Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:21 PM GMT

PDB ID	:	1JXA
Title	:	GLUCOSAMINE 6-PHOSPHATE SYNTHASE WITH GLUCOSE 6-PHOSPHATE
Authors	:	Teplyakov, A.; Obmolova, G.; Badet, B.; Badet-Denisot, M.A.
Deposited on	:	2001-09-06
Resolution	:	3.10 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:

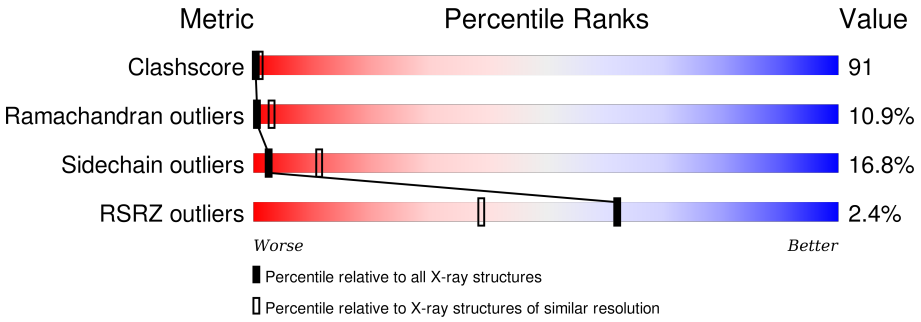
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	608	20% 54% 23%
1	B	608	17% 60% 20%
1	C	608	5% 21% 60% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14156 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.

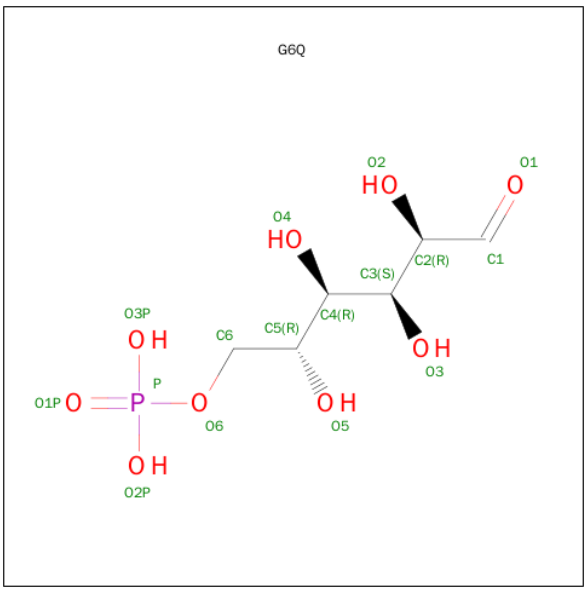
- Molecule 1 is a protein called glucosamine 6-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			
1	B	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			
1	C	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	LYS	ARG	CONFLICT	UNP P17169
B	421	LYS	ARG	CONFLICT	UNP P17169
C	421	LYS	ARG	CONFLICT	UNP P17169

- Molecule 2 is SUGAR (GLUCOSE-6-PHOSPHATE) (three-letter code: G6Q) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is water.

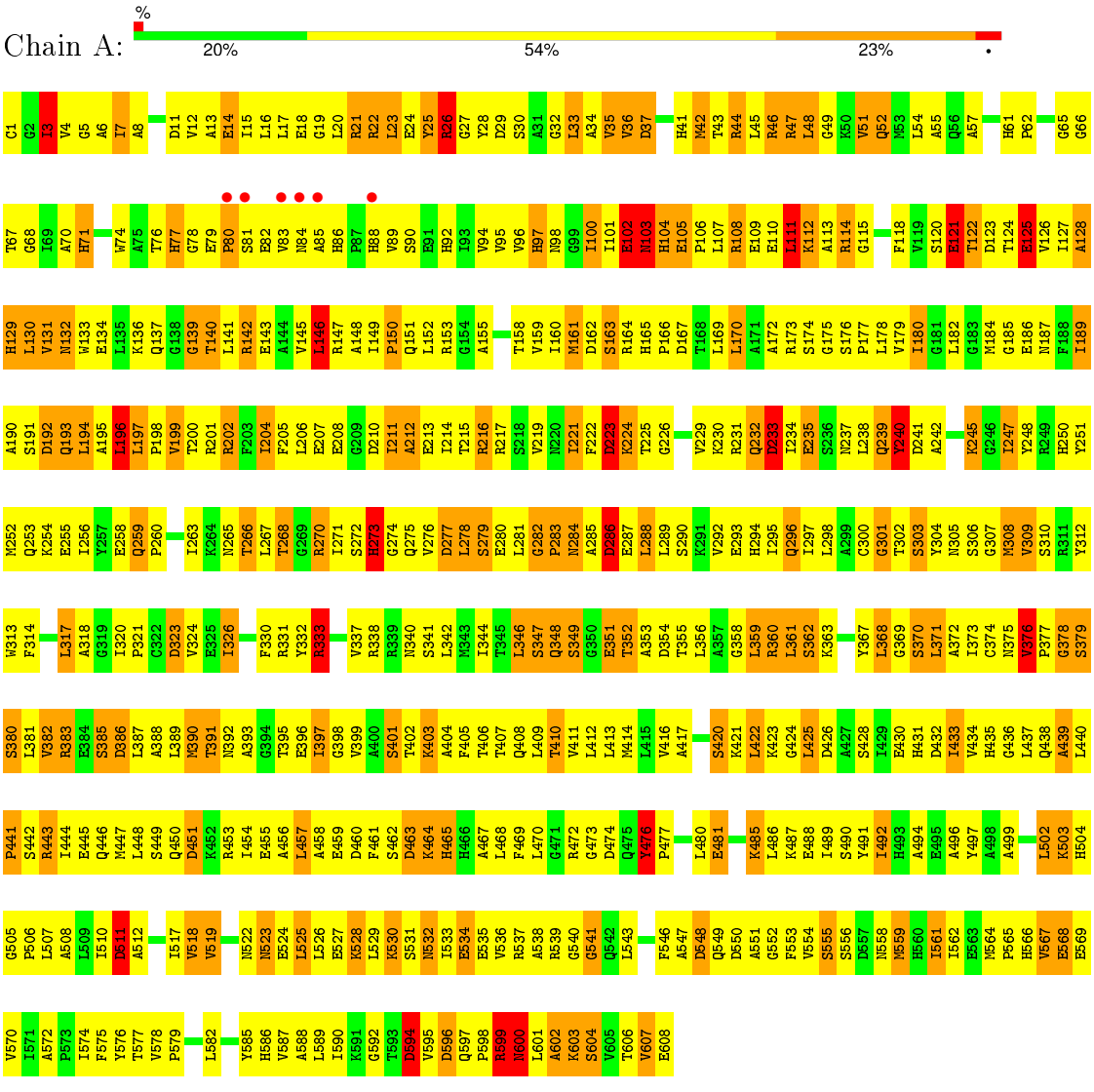
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	10	Total	O	0	0
			10	10		
3	C	3	Total	O	0	0
			3	3		

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.

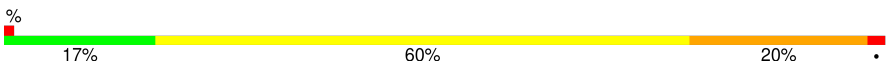
- Molecule 1: glucosamine 6-phosphate synthase

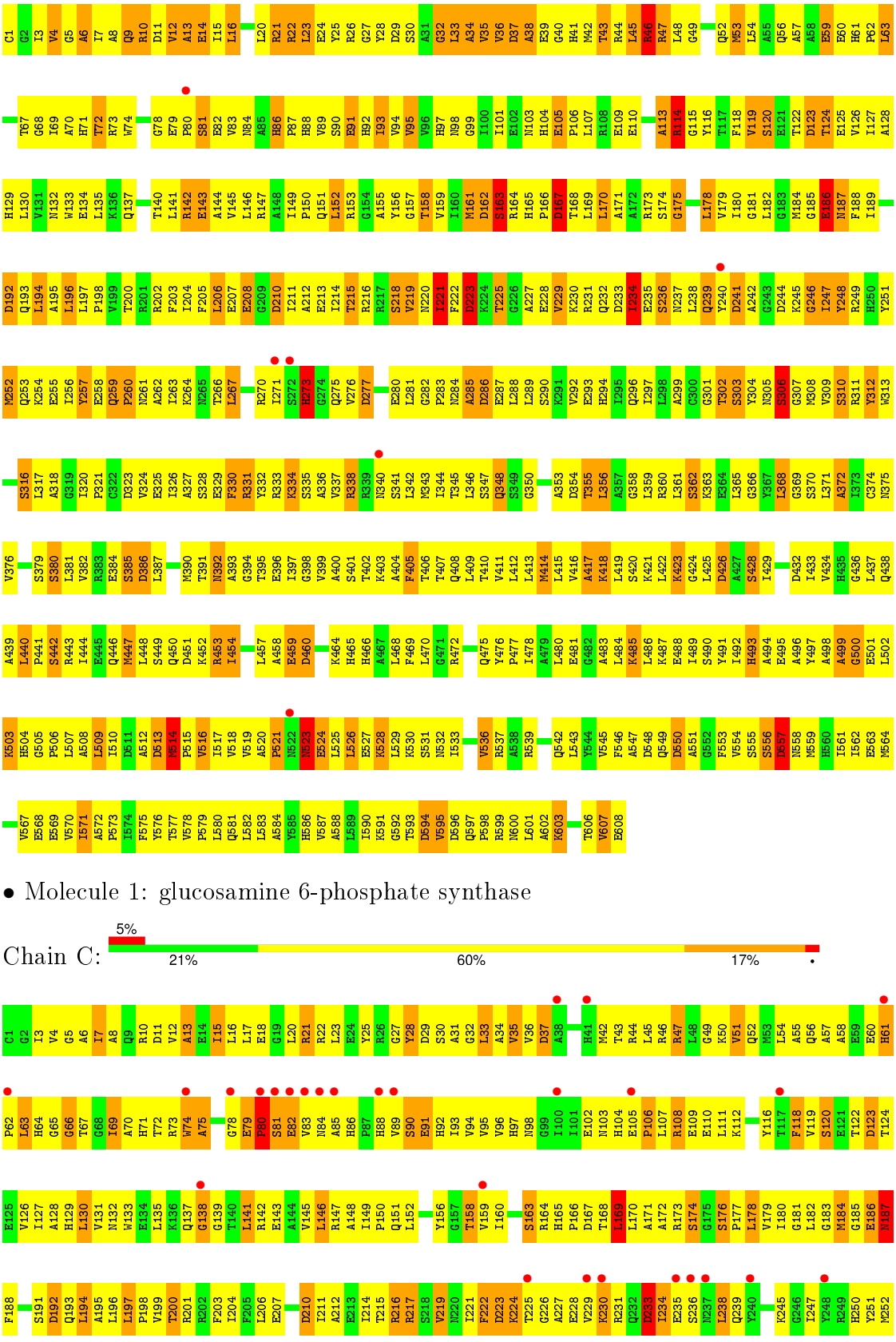
Chain A:



- Molecule 1: glucosamine 6-phosphate synthase

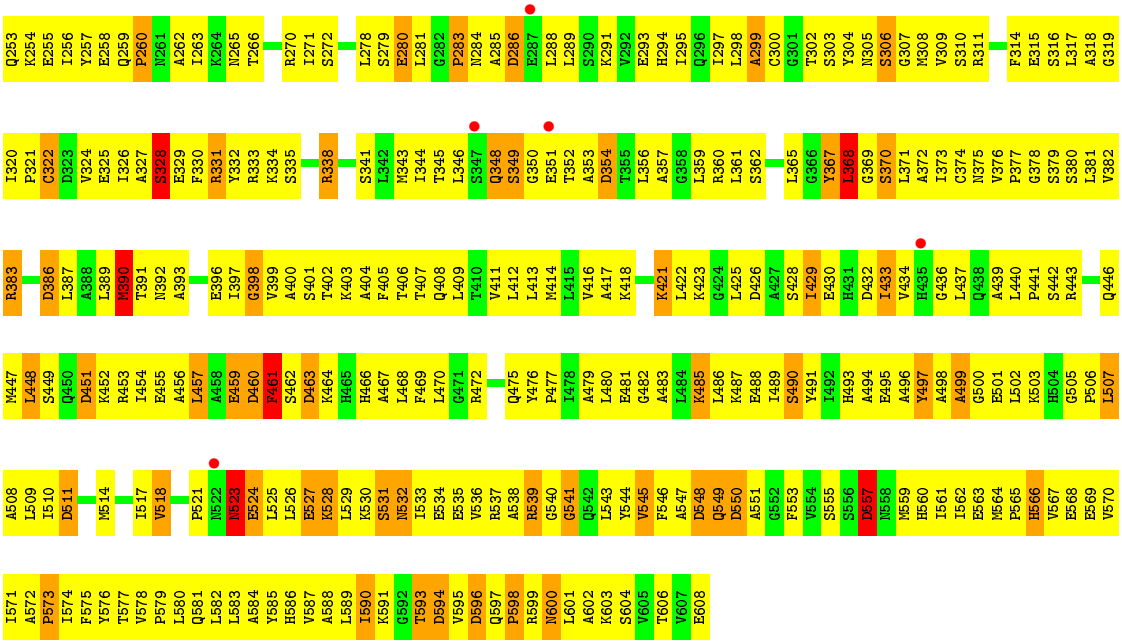
Chain B:





• Molecule 1: glucosamine 6-phosphate synthase

Chain C:


Q253 K254 E255 I256 Y257 E258 Q259 P260 N261 A262 I263 K264 N265 T266 R270 I271 S272 L278 S279 E280 L281 G282 P283 N284 A285 D286 E287 L288 L289 S290 K291 V292 E293 H294 I295 Q296 I297 L298 A299 G300 G301 T302 S303 Y304 N305 S306 G307 M308 V309 S310 R311 F314 E315 S316 L317 A318 G319
I320 P321 C322 D323 V324 E325 I326 A327 S328 E329 F330 R331 Y332 R333 K334 S335 R338 S341 L342 M343 I344 T345 L346 S347 Q348 S349 G350 E351 T352 A353 D354 T355 L356 A357 G358 L359 R360 L361 S362 L365 G366 Y367 L368 G369 S370 L371 A372 I373 C374 N375 V376 P377 G378 S379 S380 L381 V382
R383 D386 L387 A388 L389 M390 T391 N392 A393 E396 I397 G398 V399 A400 S401 T402 K403 A404 F405 T406 T407 Q408 L409 T410 V411 L412 L413 M414 L415 V416 A417 K418 K421 L422 K423 G424 L425 D426 A427 S428 I429 E430 H431 D432 I433 V434 H435 G436 L437 Q438 A439 L440 P441 S442 R443 Q446
M447 L448 S449 Q450 D451 K452 R453 I454 E455 A456 I457 A458 E459 D460 F461 S462 D463 K464 H465 H466 A467 L468 F469 L470 G471 R472 Q475 Y476 P477 I478 A479 L480 E481 G482 A483 I484 K485 L486 K487 E488 I489 S490 Y491 I492 H493 A494 E495 A496 Y497 A498 A499 G500 E501 L502 K503 H504 G505 P506 L507
A508 L509 I510 D511 M514 I517 V518 P521 N522 N523 E524 L525 L526 E527 K528 L529 K530 S531 N532 I533 E534 E535 V536 R537 A538 R539 G540 G541 Q542 L543 Y544 V545 F546 A547 D548 Q549 D550 A551 G552 F553 V554 S555 S556 D557 N558 M559 H560 I561 I562 E563 M564 P565 H566 V567 E568 E569 V570
I571 A572 P573 I574 F575 Y576 T577 V578 P579 L580 Q581 L582 L583 A584 Y585 H586 V587 A588 L589 I590 K591 G592 T593 D594 V595 D596 Q597 P598 R599 N600 L601 A602 K603 S604 V605 T606 V607 E608

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.40Å 112.40Å 185.10Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 19.97 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 92.7 (19.97-3.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 3.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.280 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 83.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 45685 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14156	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: G6Q

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	0.82	1/4776 (0.0%)	1.34	47/6467 (0.7%)
1	B	0.67	0/4776	1.10	29/6467 (0.4%)
1	C	0.51	0/4776	0.90	18/6467 (0.3%)
All	All	0.68	1/14328 (0.0%)	1.13	94/19401 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	TYR	CD1-CE1	-5.16	1.31	1.39

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	323	ASP	CB-CG-OD2	9.78	127.10	118.30
1	A	22	ARG	NE-CZ-NH1	-8.83	115.88	120.30
1	B	47	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	142	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	114	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	B	167	ASP	CB-CG-OD2	8.73	126.16	118.30
1	A	216	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	217	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	216	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	278	LEU	CB-CG-CD1	-8.58	96.42	111.00
1	B	142	ARG	NE-CZ-NH2	8.33	124.47	120.30
1	A	37	ASP	CB-CG-OD2	7.96	125.46	118.30
1	B	46	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	46	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	A	354	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	47	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	432	ASP	CB-CG-OD2	7.56	125.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	333	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	26	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	B	22	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	B	10	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	286	ASP	CB-CG-OD2	6.90	124.51	118.30
1	C	596	ASP	CB-CG-OD2	6.87	124.49	118.30
1	A	162	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	23	LEU	CB-CG-CD2	-6.56	99.85	111.00
1	A	426	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	3	ILE	CG1-CB-CG2	-6.49	97.13	111.40
1	B	460	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	223	ASP	CB-CG-OD2	6.27	123.95	118.30
1	C	80	PRO	N-CA-C	-6.27	95.80	112.10
1	A	47	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	550	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	229	VAL	CB-CA-C	-6.08	99.84	111.40
1	A	298	LEU	CB-CG-CD1	6.04	121.26	111.00
1	A	360	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	C	37	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	286	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	432	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	219	VAL	CB-CA-C	-5.88	100.23	111.40
1	C	511	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	114	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	460	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	121	GLU	N-CA-CB	-5.79	100.18	110.60
1	A	100	ILE	CG1-CB-CG2	-5.75	98.76	111.40
1	A	130	LEU	CB-CG-CD2	5.73	120.75	111.00
1	A	451	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	386	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	557	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	111	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	C	123	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	21	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	210	ASP	CB-CG-OD2	5.64	123.38	118.30
1	C	223	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	557	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	567	VAL	CB-CA-C	-5.58	100.80	111.40
1	A	233	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	432	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	354	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	286	ASP	CB-CG-OD2	5.46	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	277	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	426	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	594	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	192	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	463	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	196	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	A	577	THR	CA-CB-CG2	-5.36	104.89	112.40
1	A	277	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	382	VAL	CA-CB-CG1	-5.34	102.89	110.90
1	A	22	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	B	192	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	217	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	594	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	162	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	270	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	A	376	VAL	CB-CA-C	-5.23	101.46	111.40
1	A	352	THR	CA-CB-CG2	-5.22	105.09	112.40
1	C	192	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	196	LEU	CA-CB-CG	-5.17	103.41	115.30
1	A	204	ILE	N-CA-C	-5.17	97.06	111.00
1	A	196	LEU	CB-CG-CD1	5.15	119.75	111.00
1	B	16	LEU	CB-CG-CD1	5.14	119.74	111.00
1	A	333	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	451	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	16	LEU	CA-CB-CG	-5.13	103.51	115.30
1	A	23	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	B	323	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	386	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	37	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	A	317	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	C	233	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	223	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	599	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	C	463	ASP	CB-CG-OD2	5.03	122.82	118.30

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	4695	0	4715	862	1
1	B	4695	0	4715	918	0
1	C	4695	0	4715	826	0
2	A	16	0	10	4	0
2	B	16	0	11	2	0
3	A	26	0	0	2	0
3	B	10	0	0	2	0
3	C	3	0	0	0	0
All	All	14156	0	14166	2564	1

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 91.

