310	ASN
1	k	346	ASN
1	k	365	GLN
1	k	400	ASN
1	k	468	GLN
1	k	481	ASN
1	k	507	GLN
1	k	508	ASN
1	l	37	ASN
1	l	97	GLN
1	l	153	ASN
1	l	193	GLN
1	l	228	ASN
1	l	310	ASN
1	l	346	ASN
1	l	365	GLN
1	l	400	ASN
1	l	468	GLN
1	l	481	ASN
1	l	507	GLN

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Mol	Chain	Res	Type
1	l	508	ASN
1	m	37	ASN
1	m	97	GLN
1	m	153	ASN
1	m	193	GLN
1	m	228	ASN
1	m	310	ASN
1	m	346	ASN
1	m	365	GLN
1	m	400	ASN
1	m	468	GLN
1	m	481	ASN
1	m	507	GLN
1	m	508	ASN
1	n	37	ASN
1	n	97	GLN
1	n	153	ASN
1	n	193	GLN
1	n	228	ASN
1	n	310	ASN
1	n	346	ASN
1	n	365	GLN
1	n	400	ASN
1	n	468	GLN
1	n	481	ASN
1	n	507	GLN
1	n	508	ASN
2	q	41	GLN
2	r	41	GLN
2	t	41	GLN
2	t	100	GLN
2	u	41	GLN
2	u	56	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 14 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	A	602	3	22,29,29	1.31	2 (9%)	27,45,45	2.91	4 (14%)
4	ADP	B	602	3	22,29,29	1.37	4 (18%)	27,45,45	2.95	6 (22%)
4	ADP	C	602	3	22,29,29	1.30	4 (18%)	27,45,45	3.02	4 (14%)
4	ADP	D	602	3	22,29,29	1.58	5 (22%)	27,45,45	2.91	4 (14%)
4	ADP	E	602	3	22,29,29	1.32	3 (13%)	27,45,45	3.03	5 (18%)
4	ADP	F	602	3	22,29,29	1.29	3 (13%)	27,45,45	2.96	6 (22%)
4	ADP	G	602	3	22,29,29	1.40	5 (22%)	27,45,45	2.99	4 (14%)
5	DMS	H	601	-	3,3,3	0.22	0	3,3,3	0.65	0
5	DMS	I	601	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	J	601	-	3,3,3	0.36	0	3,3,3	0.73	0
5	DMS	K	601	-	3,3,3	0.28	0	3,3,3	0.66	0
5	DMS	L	601	-	3,3,3	0.30	0	3,3,3	0.67	0
5	DMS	M	601	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	N	701	-	3,3,3	0.25	0	3,3,3	0.63	0
4	ADP	a	602	3	22,29,29	1.38	3 (13%)	27,45,45	2.93	4 (14%)
4	ADP	b	602	3	22,29,29	1.47	5 (22%)	27,45,45	3.04	3 (11%)
4	ADP	c	602	3	22,29,29	1.54	4 (18%)	27,45,45	3.17	4 (14%)
4	ADP	d	602	3	22,29,29	1.51	5 (22%)	27,45,45	3.05	6 (22%)
4	ADP	e	602	3	22,29,29	1.56	6 (27%)	27,45,45	2.98	3 (11%)
4	ADP	f	602	3	22,29,29	1.54	4 (18%)	27,45,45	3.03	4 (14%)
4	ADP	g	602	3	22,29,29	1.46	5 (22%)	27,45,45	2.98	5 (18%)
5	DMS	h	601	-	3,3,3	0.34	0	3,3,3	0.69	0
5	DMS	i	601	-	3,3,3	0.33	0	3,3,3	0.67	0
5	DMS	j	601	-	3,3,3	0.29	0	3,3,3	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	k	601	-	3,3,3	0.30	0	3,3,3	0.65	0
5	DMS	l	601	-	3,3,3	0.32	0	3,3,3	0.66	0
5	DMS	m	601	-	3,3,3	0.25	0	3,3,3	0.59	0
5	DMS	n	701	-	3,3,3	0.25	0	3,3,3	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	602	3	-	0/12/32/32	0/3/3/3
4	ADP	B	602	3	-	0/12/32/32	0/3/3/3
4	ADP	C	602	3	-	0/12/32/32	0/3/3/3
4	ADP	D	602	3	-	0/12/32/32	0/3/3/3
4	ADP	E	602	3	-	0/12/32/32	0/3/3/3
4	ADP	F	602	3	-	0/12/32/32	0/3/3/3
4	ADP	G	602	3	-	0/12/32/32	0/3/3/3
5	DMS	H	601	-	-	0/0/0/0	0/0/0/0
5	DMS	I	601	-	-	0/0/0/0	0/0/0/0
5	DMS	J	601	-	-	0/0/0/0	0/0/0/0
5	DMS	K	601	-	-	0/0/0/0	0/0/0/0
5	DMS	L	601	-	-	0/0/0/0	0/0/0/0
5	DMS	M	601	-	-	0/0/0/0	0/0/0/0
5	DMS	N	701	-	-	0/0/0/0	0/0/0/0
4	ADP	a	602	3	-	0/12/32/32	0/3/3/3
4	ADP	b	602	3	-	0/12/32/32	0/3/3/3
4	ADP	c	602	3	-	0/12/32/32	0/3/3/3
4	ADP	d	602	3	-	0/12/32/32	0/3/3/3
4	ADP	e	602	3	-	0/12/32/32	0/3/3/3
4	ADP	f	602	3	-	0/12/32/32	0/3/3/3
4	ADP	g	602	3	-	0/12/32/32	0/3/3/3
5	DMS	h	601	-	-	0/0/0/0	0/0/0/0
5	DMS	i	601	-	-	0/0/0/0	0/0/0/0
5	DMS	j	601	-	-	0/0/0/0	0/0/0/0
5	DMS	k	601	-	-	0/0/0/0	0/0/0/0
5	DMS	l	601	-	-	0/0/0/0	0/0/0/0
5	DMS	m	601	-	-	0/0/0/0	0/0/0/0
5	DMS	n	701	-	-	0/0/0/0	0/0/0/0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	602	ADP	C5-N7	-2.43	1.31	1.39
4	g	602	ADP	C5-N7	-2.29	1.31	1.39
4	G	602	ADP	PA-O2A	-2.28	1.45	1.54
4	E	602	ADP	PA-O2A	-2.24	1.45	1.54
4	D	602	ADP	PA-O2A	-2.21	1.45	1.54
4	B	602	ADP	PA-O2A	-2.14	1.45	1.54
4	a	602	ADP	PA-O2A	-2.14	1.45	1.54
4	e	602	ADP	PA-O2A	-2.11	1.46	1.54
4	d	602	ADP	C5-N7	-2.11	1.32	1.39
4	c	602	ADP	PA-O2A	-2.08	1.46	1.54
4	C	602	ADP	PA-O2A	-2.07	1.46	1.54
4	B	602	ADP	C5-N7	-2.07	1.32	1.39
4	b	602	ADP	PA-O2A	-2.03	1.46	1.54
4	G	602	ADP	C5'-C4'	2.00	1.58	1.51
4	F	602	ADP	C4-N3	2.01	1.38	1.35
4	d	602	ADP	C2-N1	2.04	1.37	1.33
4	B	602	ADP	O4'-C1'	2.06	1.43	1.41
4	e	602	ADP	PB-O2B	2.07	1.62	1.54
4	D	602	ADP	C4-N3	2.07	1.38	1.35
4	C	602	ADP	O4'-C1'	2.09	1.43	1.41