All (2564) 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:A:100:ILE:CD1	1:A:100:ILE:CG1	1.76	1.63
1:A:304:TYR:CE1	1:A:326:ILE:HD13	1.47	1.48
1:A:304:TYR:CD1	1:A:326:ILE:CD1	2.18	1.26
1:B:484:LEU:O	1:B:485:LYS:HG2	1.27	1.25
1:B:223:ASP:OD2	1:B:225:THR:HG23	1.32	1.25
1:A:491:TYR:CZ	1:A:599:ARG:HD3	1.74	1.22
1:C:399:VAL:HG23	1:C:596:ASP:O	1.39	1.21
1:C:565:PRO:HG2	1:C:575:PHE:HZ	1.05	1.19
1:C:252:MET:SD	1:C:400:ALA:HB3	1.81	1.18
1:B:281:LEU:HD13	1:B:387:LEU:CD1	1.72	1.18
1:B:529:LEU:O	1:B:533:ILE:HG13	1.42	1.18
1:A:146:LEU:HG	1:A:211:ILE:HD12	1.25	1.18
1:B:406:THR:HA	1:B:409:LEU:HD12	1.21	1.18
1:B:356:LEU:HD11	1:B:360:ARG:CZ	1.73	1.18
1:A:304:TYR:CD1	1:A:326:ILE:HD13	1.76	1.18
1:B:502:LEU:HA	1:B:506:PRO:HG2	1.26	1.18
1:B:21:ARG:HG3	1:B:21:ARG:HH11	1.08	1.16
1:A:304:TYR:CE1	1:A:326:ILE:CD1	2.27	1.16
1:B:529:LEU:HG	1:B:533:ILE:HD11	1.28	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:O	1:A:121:GLU:HG3	1.47	1.14
1:C:440:LEU:HB3	1:C:441:PRO:HD3	1.21	1.14
1:B:22:ARG:HD3	1:B:194:LEU:O	1.46	1.13
1:B:281:LEU:CD1	1:B:387:LEU:HD13	1.79	1.13
1:B:523:ASN:ND2	1:B:525:LEU:H	1.44	1.12
1:B:48:LEU:HD21	1:B:81:SER:HB2	1.31	1.12
1:C:565:PRO:HG2	1:C:575:PHE:CZ	1.84	1.11
1:C:457:LEU:CD2	1:C:562:ILE:HD11	1.79	1.11
1:B:187:ASN:N	1:B:187:ASN:HD22	1.38	1.11
1:A:193:GLN:NE2	1:A:205:PHE:HZ	1.49	1.11
1:A:607:VAL:HG23	1:A:608:GLU:H	0.96	1.09
1:A:247:ILE:H	1:A:247:ILE:HD12	0.96	1.09
1:B:33:LEU:H	1:B:33:LEU:HD23	1.17	1.09
1:B:587:VAL:HA	1:B:590:ILE:HD12	1.33	1.09
1:B:532:ASN:O	1:B:536:VAL:HG22	1.53	1.09
1:A:383:ARG:HG2	1:A:383:ARG:HH11	1.14	1.09
1:A:607:VAL:HG23	1:A:608:GLU:N	1.65	1.08
1:B:32:GLY:H	1:B:54:LEU:HD22	1.16	1.08
1:A:346:LEU:CD2	1:A:408:GLN:HG2	1.83	1.08
1:A:470:LEU:HB2	1:A:518:VAL:CG2	1.83	1.08
1:B:313:TRP:CZ3	1:B:413:LEU:HD13	1.87	1.08
1:A:351:GLU:OE2	1:A:380:SER:HB2	1.53	1.07
1:B:537:ARG:HE	1:B:558:ASN:ND2	1.51	1.07
1:A:22:ARG:O	1:A:23:LEU:HD23	1.55	1.07
1:A:371:LEU:HD13	1:A:372:ALA:H	1.11	1.07
1:B:316:SER:OG	1:B:317:LEU:HG	1.52	1.06
1:A:185:GLY:O	1:A:216:ARG:HB3	1.53	1.06
1:A:95:VAL:HG11	1:A:127:ILE:HG21	1.28	1.06
1:B:36:VAL:HG12	1:B:37:ASP:H	1.21	1.06
1:C:375:ASN:HD21	1:C:393:ALA:HB3	1.11	1.05
1:B:146:LEU:HD12	1:B:211:ILE:HD13	1.34	1.05
1:B:187:ASN:H	1:B:187:ASN:ND2	1.53	1.05
1:C:375:ASN:HA	1:C:391:THR:OG1	1.55	1.05
1:B:142:ARG:HG2	1:B:142:ARG:NH1	1.72	1.04
1:C:375:ASN:ND2	1:C:393:ALA:HB3	1.70	1.04
1:B:523:ASN:HD21	1:B:525:LEU:HG	1.22	1.04
1:A:33:LEU:HD22	1:A:33:LEU:H	1.13	1.04
1:C:219:VAL:O	1:C:219:VAL:HG12	1.58	1.04
1:A:199:VAL:HG23	1:A:200:THR:H	1.17	1.04
1:B:230:LYS:O	1:B:231:ARG:HD3	1.56	1.04
1:A:84:ASN:HD21	1:A:122:THR:HB	1.24	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:N	1:B:54:LEU:HD22	1.70	1.03
1:B:344:ILE:HG23	1:B:371:LEU:HD23	1.40	1.03
1:A:272:SER:O	1:A:273:HIS:HB2	1.55	1.02
1:B:313:TRP:CE3	1:B:413:LEU:HD13	1.95	1.02
1:B:356:LEU:HD11	1:B:360:ARG:NE	1.74	1.02
1:C:350:GLY:HA2	1:C:381:LEU:HD12	1.36	1.02
1:A:247:ILE:N	1:A:247:ILE:HD12	1.71	1.02
1:A:84:ASN:ND2	1:A:122:THR:HB	1.74	1.02
1:A:296:GLN:HE21	1:A:296:GLN:CA	1.70	1.01
1:C:457:LEU:HD21	1:C:562:ILE:CD1	1.89	1.01
1:A:5:GLY:HA3	1:A:189:ILE:HG22	1.42	1.01
1:C:480:LEU:HD23	1:C:496:ALA:HB1	1.37	1.01
1:A:382:VAL:HG21	1:A:390:MET:CE	1.90	1.01
1:A:296:GLN:HA	1:A:296:GLN:HE21	1.18	1.01
1:B:507:LEU:HD12	1:B:510:ILE:HG12	1.37	1.01
1:A:532:ASN:H	1:A:532:ASN:ND2	1.49	1.01
1:A:250:HIS:HB3	1:A:596:ASP:OD2	1.59	1.01
1:C:27:GLY:O	1:C:29:ASP:N	1.94	1.01
1:C:7:ILE:HG21	1:C:214:ILE:HG22	1.40	1.01
1:A:296:GLN:HA	1:A:296:GLN:NE2	1.75	1.00
1:A:333:ARG:HG3	1:A:333:ARG:HH11	1.23	1.00
1:A:17:LEU:HD21	1:A:33:LEU:CD1	1.91	1.00
1:A:7:ILE:HD11	1:A:215:THR:HA	1.43	1.00
1:A:371:LEU:CD1	1:A:372:ALA:N	2.25	1.00
1:B:46:ARG:O	1:B:47:ARG:HG2	1.60	0.99
1:A:103:ASN:ND2	1:A:153:ARG:H	1.58	0.99
1:B:537:ARG:NE	1:B:558:ASN:HD21	1.58	0.99
1:B:587:VAL:HA	1:B:590:ILE:CD1	1.93	0.99
1:C:224:LYS:CD	1:C:225:THR:HG23	1.91	0.99
1:A:71:HIS:ND1	1:A:86:HIS:HB2	1.77	0.99
1:A:193:GLN:HE21	1:A:205:PHE:HZ	1.09	0.99
1:B:142:ARG:HD3	1:B:213:GLU:OE1	1.59	0.98
1:C:373:ILE:HD13	1:C:411:VAL:HG12	1.44	0.98
1:B:559:MET:CE	1:B:561:ILE:HD11	1.92	0.98
1:C:457:LEU:HD21	1:C:562:ILE:HD11	0.99	0.98
1:C:159:VAL:HG22	1:C:171:ALA:HB1	1.44	0.98
1:A:247:ILE:CD1	1:A:247:ILE:H	1.73	0.98
1:B:122:THR:O	1:B:124:THR:N	1.94	0.98
1:C:565:PRO:CG	1:C:575:PHE:HZ	1.77	0.98
1:A:388:ALA:O	1:A:389:LEU:HD12	1.64	0.98
1:C:570:VAL:HG13	1:C:571:ILE:H	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:TYR:CE1	1:A:599:ARG:HD3	1.98	0.98
1:A:111:LEU:O	1:A:113:ALA:N	1.97	0.98
1:B:179:VAL:HG23	1:B:205:PHE:HA	1.45	0.97
1:C:18:GLU:HA	1:C:21:ARG:HH11	1.26	0.97
1:A:180:ILE:HD11	1:A:214:ILE:HD11	1.43	0.97
1:C:42:MET:HE3	1:C:44:ARG:HE	1.24	0.97
1:C:79:GLU:O	1:C:81:SER:N	1.97	0.97
1:A:356:LEU:HD21	1:A:360:ARG:NH2	1.80	0.96
1:A:371:LEU:HD13	1:A:372:ALA:N	1.78	0.96
1:C:192:ASP:OD2	1:C:194:LEU:HD22	1.66	0.95
1:B:559:MET:HE3	1:B:561:ILE:HD11	1.45	0.95
1:B:34:ALA:HB2	1:B:87:PRO:HG2	1.47	0.95
1:A:95:VAL:HG11	1:A:127:ILE:CG2	1.96	0.95
1:C:146:LEU:HD11	1:C:226:GLY:HA2	1.45	0.95
1:A:189:ILE:HD12	1:A:190:ALA:H	1.32	0.95
1:C:224:LYS:HD3	1:C:225:THR:HG23	1.46	0.94
1:A:421:LYS:HE2	1:A:430:GLU:OE1	1.66	0.94
1:A:103:ASN:HD21	1:A:153:ARG:N	1.64	0.94
1:C:170:LEU:HD22	1:C:171:ALA:H	1.32	0.94
1:A:382:VAL:HG21	1:A:390:MET:HE1	1.44	0.94
1:B:259:GLN:O	1:B:262:ALA:HB3	1.68	0.94
1:A:356:LEU:HD21	1:A:360:ARG:HH21	1.29	0.94
1:B:413:LEU:HD23	1:B:437:LEU:HD21	1.48	0.94
1:A:281:LEU:HD22	1:A:387:LEU:HD12	1.50	0.94
1:A:267:LEU:HD23	1:A:414:MET:HE1	1.50	0.94
1:A:532:ASN:HD22	1:A:532:ASN:N	1.63	0.94
1:C:440:LEU:HD13	1:C:571:ILE:HD12	1.48	0.93
1:B:289:LEU:O	1:B:292:VAL:HG23	1.68	0.93
1:C:111:LEU:HD13	1:C:116:TYR:CD2	2.03	0.93
1:A:532:ASN:H	1:A:532:ASN:HD22	1.01	0.93
1:A:607:VAL:CG2	1:A:608:GLU:H	1.81	0.93
1:A:251:TYR:O	1:A:255:GLU:HG3	1.69	0.93
1:C:451:ASP:OD2	1:C:582:LEU:HD13	1.69	0.93
1:B:146:LEU:CD1	1:B:211:ILE:HD13	1.98	0.93
1:A:105:GLU:HB3	1:A:106:PRO:HD3	1.49	0.93
1:B:24:GLU:HG2	1:B:597:GLN:NE2	1.83	0.92
1:A:603:LYS:HG3	1:A:604:SER:H	1.32	0.92
1:B:572:ALA:N	1:B:573:PRO:HD2	1.84	0.92
1:A:248:TYR:CD2	1:A:254:LYS:HB2	2.04	0.92
1:B:332:TYR:CE1	1:C:528:LYS:NZ	2.37	0.92
1:C:32:GLY:HA3	1:C:86:HIS:O	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ILE:HD13	1:C:411:VAL:CG1	1.99	0.92
1:C:423:LYS:HD3	1:C:425:LEU:HG	1.51	0.92
1:B:371:LEU:HG	1:B:372:ALA:H	1.34	0.92
1:B:546:PHE:CE2	1:B:562:ILE:HD13	2.05	0.92
1:C:570:VAL:HG13	1:C:571:ILE:N	1.85	0.91
1:B:447:MET:HE3	1:B:564:MET:SD	2.11	0.91
1:B:63:LEU:HD12	1:B:63:LEU:H	1.32	0.91
1:A:36:VAL:CG1	1:A:42:MET:HA	1.99	0.91
1:C:476:TYR:HB3	1:C:477:PRO:HD3	1.49	0.91
1:C:485:LYS:HA	1:C:485:LYS:HE3	1.49	0.91
1:C:31:ALA:CB	1:C:51:VAL:HG22	1.99	0.91
1:A:146:LEU:HD21	1:A:226:GLY:HA2	1.49	0.91
1:B:186:GLU:O	1:B:186:GLU:CG	2.17	0.91
1:B:587:VAL:CA	1:B:590:ILE:HD12	2.00	0.91
1:A:84:ASN:HB2	1:A:121:GLU:OE1	1.70	0.90
1:A:33:LEU:O	1:A:33:LEU:HD23	1.71	0.90
1:C:4:VAL:HG12	1:C:4:VAL:O	1.70	0.90
1:C:182:LEU:HD11	1:C:204:ILE:CD1	2.00	0.90
1:C:252:MET:SD	1:C:400:ALA:CB	2.58	0.90
1:B:501:GLU:HG3	1:C:326:ILE:HD12	1.51	0.90
1:A:376:VAL:HG12	1:A:379:SER:OG	1.71	0.90
1:B:344:ILE:HD13	1:B:371:LEU:CD2	2.02	0.90
1:C:399:VAL:CG2	1:C:596:ASP:O	2.20	0.89
1:A:371:LEU:CD1	1:A:372:ALA:H	1.84	0.89
1:C:255:GLU:O	1:C:403:LYS:HB3	1.73	0.89
1:B:142:ARG:HH12	1:B:146:LEU:HD22	1.36	0.89
1:C:199:VAL:HG23	1:C:200:THR:HG22	1.52	0.89
1:B:286:ASP:OD2	1:B:422:LEU:HD21	1.72	0.89
1:C:524:GLU:H	1:C:524:GLU:CD	1.74	0.89
1:C:379:SER:HB2	1:C:382:VAL:HG23	1.54	0.89
1:B:33:LEU:CD2	1:B:33:LEU:H	1.85	0.89
1:A:470:LEU:HB2	1:A:518:VAL:HG22	1.55	0.89
1:B:447:MET:CE	1:B:564:MET:SD	2.60	0.89
1:B:162:ASP:O	1:B:164:ARG:N	2.06	0.88
1:B:310:SER:CB	1:B:412:LEU:HD13	2.03	0.88
1:B:502:LEU:CA	1:B:506:PRO:HG2	2.03	0.88
1:B:214:ILE:HG22	1:B:215:THR:N	1.85	0.88
1:A:33:LEU:N	1:A:33:LEU:HD22	1.82	0.88
1:A:202:ARG:HG2	1:A:202:ARG:HH11	1.38	0.88
1:A:5:GLY:CA	1:A:189:ILE:HG22	2.04	0.88
1:C:98:ASN:ND2	1:C:176:SER:OG	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD11	1:C:164:ARG:HH22	1.37	0.87
1:B:142:ARG:NH1	1:B:146:LEU:HD22	1.89	0.87
1:A:304:TYR:CG	1:A:326:ILE:HD11	2.09	0.87
1:C:440:LEU:CB	1:C:441:PRO:HD3	2.04	0.87
1:C:499:ALA:O	1:C:502:LEU:HD13	1.74	0.87
1:B:396:GLU:OE1	1:B:401:SER:OG	1.91	0.87
1:B:293:GLU:O	1:B:321:PRO:HG2	1.74	0.87
1:B:297:ILE:HB	1:B:324:VAL:HA	1.56	0.87
1:B:187:ASN:N	1:B:187:ASN:ND2	2.09	0.87
1:A:423:LYS:O	1:A:425:LEU:N	2.08	0.87
1:C:130:LEU:O	1:C:130:LEU:HD23	1.75	0.87
1:A:553:PHE:HD2	1:A:559:MET:CE	1.88	0.87
1:B:528:LYS:HD2	1:B:528:LYS:H	1.40	0.86
1:B:48:LEU:CD2	1:B:81:SER:HB2	2.03	0.86
1:C:304:TYR:CE2	1:C:308:MET:HE2	2.10	0.86
1:A:567:VAL:HG22	1:A:575:PHE:CE2	2.09	0.86
1:C:578:VAL:HB	1:C:579:PRO:HD3	1.56	0.86
1:C:413:LEU:O	1:C:416:VAL:HB	1.74	0.86
1:B:22:ARG:HD2	1:B:195:ALA:HA	1.58	0.86
1:B:142:ARG:HH12	1:B:146:LEU:CD2	1.87	0.86
1:A:110:GLU:O	1:A:113:ALA:HB3	1.75	0.86
1:B:523:ASN:ND2	1:B:525:LEU:N	2.22	0.86
1:A:193:GLN:NE2	1:A:205:PHE:CZ	2.38	0.86
1:B:90:SER:O	1:B:91:GLU:HB2	1.75	0.86