4	f	602	ADP	C2-N1	2.10	1.37	1.33
4	g	602	ADP	PB-O2B	2.11	1.62	1.54
4	a	602	ADP	C4-N3	2.16	1.38	1.35
4	g	602	ADP	C4-N3	2.16	1.38	1.35
4	G	602	ADP	C2-N1	2.18	1.38	1.33
4	b	602	ADP	C2-N1	2.22	1.38	1.33
4	e	602	ADP	C2-N1	2.26	1.38	1.33
4	C	602	ADP	C4-N3	2.30	1.39	1.35
4	E	602	ADP	C2-N3	2.35	1.36	1.32
4	E	602	ADP	C4-N3	2.38	1.39	1.35
4	c	602	ADP	C2-N1	2.48	1.38	1.33
4	e	602	ADP	C4-N3	2.49	1.39	1.35
4	f	602	ADP	C4-N3	2.49	1.39	1.35
4	G	602	ADP	C4-N3	2.51	1.39	1.35
4	d	602	ADP	C2-N3	2.61	1.36	1.32
4	A	602	ADP	C2-N3	2.67	1.36	1.32
4	d	602	ADP	O4'-C1'	2.68	1.44	1.41
4	b	602	ADP	C2-N3	2.69	1.37	1.32
4	C	602	ADP	C2-N3	2.69	1.37	1.32
4	g	602	ADP	O4'-C1'	2.77	1.44	1.41
4	D	602	ADP	PB-O2B	2.78	1.64	1.54
4	e	602	ADP	O4'-C1'	2.78	1.44	1.41
4	b	602	ADP	C4-N3	2.80	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	ADP	O4'-C1'	2.80	1.44	1.41
4	c	602	ADP	O4'-C1'	2.82	1.44	1.41
4	f	602	ADP	C2-N3	2.92	1.37	1.32
4	g	602	ADP	C2-N3	2.94	1.37	1.32
4	F	602	ADP	C2-N3	3.00	1.37	1.32
4	b	602	ADP	O4'-C1'	3.00	1.45	1.41
4	e	602	ADP	C2-N3	3.06	1.37	1.32
4	d	602	ADP	C4-N3	3.12	1.40	1.35
4	G	602	ADP	O4'-C1'	3.14	1.45	1.41
4	A	602	ADP	O4'-C1'	3.14	1.45	1.41
4	f	602	ADP	O4'-C1'	3.25	1.45	1.41
4	c	602	ADP	C2-N3	3.36	1.38	1.32
4	a	602	ADP	C2-N3	3.41	1.38	1.32
4	B	602	ADP	C2-N3	3.50	1.38	1.32
4	D	602	ADP	C2-N3	3.78	1.38	1.32

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	c	602	ADP	N3-C2-N1	-14.89	117.50	128.89
4	f	602	ADP	N3-C2-N1	-14.59	117.72	128.89
4	b	602	ADP	N3-C2-N1	-14.53	117.77	128.89
4	d	602	ADP	N3-C2-N1	-14.52	117.78	128.89
4	C	602	ADP	N3-C2-N1	-14.41	117.86	128.89
4	G	602	ADP	N3-C2-N1	-14.34	117.91	128.89
4	E	602	ADP	N3-C2-N1	-14.15	118.06	128.89
4	g	602	ADP	N3-C2-N1	-14.12	118.08	128.89
4	e	602	ADP	N3-C2-N1	-13.98	118.19	128.89
4	D	602	ADP	N3-C2-N1	-13.90	118.25	128.89
4	a	602	ADP	N3-C2-N1	-13.87	118.27	128.89
4	A	602	ADP	N3-C2-N1	-13.81	118.32	128.89
4	F	602	ADP	N3-C2-N1	-13.77	118.35	128.89
4	B	602	ADP	N3-C2-N1	-13.67	118.42	128.89
4	c	602	ADP	C4-C5-N7	-4.73	105.13	109.48
4	e	602	ADP	C4-C5-N7	-4.08	105.73	109.48
4	A	602	ADP	C4'-O4'-C1'	-3.46	105.92	109.72
4	E	602	ADP	C4'-O4'-C1'	-3.15	106.25	109.72
4	B	602	ADP	C4'-O4'-C1'	-3.08	106.34	109.72
4	C	602	ADP	C4'-O4'-C1'	-3.07	106.35	109.72
4	B	602	ADP	C4-C5-N7	-3.05	106.67	109.48
4	E	602	ADP	C4-C5-N7	-2.95	106.76	109.48
4	F	602	ADP	C4-C5-N7	-2.95	106.76	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	a	602	ADP	C4-C5-N7	-2.88	106.83	109.48
4	b	602	ADP	C4'-O4'-C1'	-2.87	106.56	109.72
4	g	602	ADP	C4-C5-N7	-2.77	106.93	109.48
4	d	602	ADP	C4-C5-N7	-2.77	106.93	109.48
4	F	602	ADP	C4'-O4'-C1'	-2.76	106.68	109.72
4	G	602	ADP	C4-C5-N7	-2.72	106.98	109.48
4	f	602	ADP	C4-C5-N7	-2.66	107.03	109.48
4	a	602	ADP	C4'-O4'-C1'	-2.43	107.05	109.72
4	G	602	ADP	C4'-O4'-C1'	-2.32	107.17	109.72
4	d	602	ADP	C4'-O4'-C1'	-2.30	107.19	109.72
4	C	602	ADP	C1'-N9-C4	-2.29	123.49	126.94
4	g	602	ADP	C4'-O4'-C1'	-2.17	107.34	109.72
4	f	602	ADP	C4'-O4'-C1'	-2.15	107.36	109.72
4	D	602	ADP	C4'-O4'-C1'	-2.14	107.37	109.72
4	D	602	ADP	C4-C5-N7	-2.02	107.62	109.48
4	d	602	ADP	C2-N1-C6	2.02	122.37	118.77
4	A	602	ADP	O4'-C4'-C5'	2.09	116.79	109.32
4	d	602	ADP	O4'-C4'-C5'	2.10	116.83	109.32
4	E	602	ADP	O4'-C4'-C5'	2.10	116.83	109.32
4	f	602	ADP	O4'-C4'-C5'	2.11	116.86	109.32
4	e	602	ADP	O4'-C4'-C5'	2.12	116.89	109.32
4	A	602	ADP	C2-N1-C6	2.12	122.55	118.77
4	d	602	ADP	O4'-C1'-N9	2.12	112.55	108.10
4	g	602	ADP	O4'-C4'-C5'	2.16	117.04	109.32
4	B	602	ADP	O3A-PA-O5'	2.19	108.74	102.94
4	C	602	ADP	O4'-C4'-C5'	2.21	117.23	109.32
4	b	602	ADP	O4'-C4'-C5'	2.24	117.34	109.32
4	G	602	ADP	O4'-C4'-C5'	2.26	117.41	109.32
4	a	602	ADP	O4'-C4'-C5'	2.27	117.44	109.32
4	D	602	ADP	O4'-C4'-C5'	2.33	117.66	109.32
4	F	602	ADP	O4'-C1'-N9	2.33	112.98	108.10
4	E	602	ADP	O3A-PA-O5'	2.34	109.15	102.94
4	F	602	ADP	O3A-PA-O5'	2.36	109.19	102.94
4	B	602	ADP	O4'-C1'-N9	2.39	113.09	108.10
4	B	602	ADP	O4'-C4'-C5'	2.39	117.88	109.32
4	c	602	ADP	O3A-PA-O5'	2.41	109.33	102.94
4	c	602	ADP	O4'-C4'-C5'	2.43	118.01	109.32
4	g	602	ADP	O3A-PA-O5'	2.46	109.47	102.94
4	F	602	ADP	O4'-C4'-C5'	2.62	118.70	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ADP	1	0
4	B	602	ADP	1	0
4	C	602	ADP	1	0
4	D	602	ADP	1	0
4	E	602	ADP	5	0
4	F	602	ADP	2	0
4	G	602	ADP	1	0
5	H	601	DMS	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	527/543 (97%)	-0.22	4 (0%) 87 81	16, 51, 95, 147	0
1	B	527/543 (97%)	-0.16	4 (0%) 87 81	15, 52, 101, 146	0
1	C	526/543 (96%)	-0.23	2 (0%) 93 90	14, 50, 101, 140	0
1	D	526/543 (96%)	-0.08	12 (2%) 64 52	14, 55, 120, 154	0
1	E	526/543 (96%)	-0.02	13 (2%) 61 48	9, 51, 127, 164	0
1	F	529/543 (97%)	-0.07	12 (2%) 64 52	17, 58, 108, 159	0
1	G	525/543 (96%)	-0.13	4 (0%) 87 81	19, 57, 106, 140	0
1	H	526/543 (96%)	-0.02	16 (3%) 54 41	26, 70, 120, 163	0
1	I	525/543 (96%)	-0.09	9 (1%) 73 63	24, 67, 121, 151	0
1	J	525/543 (96%)	-0.11	9 (1%) 73 63	14, 55, 110, 163	0
1	K	525/543 (96%)	-0.06	11 (2%) 67 56	16, 63, 120, 157	0
1	L	526/543 (96%)	-0.08	11 (2%) 67 56	23, 62, 115, 154	0
1	M	525/543 (96%)	1.94	186 (35%) 0 0	25, 95, 150, 167	0
1	N	526/543 (96%)	0.08	23 (4%) 38 26	25, 70, 124, 167	0
1	a	527/543 (97%)	0.28	38 (7%) 18 10	18, 71, 128, 157	0
1	b	526/543 (96%)	0.22	49 (9%) 11 5	18, 66, 121, 163	0
1	c	527/543 (97%)	0.15	27 (5%) 32 21	23, 72, 134, 166	0
1	d	527/543 (97%)	0.04	13 (2%) 61 48	29, 77, 118, 146	0
1	e	526/543 (96%)	0.18	21 (3%) 42 30	42, 81, 116, 155	0
1	f	527/543 (97%)	0.31	26 (4%) 33 22	45, 88, 123, 149	0
1	g	526/543 (96%)	0.22	32 (6%) 25 15	27, 88, 136, 163	0
1	h	525/543 (96%)	-0.07	7 (1%) 79 71	24, 61, 112, 150	0
1	i	525/543 (96%)	0.10	25 (4%) 34 23	28, 76, 125, 160	0
1	j	525/543 (96%)	0.23	30 (5%) 27 17	32, 79, 125, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	k	525/543 (96%)	0.51	61 (11%) 6 3	37, 94, 135, 158	0
1	l	525/543 (96%)	1.02	114 (21%) 1 1	48, 106, 143, 162	0
1	m	525/543 (96%)	1.55	164 (31%) 1 0	56, 104, 146, 174	0
1	n	525/543 (96%)	0.11	30 (5%) 27 17	37, 79, 130, 158	0
2	O	96/100 (96%)	0.64	12 (12%) 5 2	59, 109, 142, 146	0
2	P	94/100 (94%)	0.54	7 (7%) 17 9	69, 108, 142, 146	0
2	Q	96/100 (96%)	0.63	9 (9%) 11 5	60, 108, 142, 149	0
2	R	96/100 (96%)	0.42	7 (7%) 18 10	60, 99, 134, 151	0
2	S	96/100 (96%)	0.76	14 (14%) 3 2	61, 107, 140, 150	0
2	T	96/100 (96%)	0.76	12 (12%) 5 2	65, 106, 141, 154	0
2	U	96/100 (96%)	0.73	10 (10%) 8 4	55, 107, 142, 148	0
2	o	96/100 (96%)	1.42	28 (29%) 1 0	86, 116, 152, 164	0
2	p	96/100 (96%)	0.84	14 (14%) 3 2	80, 112, 146, 150	0
2	q	96/100 (96%)	0.51	6 (6%) 23 14	45, 101, 141, 157	0
2	r	96/100 (96%)	0.67	9 (9%) 11 5	60, 109, 141, 150	0
2	s	96/100 (96%)	0.84	15 (15%) 3 1	73, 114, 143, 150	0
2	t	96/100 (96%)	0.70	16 (16%) 2 1	82, 118, 147, 159	0
2	u	96/100 (96%)	0.92	17 (17%) 2 1	83, 122, 153, 167	0
All	All	16067/16604 (96%)	0.24	1129 (7%) 19 11	9, 76, 133, 174	0

All (1129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	294	VAL	17.3
1	M	291	ILE	17.1
1	M	273	ALA	16.0
1	M	247	LEU	15.6
1	M	246	LEU	13.5
1	M	290	ASP	13.0
1	m	271	SER	12.8
1	M	219	ILE	12.8
1	m	356	ASP	12.4
1	M	332	VAL	11.8
1	M	199	ILE	11.8
1	m	355	THR	11.0
1	M	229	VAL	10.7

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Mol	Chain	Res	Type	RSRZ
1	M	295	THR	10.7
1	M	260	THR	10.3
1	M	200	SER	10.2
1	m	261	LEU	10.0
1	M	279	GLY	9.9
1	M	315	MET	9.6
1	M	375	VAL	9.6
1	m	236	LEU	9.6
1	M	245	PRO	9.6
1	M	371	LEU	9.3
1	M	217	ALA	9.2
1	M	368	LEU	9.2
1	M	264	ASN	9.1
1	M	299	VAL	8.9
1	M	222	VAL	8.7
1	M	306	PHE	8.7
1	M	330	THR	8.6
1	m	315	MET	8.6
1	M	262	VAL	8.6
1	M	283	ARG	8.5
1	m	298	THR	8.5
1	M	234	PRO	8.4
1	M	209	THR	8.4
1	M	192	TYR	8.3
1	m	319	ALA	8.3
1	m	257	ALA	8.2
1	M	208	GLU	8.2
1	m	234	PRO	8.2
1	m	217	ALA	8.2
1	M	354	THR	8.1
1	M	356	ASP	8.0
1	M	215	GLU	8.0
1	m	214	LEU	8.0
1	M	171	GLU	7.9
1	M	189	VAL	7.9
1	M	259	ALA	7.9
1	M	266	LEU	7.8
1	m	210	MET	7.7
1	M	357	SER	7.7
1	l	357	SER	7.7
1	m	291	ILE	7.7
1	m	273	ALA	7.6

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Mol	Chain	Res	Type	RSRZ
1	M	193	GLN	7.5
1	M	280	PHE	7.5
1	l	304	LEU	7.4
1	H	527	PRO	7.4
1	m	316	LEU	7.4
1	m	264	ASN	7.4
1	M	270	LEU	7.3
1	k	527	PRO	7.3
1	M	233	LEU	7.3