1:C:480:LEU:HD23	1:C:496:ALA:CB	2.05	0.86
1:A:276:VAL:CG2	1:A:414:MET:HG2	2.05	0.85
1:C:485:LYS:CA	1:C:485:LYS:HE3	2.06	0.85
1:C:499:ALA:HB1	1:C:532:ASN:OD1	1.75	0.85
1:B:142:ARG:HH11	1:B:142:ARG:CG	1.83	0.85
1:C:294:HIS:NE2	1:C:338:ARG:HD2	1.91	0.85
1:C:373:ILE:CD1	1:C:411:VAL:HG12	2.05	0.85
1:C:343:MET:C	1:C:344:ILE:HD12	1.97	0.85
1:A:207:GLU:HG3	1:A:231:ARG:NH1	1.92	0.85
1:A:105:GLU:OE2	1:A:109:GLU:HG2	1.77	0.85
1:A:510:ILE:HD13	1:A:536:VAL:HB	1.59	0.85
1:A:267:LEU:CD2	1:A:414:MET:CE	2.55	0.85
1:B:186:GLU:HG3	1:B:186:GLU:O	1.74	0.85
1:B:221:ILE:H	1:B:221:ILE:HD12	1.41	0.85
1:B:229:VAL:HG21	1:B:231:ARG:HE	1.39	0.84
1:C:221:ILE:O	1:C:228:GLU:HG3	1.77	0.84
1:C:111:LEU:HB3	1:C:116:TYR:HD2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:SER:HA	1:C:49:GLY:O	1.78	0.84
1:B:313:TRP:CE3	1:B:413:LEU:CD1	2.59	0.84
1:B:130:LEU:HD23	1:B:152:LEU:HD21	1.57	0.84
1:A:567:VAL:HG12	1:A:568:GLU:H	1.41	0.84
1:B:469:PHE:CE1	1:B:517:ILE:HD13	2.11	0.84
1:C:440:LEU:HB3	1:C:441:PRO:CD	2.05	0.84
1:B:600:ASN:CG	1:C:539:ARG:HG3	1.97	0.84
1:B:355:THR:O	1:B:358:GLY:N	2.10	0.84
1:A:279:SER:O	1:A:281:LEU:N	2.10	0.84
1:B:142:ARG:HG2	1:B:142:ARG:HH11	1.34	0.84
1:C:4:VAL:O	1:C:16:LEU:HD22	1.77	0.84
1:A:128:ALA:O	1:A:130:LEU:N	2.10	0.84
1:A:455:GLU:HG3	1:A:586:HIS:CE1	2.10	0.84
1:B:25:TYR:CE2	1:B:26:ARG:HG3	2.12	0.84
1:A:376:VAL:HG12	1:A:376:VAL:O	1.77	0.84
1:C:149:ILE:H	1:C:150:PRO:HD2	1.42	0.84
1:A:510:ILE:CD1	1:A:536:VAL:HB	2.08	0.84
1:C:230:LYS:O	1:C:231:ARG:HD3	1.76	0.84
1:B:520:ALA:HB2	1:B:529:LEU:CD2	2.07	0.84
1:A:346:LEU:HD22	1:A:408:GLN:HG2	1.58	0.84
1:B:458:ALA:O	1:B:460:ASP:N	2.11	0.84
1:B:484:LEU:O	1:B:485:LYS:CG	2.21	0.83
1:A:304:TYR:CG	1:A:326:ILE:CD1	2.60	0.83
1:B:33:LEU:HD23	1:B:33:LEU:N	1.91	0.83
1:B:147:ARG:O	1:B:150:PRO:HD2	1.78	0.83
1:C:278:LEU:HD12	1:C:418:LYS:HG2	1.58	0.83
1:A:140:THR:HG23	1:A:143:GLU:OE1	1.78	0.83
1:B:310:SER:OG	1:B:412:LEU:HD13	1.79	0.83
1:A:25:TYR:HE1	1:A:26:ARG:HG2	1.40	0.83
1:A:398:GLY:O	1:A:603:LYS:HD2	1.78	0.83
1:C:54:LEU:HD12	1:C:54:LEU:O	1.77	0.83
1:C:491:TYR:CZ	1:C:599:ARG:HD3	2.13	0.83
1:C:325:GLU:OE1	1:C:330:PHE:HB2	1.78	0.83
1:A:110:GLU:O	1:A:111:LEU:O	1.97	0.83
1:C:36:VAL:CG1	1:C:166:PRO:HB3	2.09	0.83
1:A:567:VAL:HG12	1:A:568:GLU:N	1.94	0.83
1:A:36:VAL:HG13	1:A:42:MET:HA	1.59	0.83
1:A:304:TYR:CD2	1:A:326:ILE:HD11	2.13	0.82
1:A:142:ARG:HD2	1:A:222:PHE:CZ	2.15	0.82
1:A:383:ARG:HH11	1:A:383:ARG:CG	1.92	0.82
1:A:25:TYR:CD1	1:A:26:ARG:N	2.48	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:HIS:HB3	1:B:341:SER:OG	1.80	0.82
1:A:559:MET:CE	1:A:561:ILE:HD11	2.09	0.82
1:A:199:VAL:HG23	1:A:200:THR:N	1.94	0.82
1:A:263:ILE:HD11	1:A:406:THR:CG2	2.10	0.81
1:B:310:SER:HB2	1:B:412:LEU:HD13	1.61	0.81
1:A:386:ASP:O	1:A:387:LEU:HD22	1.80	0.81
1:B:523:ASN:HD22	1:B:524:GLU:N	1.78	0.81
1:A:164:ARG:O	1:A:165:HIS:ND1	2.13	0.81
1:B:93:ILE:HG22	1:B:93:ILE:O	1.79	0.81
1:A:371:LEU:HD12	1:A:372:ALA:N	1.96	0.81
1:C:20:LEU:HB3	1:C:51:VAL:HG21	1.63	0.81
1:B:468:LEU:CD1	1:B:497:TYR:HD2	1.93	0.81
1:A:266:THR:HG23	1:A:391:THR:O	1.81	0.81
1:B:173:ARG:HG2	1:B:208:GLU:HA	1.63	0.81
1:A:294:HIS:CE1	1:A:338:ARG:HG2	2.16	0.81
1:B:396:GLU:OE2	1:B:401:SER:HA	1.81	0.81
1:C:149:ILE:N	1:C:150:PRO:HD2	1.93	0.81
1:C:506:PRO:C	1:C:508:ALA:H	1.83	0.81
1:B:297:ILE:HD12	1:B:324:VAL:HG22	1.63	0.81
1:A:529:LEU:HA	1:A:532:ASN:HD21	1.46	0.81
1:B:545:VAL:HB	1:B:561:ILE:HD13	1.63	0.80
1:C:305:ASN:ND2	1:C:481:GLU:OE1	2.13	0.80
1:A:21:ARG:HG2	1:A:51:VAL:HG11	1.61	0.80
1:A:17:LEU:HD21	1:A:33:LEU:HD13	1.61	0.80
1:B:122:THR:C	1:B:124:THR:H	1.82	0.80
1:B:1:CYS:N	1:B:26:ARG:O	2.15	0.80
1:A:7:ILE:HD11	1:A:215:THR:CA	2.11	0.80
1:B:214:ILE:O	1:B:215:THR:HG22	1.81	0.80
1:B:371:LEU:HG	1:B:372:ALA:N	1.91	0.80
1:B:600:ASN:ND2	1:C:539:ARG:HG3	1.96	0.80
1:B:126:VAL:HG13	1:B:127:ILE:N	1.97	0.80
1:C:353:ALA:HB1	1:C:608:GLU:OE1	1.81	0.80
1:B:118:PHE:O	1:B:120:SER:N	2.14	0.80
1:B:140:THR:HG23	1:B:143:GLU:OE1	1.81	0.80
1:A:331:ARG:HD3	1:A:332:TYR:CE2	2.16	0.80
1:C:82:GLU:HG3	1:C:83:VAL:H	1.47	0.80
1:A:84:ASN:ND2	1:A:121:GLU:O	2.13	0.80
1:A:607:VAL:CG2	1:A:608:GLU:N	2.38	0.80
1:B:476:TYR:HB3	1:B:477:PRO:HD3	1.63	0.80
1:A:121:GLU:O	1:A:121:GLU:CG	2.24	0.80
1:C:69:ILE:HD11	1:C:94:VAL:HG12	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:ARG:HE	1:B:558:ASN:HD21	0.81	0.80
1:C:36:VAL:HG12	1:C:166:PRO:CB	2.12	0.80
1:B:485:LYS:O	1:B:488:GLU:N	2.14	0.80
1:A:599:ARG:HG3	1:A:600:ASN:OD1	1.82	0.80
1:C:90:SER:HA	1:C:129:HIS:CE1	2.17	0.80
1:A:149:ILE:HB	1:A:150:PRO:HD3	1.63	0.80
1:A:308:MET:O	1:A:310:SER:N	2.16	0.79
1:A:481:GLU:OE1	1:A:481:GLU:HA	1.80	0.79
1:B:90:SER:HB2	1:B:129:HIS:ND1	1.97	0.79
1:A:356:LEU:HD12	1:A:381:LEU:HD23	1.64	0.79
1:B:270:ARG:HD3	1:B:414:MET:CE	2.12	0.79
1:A:182:LEU:HD11	1:A:204:ILE:HD11	1.64	0.79
1:B:344:ILE:HD13	1:B:371:LEU:HD23	1.62	0.79
1:A:447:MET:CE	1:A:564:MET:SD	2.70	0.79
1:A:396:GLU:HG2	1:A:603:LYS:HZ2	1.47	0.79
1:C:159:VAL:HG22	1:C:171:ALA:CB	2.11	0.79
1:A:481:GLU:OE2	1:A:485:LYS:HE2	1.83	0.79
1:A:276:VAL:HG23	1:A:414:MET:HG2	1.63	0.79
1:C:371:LEU:HA	1:C:387:LEU:HB2	1.64	0.79
1:B:433:ILE:HG13	1:B:570:VAL:HG21	1.62	0.79
1:B:276:VAL:HG13	1:B:434:VAL:HG22	1.64	0.79
1:A:382:VAL:O	1:A:382:VAL:HG12	1.82	0.79
1:C:35:VAL:HA	1:C:67:THR:O	1.81	0.79
1:B:97:HIS:HB2	1:B:158:THR:HB	1.64	0.79
1:A:223:ASP:OD1	1:A:223:ASP:C	2.21	0.79
1:B:523:ASN:HD21	1:B:525:LEU:CG	1.96	0.79
1:B:413:LEU:HA	1:B:416:VAL:HG23	1.65	0.78
1:C:447:MET:HE1	1:C:579:PRO:HD3	1.64	0.78
1:A:470:LEU:HB2	1:A:518:VAL:HG23	1.64	0.78
1:B:229:VAL:CG2	1:B:231:ARG:HE	1.95	0.78
1:C:371:LEU:HD23	1:C:372:ALA:N	1.97	0.78
1:C:359:LEU:HD23	1:C:381:LEU:HD23	1.64	0.78
1:A:410:THR:HG23	1:A:437:LEU:CD2	2.12	0.78
1:C:532:ASN:H	1:C:532:ASN:HD22	1.28	0.78
1:A:536:VAL:CG2	1:A:543:LEU:HD11	2.12	0.78
1:A:333:ARG:NH1	1:A:333:ARG:HG3	1.92	0.78
1:A:447:MET:HE1	1:A:564:MET:SD	2.23	0.78
1:B:483:ALA:O	1:B:487:LYS:HB3	1.83	0.78
1:A:28:TYR:CZ	1:A:597:GLN:HB3	2.18	0.78
1:C:234:ILE:CD1	1:C:236:SER:H	1.95	0.78
1:B:169:LEU:O	1:B:170:LEU:HD22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:GLU:OE2	1:C:485:LYS:NZ	2.15	0.78
1:A:399:VAL:HG23	1:A:596:ASP:O	1.83	0.78
1:B:520:ALA:HB2	1:B:529:LEU:HD21	1.64	0.78
1:A:42:MET:HG3	1:A:43:THR:N	1.99	0.78
1:A:440:LEU:HB3	1:A:441:PRO:HD3	1.66	0.78
1:C:517:ILE:HD12	1:C:544:TYR:HB2	1.66	0.78
1:A:533:ILE:HG23	1:A:543:LEU:CD2	2.14	0.78
1:B:440:LEU:HB3	1:B:441:PRO:HD3	1.65	0.78
1:C:263:ILE:HG21	1:C:440:LEU:HD23	1.66	0.78
1:C:502:LEU:HB3	1:C:507:LEU:HB2	1.66	0.78
1:C:578:VAL:HB	1:C:579:PRO:CD	2.13	0.78
1:C:182:LEU:HD11	1:C:204:ILE:HD11	1.64	0.78
1:B:302:THR:OG1	1:B:481:GLU:OE2	2.00	0.78
1:B:470:LEU:HB2	1:B:518:VAL:HG22	1.63	0.77
1:B:221:ILE:HG22	1:B:222:PHE:N	1.99	0.77
1:C:486:LEU:HG	1:C:486:LEU:O	1.84	0.77
1:B:469:PHE:C	1:B:470:LEU:HD23	2.05	0.77
1:A:383:ARG:NH1	1:A:383:ARG:HG2	1.95	0.77
1:B:468:LEU:HD23	1:B:516:VAL:HG22	1.65	0.77
1:B:80:PRO:O	1:B:84:ASN:OD1	2.03	0.77
1:B:179:VAL:HG23	1:B:205:PHE:CA	2.13	0.77
1:B:267:LEU:HA	1:B:414:MET:SD	2.25	0.77
1:B:22:ARG:HG3	1:B:22:ARG:NH1	1.99	0.77
1:B:230:LYS:O	1:B:231:ARG:CD	2.32	0.77
1:A:279:SER:C	1:A:281:LEU:H	1.86	0.77
1:C:507:LEU:O	1:C:507:LEU:HG	1.83	0.77
1:A:146:LEU:CD2	1:A:226:GLY:HA2	2.13	0.77
1:C:193:GLN:O	1:C:197:LEU:HG	1.84	0.77
1:C:294:HIS:CD2	1:C:338:ARG:HD2	2.18	0.77
1:A:95:VAL:HG21	1:A:127:ILE:HG22	1.65	0.77
1:B:36:VAL:HG12	1:B:37:ASP:N	1.99	0.77
1:B:256:ILE:O	1:B:259:GLN:HB2	1.85	0.77
1:C:281:LEU:HD13	1:C:387:LEU:HD22	1.66	0.77
1:A:5:GLY:HA3	1:A:189:ILE:CG2	2.15	0.77
1:A:25:TYR:CE1	1:A:26:ARG:HG2	2.21	0.76
1:B:594:ASP:HB3	1:B:597:GLN:O	1.85	0.76
1:B:393:ALA:O	1:B:403:LYS:NZ	2.15	0.76
1:C:42:MET:CE	1:C:44:ARG:HB2	2.14	0.76
1:A:207:GLU:HG3	1:A:231:ARG:CZ	2.15	0.76
1:B:329:GLU:OE2	1:C:472:ARG:HG3	1.84	0.76
1:A:491:TYR:CE1	1:A:599:ARG:CD	2.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:HG23	1:A:437:LEU:HD22	1.66	0.76
1:C:281:LEU:HD21	1:C:389:LEU:HD21	1.67	0.76
1:B:517:ILE:HG23	1:B:546:PHE:HE1	1.51	0.76
1:A:314:PHE:O	1:A:318:ALA:HB3	1.85	0.76
1:B:501:GLU:CG	1:C:326:ILE:HD12	2.15	0.76
1:A:247:ILE:N	1:A:247:ILE:CD1	2.39	0.76
1:B:140:THR:O	1:B:143:GLU:N	2.19	0.76
1:A:8:ALA:HB2	1:A:186:GLU:HB2	1.67	0.76
1:A:173:ARG:HD2	1:A:177:PRO:HA	1.68	0.76
1:A:20:LEU:HB3	1:A:51:VAL:HG21	1.68	0.76
1:B:21:ARG:HG3	1:B:21:ARG:NH1	1.88	0.76
1:A:265:ASN:O	1:A:268:THR:HB	1.86	0.76
1:A:476:TYR:HB3	1:A:477:PRO:HD3	1.68	0.76
1:B:15:ILE:HG21	1:B:188:PHE:CE2	2.21	0.76
1:A:548:ASP:OD1	1:A:550:ASP:N	2.18	0.76
1:A:33:LEU:C	1:A:33:LEU:HD23	2.03	0.75
1:C:251:TYR:CD1	1:C:397:ILE:HG21	2.21	0.75
1:C:299:ALA:HB1	1:C:303:SER:CB	2.17	0.75
1:C:380:SER:O	1:C:383:ARG:HB2	1.87	0.75
1:A:199:VAL:CG2	1:A:200:THR:H	1.98	0.75
1:A:524:GLU:HG2	1:A:525:LEU:HD23	1.68	0.75
1:C:141:LEU:CD2	1:C:168:THR:OG1	2.34	0.75
1:B:447:MET:CE	1:B:564:MET:CE	2.64	0.75
1:C:263:ILE:O	1:C:266:THR:HB	1.86	0.75
1:A:192:ASP:OD2	1:A:194:LEU:CB	2.34	0.75
1:C:216:ARG:HH21	1:C:217:ARG:NH2	1.83	0.75
1:C:506:PRO:O	1:C:508:ALA:N	2.20	0.75
1:A:522:ASN:O	1:A:522:ASN:CG	2.18	0.75
1:C:61:HIS:H	1:C:62:PRO:HD3	1.51	0.75
1:A:96:VAL:HG23	1:A:96:VAL:O	1.85	0.75