1	M	343	ALA	7.3
1	m	371	LEU	7.2
1	M	263	VAL	7.2
1	M	298	THR	7.2
1	m	209	THR	7.2
1	M	202	TYR	7.0
1	M	367	ARG	7.0
1	l	359	TYR	6.9
1	m	235	ILE	6.9
1	m	280	PHE	6.9
1	M	218	PHE	6.9
1	m	266	LEU	6.9
1	M	227	SER	6.9
1	L	527	PRO	6.8
1	m	357	SER	6.8
1	m	245	PRO	6.8
1	m	260	THR	6.8
1	m	233	LEU	6.8
1	M	327	ASP	6.7
1	L	528	GLU	6.7
1	M	213	VAL	6.7
1	m	265	LYS	6.6
1	m	279	GLY	6.6
1	M	232	LEU	6.6
1	M	251	GLU	6.6
1	m	288	LEU	6.5
1	m	262	VAL	6.5
1	N	527	PRO	6.5
1	m	253	VAL	6.5
1	m	201	PRO	6.5
1	M	257	ALA	6.5
1	k	358	GLU	6.4
1	m	215	GLU	6.4

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Mol	Chain	Res	Type	RSRZ
1	m	263	VAL	6.4
1	k	214	LEU	6.4
1	M	268	GLY	6.4
1	m	270	LEU	6.3
1	M	255	GLY	6.3
1	m	232	LEU	6.3
1	N	528	GLU	6.3
1	m	299	VAL	6.3
1	M	201	PRO	6.2
1	l	191	GLY	6.2
1	M	274	ALA	6.2
1	m	382	ALA	6.2
1	M	314	SER	6.2
1	M	350	LYS	6.1
1	a	332	VAL	6.1
2	T	24	PRO	6.1
1	j	368	LEU	6.1
1	m	192	TYR	6.1
1	M	282	ASP	6.0
2	o	24	PRO	6.0
1	m	237	GLU	6.0
1	b	362	GLU	6.0
2	o	44	LYS	6.0
1	M	258	LEU	6.0
1	M	322	VAL	6.0
2	u	6	THR	6.0
1	m	255	GLY	5.9
1	m	294	VAL	5.9
1	M	214	LEU	5.9
1	M	253	VAL	5.9
1	m	267	ARG	5.9
1	A	529	LYS	5.8
1	l	375	VAL	5.8
1	i	356	ASP	5.8
1	M	382	ALA	5.8
1	M	252	ASP	5.8
2	s	100	GLN	5.7
1	k	371	LEU	5.7
1	M	300	ILE	5.7
1	M	173	ILE	5.7
1	k	357	SER	5.7
1	M	318	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
1	m	360	ALA	5.6
1	M	239	VAL	5.6
1	k	355	THR	5.6
1	l	168	VAL	5.6
1	m	200	SER	5.6
1	a	529	LYS	5.6
1	m	247	LEU	5.6
1	M	265	LYS	5.5
1	m	348	ILE	5.5
1	M	267	ARG	5.5
1	M	244	LYS	5.5
1	n	527	PRO	5.5
1	M	359	TYR	5.4
1	M	355	THR	5.4
1	m	203	PHE	5.4
1	M	311	ALA	5.3
1	m	325	THR	5.3
1	m	292	ALA	5.3
1	m	246	LEU	5.3
1	m	306	PHE	5.3
1	c	208	GLU	5.3
1	l	395	PHE	5.3
1	c	270	LEU	5.3
1	M	254	GLU	5.3
1	c	529	LYS	5.2
1	m	222	VAL	5.2
1	M	230	ARG	5.2
1	a	279	GLY	5.2
2	s	57	GLY	5.2
1	M	236	LEU	5.2
1	m	202	TYR	5.2
1	F	530	LYS	5.2
1	l	370	LYS	5.2
1	m	258	LEU	5.1
2	o	99	LEU	5.1
1	N	266	LEU	5.1
2	U	24	PRO	5.1
1	M	271	SER	5.1
1	m	241	GLN	5.1
1	L	304	LEU	5.0
1	a	278	PRO	5.0
1	h	527	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	b	226	VAL	5.0
1	l	348	ILE	5.0
1	m	313	LEU	5.0
1	m	311	ALA	5.0
1	M	289	LYS	5.0
1	M	320	GLU	5.0
1	g	339	GLU	5.0
1	m	354	THR	5.0
1	M	341	ILE	5.0
1	m	256	GLU	5.0
1	m	374	GLY	5.0
2	Q	28	GLY	5.0
1	a	277	ALA	5.0
1	M	328	GLU	4.9
1	f	529	LYS	4.9
1	c	528	GLU	4.9
1	m	295	THR	4.9
1	M	331	ILE	4.9
1	m	208	GLU	4.9
1	M	346	ASN	4.9
1	M	269	THR	4.9
1	l	345	ILE	4.8
1	a	300	ILE	4.8
1	m	219	ILE	4.8
1	k	368	LEU	4.8
1	M	305	GLY	4.8
1	N	359	TYR	4.8
2	o	69	ILE	4.8
1	m	305	GLY	4.8
1	b	303	GLU	4.8
1	m	297	GLY	4.8
1	M	206	ASN	4.8
1	K	527	PRO	4.7
1	i	355	THR	4.7
1	M	365	GLN	4.7
1	N	526	LYS	4.7
2	R	5	LYS	4.7
1	M	292	ALA	4.7
1	f	527	PRO	4.7
2	o	39	LYS	4.7
1	D	528	GLU	4.7
1	k	304	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	m	268	GLY	4.7
1	m	350	LYS	4.7
1	M	228	ASN	4.6
1	c	351	GLU	4.6
1	l	223	GLU	4.6
1	m	375	VAL	4.6
1	M	261	LEU	4.6
1	M	216	ASP	4.6
1	M	242	THR	4.6
1	m	243	GLY	4.6
1	m	340	ASP	4.5
1	l	173	ILE	4.5
1	N	44	PHE	4.5
1	c	280	PHE	4.5
1	j	182	LEU	4.5
1	M	256	GLU	4.5
1	b	528	GLU	4.5
1	J	527	PRO	4.5
1	g	280	PHE	4.5
1	n	354	THR	4.4
1	N	368	LEU	4.4
1	m	283	ARG	4.4
1	M	363	LYS	4.4
2	T	39	LYS	4.4
1	M	210	MET	4.4
1	m	300	ILE	4.4
1	E	270	LEU	4.4
1	e	374	GLY	4.4
1	m	239	VAL	4.4
1	m	314	SER	4.4
1	b	329	THR	4.4
1	m	216	ASP	4.4
1	M	226	VAL	4.4
1	M	339	GLU	4.4
1	m	290	ASP	4.3
1	m	312	THR	4.3
2	o	31	VAL	4.3
1	M	304	LEU	4.3
1	b	368	LEU	4.3
1	h	3	ALA	4.3
2	u	5	LYS	4.3
1	l	366	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	m	346	ASN	4.3
2	o	43	GLY	4.3
1	f	364	LEU	4.3
1	l	257	ALA	4.3
2	p	94	ASP	4.3
1	D	358	GLU	4.3
1	M	353	GLU	4.3
1	m	334	GLY	4.3
1	M	361	ARG	4.3
1	m	212	ALA	4.3
1	m	278	PRO	4.3
1	m	171	GLU	4.3
1	m	368	LEU	4.3
1	m	364	LEU	4.2
1	M	156	GLU	4.2
1	M	342	GLU	4.2
1	b	352	LEU	4.2
1	l	264	ASN	4.2
1	j	355	THR	4.2
1	l	350	LYS	4.2
2	p	88	VAL	4.2
1	m	308	LEU	4.2
1	M	347	GLY	4.2
1	F	531	GLU	4.2
1	m	303	GLU	4.2
1	M	297	GLY	4.2
1	b	275	VAL	4.2
1	k	187	LYS	4.1
1	B	374	GLY	4.1
1	b	227	SER	4.1
1	m	345	ILE	4.1
1	m	373	GLY	4.1
2	T	38	GLU	4.1