1:B:200:THR:HG23	1:B:203:PHE:HE1	1.51	0.75
1:C:31:ALA:HB2	1:C:51:VAL:HG22	1.68	0.75
1:A:477:PRO:HA	1:A:480:LEU:HB2	1.68	0.75
1:B:516:VAL:HB	1:B:543:LEU:HD23	1.68	0.75
1:C:409:LEU:HA	1:C:412:LEU:HD12	1.66	0.75
1:C:238:LEU:H	1:C:238:LEU:HD12	1.52	0.75
1:B:52:GLN:HA	1:B:52:GLN:OE1	1.84	0.75
1:B:521:PRO:O	1:B:526:LEU:HD22	1.86	0.75
1:C:404:ALA:O	1:C:408:GLN:HG3	1.86	0.75
1:B:3:ILE:HD11	1:B:98:ASN:N	2.01	0.75
1:B:234:ILE:HD12	1:B:235:GLU:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:HD13	1:B:387:LEU:HD13	0.84	0.74
1:B:297:ILE:HD12	1:B:324:VAL:CG2	2.17	0.74
1:A:267:LEU:CD2	1:A:414:MET:HE1	2.17	0.74
1:B:391:THR:O	1:B:392:ASN:C	2.26	0.74
1:B:293:GLU:O	1:B:321:PRO:CG	2.34	0.74
1:C:60:GLU:O	1:C:61:HIS:HB2	1.87	0.74
1:A:196:LEU:C	1:A:198:PRO:HD2	2.08	0.74
1:B:510:ILE:HD13	1:B:510:ILE:N	1.99	0.74
1:A:21:ARG:HG2	1:A:51:VAL:CG1	2.18	0.74
1:B:305:ASN:O	1:B:306:SER:C	2.26	0.74
1:A:32:GLY:HA2	1:A:54:LEU:HD11	1.69	0.74
1:A:308:MET:O	1:A:309:VAL:C	2.23	0.74
1:B:559:MET:O	1:B:559:MET:CG	2.35	0.74
1:C:399:VAL:HG13	1:C:602:ALA:O	1.86	0.74
1:B:182:LEU:HD11	1:B:204:ILE:HD11	1.68	0.74
1:A:553:PHE:HD2	1:A:559:MET:HE1	1.50	0.74
1:B:169:LEU:O	1:B:170:LEU:CD2	2.35	0.74
1:C:543:LEU:HD13	1:C:559:MET:CE	2.18	0.73
1:C:346:LEU:HD22	1:C:408:GLN:OE1	1.88	0.73
1:A:255:GLU:OE1	1:A:397:ILE:N	2.20	0.73
1:B:221:ILE:H	1:B:221:ILE:CD1	1.99	0.73
1:A:606:THR:O	1:A:607:VAL:O	2.05	0.73
1:A:304:TYR:CZ	1:A:326:ILE:HD13	2.22	0.73
1:A:536:VAL:HG23	1:A:543:LEU:HD11	1.71	0.73
1:C:145:VAL:HG11	1:C:170:LEU:HD11	1.71	0.73
1:A:142:ARG:HD2	1:A:222:PHE:CE1	2.22	0.73
1:C:351:GLU:HG2	1:C:380:SER:HB2	1.69	0.73
1:A:36:VAL:HG12	1:A:41:HIS:O	1.89	0.73
1:A:391:THR:HG22	1:A:407:THR:HB	1.69	0.73
1:C:17:LEU:HD21	1:C:33:LEU:CD1	2.17	0.73
1:B:21:ARG:CG	1:B:21:ARG:HH11	1.94	0.73
1:C:141:LEU:HD22	1:C:168:THR:OG1	1.88	0.73
1:B:27:GLY:HA2	1:B:74:TRP:HB2	1.70	0.73
1:C:413:LEU:CD2	1:C:571:ILE:HG22	2.18	0.73
1:C:399:VAL:HG21	1:C:598:PRO:HD2	1.70	0.73
1:B:88:HIS:HB2	1:B:124:THR:CG2	2.19	0.73
1:B:146:LEU:HD12	1:B:211:ILE:CD1	2.16	0.73
1:A:103:ASN:HD21	1:A:153:ARG:H	0.81	0.73
1:A:100:ILE:CD1	1:A:607:VAL:HA	2.19	0.73
1:A:372:ALA:HB2	1:A:385:SER:OG	1.89	0.73
1:C:599:ARG:HG3	1:C:600:ASN:ND2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:NE2	1:C:97:HIS:O	2.21	0.73
1:B:214:ILE:CG2	1:B:215:THR:N	2.52	0.73
1:A:267:LEU:HD23	1:A:414:MET:CE	2.19	0.72
1:A:165:HIS:HB3	1:A:167:ASP:OD1	1.88	0.72
1:C:386:ASP:O	1:C:387:LEU:HG	1.89	0.72
1:A:546:PHE:CE1	1:A:562:ILE:HD12	2.23	0.72
1:A:373:ILE:HD13	1:A:411:VAL:CG1	2.20	0.72
1:A:52:GLN:HA	1:A:52:GLN:HE21	1.52	0.72
1:A:307:GLY:O	1:A:310:SER:OG	2.06	0.72
1:B:400:ALA:HA	2:B:701:G6Q:C1	2.19	0.72
1:A:136:LYS:HB2	1:A:137:GLN:HE21	1.53	0.72
1:A:304:TYR:CZ	1:A:326:ILE:CD1	2.72	0.72
1:C:263:ILE:HD12	1:C:440:LEU:HD21	1.71	0.72
1:A:399:VAL:HA	1:A:603:LYS:HB2	1.70	0.72
1:A:165:HIS:O	1:A:167:ASP:N	2.20	0.72
1:C:7:ILE:HD11	1:C:167:ASP:O	1.89	0.72
1:C:533:ILE:O	1:C:536:VAL:HG22	1.90	0.72
1:C:88:HIS:HE1	1:C:122:THR:HG21	1.55	0.72
1:C:17:LEU:HD21	1:C:33:LEU:HD13	1.70	0.72
1:B:276:VAL:HG21	1:B:417:ALA:HB3	1.72	0.72
1:B:457:LEU:CD2	1:B:562:ILE:HD11	2.20	0.72
1:B:446:GLN:O	1:B:449:SER:OG	2.07	0.72
1:B:301:GLY:O	1:B:304:TYR:HB3	1.89	0.72
1:C:20:LEU:HB2	1:C:51:VAL:HG11	1.70	0.72
1:A:331:ARG:HG3	1:A:332:TYR:N	2.05	0.72
1:C:566:HIS:O	1:C:567:VAL:HG13	1.89	0.72
1:B:24:GLU:HG2	1:B:597:GLN:HE21	1.53	0.71
1:A:376:VAL:HG12	1:A:379:SER:HG	1.54	0.71
1:B:529:LEU:HG	1:B:533:ILE:CD1	2.15	0.71
1:A:267:LEU:HD22	1:A:414:MET:CE	2.20	0.71
1:B:415:LEU:HD11	1:B:419:LEU:HD11	1.69	0.71
1:C:309:VAL:HG22	1:C:477:PRO:HB2	1.72	0.71
1:C:31:ALA:O	1:C:54:LEU:CD2	2.39	0.71
1:B:214:ILE:C	1:B:215:THR:HG22	2.10	0.71
1:B:248:TYR:CE2	1:B:254:LYS:HG3	2.26	0.71
1:B:294:HIS:CG	1:B:341:SER:HG	2.08	0.71
1:B:45:LEU:HD11	1:B:57:ALA:HB1	1.73	0.71
1:B:294:HIS:CG	1:B:341:SER:OG	2.43	0.71
1:A:25:TYR:HD1	1:A:26:ARG:N	1.89	0.71
1:A:202:ARG:CG	1:A:202:ARG:HH11	2.02	0.71
1:B:276:VAL:HG21	1:B:417:ALA:CB	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ASN:ND2	1:B:375:ASN:O	2.24	0.71
1:B:469:PHE:O	1:B:470:LEU:HD23	1.90	0.71
1:B:447:MET:HE1	1:B:564:MET:CE	2.20	0.71
1:A:245:LYS:HG2	1:A:251:TYR:CE1	2.25	0.71
1:C:98:ASN:O	1:C:156:TYR:HA	1.91	0.71
1:C:180:ILE:CD1	1:C:206:LEU:HD21	2.21	0.71
1:A:20:LEU:HD21	1:A:71:HIS:H	1.54	0.71
1:B:537:ARG:NE	1:B:558:ASN:ND2	2.27	0.71
1:A:525:LEU:HD23	1:A:525:LEU:N	2.05	0.71
1:A:294:HIS:ND1	1:A:338:ARG:HG2	2.05	0.71
1:B:559:MET:O	1:B:559:MET:HG2	1.91	0.71
1:C:447:MET:CE	1:C:579:PRO:HD3	2.21	0.71
1:B:63:LEU:HD12	1:B:63:LEU:N	2.06	0.71
1:B:583:LEU:O	1:B:587:VAL:HG23	1.91	0.70
1:A:70:ALA:O	1:A:71:HIS:HB2	1.91	0.70
1:B:263:ILE:HD12	1:B:444:ILE:CD1	2.21	0.70
1:A:522:ASN:OD1	1:A:522:ASN:O	2.09	0.70
1:B:559:MET:HE2	1:B:561:ILE:HD11	1.72	0.70
1:A:20:LEU:HD21	1:A:71:HIS:N	2.05	0.70
1:B:254:LYS:O	1:B:258:GLU:HB2	1.90	0.70
1:B:344:ILE:HD13	1:B:371:LEU:HD22	1.71	0.70
1:B:523:ASN:HD22	1:B:523:ASN:C	1.94	0.70
1:B:526:LEU:HD12	1:B:526:LEU:O	1.91	0.70
1:A:401:SER:O	1:A:485:LYS:HE3	1.90	0.70
1:C:413:LEU:HD21	1:C:571:ILE:HG22	1.72	0.70
1:A:33:LEU:HA	1:A:70:ALA:HA	1.72	0.70
1:A:423:LYS:O	1:A:425:LEU:HD23	1.91	0.70
1:B:468:LEU:CD1	1:B:497:TYR:CD2	2.75	0.70
1:C:536:VAL:HG23	1:C:537:ARG:N	2.07	0.70
1:A:189:ILE:HD12	1:A:190:ALA:N	2.04	0.70
1:B:22:ARG:CD	1:B:194:LEU:O	2.33	0.70
1:A:333:ARG:NH1	1:A:333:ARG:CG	2.52	0.70
1:A:353:ALA:CB	1:A:608:GLU:HA	2.22	0.70
1:C:457:LEU:CD2	1:C:562:ILE:CD1	2.61	0.70
1:C:570:VAL:CG1	1:C:571:ILE:H	2.04	0.70
1:C:151:GLN:O	1:C:152:LEU:HD23	1.90	0.70
1:B:342:LEU:HD12	1:B:369:GLY:O	1.92	0.70
1:A:101:ILE:HD12	1:A:152:LEU:HD22	1.74	0.70
1:C:543:LEU:HD13	1:C:559:MET:HE2	1.74	0.70
1:A:33:LEU:N	1:A:33:LEU:CD2	2.52	0.70
1:C:79:GLU:C	1:C:81:SER:N	2.45	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:CB	1:A:186:GLU:HB3	2.22	0.70
1:A:7:ILE:HG12	1:A:7:ILE:O	1.90	0.70
1:B:475:GLN:HE21	1:B:519:VAL:CG2	2.04	0.69
1:A:95:VAL:CG1	1:A:127:ILE:HG21	2.16	0.69
1:C:36:VAL:HG12	1:C:166:PRO:HB3	1.71	0.69
1:C:251:TYR:CE1	1:C:397:ILE:HG21	2.27	0.69
1:C:403:LYS:O	1:C:407:THR:HG23	1.92	0.69
1:C:156:TYR:CE1	1:C:174:SER:HB3	2.27	0.69
1:C:104:HIS:O	1:C:108:ARG:HB2	1.92	0.69
1:A:146:LEU:HG	1:A:211:ILE:CD1	2.16	0.69
1:B:142:ARG:O	1:B:146:LEU:HB2	1.92	0.69
1:B:182:LEU:HD21	1:B:204:ILE:HD12	1.74	0.69
1:C:251:TYR:CG	1:C:397:ILE:HG21	2.27	0.69
1:A:105:GLU:H	1:A:106:PRO:HD2	1.55	0.69
1:C:482:GLY:HA3	1:C:580:LEU:HD13	1.73	0.69
1:A:304:TYR:CD1	1:A:326:ILE:HD11	2.17	0.69
1:C:553:PHE:HB3	1:C:561:ILE:CD1	2.23	0.69
1:B:126:VAL:HG13	1:B:127:ILE:H	1.55	0.69
1:B:25:TYR:CE2	1:B:26:ARG:CG	2.75	0.69
1:A:534:GLU:OE1	1:A:534:GLU:HA	1.93	0.69
1:B:289:LEU:O	1:B:292:VAL:CG2	2.40	0.69
1:A:14:GLU:O	1:A:14:GLU:HG2	1.90	0.69
1:B:223:ASP:OD2	1:B:225:THR:CG2	2.26	0.69
1:B:42:MET:CE	1:B:94:VAL:CG2	2.70	0.69
1:B:501:GLU:OE2	1:B:504:HIS:CD2	2.46	0.69
1:B:529:LEU:CG	1:B:533:ILE:HD11	2.17	0.69
1:C:356:LEU:CD1	1:C:380:SER:HB3	2.22	0.69
1:C:480:LEU:CD2	1:C:496:ALA:CB	2.71	0.69
1:B:164:ARG:O	1:B:165:HIS:HD2	1.76	0.69
1:C:327:ALA:O	1:C:329:GLU:N	2.23	0.69
1:C:487:LYS:O	1:C:489:ILE:N	2.26	0.69
1:A:239:GLN:O	1:A:240:TYR:C	2.31	0.69
1:C:127:ILE:HG22	1:C:152:LEU:CD1	2.22	0.69
1:B:517:ILE:HG23	1:B:546:PHE:CE1	2.28	0.69
1:A:197:LEU:N	1:A:198:PRO:CD	2.55	0.69
1:A:185:GLY:O	1:A:216:ARG:CB	2.38	0.69
1:B:24:GLU:CD	1:B:597:GLN:HE22	1.95	0.69
1:A:192:ASP:OD2	1:A:194:LEU:HB2	1.92	0.68
1:B:33:LEU:CD2	1:B:33:LEU:N	2.50	0.68
1:A:568:GLU:N	1:A:568:GLU:OE1	2.26	0.68
1:C:104:HIS:CG	1:C:123:ASP:HA	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LEU:HD12	1:B:506:PRO:HB2	1.75	0.68
1:C:6:ALA:HB1	1:C:12:VAL:HG11	1.75	0.68
1:A:421:LYS:CE	1:A:430:GLU:OE1	2.41	0.68
1:C:234:ILE:HD12	1:C:236:SER:H	1.57	0.68
1:A:304:TYR:O	1:A:305:ASN:C	2.32	0.68
1:B:577:THR:HA	1:B:580:LEU:HD12	1.74	0.68
1:C:576:TYR:O	1:C:579:PRO:HD2	1.92	0.68
1:C:460:ASP:O	1:C:460:ASP:OD1	2.10	0.68
1:A:172:ALA:O	1:A:178:LEU:HD12	1.92	0.68
1:B:329:GLU:O	1:B:330:PHE:C	2.30	0.68
1:C:127:ILE:HG22	1:C:152:LEU:HD11	1.75	0.68
1:B:263:ILE:CD1	1:B:444:ILE:CD1	2.71	0.68
1:B:501:GLU:HA	1:B:504:HIS:HD2	1.57	0.68
1:A:25:TYR:CE2	1:A:397:ILE:HD12	2.28	0.68
1:B:601:LEU:HD11	1:C:505:GLY:HA2	1.76	0.68
1:A:443:ARG:O	1:A:446:GLN:HB3	1.94	0.68
1:A:304:TYR:O	1:A:307:GLY:N	2.26	0.68
1:A:192:ASP:OD2	1:A:194:LEU:HB3	1.94	0.68
1:A:212:ALA:HA	1:A:221:ILE:HA	1.76	0.68
1:A:4:VAL:HG12	1:A:5:GLY:N	2.09	0.68
1:C:179:VAL:O	1:C:179:VAL:HG13	1.94	0.68
1:C:139:GLY:HA2	1:C:143:GLU:HB3	1.76	0.68
1:A:313:TRP:HA	1:A:317:LEU:HD12	1.76	0.68
1:C:399:VAL:CG1	1:C:602:ALA:O	2.41	0.68
1:C:118:PHE:HD1	1:C:118:PHE:H	1.42	0.68
1:B:468:LEU:O	1:B:516:VAL:HA	1.94	0.68
1:C:570:VAL:HG13	1:C:571:ILE:HG23	1.75	0.68
1:A:396:GLU:OE1	1:A:603:LYS:NZ	2.22	0.68
1:A:34:ALA:O	1:A:68:GLY:HA2	1.94	0.68
1:B:95:VAL:O	1:B:95:VAL:HG12	1.94	0.68
1:A:107:LEU:O	1:A:109:GLU:N	2.27	0.68
1:B:516:VAL:HB	1:B:543:LEU:CD2	2.23	0.67
1:C:199:VAL:CG2	1:C:200:THR:HG22	2.24	0.67
1:C:461:PHE:HZ	1:C:517:ILE:HD11	1.59	0.67
1:C:139:GLY:CA	1:C:143:GLU:HB3	2.25	0.67
1:C:343:MET:HE2	1:C:367:TYR:CE2	2.29	0.67