1	k	356	ASP	4.1
1	l	181	SER	4.1
1	M	293	ALA	4.1
2	t	73	ALA	4.1
1	m	178	GLU	4.1
1	G	374	GLY	4.1
1	M	360	ALA	4.1
1	M	376	ALA	4.1
1	m	249	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	529	LYS	4.0
1	m	274	ALA	4.0
2	r	56	ASN	4.0
1	M	172	GLY	4.0
1	k	270	LEU	4.0
1	l	142	LYS	4.0
2	r	37	LYS	4.0
1	E	244	LYS	4.0
1	l	371	LEU	4.0
2	S	44	LYS	4.0
1	l	527	PRO	3.9
1	l	226	VAL	3.9
1	N	373	GLY	3.9
1	M	225	LYS	3.9
2	p	90	LEU	3.9
1	m	254	GLU	3.9
1	M	366	GLU	3.9
1	m	347	GLY	3.9
1	M	384	THR	3.9
1	f	354	THR	3.9
1	l	248	ILE	3.9
2	o	87	TYR	3.9
1	c	365	GLN	3.9
1	l	227	SER	3.9
1	n	357	SER	3.9
1	K	183	GLU	3.9
1	f	353	GLU	3.9
1	m	160	LEU	3.9
1	l	230	ARG	3.9
1	f	322	VAL	3.8
1	k	352	LEU	3.8
1	M	326	LYS	3.8
1	M	240	ALA	3.8
1	m	287	MET	3.8
1	n	3	ALA	3.8
1	M	395	PHE	3.8
1	n	355	THR	3.8
1	l	360	ALA	3.8
1	E	356	ASP	3.8
1	m	250	ALA	3.8
1	M	358	GLU	3.8
1	m	3	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	44	PHE	3.7
1	c	359	TYR	3.7
1	M	278	PRO	3.7
1	l	189	VAL	3.7
1	M	281	GLY	3.7
1	k	185	GLU	3.7
1	M	272	VAL	3.7
1	j	348	ILE	3.7
1	l	138	VAL	3.7
1	M	178	GLU	3.7
1	M	351	GLU	3.7
1	N	356	ASP	3.7
1	l	183	GLU	3.7
1	m	213	VAL	3.7
1	M	352	LEU	3.7
1	F	356	ASP	3.7
1	l	182	LEU	3.6
1	n	371	LEU	3.6
2	u	9	LYS	3.6
1	M	526	LYS	3.6
1	l	167	LYS	3.6
1	M	329	THR	3.6
1	L	526	LYS	3.6
1	m	341	ILE	3.6
1	l	267	ARG	3.6
1	k	381	GLY	3.6
1	M	221	ILE	3.6
1	B	302	GLU	3.6
1	N	354	THR	3.6
1	h	270	LEU	3.6
1	l	169	GLY	3.6
1	N	363	LYS	3.6
1	j	186	LEU	3.6
1	m	44	PHE	3.6
1	H	528	GLU	3.6
1	g	190	GLU	3.6
1	k	213	VAL	3.6
1	l	139	GLU	3.6
2	U	100	GLN	3.6
1	k	383	ALA	3.6
1	l	221	ILE	3.6
2	o	100	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	340	ASP	3.6
2	p	20	ILE	3.6
1	f	352	LEU	3.6
1	l	266	LEU	3.6
2	S	20	ILE	3.6
2	U	83	ASP	3.6
1	a	337	LYS	3.6
1	l	330	THR	3.5
2	O	34	ASP	3.5
1	D	278	PRO	3.5
1	M	381	GLY	3.5
1	l	362	GLU	3.5
1	b	371	LEU	3.5
1	f	371	LEU	3.5
1	M	310	ASN	3.5
1	b	339	GLU	3.5
1	b	205	THR	3.5
1	M	307	LYS	3.5
1	l	256	GLU	3.5
2	u	55	GLU	3.5
1	N	371	LEU	3.5
1	l	299	VAL	3.5
1	m	199	ILE	3.5
1	m	302	GLU	3.5
1	n	283	ARG	3.5
1	b	204	VAL	3.5
1	k	178	GLU	3.5
1	n	356	ASP	3.5
1	l	355	THR	3.5
1	F	364	LEU	3.5
1	l	352	LEU	3.5
2	S	29	GLY	3.5
1	N	3	ALA	3.5
1	c	358	GLU	3.4
1	m	227	SER	3.4
1	E	349	LYS	3.4
1	f	241	GLN	3.4
1	l	373	GLY	3.4
2	T	23	GLU	3.4
1	l	192	TYR	3.4
1	I	3	ALA	3.4
1	l	526	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	n	266	LEU	3.4
2	S	31	VAL	3.4
1	i	354	THR	3.4
1	M	387	GLU	3.4
2	t	36	ALA	3.4
1	l	308	LEU	3.4
1	k	167	LYS	3.4
1	m	242	THR	3.4
1	M	364	LEU	3.4
1	H	382	ALA	3.4
1	g	187	LYS	3.4
1	m	526	LYS	3.4
2	u	15	VAL	3.4
2	q	75	TYR	3.4
1	m	361	ARG	3.4
2	S	74	LYS	3.4
1	b	313	LEU	3.3
1	m	186	LEU	3.3
1	b	208	GLU	3.3
1	j	474	LYS	3.3
1	n	257	ALA	3.3
1	L	182	LEU	3.3
1	l	213	VAL	3.3
1	I	280	PHE	3.3
1	n	282	ASP	3.3
2	t	100	GLN	3.3
1	j	350	LYS	3.3
1	a	241	GLN	3.3
1	M	248	ILE	3.3
1	E	280	PHE	3.2
2	r	75	TYR	3.2
1	l	367	ARG	3.2
1	J	526	LYS	3.2
1	k	269	THR	3.2
2	p	33	PRO	3.2
1	b	300	ILE	3.2
1	c	345	ILE	3.2
1	d	472	GLU	3.2
1	l	356	ASP	3.2
1	l	272	VAL	3.2
1	c	348	ILE	3.2
1	m	182	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	m	252	ASP	3.2
1	E	205	THR	3.2
1	e	280	PHE	3.2
1	D	304	LEU	3.2
2	S	94	ASP	3.2
1	a	528	GLU	3.2
1	l	242	THR	3.2
1	l	280	PHE	3.2
1	m	362	GLU	3.2
1	g	364	LEU	3.2
2	S	59	ARG	3.1
1	M	237	GLU	3.1
1	k	322	VAL	3.1
1	m	204	VAL	3.1
1	m	223	GLU	3.1
1	k	348	ILE	3.1
2	u	96	LEU	3.1
2	R	83	ASP	3.1
1	M	243	GLY	3.1
1	M	362	GLU	3.1
1	j	358	GLU	3.1
2	o	21	GLU	3.1
1	l	188	PHE	3.1
2	s	7	VAL	3.1
1	l	3	ALA	3.1
1	g	359	TYR	3.1
1	j	371	LEU	3.1
1	e	171	GLU	3.1
2	P	29	GLY	3.1
1	k	526	LYS	3.1
2	S	54	LEU	3.1
2	T	70	VAL	3.1
1	M	370	LYS	3.1
1	H	270	LEU	3.1
1	k	359	TYR	3.1
1	l	145	GLU	3.1
1	l	285	LYS	3.1
1	m	259	ALA	3.1
1	b	358	GLU	3.1
1	I	350	LYS	3.1
2	o	17	VAL	3.1
2	u	19	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	l	244	LYS	3.1
2	o	37	LYS	3.1
1	N	353	GLU	3.1
1	f	361	ARG	3.1
1	i	283	ARG	3.1
1	N	355	THR	3.1
2	u	22	GLU	3.1
2	t	46	ILE	3.1
1	n	368	LEU	3.1
2	O	84	GLY	3.1
1	B	171	GLU	3.0
1	a	314	SER	3.0
1	k	330	THR	3.0
1	l	361	ARG	3.0
1	M	224	LYS	3.0
1	M	345	ILE	3.0
1	k	321	ARG	3.0