1:A:491:TYR:CZ	1:A:599:ARG:CD	2.67	0.67
1:A:237:ASN:O	1:A:239:GLN:N	2.24	0.67
1:C:42:MET:HE2	1:C:44:ARG:HB2	1.75	0.67
1:C:17:LEU:CD2	1:C:33:LEU:HD13	2.24	0.67
1:A:145:VAL:O	1:A:147:ARG:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ASP:OD2	1:B:41:HIS:HB2	1.94	0.67
1:A:164:ARG:C	1:A:165:HIS:ND1	2.48	0.67
1:A:197:LEU:HD11	1:A:239:GLN:HB3	1.77	0.67
1:A:376:VAL:O	1:A:379:SER:OG	2.12	0.67
1:A:351:GLU:OE2	1:A:380:SER:CB	2.39	0.67
1:C:204:ILE:HG12	1:C:233:ASP:HB3	1.77	0.67
1:A:342:LEU:HD12	1:A:369:GLY:O	1.94	0.67
1:C:299:ALA:HB1	1:C:303:SER:HB2	1.76	0.67
1:B:194:LEU:HD23	1:B:194:LEU:O	1.94	0.67
1:A:567:VAL:HG22	1:A:575:PHE:CD2	2.29	0.67
1:C:486:LEU:HD12	1:C:490:SER:OG	1.93	0.67
1:A:8:ALA:HB1	1:A:186:GLU:HB3	1.76	0.67
1:B:402:THR:OG1	1:B:403:LYS:N	2.28	0.67
1:B:457:LEU:HD21	1:B:562:ILE:HD11	1.77	0.67
1:B:42:MET:SD	1:B:43:THR:N	2.67	0.67
1:A:281:LEU:HD22	1:A:387:LEU:CD1	2.22	0.67
1:A:454:ILE:HA	1:A:457:LEU:HD23	1.76	0.67
1:A:15:ILE:O	1:A:16:LEU:C	2.32	0.67
1:B:45:LEU:HG	1:B:45:LEU:O	1.93	0.67
1:A:382:VAL:HG21	1:A:390:MET:HE3	1.74	0.67
1:C:7:ILE:O	1:C:7:ILE:HG23	1.95	0.67
1:B:520:ALA:CB	1:B:529:LEU:HD23	2.25	0.67
1:C:306:SER:HB2	1:C:346:LEU:HD13	1.76	0.67
1:C:533:ILE:O	1:C:536:VAL:CG2	2.43	0.67
1:C:288:LEU:HD11	1:C:368:LEU:HD21	1.77	0.67
1:B:306:SER:OG	1:B:346:LEU:HD13	1.95	0.66
1:C:156:TYR:CE2	1:C:158:THR:HG22	2.29	0.66
1:B:9:GLN:O	1:B:9:GLN:OE1	2.13	0.66
1:A:248:TYR:CD2	1:A:254:LYS:CB	2.77	0.66
1:A:200:THR:OG1	1:A:201:ARG:N	2.26	0.66
1:A:54:LEU:O	1:A:57:ALA:N	2.27	0.66
1:C:578:VAL:O	1:C:581:GLN:HB2	1.95	0.66
1:C:476:TYR:O	1:C:479:ALA:HB3	1.96	0.66
1:C:524:GLU:N	1:C:524:GLU:CD	2.49	0.66
1:A:485:LYS:O	1:A:488:GLU:N	2.28	0.66
1:C:18:GLU:CA	1:C:21:ARG:HH11	2.07	0.66
1:B:270:ARG:NE	1:B:280:GLU:OE1	2.28	0.66
1:B:413:LEU:HA	1:B:416:VAL:CG2	2.24	0.66
1:A:197:LEU:N	1:A:198:PRO:HD2	2.10	0.66
1:C:472:ARG:HD2	1:C:525:LEU:HD22	1.78	0.66
1:A:346:LEU:HD21	1:A:408:GLN:HG2	1.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:CA	1:A:532:ASN:HD21	2.09	0.66
1:B:290:SER:OG	1:B:422:LEU:HD13	1.95	0.66
1:B:513:ASP:O	1:B:514:MET:HB2	1.95	0.66
1:A:196:LEU:N	1:A:196:LEU:HD23	2.10	0.66
1:B:22:ARG:CD	1:B:195:ALA:HA	2.25	0.66
1:C:170:LEU:HD13	1:C:171:ALA:N	2.10	0.66
1:B:200:THR:HG23	1:B:203:PHE:CE1	2.30	0.66
1:A:134:GLU:O	1:A:147:ARG:NH2	2.28	0.66
1:B:486:LEU:O	1:B:490:SER:HB3	1.95	0.66
1:B:502:LEU:O	1:B:506:PRO:HD2	1.95	0.66
1:B:520:ALA:HB2	1:B:529:LEU:HD23	1.78	0.66
1:A:88:HIS:HD2	1:A:124:THR:CG2	2.09	0.66
1:C:90:SER:HG	1:C:129:HIS:CE1	2.13	0.66
1:C:107:LEU:HA	1:C:110:GLU:HB3	1.75	0.66
1:B:399:VAL:HA	1:B:603:LYS:HD2	1.78	0.66
1:A:434:VAL:HG12	1:A:435:HIS:N	2.11	0.66
1:B:576:TYR:O	1:B:579:PRO:HG2	1.96	0.66
1:B:88:HIS:HB2	1:B:124:THR:HG22	1.77	0.66
1:B:56:GLN:O	1:B:57:ALA:C	2.31	0.66
1:B:187:ASN:HD22	1:B:187:ASN:H	0.74	0.66
1:C:95:VAL:HG21	1:C:128:ALA:HA	1.78	0.66
1:B:234:ILE:CG1	1:B:235:GLU:N	2.59	0.66
1:A:399:VAL:HG21	1:A:597:GLN:HA	1.77	0.65
1:C:251:TYR:CD2	1:C:397:ILE:HG21	2.31	0.65
1:A:107:LEU:O	1:A:108:ARG:C	2.33	0.65
1:C:304:TYR:CZ	1:C:308:MET:HE2	2.31	0.65
1:C:204:ILE:HG23	1:C:231:ARG:HB2	1.78	0.65
1:C:283:PRO:HG2	1:C:284:ASN:H	1.60	0.65
1:B:502:LEU:HG	1:B:507:LEU:HB2	1.78	0.65
1:A:121:GLU:O	1:A:122:THR:HB	1.96	0.65
1:C:201:ARG:O	1:C:203:PHE:CD2	2.50	0.65
1:A:204:ILE:HG13	1:A:233:ASP:HB3	1.77	0.65
1:C:368:LEU:HD23	1:C:369:GLY:N	2.11	0.65
1:A:388:ALA:C	1:A:389:LEU:HD12	2.16	0.65
1:A:437:LEU:O	1:A:439:ALA:N	2.27	0.65
1:B:263:ILE:HD12	1:B:444:ILE:HD12	1.79	0.65
1:C:197:LEU:H	1:C:198:PRO:CD	2.09	0.65
1:B:162:ASP:C	1:B:164:ARG:H	1.99	0.65
1:A:559:MET:HE2	1:A:561:ILE:HD11	1.78	0.65
1:A:136:LYS:HB2	1:A:137:GLN:NE2	2.10	0.65
1:C:28:TYR:O	1:C:50:LYS:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LEU:C	1:B:415:LEU:H	1.98	0.65
1:A:396:GLU:HG2	1:A:603:LYS:NZ	2.10	0.65
1:A:511:ASP:C	1:A:511:ASP:OD1	2.33	0.65
1:A:48:LEU:HD13	1:A:82:GLU:HG3	1.77	0.65
1:A:305:ASN:ND2	1:A:481:GLU:HA	2.12	0.65
1:B:252:MET:CE	1:B:489:ILE:HD13	2.27	0.65
1:A:559:MET:HE3	1:A:561:ILE:HD11	1.78	0.65
1:A:346:LEU:HD11	1:A:412:LEU:HD11	1.78	0.65
1:A:273:HIS:O	1:A:275:GLN:N	2.29	0.65
1:A:480:LEU:HD23	1:A:496:ALA:HB3	1.79	0.65
1:B:311:ARG:O	1:B:313:TRP:N	2.30	0.65
1:B:572:ALA:HB3	1:B:573:PRO:CD	2.27	0.65
1:C:412:LEU:O	1:C:416:VAL:HG23	1.97	0.65
1:A:221:ILE:HG22	1:A:229:VAL:HB	1.78	0.65
1:A:182:LEU:HD11	1:A:204:ILE:CD1	2.27	0.65
1:C:295:ILE:O	1:C:295:ILE:HG22	1.96	0.65
1:C:373:ILE:CD1	1:C:411:VAL:CG1	2.70	0.65
1:C:447:MET:O	1:C:449:SER:N	2.30	0.65
1:A:602:ALA:O	1:A:603:LYS:O	2.15	0.65
1:C:476:TYR:CB	1:C:477:PRO:HD3	2.24	0.65
1:B:294:HIS:CB	1:B:341:SER:OG	2.45	0.65
1:A:447:MET:HE3	1:A:564:MET:SD	2.36	0.65
1:B:231:ARG:HA	3:B:706:HOH:O	1.95	0.65
1:B:185:GLY:O	1:B:186:GLU:HB3	1.97	0.65
1:B:235:GLU:O	1:B:236:SER:O	2.15	0.65
1:C:104:HIS:NE2	1:C:108:ARG:HG3	2.11	0.65
1:A:229:VAL:HG11	1:A:231:ARG:CZ	2.26	0.64
1:B:229:VAL:HG11	1:B:231:ARG:HH21	1.61	0.64
1:A:103:ASN:O	1:A:106:PRO:HD2	1.97	0.64
1:C:31:ALA:O	1:C:54:LEU:HD22	1.96	0.64
1:A:141:LEU:C	1:A:143:GLU:H	2.00	0.64
1:A:324:VAL:HG12	1:A:324:VAL:O	1.95	0.64
1:A:603:LYS:CG	1:A:604:SER:H	2.09	0.64
1:A:8:ALA:HB2	1:A:186:GLU:CB	2.26	0.64
1:B:492:ILE:O	1:B:494:ALA:N	2.29	0.64
1:A:248:TYR:CG	1:A:254:LYS:HB2	2.31	0.64
1:A:234:ILE:HD12	1:A:235:GLU:O	1.97	0.64
1:A:382:VAL:CG2	1:A:390:MET:HE3	2.28	0.64
1:A:105:GLU:HB3	1:A:106:PRO:CD	2.27	0.64
1:C:506:PRO:C	1:C:508:ALA:N	2.49	0.64
1:C:219:VAL:O	1:C:219:VAL:CG1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:CE1	1:C:122:THR:HG21	2.32	0.64
1:B:179:VAL:HG13	1:B:179:VAL:O	1.97	0.64
1:B:24:GLU:CG	1:B:597:GLN:NE2	2.58	0.64
1:C:158:THR:HG23	1:C:172:ALA:O	1.97	0.64
1:B:524:GLU:CD	1:B:524:GLU:H	2.01	0.64
1:B:78:GLY:H	1:C:538:ALA:HB2	1.63	0.64
1:B:90:SER:CB	1:B:129:HIS:ND1	2.60	0.64
1:A:32:GLY:HA2	1:A:54:LEU:HD21	1.77	0.64
1:B:42:MET:HG3	1:B:163:SER:HB3	1.80	0.64
1:B:289:LEU:C	1:B:292:VAL:HG23	2.16	0.64
1:C:179:VAL:CG2	1:C:203:PHE:HB3	2.27	0.64
1:A:292:VAL:HG21	1:A:342:LEU:HB2	1.78	0.64
1:A:304:TYR:CD1	1:A:326:ILE:HD12	2.29	0.64
1:C:356:LEU:HD11	1:C:380:SER:HB3	1.79	0.64
1:A:374:CYS:HB3	1:A:390:MET:HE3	1.80	0.64
1:A:578:VAL:N	1:A:579:PRO:HD2	2.12	0.64
1:B:359:LEU:HA	1:B:362:SER:HB3	1.79	0.64
1:B:475:GLN:HE21	1:B:519:VAL:HG21	1.63	0.64
1:B:587:VAL:O	1:B:590:ILE:HD12	1.98	0.64
1:C:448:LEU:O	1:C:451:ASP:OD1	2.15	0.64
1:B:71:HIS:ND1	1:B:72:THR:N	2.46	0.64
1:C:7:ILE:HG21	1:C:214:ILE:CG2	2.21	0.64
1:B:220:ASN:O	1:B:222:PHE:CD2	2.51	0.64
1:B:310:SER:HB2	1:B:412:LEU:CD1	2.28	0.63
1:A:36:VAL:HG12	1:A:41:HIS:C	2.19	0.63
1:B:14:GLU:O	1:B:15:ILE:C	2.34	0.63
1:B:413:LEU:O	1:B:415:LEU:N	2.31	0.63
1:C:565:PRO:O	1:C:566:HIS:O	2.17	0.63
1:A:382:VAL:CG2	1:A:390:MET:CE	2.72	0.63
1:B:379:SER:O	1:B:382:VAL:N	2.18	0.63
1:A:33:LEU:C	1:A:33:LEU:CD2	2.67	0.63
1:A:383:ARG:NH1	1:A:383:ARG:CG	2.57	0.63
1:A:185:GLY:O	1:A:216:ARG:O	2.16	0.63
1:C:50:LYS:O	1:C:52:GLN:N	2.30	0.63
1:A:304:TYR:CE2	1:A:326:ILE:HD11	2.33	0.63
1:B:413:LEU:O	1:B:416:VAL:N	2.27	0.63
1:B:89:VAL:HG12	1:B:94:VAL:HG13	1.81	0.63
1:B:42:MET:CE	1:B:94:VAL:HG21	2.26	0.63
1:B:316:SER:HG	1:B:317:LEU:HG	1.62	0.63
1:C:486:LEU:O	1:C:490:SER:HB2	1.98	0.63
1:B:105:GLU:HB3	1:B:106:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:OE1	1:A:481:GLU:CA	2.46	0.63
1:A:15:ILE:O	1:A:18:GLU:N	2.31	0.63
1:A:536:VAL:HG21	1:A:543:LEU:HD11	1.80	0.63
1:A:111:LEU:O	1:A:112:LYS:C	2.36	0.63
1:C:107:LEU:O	1:C:109:GLU:N	2.31	0.63
1:B:594:ASP:CB	1:B:597:GLN:O	2.46	0.63
1:C:234:ILE:HD12	1:C:235:GLU:N	2.14	0.63
1:B:251:TYR:CD2	1:B:397:ILE:HG21	2.34	0.63
1:B:485:LYS:O	1:B:486:LEU:C	2.37	0.63
1:C:564:MET:HB3	1:C:565:PRO:HD2	1.79	0.63
1:C:370:SER:HG	1:C:386:ASP:H	1.45	0.63
1:B:398:GLY:O	1:B:603:LYS:NZ	2.28	0.63
1:C:327:ALA:C	1:C:329:GLU:H	2.01	0.63
1:C:36:VAL:HG11	1:C:166:PRO:HB3	1.79	0.63
1:A:110:GLU:O	1:A:113:ALA:CB	2.44	0.63
1:B:503:LYS:HE3	1:B:503:LYS:HA	1.81	0.63
1:B:391:THR:HG22	1:B:411:VAL:HG21	1.80	0.62
1:B:470:LEU:CB	1:B:518:VAL:HG22	2.29	0.62
1:A:74:TRP:CE3	1:A:602:ALA:HB3	2.33	0.62
1:C:182:LEU:HD11	1:C:204:ILE:HD12	1.77	0.62
1:C:299:ALA:HB1	1:C:303:SER:HB3	1.81	0.62
1:A:251:TYR:HB3	1:A:255:GLU:OE2	1.99	0.62
1:A:102:GLU:N	1:A:153:ARG:O	2.30	0.62
1:C:3:ILE:HD11	1:C:98:ASN:HB2	1.79	0.62
1:A:338:ARG:N	1:A:338:ARG:HD3	2.14	0.62
1:B:475:GLN:NE2	1:B:519:VAL:HG21	2.15	0.62
1:B:518:VAL:HG11	1:B:529:LEU:HD11	1.80	0.62
1:C:251:TYR:CG	1:C:397:ILE:CG2	2.82	0.62
1:C:216:ARG:HH21	1:C:217:ARG:HH22	1.47	0.62
1:C:105:GLU:HB2	1:C:106:PRO:HD3	1.80	0.62
1:A:207:GLU:HG2	1:A:231:ARG:HD2	1.80	0.62
1:B:37:ASP:C	1:B:37:ASP:OD1	2.37	0.62
1:B:15:ILE:HG21	1:B:188:PHE:HE2	1.63	0.62
1:A:32:GLY:HA2	1:A:54:LEU:CD1	2.29	0.62
1:C:23:LEU:O	1:C:23:LEU:HD12	1.99	0.62
1:A:76:THR:C	1:A:78:GLY:H	2.03	0.62
1:A:120:SER:OG	1:A:121:GLU:HG2	1.99	0.62
1:C:80:PRO:O	1:C:84:ASN:OD1	2.17	0.62
1:B:539:ARG:HB3	1:C:600:ASN:OD1	1.98	0.62
1:A:8:ALA:CB	1:A:186:GLU:CB	2.77	0.62
1:C:521:PRO:HA	1:C:548:ASP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:LEU:CD1	1:B:510:ILE:HG12	2.22	0.62
1:A:237:ASN:C	1:A:239:GLN:H	2.03	0.62