1	b	277	ALA	3.0
1	l	382	ALA	3.0
1	m	142	LYS	3.0
2	u	75	TYR	3.0
1	i	260	THR	3.0
1	l	268	GLY	3.0
2	O	76	GLY	3.0
1	m	304	LEU	3.0
1	l	245	PRO	3.0
1	b	337	LYS	3.0
1	j	187	LYS	3.0
1	M	175	THR	3.0
1	k	305	GLY	3.0
1	E	358	GLU	3.0
1	b	194	PHE	3.0
1	l	229	VAL	3.0
1	m	176	VAL	3.0
1	e	303	GLU	3.0
1	e	351	GLU	3.0
1	m	269	THR	3.0
1	c	360	ALA	3.0
2	u	56	ASN	3.0
1	a	348	ILE	3.0
1	M	152	ALA	3.0
1	g	165	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	k	361	ARG	3.0
1	l	155	PRO	3.0
1	l	228	ASN	3.0
2	O	28	GLY	3.0
1	j	379	ARG	3.0
1	l	289	LYS	3.0
1	g	188	PHE	3.0
1	m	395	PHE	3.0
1	K	355	THR	2.9
1	f	528	GLU	2.9
1	j	347	GLY	2.9
1	a	361	ARG	2.9
1	M	348	ILE	2.9
2	o	89	ILE	2.9
1	l	260	THR	2.9
1	l	353	GLU	2.9
1	m	207	PRO	2.9
2	q	40	PRO	2.9
2	o	42	LYS	2.9
1	I	356	ASP	2.9
1	j	351	GLU	2.9
1	l	474	LYS	2.9
2	R	74	LYS	2.9
1	M	312	THR	2.9
1	D	302	GLU	2.9
1	a	358	GLU	2.9
1	m	301	SER	2.9
1	M	323	ARG	2.9
1	K	368	LEU	2.9
1	l	233	LEU	2.9
1	m	188	PHE	2.9
2	O	100	GLN	2.9
1	j	357	SER	2.9
2	P	46	ILE	2.9
2	O	99	LEU	2.9
1	a	226	VAL	2.9
1	m	138	VAL	2.9
2	t	5	LYS	2.9
1	k	331	ILE	2.9
1	l	179	SER	2.9
1	a	362	GLU	2.9
1	e	208	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	k	191	GLY	2.9
1	M	220	LEU	2.9
1	l	236	LEU	2.9
1	M	374	GLY	2.9
1	g	228	ASN	2.9
1	f	332	VAL	2.8
1	a	247	LEU	2.8
1	e	354	THR	2.8
1	j	226	VAL	2.8
1	k	380	VAL	2.8
1	l	222	VAL	2.8
1	M	198	TYR	2.8
1	M	288	LEU	2.8
1	l	363	LYS	2.8
1	m	220	LEU	2.8
2	p	8	ILE	2.8
1	b	209	THR	2.8
1	b	340	ASP	2.8
1	g	161	ILE	2.8
1	m	136	ILE	2.8
1	a	306	PHE	2.8
1	I	230	ARG	2.8
1	m	251	GLU	2.8
2	o	70	VAL	2.8
1	k	354	THR	2.8
1	a	192	TYR	2.8
2	o	83	ASP	2.8
1	a	303	GLU	2.8
1	b	253	VAL	2.8
1	i	241	GLN	2.8
1	n	350	LYS	2.8
1	N	352	LEU	2.8
1	G	372	ALA	2.8
2	s	33	PRO	2.8
1	b	324	ILE	2.8
1	l	214	LEU	2.8
2	U	82	ILE	2.8
2	o	82	ILE	2.8
1	k	332	VAL	2.8
1	M	190	GLU	2.8
1	j	428	LEU	2.8
1	k	261	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	i	250	ALA	2.8
1	b	251	GLU	2.8
1	m	185	GLU	2.8
2	o	20	ILE	2.8
2	R	6	THR	2.8
2	t	70	VAL	2.8
1	C	303	GLU	2.7
1	H	280	PHE	2.7
1	a	236	LEU	2.7
1	D	360	ALA	2.7
1	f	143	ALA	2.7
1	M	275	VAL	2.7
2	R	7	VAL	2.7
1	a	342	GLU	2.7
1	g	305	GLY	2.7
1	M	344	ARG	2.7
1	g	341	ILE	2.7
2	q	68	ASP	2.7
1	m	159	LYS	2.7
1	M	319	ALA	2.7
1	k	382	ALA	2.7
2	u	87	TYR	2.7
1	c	198	TYR	2.7
1	j	260	THR	2.7
1	m	358	GLU	2.7
1	M	196	LYS	2.7
1	M	391	LYS	2.7
2	t	8	ILE	2.7
1	A	302	GLU	2.7
1	m	339	GLU	2.7
1	c	243	GLY	2.7
2	q	5	LYS	2.7
1	H	371	LEU	2.7
1	m	248	ILE	2.7
1	H	3	ALA	2.7
1	e	185	GLU	2.7
2	p	6	THR	2.7
1	F	474	LYS	2.7
1	e	188	PHE	2.7
1	j	262	VAL	2.7
1	l	224	LYS	2.7
2	o	30	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	n	376	ALA	2.7
1	e	244	LYS	2.6
1	h	306	PHE	2.6
1	g	313	LEU	2.6
1	n	287	MET	2.6
1	D	216	ASP	2.6
2	u	7	VAL	2.6
2	U	81	GLU	2.6
1	N	364	LEU	2.6
1	l	364	LEU	2.6
1	b	221	ILE	2.6
1	k	5	ILE	2.6
1	H	355	THR	2.6
1	l	354	THR	2.6
1	m	184	THR	2.6
2	s	6	THR	2.6
1	a	308	LEU	2.6
1	M	527	PRO	2.6
1	b	191	GLY	2.6
1	g	347	GLY	2.6
1	a	242	THR	2.6
1	a	298	THR	2.6
1	D	371	LEU	2.6
2	t	99	LEU	2.6
1	k	474	LYS	2.6
2	o	8	ILE	2.6
1	d	527	PRO	2.6
1	j	527	PRO	2.6
1	m	527	PRO	2.6
1	k	215	GLU	2.6
1	k	272	VAL	2.6
1	J	368	LEU	2.6
2	s	8	ILE	2.6
1	M	241	GLN	2.6
2	r	94	ASP	2.6
1	l	358	GLU	2.6
1	l	387	GLU	2.6
1	c	242	THR	2.6
1	m	289	LYS	2.6
2	T	44	LYS	2.6
1	i	368	LEU	2.6
1	D	279	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	333	GLY	2.6
1	g	185	GLU	2.6
1	n	526	LYS	2.6
2	t	37	LYS	2.6
1	j	332	VAL	2.6
1	l	136	ILE	2.6
1	g	356	ASP	2.6
2	t	83	ASP	2.6
1	m	66	LEU	2.6
1	e	528	GLU	2.6
1	g	362	GLU	2.6
1	l	336	GLY	2.6
2	s	29	GLY	2.6
1	m	310	ASN	2.6
1	g	138	VAL	2.6
1	E	208	GLU	2.5
1	a	371	LEU	2.5
1	g	366	GLU	2.5
2	s	99	LEU	2.5
1	e	360	ALA	2.5
2	Q	56	ASN	2.5
1	l	318	ARG	2.5
1	c	211	GLU	2.5
2	S	99	LEU	2.5
1	m	417	THR	2.5
1	n	348	ILE	2.5
2	o	6	THR	2.5
2	S	24	PRO	2.5
1	e	302	GLU	2.5
1	M	191	GLY	2.5
1	a	305	GLY	2.5
1	i	347	GLY	2.5
1	m	321	ARG	2.5
1	b	265	LYS	2.5
1	K	262	VAL	2.5
1	M	203	PHE	2.5
2	u	88	VAL	2.5
1	N	270	LEU	2.5
1	l	283	ARG	2.5
1	m	173	ILE	2.5
2	o	5	LYS	2.5
1	g	325	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	i	179	SER	2.5