1:A:111:LEU:O	1:A:114:ARG:N	2.33	0.62
1:A:17:LEU:CD2	1:A:33:LEU:CD1	2.72	0.62
1:C:245:LYS:O	1:C:254:LYS:HD3	1.99	0.62
1:B:129:HIS:O	1:B:132:ASN:HB3	2.00	0.62
1:A:141:LEU:HD23	1:A:170:LEU:HD23	1.80	0.62
1:A:569:GLU:HA	1:A:572:ALA:HB2	1.82	0.62
1:C:185:GLY:HA2	1:C:217:ARG:HG3	1.81	0.62
1:A:103:ASN:O	1:A:105:GLU:N	2.32	0.62
1:B:477:PRO:HA	1:B:480:LEU:HD12	1.81	0.62
1:B:516:VAL:HG12	1:B:516:VAL:O	1.98	0.62
1:C:341:SER:OG	1:C:367:TYR:CD2	2.53	0.62
1:A:510:ILE:CD1	1:A:536:VAL:CG1	2.77	0.62
1:C:170:LEU:HD22	1:C:171:ALA:N	2.11	0.62
1:B:182:LEU:HD21	1:B:204:ILE:CD1	2.29	0.62
1:C:158:THR:OG1	1:C:160:ILE:HD12	1.99	0.62
1:B:178:LEU:CD1	1:B:189:ILE:HD11	2.30	0.62
1:A:89:VAL:HG23	1:A:89:VAL:O	1.98	0.62
1:C:544:TYR:CE2	1:C:560:HIS:HD2	2.18	0.62
1:B:607:VAL:O	1:B:608:GLU:C	2.38	0.62
1:B:359:LEU:HD11	1:B:381:LEU:HD12	1.82	0.61
1:C:359:LEU:O	1:C:362:SER:OG	2.18	0.61
1:C:224:LYS:HD3	1:C:225:THR:N	2.15	0.61
1:A:553:PHE:CD2	1:A:559:MET:CE	2.77	0.61
1:C:234:ILE:HD13	1:C:236:SER:H	1.65	0.61
1:A:489:ILE:HG13	1:A:588:ALA:HB2	1.81	0.61
1:A:205:PHE:HE2	1:A:234:ILE:HD11	1.66	0.61
1:C:42:MET:HE3	1:C:44:ARG:NE	2.07	0.61
1:A:347:SER:HB2	1:A:381:LEU:CD1	2.30	0.61
1:A:356:LEU:HA	1:A:381:LEU:HD21	1.82	0.61
1:B:305:ASN:O	1:B:306:SER:O	2.17	0.61
1:B:587:VAL:C	1:B:590:ILE:HD12	2.20	0.61
1:A:239:GLN:O	1:A:241:ASP:N	2.33	0.61
1:A:510:ILE:CD1	1:A:536:VAL:CB	2.79	0.61
1:B:439:ALA:O	1:B:443:ARG:HG2	2.00	0.61
1:A:310:SER:O	1:A:313:TRP:N	2.34	0.61
1:B:124:THR:O	1:B:127:ILE:N	2.33	0.61
1:C:565:PRO:O	1:C:566:HIS:C	2.39	0.61
1:B:42:MET:HE1	1:B:94:VAL:CG2	2.31	0.61
1:C:251:TYR:CZ	1:C:397:ILE:HG21	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASN:HA	1:A:391:THR:OG1	2.00	0.61
1:C:180:ILE:HD11	1:C:206:LEU:HD21	1.82	0.61
1:A:529:LEU:O	1:A:532:ASN:ND2	2.33	0.61
1:B:220:ASN:O	1:B:222:PHE:CE2	2.53	0.61
1:C:173:ARG:HG3	1:C:178:LEU:HB2	1.81	0.61
1:A:342:LEU:O	1:A:342:LEU:HG	2.00	0.61
1:B:572:ALA:N	1:B:573:PRO:CD	2.60	0.61
1:C:467:ALA:O	1:C:494:ALA:HA	2.00	0.61
1:A:17:LEU:CD2	1:A:33:LEU:HD13	2.31	0.61
1:C:90:SER:O	1:C:91:GLU:HB2	2.01	0.61
1:B:3:ILE:O	1:B:4:VAL:CG2	2.49	0.61
1:A:485:LYS:O	1:A:486:LEU:C	2.37	0.61
1:B:528:LYS:O	1:B:531:SER:HB3	2.01	0.61
1:C:263:ILE:CG2	1:C:440:LEU:HD23	2.31	0.61
1:C:545:VAL:HB	1:C:561:ILE:HD13	1.81	0.61
1:B:192:ASP:OD1	1:B:194:LEU:HB2	2.00	0.61
1:B:186:GLU:HG2	1:B:186:GLU:O	2.00	0.61
1:A:469:PHE:CZ	1:A:517:ILE:HD13	2.36	0.61
1:A:453:ARG:O	1:A:456:ALA:HB3	2.00	0.61
1:C:250:HIS:HB3	1:C:596:ASP:OD1	2.00	0.61
1:B:42:MET:HE2	1:B:94:VAL:CG2	2.31	0.61
1:A:276:VAL:HG12	1:A:430:GLU:OE2	2.01	0.61
1:B:63:LEU:CD1	1:B:63:LEU:H	2.09	0.61
1:A:204:ILE:CG1	1:A:233:ASP:HB3	2.31	0.61
1:C:28:TYR:HB2	1:C:50:LYS:HD3	1.82	0.61
1:A:448:LEU:C	1:A:450:GLN:H	2.04	0.61
1:B:549:GLN:HA	1:B:563:GLU:OE2	2.01	0.61
1:C:485:LYS:O	1:C:584:ALA:HB1	2.00	0.61
1:C:529:LEU:HA	1:C:532:ASN:ND2	2.16	0.61
1:A:272:SER:O	1:A:273:HIS:CB	2.40	0.61
1:C:111:LEU:HB3	1:C:116:TYR:CD2	2.31	0.61
1:C:318:ALA:C	1:C:320:ILE:H	2.02	0.61
1:B:167:ASP:OD1	1:B:167:ASP:C	2.39	0.61
1:C:359:LEU:HD23	1:C:381:LEU:CD2	2.31	0.60
1:B:130:LEU:CD2	1:B:152:LEU:HD21	2.28	0.60
1:C:4:VAL:CG1	1:C:4:VAL:O	2.43	0.60
1:B:294:HIS:ND1	1:B:341:SER:OG	2.35	0.60
1:B:122:THR:C	1:B:124:THR:N	2.49	0.60
1:B:22:ARG:CG	1:B:22:ARG:HH11	2.13	0.60
1:A:276:VAL:HG21	1:A:414:MET:HG2	1.81	0.60
1:B:214:ILE:C	1:B:215:THR:CG2	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HG21	1:C:131:VAL:HB	1.83	0.60
1:B:270:ARG:HD3	1:B:414:MET:HE1	1.80	0.60
1:C:12:VAL:O	1:C:13:ALA:C	2.39	0.60
1:C:42:MET:HE3	1:C:44:ARG:HB2	1.83	0.60
1:B:338:ARG:NE	1:C:321:PRO:HB3	2.15	0.60
1:A:128:ALA:C	1:A:130:LEU:H	2.05	0.60
1:A:603:LYS:HG3	1:A:604:SER:N	2.10	0.60
1:A:503:LYS:HD3	1:A:535:GLU:CD	2.22	0.60
1:A:510:ILE:HD11	1:A:536:VAL:CG1	2.31	0.60
1:A:3:ILE:HG22	1:A:191:SER:HB3	1.82	0.60
1:C:279:SER:O	1:C:280:GLU:C	2.40	0.60
1:A:207:GLU:N	1:A:210:ASP:OD2	2.34	0.60
1:B:105:GLU:H	1:B:106:PRO:HD2	1.66	0.60
1:C:399:VAL:HG13	1:C:603:LYS:HA	1.83	0.60
1:A:472:ARG:HG2	1:A:525:LEU:HD12	1.83	0.60
1:B:493:HIS:CD2	1:C:466:HIS:ND1	2.70	0.60
1:C:555:SER:OG	1:C:561:ILE:HB	2.01	0.60
1:A:180:ILE:CD1	1:A:214:ILE:HD11	2.23	0.60
1:A:279:SER:C	1:A:281:LEU:N	2.51	0.60
1:C:255:GLU:OE2	1:C:397:ILE:N	2.33	0.60
1:C:69:ILE:HG21	1:C:159:VAL:HG12	1.83	0.60
1:B:294:HIS:O	1:B:341:SER:HA	2.01	0.60
1:B:67:THR:OG1	1:B:166:PRO:O	2.17	0.60
1:B:113:ALA:O	1:B:115:GLY:N	2.34	0.60
1:C:29:ASP:OD2	1:C:75:ALA:N	2.33	0.60
1:B:329:GLU:O	1:B:330:PHE:O	2.20	0.60
1:B:1:CYS:HA	1:B:72:THR:O	2.02	0.60
1:A:103:ASN:C	1:A:105:GLU:H	2.05	0.60
1:A:133:TRP:CZ3	1:A:134:GLU:OE2	2.55	0.60
1:B:454:ILE:O	1:B:457:LEU:HB3	2.01	0.60
1:C:178:LEU:HB3	1:C:206:LEU:HD12	1.82	0.60
1:B:520:ALA:CB	1:B:529:LEU:CD2	2.80	0.60
1:B:572:ALA:H	1:B:573:PRO:HD2	1.67	0.60
1:A:175:GLY:N	1:A:208:GLU:OE2	2.34	0.60
1:B:152:LEU:N	1:B:152:LEU:HD23	2.17	0.60
1:C:251:TYR:CE2	1:C:397:ILE:HG21	2.37	0.60
1:C:44:ARG:HD3	1:C:46:ARG:HD3	1.84	0.60
1:C:95:VAL:O	1:C:96:VAL:HG13	2.01	0.60
1:B:214:ILE:HG22	1:B:215:THR:H	1.66	0.60
1:C:286:ASP:OD1	1:C:422:LEU:HD11	2.02	0.60
1:A:353:ALA:HB1	1:A:608:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:TRP:CZ3	1:C:602:ALA:HB2	2.37	0.59
1:B:228:GLU:HG2	1:B:229:VAL:H	1.66	0.59
1:B:594:ASP:O	1:B:595:VAL:C	2.39	0.59
1:B:32:GLY:HA3	1:B:46:ARG:HA	1.84	0.59
1:C:18:GLU:OE2	1:C:21:ARG:NH1	2.35	0.59
1:B:394:GLY:HA3	1:B:403:LYS:NZ	2.17	0.59
1:B:454:ILE:HD12	1:B:582:LEU:HD12	1.84	0.59
1:B:487:LYS:HD3	1:C:509:LEU:HD11	1.84	0.59
1:C:565:PRO:O	1:C:567:VAL:HG13	2.02	0.59
1:B:118:PHE:C	1:B:120:SER:H	2.04	0.59
1:B:32:GLY:CA	1:B:54:LEU:HD22	2.31	0.59
1:A:371:LEU:CD1	1:A:371:LEU:C	2.66	0.59
1:C:33:LEU:HA	1:C:70:ALA:HA	1.85	0.59
1:C:135:LEU:HD11	1:C:164:ARG:NH2	2.12	0.59
1:A:20:LEU:O	1:A:21:ARG:C	2.39	0.59
1:B:221:ILE:HG22	1:B:222:PHE:H	1.65	0.59
1:A:434:VAL:O	1:A:435:HIS:C	2.41	0.59
1:A:18:GLU:OE1	1:A:18:GLU:HA	2.02	0.59
1:A:510:ILE:CG2	1:A:511:ASP:N	2.65	0.59
1:B:241:ASP:HB3	1:B:244:ASP:O	2.03	0.59
1:B:421:LYS:O	1:B:424:GLY:N	2.36	0.59
1:B:334:LYS:HD2	1:B:334:LYS:C	2.23	0.59
1:A:312:TYR:CZ	1:A:473:GLY:O	2.56	0.59
1:A:474:ASP:C	1:A:474:ASP:OD1	2.40	0.59
1:C:594:ASP:HB3	1:C:597:GLN:O	2.02	0.59
1:A:297:ILE:HB	1:A:324:VAL:HA	1.84	0.59
1:B:359:LEU:HD13	1:B:384:GLU:O	2.02	0.59
1:B:447:MET:HE3	1:B:564:MET:CE	2.29	0.59
1:B:501:GLU:CG	1:C:326:ILE:HG21	2.32	0.59
1:B:42:MET:CE	1:B:94:VAL:HG22	2.33	0.59
1:B:254:LYS:O	1:B:258:GLU:CB	2.51	0.59
1:B:344:ILE:CG2	1:B:371:LEU:HD23	2.25	0.59
1:A:531:SER:O	1:A:534:GLU:N	2.36	0.59
1:C:234:ILE:CD1	1:C:238:LEU:HD11	2.33	0.59
1:C:173:ARG:HB2	1:C:178:LEU:HD13	1.85	0.59
1:B:436:GLY:O	1:B:571:ILE:HD13	2.02	0.59
1:A:102:GLU:O	1:A:104:HIS:N	2.36	0.59
1:C:130:LEU:HD22	1:C:148:ALA:HB1	1.83	0.59
1:C:20:LEU:CB	1:C:51:VAL:HG11	2.32	0.59
1:A:20:LEU:CB	1:A:51:VAL:HG21	2.33	0.59
1:A:149:ILE:O	1:A:151:GLN:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASN:O	1:B:264:LYS:HB3	2.03	0.59
1:A:187:ASN:ND2	1:A:219:VAL:HG22	2.18	0.59
1:B:468:LEU:HD13	1:B:497:TYR:CD2	2.38	0.58
1:C:343:MET:CE	1:C:367:TYR:CE2	2.85	0.58
1:A:526:LEU:O	1:A:529:LEU:HB3	2.03	0.58
1:B:14:GLU:HG2	1:B:15:ILE:N	2.18	0.58
1:C:265:ASN:O	1:C:392:ASN:HB2	2.03	0.58
1:B:276:VAL:HG23	1:B:276:VAL:O	2.03	0.58
1:B:304:TYR:CE2	1:B:308:MET:HE2	2.37	0.58
1:B:419:LEU:O	1:B:423:LYS:HG2	2.02	0.58
1:A:13:ALA:O	1:A:15:ILE:N	2.36	0.58
1:C:224:LYS:HD2	1:C:225:THR:HG23	1.84	0.58
1:C:308:MET:HB2	1:C:477:PRO:HB3	1.85	0.58
1:A:318:ALA:HB1	1:A:320:ILE:HG13	1.84	0.58
1:B:29:ASP:O	1:B:49:GLY:N	2.25	0.58
1:A:519:VAL:HG12	1:A:576:TYR:HD2	1.67	0.58
1:B:404:ALA:HA	1:B:407:THR:HG1	1.68	0.58
1:B:578:VAL:N	1:B:579:PRO:HD2	2.18	0.58
1:C:263:ILE:HD12	1:C:440:LEU:CD2	2.33	0.58
1:A:221:ILE:HG21	1:A:231:ARG:HG2	1.84	0.58
1:A:373:ILE:HD13	1:A:411:VAL:HG11	1.85	0.58
1:A:105:GLU:H	1:A:106:PRO:CD	2.16	0.58
1:C:18:GLU:HA	1:C:21:ARG:NH1	2.09	0.58
1:C:90:SER:OG	1:C:129:HIS:ND1	2.35	0.58
1:C:371:LEU:HD11	1:C:389:LEU:HD11	1.84	0.58
1:A:268:THR:O	1:A:268:THR:HG22	2.02	0.58
1:A:32:GLY:HA2	1:A:54:LEU:CD2	2.33	0.58
1:A:503:LYS:HD3	1:A:535:GLU:OE2	2.03	0.58
1:B:240:TYR:CE1	1:B:241:ASP:HB2	2.37	0.58
1:B:263:ILE:CD1	1:B:444:ILE:HD11	2.33	0.58
1:C:418:LYS:O	1:C:422:LEU:HB2	2.03	0.58
1:A:47:ARG:NE	1:A:57:ALA:HB2	2.18	0.58
1:B:273:HIS:O	1:B:275:GLN:HG3	2.03	0.58
1:B:523:ASN:OD1	1:B:525:LEU:HB2	2.03	0.58
1:A:270:ARG:O	1:A:277:ASP:N	2.32	0.58
1:A:375:ASN:OD1	1:A:393:ALA:HB3	2.04	0.58
1:C:318:ALA:O	1:C:320:ILE:N	2.37	0.58
1:A:551:ALA:CB	1:A:553:PHE:HD1	2.17	0.58
1:C:311:ARG:HA	1:C:322:CYS:SG	2.44	0.58
1:B:343:MET:HB3	1:B:370:SER:CB	2.32	0.58
1:B:356:LEU:CD1	1:B:360:ARG:NE	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:N	1:C:198:PRO:CD	2.66	0.58
1:A:128:ALA:C	1:A:130:LEU:N	2.55	0.58
1:B:546:PHE:CE2	1:B:562:ILE:CD1	2.83	0.58
1:A:491:TYR:CG	1:A:599:ARG:NH1	2.71	0.58
1:A:161:MET:HB2	1:A:169:LEU:HD23	1.86	0.58
1:A:36:VAL:HG12	1:A:42:MET:HA	1.85	0.58
1:A:510:ILE:CD1	1:A:536:VAL:HG12	2.34	0.58
1:C:184:MET:HA	1:C:184:MET:HE2	1.85	0.58
1:C:5:GLY:HA2	1:C:69:ILE:HA	1.84	0.58
1:B:221:ILE:CG2	1:B:222:PHE:N	2.66	0.58