1	j	354	THR	2.5
1	k	375	VAL	2.5
1	i	304	LEU	2.5
1	l	296	GLY	2.5
1	M	238	GLN	2.5
1	b	338	LYS	2.5
2	T	30	ILE	2.5
1	c	188	PHE	2.5
1	g	44	PHE	2.5
1	n	44	PHE	2.5
1	d	305	GLY	2.5
1	L	3	ALA	2.5
1	M	144	ILE	2.5
1	l	249	ILE	2.5
1	m	221	ILE	2.5
1	M	165	MET	2.5
2	o	16	VAL	2.5
1	k	182	LEU	2.5
1	A	528	GLU	2.5
1	l	334	GLY	2.5
2	u	70	VAL	2.5
1	M	212	ALA	2.5
1	m	324	ILE	2.5
1	L	381	GLY	2.5
1	M	325	THR	2.4
1	N	358	GLU	2.4
1	m	198	TYR	2.4
1	a	326	LYS	2.4
1	E	44	PHE	2.4
1	h	44	PHE	2.4
1	g	315	MET	2.4
1	j	373	GLY	2.4
1	d	323	ARG	2.4
1	i	185	GLU	2.4
2	p	38	GLU	2.4
2	O	27	LYS	2.4
1	m	343	ALA	2.4
2	r	20	ILE	2.4
1	M	321	ARG	2.4
1	l	381	GLY	2.4
1	l	380	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	256	GLU	2.4
1	d	302	GLU	2.4
1	b	201	PRO	2.4
1	k	280	PHE	2.4
1	J	303	GLU	2.4
1	m	320	GLU	2.4
2	Q	99	LEU	2.4
1	b	351	GLU	2.4
2	r	34	ASP	2.4
1	J	3	ALA	2.4
1	M	148	ALA	2.4
1	M	383	ALA	2.4
2	P	36	ALA	2.4
2	O	8	ILE	2.4
1	d	529	LYS	2.4
1	i	350	LYS	2.4
1	m	478	TYR	2.4
1	F	358	GLU	2.4
1	H	358	GLU	2.4
1	f	368	LEU	2.4
1	k	148	ALA	2.4
1	g	527	PRO	2.4
1	c	362	GLU	2.4
1	k	44	PHE	2.4
1	n	183	GLU	2.4
1	g	230	ARG	2.4
1	m	380	VAL	2.4
1	L	261	LEU	2.4
1	b	363	LYS	2.4
1	M	143	ALA	2.4
1	k	120	ILE	2.4
1	A	527	PRO	2.4
1	H	303	GLU	2.4
1	M	303	GLU	2.4
1	a	251	GLU	2.4
1	f	373	GLY	2.4
1	k	334	GLY	2.4
1	N	357	SER	2.4
1	i	357	SER	2.4
1	N	267	ARG	2.4
1	k	267	ARG	2.4
1	l	306	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	p	87	TYR	2.4
1	m	62	LEU	2.4
1	l	250	ALA	2.4
1	m	383	ALA	2.4
1	k	34	ARG	2.4
1	i	395	PHE	2.4
1	J	356	ASP	2.4
2	T	71	VAL	2.4
1	M	316	LEU	2.3
1	e	270	LEU	2.3
1	M	211	GLU	2.3
1	i	230	ARG	2.3
1	i	351	GLU	2.3
2	o	38	GLU	2.3
1	j	334	GLY	2.3
1	D	44	PHE	2.3
2	s	53	VAL	2.3
1	k	364	LEU	2.3
1	l	384	THR	2.3
1	n	364	LEU	2.3
2	s	54	LEU	2.3
1	b	215	GLU	2.3
1	c	241	GLN	2.3
2	u	57	GLY	2.3
1	K	44	PHE	2.3
1	a	218	PHE	2.3
1	b	44	PHE	2.3
1	b	266	LEU	2.3
1	b	359	TYR	2.3
2	S	96	LEU	2.3
2	u	99	LEU	2.3
2	Q	100	GLN	2.3
1	a	373	GLY	2.3
1	e	306	PHE	2.3
1	k	6	LEU	2.3
1	l	85	ALA	2.3
1	i	341	ILE	2.3
1	l	144	ILE	2.3
1	i	280	PHE	2.3
1	c	244	LYS	2.3
1	e	186	LEU	2.3
1	j	352	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	3	ALA	2.3
1	f	280	PHE	2.3
2	t	98	VAL	2.3
1	l	482	ALA	2.3
2	t	97	ALA	2.3
1	n	341	ILE	2.3
1	f	474	LYS	2.3
1	k	260	THR	2.3
1	l	263	VAL	2.3
1	i	232	LEU	2.3
1	f	357	SER	2.3
1	j	376	ALA	2.3
1	j	460	TYR	2.3
1	m	240	ALA	2.3
1	a	221	ILE	2.3
1	e	144	ILE	2.3
1	m	272	VAL	2.3
1	c	356	ASP	2.3
1	e	527	PRO	2.3
1	g	374	GLY	2.3
1	i	282	ASP	2.3
1	l	193	GLN	2.3
1	c	363	LYS	2.3
1	H	348	ILE	2.3
1	a	203	PHE	2.3
2	O	60	VAL	2.3
1	E	245	PRO	2.3
1	G	373	GLY	2.3
1	M	170	LYS	2.3
1	a	356	ASP	2.2
2	p	84	GLY	2.3
1	K	250	ALA	2.2
1	n	361	ARG	2.2
2	s	20	ILE	2.2
1	K	187	LYS	2.2
1	a	204	VAL	2.2
1	c	197	GLY	2.2
1	l	232	LEU	2.2
1	b	240	ALA	2.2
1	b	353	GLU	2.2
2	o	22	GLU	2.2
1	b	192	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	l	161	ILE	2.2
1	n	173	ILE	2.2
1	E	326	LYS	2.2
1	l	391	LYS	2.2
2	t	71	VAL	2.2
1	b	232	LEU	2.2
1	k	175	THR	2.2
2	P	99	LEU	2.2
1	l	148	ALA	2.2
2	Q	94	ASP	2.2
2	P	69	ILE	2.2
1	a	340	ASP	2.2
1	b	282	ASP	2.2
1	f	355	THR	2.2
1	M	285	LYS	2.2
1	h	348	ILE	2.2
1	k	339	GLU	2.2
1	n	270	LEU	2.2
1	a	245	PRO	2.2
1	d	331	ILE	2.2
2	Q	20	ILE	2.2
1	f	165	MET	2.2
1	g	485	GLY	2.2
1	B	368	LEU	2.2
1	g	308	LEU	2.2
1	b	195	ASP	2.2
1	j	280	PHE	2.2
1	n	199	ILE	2.2
1	f	358	GLU	2.2
1	k	244	LYS	2.2
1	k	366	GLU	2.2
2	U	44	LYS	2.2
2	S	71	VAL	2.2
2	t	64	VAL	2.2
1	a	327	ASP	2.2
1	m	327	ASP	2.2
2	p	36	ALA	2.2
1	I	355	THR	2.2
1	m	384	THR	2.2
1	L	302	GLU	2.2
1	d	358	GLU	2.2
2	t	43	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	m	218	PHE	2.2
1	F	348	ILE	2.2
1	b	249	ILE	2.2
1	c	207	PRO	2.2
1	l	131	ILE	2.2
1	l	178	GLU	2.2
2	O	69	ILE	2.2
1	M	296	GLY	2.2
1	l	298	THR	2.2
1	d	247	LEU	2.2
1	m	275	VAL	2.2
2	O	64	VAL	2.2
2	p	71	VAL	2.2
2	r	31	VAL	2.2
1	k	3	ALA	2.2
1	g	363	LYS	2.1
2	U	74	LYS	2.1
1	F	208	GLU	2.1
1	M	286	GLU	2.1
1	e	358	GLU	2.1
1	I	283	ARG	2.1
2	r	100	GLN	2.1
2	s	32	LEU	2.1
1	N	43	LYS	2.1
2	P	75	TYR	2.1
1	L	356	ASP	2.1
1	m	187	LYS	2.1
1	m	332	VAL	2.1
2	T	42	LYS	2.1
2	o	15	VAL	2.1