1:B:168:THR:HG22	1:B:169:LEU:N	2.19	0.58
1:C:11:ASP:OD1	1:C:65:GLY:O	2.22	0.58
1:A:355:THR:O	1:A:355:THR:HG22	2.04	0.58
1:A:305:ASN:O	1:A:308:MET:HB2	2.03	0.58
1:C:565:PRO:CG	1:C:575:PHE:CZ	2.65	0.58
1:A:436:GLY:O	1:A:437:LEU:C	2.43	0.58
1:C:80:PRO:O	1:C:84:ASN:CG	2.42	0.58
1:C:476:TYR:HB3	1:C:477:PRO:CD	2.29	0.58
1:A:356:LEU:HD21	1:A:360:ARG:CZ	2.33	0.58
1:A:88:HIS:HD2	1:A:124:THR:HG21	1.68	0.58
1:A:84:ASN:HB2	1:A:121:GLU:CD	2.24	0.58
1:B:331:ARG:HA	1:B:361:LEU:HD22	1.86	0.58
1:A:523:ASN:HD22	1:A:524:GLU:N	2.02	0.58
1:B:453:ARG:NH1	1:B:453:ARG:HG3	2.19	0.57
1:B:523:ASN:HD22	1:B:525:LEU:H	1.44	0.57
1:B:526:LEU:HD11	1:B:553:PHE:HE1	1.68	0.57
1:C:300:CYS:H	1:C:303:SER:HB2	1.68	0.57
1:A:161:MET:HB2	1:A:169:LEU:CD2	2.34	0.57
1:A:530:LYS:O	1:A:530:LYS:HD2	2.03	0.57
1:A:97:HIS:C	1:A:97:HIS:ND1	2.57	0.57
1:B:346:LEU:HD22	1:B:408:GLN:HG2	1.85	0.57
1:B:343:MET:HB3	1:B:370:SER:HA	1.85	0.57
1:A:382:VAL:CG1	1:A:382:VAL:O	2.52	0.57
1:C:118:PHE:CD1	1:C:118:PHE:N	2.72	0.57
1:C:278:LEU:HD21	1:C:414:MET:HE3	1.86	0.57
1:B:98:ASN:O	1:B:157:GLY:N	2.36	0.57
1:A:79:GLU:O	1:A:81:SER:N	2.37	0.57
1:B:523:ASN:C	1:B:523:ASN:ND2	2.56	0.57
1:A:192:ASP:O	1:A:194:LEU:N	2.37	0.57
1:B:36:VAL:HG21	1:B:163:SER:HA	1.87	0.57
1:A:409:LEU:CD1	1:A:574:ILE:HG12	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HA	1:C:171:ALA:HA	1.85	0.57
1:C:74:TRP:CH2	1:C:602:ALA:HB2	2.40	0.57
1:A:532:ASN:ND2	1:A:532:ASN:N	2.23	0.57
1:C:80:PRO:HG2	1:C:84:ASN:ND2	2.19	0.57
1:A:164:ARG:O	1:A:165:HIS:CG	2.57	0.57
1:B:3:ILE:O	1:B:4:VAL:HG23	2.04	0.57
1:C:346:LEU:HD22	1:C:408:GLN:HB3	1.86	0.57
1:A:255:GLU:OE2	1:A:398:GLY:N	2.37	0.57
1:C:159:VAL:HG13	1:C:171:ALA:HB2	1.87	0.57
1:C:71:HIS:HD2	1:C:96:VAL:HB	1.69	0.57
1:B:24:GLU:CG	1:B:597:GLN:HE22	2.16	0.57
1:C:587:VAL:O	1:C:590:ILE:HG22	2.04	0.57
1:C:532:ASN:H	1:C:532:ASN:ND2	2.01	0.57
1:A:155:ALA:HB1	1:A:175:GLY:HA3	1.86	0.57
1:B:238:LEU:HD11	1:B:240:TYR:HE2	1.69	0.57
1:B:337:VAL:O	1:B:337:VAL:HG23	2.04	0.57
1:B:3:ILE:HG22	1:B:4:VAL:N	2.19	0.57
1:A:46:ARG:HD2	1:A:82:GLU:O	2.04	0.57
1:A:304:TYR:CE1	1:A:326:ILE:HD11	2.36	0.57
1:B:318:ALA:O	1:B:423:LYS:HE3	2.05	0.57
1:B:559:MET:HE3	1:B:561:ILE:CD1	2.26	0.57
1:C:564:MET:HG3	1:C:576:TYR:CE1	2.40	0.57
1:A:7:ILE:HD13	1:A:214:ILE:HG22	1.87	0.57
1:B:406:THR:O	1:B:409:LEU:HB2	2.04	0.57
1:A:90:SER:HB3	1:A:128:ALA:HB1	1.84	0.57
1:B:134:GLU:OE1	1:B:134:GLU:HA	2.04	0.57
1:C:549:GLN:HB2	1:C:564:MET:O	2.05	0.57
1:B:193:GLN:O	1:B:195:ALA:N	2.38	0.57
1:A:344:ILE:HG22	1:A:344:ILE:O	2.03	0.57
1:A:540:GLY:O	1:A:541:GLY:C	2.41	0.57
1:B:417:ALA:O	1:B:419:LEU:N	2.38	0.57
1:B:515:PRO:O	1:B:516:VAL:HG23	2.05	0.57
1:C:350:GLY:CA	1:C:381:LEU:HD12	2.24	0.57
1:A:202:ARG:NH1	1:A:202:ARG:CG	2.64	0.57
1:B:140:THR:O	1:B:141:LEU:C	2.43	0.57
1:A:330:PHE:C	1:A:330:PHE:CD1	2.78	0.57
1:A:305:ASN:ND2	1:A:481:GLU:OE1	2.38	0.57
1:A:28:TYR:CE1	1:A:597:GLN:HB3	2.40	0.57
1:C:130:LEU:HD13	1:C:152:LEU:HD11	1.87	0.57
1:A:447:MET:CE	1:A:575:PHE:CE1	2.88	0.57
1:A:507:LEU:HD12	1:A:507:LEU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:SER:O	1:B:381:LEU:N	2.38	0.56
1:A:585:TYR:O	1:A:588:ALA:HB3	2.05	0.56
1:B:331:ARG:HG3	1:B:332:TYR:N	2.20	0.56
1:C:36:VAL:O	1:C:36:VAL:HG12	2.04	0.56
1:A:110:GLU:O	1:A:111:LEU:C	2.42	0.56
1:C:197:LEU:HD23	1:C:203:PHE:HZ	1.70	0.56
1:C:289:LEU:O	1:C:422:LEU:HD22	2.05	0.56
1:B:86:HIS:N	1:B:86:HIS:CD2	2.73	0.56
1:C:533:ILE:HG22	1:C:559:MET:CE	2.36	0.56
1:A:598:PRO:CG	1:A:601:LEU:HD12	2.35	0.56
1:A:7:ILE:CD1	1:A:215:THR:CA	2.82	0.56
1:B:44:ARG:CZ	1:B:46:ARG:HH21	2.17	0.56
1:A:440:LEU:CD2	1:A:574:ILE:HD12	2.35	0.56
1:C:309:VAL:CG2	1:C:477:PRO:HB2	2.35	0.56
1:B:3:ILE:C	1:B:4:VAL:HG23	2.26	0.56
1:C:283:PRO:CG	1:C:284:ASN:H	2.18	0.56
1:A:296:GLN:NE2	1:A:296:GLN:CA	2.40	0.56
1:B:309:VAL:HG21	1:B:478:ILE:HD11	1.88	0.56
1:B:498:ALA:O	1:B:500:GLY:N	2.38	0.56
1:C:379:SER:CB	1:C:382:VAL:HG23	2.31	0.56
1:B:127:ILE:HG12	1:B:152:LEU:CD1	2.36	0.56
1:A:346:LEU:O	1:A:408:GLN:NE2	2.37	0.56
1:C:348:GLN:HG2	1:C:375:ASN:HB3	1.86	0.56
1:C:187:ASN:O	1:C:188:PHE:CG	2.59	0.56
1:C:130:LEU:CD1	1:C:152:LEU:HD21	2.36	0.56
1:B:92:HIS:CD2	1:B:164:ARG:HE	2.24	0.56
1:A:447:MET:HE2	1:A:575:PHE:CE1	2.39	0.56
1:A:184:MET:C	1:A:186:GLU:H	2.09	0.56
1:C:107:LEU:HA	1:C:110:GLU:CB	2.34	0.56
1:C:28:TYR:HB2	1:C:50:LYS:CD	2.35	0.56
1:B:60:GLU:O	1:B:62:PRO:HD3	2.05	0.56
1:B:249:ARG:O	1:B:249:ARG:HG2	2.04	0.56
1:B:586:HIS:O	1:B:590:ILE:CD1	2.53	0.56
1:C:149:ILE:N	1:C:150:PRO:CD	2.65	0.56
1:B:234:ILE:HG13	1:B:235:GLU:N	2.20	0.56
1:B:433:ILE:CG1	1:B:570:VAL:HG21	2.35	0.56
1:A:71:HIS:CE1	1:A:86:HIS:CG	2.94	0.56
1:B:338:ARG:NH2	1:C:315:GLU:OE2	2.39	0.56
1:A:76:THR:O	1:A:78:GLY:N	2.38	0.56
1:B:425:LEU:HG	1:B:426:ASP:H	1.71	0.56
1:B:468:LEU:HD11	1:B:470:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LEU:HD23	1:B:516:VAL:CG2	2.36	0.56
1:C:447:MET:C	1:C:449:SER:N	2.58	0.56
1:A:70:ALA:O	1:A:71:HIS:CB	2.53	0.56
1:C:216:ARG:NH2	1:C:217:ARG:NH2	2.52	0.56
1:A:263:ILE:HD11	1:A:406:THR:HG21	1.85	0.56
1:B:133:TRP:O	1:B:137:GLN:HG2	2.05	0.56
1:A:277:ASP:OD1	1:A:277:ASP:C	2.44	0.56
1:C:141:LEU:HD21	1:C:168:THR:OG1	2.05	0.56
1:A:102:GLU:C	1:A:104:HIS:H	2.08	0.56
1:B:253:GLN:O	1:B:256:ILE:N	2.38	0.56
1:A:553:PHE:CD2	1:A:559:MET:HE3	2.41	0.56
1:C:82:GLU:HG3	1:C:83:VAL:N	2.18	0.56
1:A:476:TYR:N	1:A:477:PRO:CD	2.68	0.56
1:C:47:ARG:HE	1:C:47:ARG:HA	1.70	0.56
1:B:276:VAL:CG1	1:B:434:VAL:HG22	2.32	0.56
1:B:447:MET:HG2	1:B:575:PHE:CZ	2.40	0.56
1:A:28:TYR:HE1	1:A:602:ALA:HA	1.70	0.56
1:C:15:ILE:HD11	1:C:199:VAL:HG11	1.88	0.56
1:C:480:LEU:HA	1:C:496:ALA:HB2	1.88	0.56
1:C:185:GLY:CA	1:C:217:ARG:HG3	2.36	0.56
1:A:145:VAL:C	1:A:147:ARG:H	2.09	0.56
1:A:165:HIS:C	1:A:167:ASP:H	2.07	0.56
1:B:283:PRO:C	1:B:285:ALA:H	2.09	0.56
1:A:313:TRP:CA	1:A:317:LEU:HD12	2.36	0.56
1:A:485:LYS:NZ	2:A:700:G6Q:O1	2.39	0.56
1:B:466:HIS:CE1	1:C:466:HIS:CE1	2.94	0.56
1:C:566:HIS:O	1:C:567:VAL:CG1	2.54	0.56
1:A:25:TYR:HE2	1:A:397:ILE:HD12	1.71	0.56
1:B:79:GLU:O	1:B:80:PRO:C	2.44	0.56
1:C:480:LEU:HA	1:C:496:ALA:CB	2.36	0.56
1:C:42:MET:CG	1:C:43:THR:N	2.68	0.56
1:B:134:GLU:O	1:B:147:ARG:NH2	2.34	0.56
1:B:484:LEU:C	1:B:485:LYS:HG2	2.18	0.56
1:B:501:GLU:CD	1:C:326:ILE:HD12	2.25	0.56
1:A:371:LEU:HD12	1:A:371:LEU:C	2.25	0.56
1:A:373:ILE:HD13	1:A:411:VAL:HG12	1.87	0.56
1:C:36:VAL:CG1	1:C:166:PRO:CB	2.76	0.56
1:C:156:TYR:HE2	1:C:158:THR:HG22	1.71	0.56
1:B:8:ALA:O	1:B:216:ARG:HD3	2.06	0.56
1:C:47:ARG:NE	1:C:47:ARG:HA	2.21	0.56
1:A:347:SER:OG	2:A:700:G6Q:O2P	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:LEU:HD12	1:C:502:LEU:N	2.21	0.55
1:B:252:MET:HE2	1:B:489:ILE:HD13	1.88	0.55
1:C:3:ILE:CD1	1:C:98:ASN:HB2	2.35	0.55
1:B:286:ASP:CB	1:B:422:LEU:HD11	2.36	0.55
1:B:162:ASP:C	1:B:162:ASP:OD1	2.43	0.55
1:A:259:GLN:O	1:A:263:ILE:HG13	2.07	0.55
1:C:544:TYR:CE2	1:C:560:HIS:CD2	2.93	0.55
1:B:159:VAL:HG22	1:B:171:ALA:HB2	1.88	0.55
1:C:487:LYS:C	1:C:489:ILE:H	2.08	0.55
1:C:543:LEU:CD1	1:C:559:MET:HE3	2.35	0.55
1:A:122:THR:OG1	1:A:123:ASP:N	2.39	0.55
1:A:375:ASN:HD21	1:A:393:ALA:HB3	1.71	0.55
1:C:179:VAL:HG21	1:C:203:PHE:HB3	1.89	0.55
1:B:5:GLY:CA	1:B:189:ILE:HG23	2.36	0.55
1:C:8:ALA:HA	1:C:186:GLU:HA	1.86	0.55
1:A:338:ARG:HD3	1:A:338:ARG:H	1.71	0.55
1:B:468:LEU:HD12	1:B:497:TYR:HD2	1.68	0.55
1:A:413:LEU:HG	1:A:433:ILE:CG2	2.36	0.55
1:A:318:ALA:CB	1:A:320:ILE:HG13	2.35	0.55
1:B:99:GLY:HA3	1:B:156:TYR:HA	1.88	0.55
1:B:24:GLU:OE2	1:B:597:GLN:NE2	2.26	0.55
1:C:297:ILE:HD12	1:C:324:VAL:HG22	1.88	0.55
1:B:221:ILE:N	1:B:221:ILE:HD12	2.15	0.55
1:C:517:ILE:CD1	1:C:544:TYR:HB2	2.35	0.55
1:C:330:PHE:C	1:C:332:TYR:H	2.09	0.55
1:B:101:ILE:N	1:B:123:ASP:OD2	2.39	0.55
1:B:20:LEU:O	1:B:21:ARG:C	2.45	0.55
1:B:259:GLN:N	1:B:260:PRO:HD2	2.21	0.55
1:C:56:GLN:O	1:C:60:GLU:HB2	2.07	0.55
1:A:282:GLY:O	1:A:284:ASN:N	2.40	0.55
1:B:476:TYR:CD1	1:B:498:ALA:HB2	2.40	0.55
1:A:437:LEU:C	1:A:439:ALA:H	2.08	0.55
1:B:164:ARG:O	1:B:165:HIS:CD2	2.59	0.55
1:C:61:HIS:N	1:C:62:PRO:HD3	2.20	0.55
1:B:480:LEU:HA	1:B:496:ALA:CB	2.36	0.55
1:B:486:LEU:O	1:B:490:SER:CB	2.55	0.55
1:A:7:ILE:CD1	1:A:215:THR:HA	2.29	0.55
1:A:254:LYS:O	1:A:258:GLU:HG3	2.06	0.55
1:C:476:TYR:O	1:C:479:ALA:N	2.40	0.55
1:B:234:ILE:CD1	1:B:235:GLU:H	2.19	0.55
1:B:447:MET:HE1	1:B:564:MET:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:THR:HG21	1:C:381:LEU:HD22	1.89	0.55
1:A:210:ASP:OD1	1:A:231:ARG:NH2	2.38	0.55
1:B:126:VAL:CG1	1:B:127:ILE:N	2.69	0.55
1:C:216:ARG:HE	1:C:217:ARG:CZ	2.19	0.55
1:C:126:VAL:HG23	1:C:127:ILE:N	2.20	0.55
1:C:80:PRO:HB2	1:C:84:ASN:OD1	2.07	0.55
1:B:237:ASN:C	1:B:239:GLN:HE22	2.10	0.55
1:A:486:LEU:HD21	1:A:492:ILE:HG21	1.89	0.55
1:B:413:LEU:CD2	1:B:571:ILE:HG22	2.37	0.55
1:A:206:LEU:HD22	1:A:210:ASP:CB	2.36	0.55
1:C:197:LEU:H	1:C:198:PRO:HD2	1.72	0.55
1:C:204:ILE:CG1	1:C:233:ASP:HB3	2.36	0.55
1:A:131:VAL:O	1:A:134:GLU:HB2	2.06	0.55
1:A:118:PHE:N	1:A:118:PHE:CD1	2.74	0.55
1:C:79:GLU:HB3	1:C:81:SER:OG	2.08	0.55
1:B:334:LYS:CD	1:B:335:SER:N	2.70	0.55
1:C:370:SER:HG	1:C:386:ASP:N	2.05	0.55
1:B:526:LEU:HD11	1:B:553:PHE:CE1	2.41	0.54
1:A:37:ASP:HA	1:A:65:GLY:HA2	1.89	0.54