2	s	44	LYS	2.1
1	d	270	LEU	2.1
1	i	258	LEU	2.1
1	l	65	HIS	2.1
2	Q	54	LEU	2.1
2	Q	90	LEU	2.1
1	g	358	GLU	2.1
1	l	487	PHE	2.1
1	m	331	ILE	2.1
1	C	170	LYS	2.1
1	d	337	LYS	2.1
1	l	278	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	T	25	LYS	2.1
1	D	332	VAL	2.1
1	k	189	VAL	2.1
2	o	58	GLN	2.1
1	n	258	LEU	2.1
1	M	185	GLU	2.1
2	U	36	ALA	2.1
2	o	73	ALA	2.1
1	c	314	SER	2.1
2	t	42	LYS	2.1
1	H	236	LEU	2.1
1	i	186	LEU	2.1
1	J	183	GLU	2.1
1	b	342	GLU	2.1
1	M	184	THR	2.1
1	f	473	THR	2.1
1	l	500	LYS	2.1
1	m	326	LYS	2.1
1	m	359	TYR	2.1
1	e	239	VAL	2.1
2	U	17	VAL	2.1
2	p	93	ARG	2.1
1	i	308	LEU	2.1
1	b	203	PHE	2.1
1	c	206	ASN	2.1
1	b	301	SER	2.1
1	j	5	ILE	2.1
1	E	527	PRO	2.1
1	M	207	PRO	2.1
1	l	316	LEU	2.1
1	n	375	VAL	2.1
2	U	70	VAL	2.1
1	E	306	PHE	2.1
1	J	280	PHE	2.1
1	J	361	ARG	2.1
1	M	136	ILE	2.1
2	u	8	ILE	2.1
1	b	241	GLN	2.1
1	c	171	GLU	2.1
1	d	241	GLN	2.1
1	n	187	LYS	2.1
2	Q	38	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	261	LEU	2.1
1	l	261	LEU	2.1
2	p	32	LEU	2.1
1	l	274	ALA	2.1
2	s	73	ALA	2.1
1	h	267	ARG	2.1
1	M	195	ASP	2.1
1	j	183	GLU	2.1
2	R	75	TYR	2.1
1	m	206	ASN	2.1
2	q	25	LYS	2.1
1	I	232	LEU	2.1
1	i	263	VAL	2.1
1	k	399	LEU	2.1
1	k	428	LEU	2.1
1	m	226	VAL	2.1
1	f	360	ALA	2.1
1	n	360	ALA	2.1
1	G	280	PHE	2.0
1	d	44	PHE	2.0
1	j	333	GLY	2.0
1	D	320	GLU	2.0
1	b	355	THR	2.0
2	T	20	ILE	2.0
1	f	475	ASN	2.0
2	P	100	GLN	2.0
1	m	381	GLY	2.0
1	F	350	LYS	2.0
1	H	526	LYS	2.0
1	K	363	LYS	2.0
1	a	350	LYS	2.0
1	g	490	MET	2.0
2	s	37	LYS	2.0
1	M	231	GLU	2.0
1	f	342	GLU	2.0
1	F	355	THR	2.0
1	l	160	LEU	2.0
1	l	247	LEU	2.0
2	S	53	VAL	2.0
1	k	212	ALA	2.0
1	l	301	SER	2.0
1	M	249	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	g	331	ILE	2.0
1	H	142	LYS	2.0
1	g	332	VAL	2.0
1	k	149	THR	2.0
1	k	186	LEU	2.0
1	n	285	LYS	2.0
2	S	70	VAL	2.0
2	T	37	LYS	2.0
1	L	44	PHE	2.0
1	f	487	PHE	2.0
1	m	194	PHE	2.0
1	M	223	GLU	2.0
1	l	385	GLU	2.0
1	m	211	GLU	2.0
1	N	65	HIS	2.0
2	O	94	ASP	2.0
2	R	94	ASP	2.0
2	q	46	ILE	2.0
2	r	89	ILE	2.0
1	F	352	LEU	2.0
1	K	182	LEU	2.0
1	e	60	VAL	2.0
1	b	343	ALA	2.0
1	l	200	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	n	701	4/4	0.88	0.27	5.15	69,85,87,99	0
5	DMS	j	601	4/4	0.79	0.29	3.36	82,83,101,117	0
5	DMS	k	601	4/4	0.88	0.25	3.16	89,96,103,115	0
5	DMS	m	601	4/4	0.94	0.23	2.96	82,92,95,105	0
5	DMS	J	601	4/4	0.85	0.24	2.95	39,53,65,90	0
5	DMS	h	601	4/4	0.93	0.22	2.86	52,58,85,96	0
5	DMS	l	601	4/4	0.88	0.24	2.30	63,95,106,125	0
5	DMS	i	601	4/4	0.94	0.22	2.24	27,32,40,87	0
5	DMS	L	601	4/4	0.90	0.24	2.18	39,58,61,94	0
5	DMS	H	601	4/4	0.91	0.24	2.15	24,28,74,96	0
4	ADP	f	602	27/27	0.91	0.28	1.93	47,93,109,116	0
5	DMS	I	601	4/4	0.95	0.20	1.76	37,58,66,93	0
5	DMS	M	601	4/4	0.93	0.20	1.51	26,29,60,79	0
4	ADP	B	602	27/27	0.96	0.23	1.47	18,54,75,80	0
4	ADP	d	602	27/27	0.93	0.23	1.41	45,72,87,93	0
4	ADP	g	602	27/27	0.92	0.26	1.29	56,84,98,103	0
4	ADP	a	602	27/27	0.94	0.24	1.24	21,70,81,90	0
4	ADP	c	602	27/27	0.94	0.23	1.14	24,67,80,102	0
4	ADP	D	602	27/27	0.95	0.21	1.12	1,38,64,69	0
4	ADP	G	602	27/27	0.96	0.21	0.93	1,61,76,85	0
4	ADP	e	602	27/27	0.94	0.23	0.92	48,78,103,108	0
4	ADP	F	602	27/27	0.97	0.21	0.75	23,51,75,88	0
4	ADP	b	602	27/27	0.96	0.20	0.70	13,58,79,85	0
5	DMS	K	601	4/4	0.91	0.18	0.69	43,44,76,91	0
4	ADP	E	602	27/27	0.96	0.20	0.59	12,44,74,80	0
4	ADP	A	602	27/27	0.97	0.21	0.42	1,47,68,77	0
5	DMS	N	701	4/4	0.98	0.16	0.32	53,57,64,90	0
4	ADP	C	602	27/27	0.96	0.19	0.03	1,34,70,78	0
3	MG	f	601	1/1	0.90	0.51	-	70,70,70,70	0
3	MG	G	601	1/1	0.97	0.21	-	29,29,29,29	0
3	MG	F	601	1/1	0.96	0.27	-	25,25,25,25	0
3	MG	a	601	1/1	0.96	0.34	-	54,54,54,54	0
3	MG	d	601	1/1	0.75	0.40	-	68,68,68,68	0
3	MG	b	601	1/1	0.90	0.28	-	53,53,53,53	0
3	MG	c	601	1/1	0.89	0.33	-	51,51,51,51	0
3	MG	g	601	1/1	0.92	0.54	-	66,66,66,66	0
3	MG	e	601	1/1	0.82	0.32	-	62,62,62,62	0
3	MG	C	601	1/1	0.92	0.21	-	28,28,28,28	0
3	MG	A	601	1/1	0.94	0.25	-	27,27,27,27	0
3	MG	E	601	1/1	0.95	0.22	-	20,20,20,20	0
3	MG	D	601	1/1	0.95	0.24	-	29,29,29,29	0
3	MG	B	601	1/1	0.95	0.32	-	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.