1:B:444:ILE:O	1:B:448:LEU:HG	2.07	0.54
1:A:567:VAL:CG2	1:A:575:PHE:CD2	2.89	0.54
1:A:486:LEU:HD11	1:A:587:VAL:HG11	1.88	0.54
1:B:304:TYR:O	1:B:305:ASN:C	2.44	0.54
1:A:602:ALA:O	1:A:603:LYS:C	2.44	0.54
1:B:110:GLU:OE2	1:B:114:ARG:NH2	2.41	0.54
1:C:376:VAL:HG13	1:C:377:PRO:HD2	1.89	0.54
1:C:443:ARG:O	1:C:446:GLN:N	2.40	0.54
1:A:399:VAL:CG2	1:A:596:ASP:O	2.56	0.54
1:B:45:LEU:HD21	1:B:57:ALA:HB3	1.90	0.54
1:A:510:ILE:HG22	1:A:511:ASP:N	2.22	0.54
1:C:486:LEU:O	1:C:490:SER:CB	2.55	0.54
1:C:523:ASN:ND2	1:C:569:GLU:OE2	2.41	0.54
1:C:434:VAL:C	1:C:436:GLY:H	2.08	0.54
1:B:313:TRP:HZ2	1:B:573:PRO:HG3	1.71	0.54
1:B:350:GLY:O	1:B:381:LEU:CB	2.56	0.54
1:A:371:LEU:HD22	1:A:387:LEU:HB3	1.89	0.54
1:A:414:MET:HE3	1:A:437:LEU:HD13	1.89	0.54
1:A:348:GLN:C	1:A:348:GLN:NE2	2.61	0.54
1:C:286:ASP:OD1	1:C:422:LEU:CD1	2.55	0.54
1:B:271:ILE:HG21	1:B:438:GLN:NE2	2.22	0.54
1:A:461:PHE:O	1:A:462:SER:C	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ASN:OD1	1:A:600:ASN:N	2.40	0.54
1:A:42:MET:O	1:A:43:THR:OG1	2.21	0.54
1:A:523:ASN:HD22	1:A:524:GLU:H	1.53	0.54
1:C:95:VAL:CG1	1:C:96:VAL:N	2.71	0.54
1:C:304:TYR:OH	1:C:308:MET:CE	2.56	0.54
1:C:234:ILE:HD12	1:C:236:SER:N	2.23	0.54
1:C:456:ALA:HA	1:C:459:GLU:OE2	2.08	0.54
1:C:572:ALA:N	1:C:573:PRO:CD	2.70	0.54
1:B:162:ASP:OD1	1:B:164:ARG:HB2	2.08	0.54
1:A:455:GLU:HG3	1:A:586:HIS:ND1	2.21	0.54
1:A:44:ARG:O	1:A:45:LEU:HD12	2.06	0.54
1:C:356:LEU:HD21	1:C:360:ARG:NH2	2.22	0.54
1:A:430:GLU:O	1:A:431:HIS:C	2.43	0.54
1:B:12:VAL:O	1:B:16:LEU:HB2	2.07	0.54
1:A:606:THR:C	1:A:607:VAL:O	2.43	0.54
1:B:413:LEU:CA	1:B:416:VAL:HG23	2.35	0.54
1:C:443:ARG:HB3	1:C:575:PHE:CE1	2.43	0.54
1:C:547:ALA:HB2	1:C:553:PHE:CD2	2.42	0.54
1:C:567:VAL:HG11	1:C:575:PHE:CD2	2.42	0.54
1:A:25:TYR:CD1	1:A:25:TYR:C	2.81	0.54
1:A:6:ALA:O	1:A:169:LEU:HD11	2.08	0.54
1:A:441:PRO:O	1:A:445:GLU:HG3	2.07	0.54
1:C:270:ARG:O	1:C:271:ILE:HD13	2.08	0.54
1:C:278:LEU:HD12	1:C:418:LYS:CG	2.35	0.54
1:B:28:TYR:CE1	1:B:602:ALA:HA	2.42	0.54
1:C:281:LEU:HD13	1:C:387:LEU:CD2	2.36	0.54
1:C:28:TYR:C	1:C:50:LYS:HB3	2.28	0.54
1:A:448:LEU:O	1:A:450:GLN:N	2.37	0.54
1:C:523:ASN:CG	1:C:569:GLU:OE2	2.46	0.54
1:B:346:LEU:HD22	1:B:408:GLN:CG	2.38	0.54
1:B:549:GLN:HG3	1:B:550:ASP:N	2.23	0.54
1:B:118:PHE:CD2	1:B:125:GLU:HG2	2.43	0.54
1:B:490:SER:OG	1:B:587:VAL:HG12	2.08	0.54
1:B:546:PHE:CD2	1:B:562:ILE:HD13	2.43	0.54
1:C:330:PHE:O	1:C:332:TYR:N	2.41	0.54
1:A:124:THR:C	1:A:126:VAL:H	2.10	0.54
1:A:180:ILE:HG13	1:A:189:ILE:HD13	1.90	0.54
1:A:346:LEU:HD22	1:A:408:GLN:HE21	1.73	0.54
1:C:251:TYR:CD2	1:C:397:ILE:CG2	2.91	0.54
1:A:393:ALA:O	1:A:403:LYS:NZ	2.37	0.54
1:C:184:MET:HE1	1:C:185:GLY:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ILE:HG13	1:C:128:ALA:N	2.23	0.54
1:A:553:PHE:HB3	1:A:561:ILE:HG13	1.89	0.54
1:A:133:TRP:O	1:A:137:GLN:HG2	2.08	0.54
1:C:505:GLY:O	1:C:508:ALA:HB2	2.08	0.54
1:A:253:GLN:HB2	1:A:585:TYR:CZ	2.43	0.53
1:B:33:LEU:HG	1:B:34:ALA:N	2.22	0.53
1:C:95:VAL:CG2	1:C:128:ALA:HA	2.38	0.53
1:A:314:PHE:CE1	1:A:416:VAL:HG22	2.43	0.53
1:B:236:SER:OG	1:B:237:ASN:N	2.41	0.53
1:A:302:THR:HG23	1:A:405:PHE:CD1	2.44	0.53
1:A:250:HIS:CB	1:A:596:ASP:OD2	2.44	0.53
1:A:28:TYR:CZ	1:A:597:GLN:CB	2.89	0.53
1:C:224:LYS:NZ	1:C:225:THR:HG23	2.24	0.53
1:B:246:GLY:O	1:B:247:ILE:C	2.46	0.53
1:B:334:LYS:HD2	1:B:335:SER:N	2.24	0.53
1:B:340:ASN:HB3	1:B:368:LEU:HD11	1.90	0.53
1:A:54:LEU:O	1:A:55:ALA:C	2.46	0.53
1:A:302:THR:CG2	1:A:405:PHE:CD1	2.91	0.53
1:C:507:LEU:O	1:C:507:LEU:CG	2.53	0.53
1:A:178:LEU:HD23	1:A:190:ALA:O	2.08	0.53
1:A:348:GLN:NE2	1:A:349:SER:N	2.55	0.53
1:B:90:SER:HB2	1:B:129:HIS:CE1	2.42	0.53
1:A:97:HIS:HA	1:A:158:THR:HA	1.91	0.53
1:B:404:ALA:HA	1:B:407:THR:OG1	2.08	0.53
1:B:497:TYR:CE1	1:B:506:PRO:HB3	2.44	0.53
1:C:310:SER:HB3	1:C:412:LEU:HD13	1.90	0.53
1:A:491:TYR:CE1	1:A:599:ARG:HG2	2.43	0.53
1:B:22:ARG:HD2	1:B:195:ALA:CA	2.35	0.53
1:A:267:LEU:HD21	1:A:437:LEU:HD22	1.90	0.53
1:B:10:ARG:NH2	1:B:186:GLU:OE2	2.31	0.53
1:C:456:ALA:HB1	1:C:459:GLU:OE2	2.09	0.53
1:B:311:ARG:C	1:B:313:TRP:H	2.12	0.53
1:B:505:GLY:N	1:B:506:PRO:CD	2.72	0.53
1:A:229:VAL:HG12	1:A:230:LYS:N	2.24	0.53
1:B:44:ARG:HD2	1:B:87:PRO:O	2.08	0.53
1:A:511:ASP:OD1	1:A:512:ALA:N	2.41	0.53
1:C:375:ASN:CA	1:C:391:THR:OG1	2.43	0.53
1:C:69:ILE:HG13	1:C:96:VAL:HG22	1.90	0.53
1:C:107:LEU:O	1:C:108:ARG:C	2.47	0.53
1:B:105:GLU:C	1:B:107:LEU:H	2.12	0.53
1:C:95:VAL:HG11	1:C:127:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:CD1	1:B:240:TYR:HE2	2.22	0.53
1:B:214:ILE:CG2	1:B:215:THR:H	2.17	0.53
1:A:134:GLU:OE1	1:A:147:ARG:HB2	2.08	0.53
1:B:14:GLU:HG2	1:B:15:ILE:H	1.73	0.53
1:A:100:ILE:HD12	1:A:607:VAL:HA	1.90	0.53
1:A:16:LEU:HD11	1:A:68:GLY:HA3	1.90	0.53
1:B:44:ARG:NH1	1:B:89:VAL:HG13	2.24	0.53
1:A:414:MET:HG3	1:A:437:LEU:CD1	2.39	0.53
1:C:137:GLN:O	1:C:138:GLY:O	2.27	0.53
1:C:45:LEU:HD21	1:C:57:ALA:O	2.09	0.53
1:B:350:GLY:O	1:B:381:LEU:HB2	2.08	0.53
1:A:491:TYR:OH	1:A:599:ARG:HD3	2.07	0.53
1:B:33:LEU:HA	1:B:70:ALA:HA	1.91	0.53
1:A:346:LEU:HD22	1:A:408:GLN:CG	2.35	0.53
1:B:207:GLU:O	1:B:210:ASP:HB2	2.08	0.53
1:B:601:LEU:HD22	1:C:503:LYS:O	2.09	0.53
1:C:417:ALA:HB2	1:C:433:ILE:HG21	1.91	0.53
1:C:455:GLU:HG3	1:C:586:HIS:CE1	2.44	0.53
1:A:304:TYR:CE1	1:A:324:VAL:O	2.62	0.53
1:A:294:HIS:HD2	1:A:321:PRO:O	1.92	0.53
1:B:405:PHE:CE2	1:B:481:GLU:HG2	2.43	0.53
1:B:499:ALA:C	1:B:501:GLU:H	2.13	0.53
1:B:500:GLY:HA3	1:C:328:SER:OG	2.09	0.53
1:C:379:SER:O	1:C:382:VAL:N	2.42	0.53
1:A:13:ALA:C	1:A:15:ILE:H	2.12	0.53
1:A:4:VAL:CG1	1:A:5:GLY:N	2.72	0.53
1:B:79:GLU:HB3	1:B:80:PRO:HD2	1.91	0.53
1:B:42:MET:HE1	1:B:94:VAL:HG21	1.87	0.53
1:C:236:SER:O	1:C:238:LEU:HD12	2.09	0.53
1:C:288:LEU:HD11	1:C:368:LEU:CD2	2.39	0.53
1:B:498:ALA:O	1:B:499:ALA:C	2.46	0.53
1:C:344:ILE:CG2	1:C:345:THR:N	2.71	0.53
1:C:533:ILE:HG22	1:C:559:MET:HE1	1.91	0.53
1:A:18:GLU:HG3	1:A:22:ARG:HD2	1.90	0.53
1:B:228:GLU:CG	1:B:229:VAL:H	2.22	0.53
1:B:287:GLU:HB3	1:B:288:LEU:HD12	1.90	0.53
1:A:551:ALA:HB1	1:A:553:PHE:CD1	2.43	0.53
1:B:207:GLU:O	1:B:208:GLU:C	2.45	0.53
1:B:168:THR:HG22	1:B:169:LEU:O	2.09	0.53
1:A:450:GLN:O	1:A:451:ASP:C	2.47	0.53
1:A:293:GLU:HB2	1:A:340:ASN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:TYR:CZ	1:A:326:ILE:HD11	2.43	0.52
1:C:572:ALA:N	1:C:573:PRO:HD2	2.24	0.52
1:A:206:LEU:HD22	1:A:210:ASP:HB2	1.91	0.52
1:B:25:TYR:CD2	1:B:26:ARG:HG3	2.44	0.52
1:C:256:ILE:HG22	1:C:257:TYR:N	2.22	0.52
1:A:529:LEU:HA	1:A:532:ASN:ND2	2.19	0.52
1:C:42:MET:HG2	1:C:43:THR:N	2.25	0.52
1:B:92:HIS:CD2	1:B:164:ARG:NE	2.77	0.52
1:A:141:LEU:C	1:A:143:GLU:N	2.63	0.52
1:C:548:ASP:O	1:C:550:ASP:N	2.42	0.52
1:C:300:CYS:SG	1:C:327:ALA:HB3	2.48	0.52
1:C:405:PHE:HA	1:C:408:GLN:NE2	2.24	0.52
1:C:440:LEU:HD13	1:C:571:ILE:CD1	2.30	0.52
1:A:95:VAL:HG12	1:A:96:VAL:N	2.23	0.52
1:B:25:TYR:CZ	1:B:26:ARG:HG3	2.44	0.52
1:A:346:LEU:HD22	1:A:408:GLN:NE2	2.24	0.52
1:B:334:LYS:CD	1:B:334:LYS:C	2.78	0.52
1:C:599:ARG:O	1:C:601:LEU:N	2.42	0.52
1:B:168:THR:CG2	1:B:169:LEU:N	2.73	0.52
1:B:155:ALA:HB1	1:B:175:GLY:HA3	1.91	0.52
1:B:346:LEU:CD2	1:B:408:GLN:HG2	2.39	0.52
1:B:348:GLN:O	1:B:376:VAL:HG23	2.09	0.52
1:B:528:LYS:H	1:B:528:LYS:CD	2.18	0.52
1:B:101:ILE:O	1:B:104:HIS:HB3	2.10	0.52
1:A:103:ASN:ND2	1:A:103:ASN:N	2.56	0.52
1:A:141:LEU:CD2	1:A:170:LEU:HD23	2.40	0.52
1:C:456:ALA:CB	1:C:459:GLU:OE2	2.57	0.52
1:C:314:PHE:CE1	1:C:416:VAL:HG22	2.45	0.52
1:B:22:ARG:HG2	1:B:194:LEU:HD22	1.91	0.52
1:A:275:GLN:OE1	1:A:421:LYS:NZ	2.36	0.52
1:A:375:ASN:ND2	1:A:393:ALA:HB3	2.23	0.52
1:B:483:ALA:O	1:B:487:LYS:HE3	2.09	0.52
1:C:564:MET:HG3	1:C:576:TYR:HE1	1.74	0.52
1:B:22:ARG:CG	1:B:22:ARG:NH1	2.58	0.52
1:A:277:ASP:OD1	1:A:278:LEU:N	2.43	0.52
1:B:539:ARG:HD2	1:C:600:ASN:OD1	2.09	0.52
1:A:331:ARG:HD3	1:A:332:TYR:CZ	2.44	0.52
1:C:537:ARG:HG3	1:C:543:LEU:HD12	1.91	0.52
1:A:26:ARG:HE	1:A:604:SER:HB3	1.75	0.52
1:C:188:PHE:CE2	1:C:199:VAL:HG23	2.45	0.52
1:A:410:THR:CG2	1:A:437:LEU:HD22	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:THR:HG22	1:A:407:THR:CB	2.39	0.52
1:B:164:ARG:C	1:B:165:HIS:CD2	2.83	0.52
1:C:206:LEU:HB3	1:C:210:ASP:CG	2.30	0.52
1:A:296:GLN:C	1:A:296:GLN:HE21	2.13	0.52
1:B:501:GLU:HA	1:B:504:HIS:CD2	2.43	0.52
1:B:553:PHE:CD2	1:B:561:ILE:HD12	2.45	0.52
1:C:344:ILE:HG22	1:C:345:THR:N	2.24	0.52
1:B:34:ALA:CB	1:B:87:PRO:HG2	2.31	0.52
1:C:188:PHE:HD2	1:C:200:THR:HG21	1.75	0.52
1:B:228:GLU:HG2	1:B:229:VAL:N	2.24	0.52
1:A:267:LEU:HD21	1:A:410:THR:CG2	2.40	0.52
1:C:111:LEU:HB2	1:C:118:PHE:CE1	2.45	0.52
1:B:221:ILE:CG2	1:B:222:PHE:H	2.21	0.52
1:B:3:ILE:CD1	1:B:98:ASN:HB3	2.39	0.52
1:B:3:ILE:CD1	1:B:98:ASN:CB	2.87	0.52
1:A:47:ARG:CZ	1:A:57:ALA:CB	2.87	0.52
1:B:276:VAL:HG13	1:B:434:VAL:CG2	2.38	0.52
1:C:409:LEU:HD23	1:C:412:LEU:HD12	1.92	0.52
1:A:173:ARG:HG3	1:A:178:LEU:HB2	1.92	0.52
1:A:96:VAL:CG2	1:A:96:VAL:O	2.55	0.52
1:B:42:MET:HE2	1:B:94:VAL:HG21	1.89	0.52
1:A:414:MET:HG3	1:A:437:LEU:HD13	1.92	0.52
1:C:234:ILE:HD13	1:C:238:LEU:HD11	1.91	0.52
1:B:470:LEU:HB2	1:B:518:VAL:CG2	2.38	0.52
1:A:599:ARG:O	1:A:601:LEU:HG	2.10	0.52
1:B:38:ALA:HB3	1:B:39:GLU:CD	2.30	0.52
1:B:193:GLN:C	1:B:195:ALA:N	2.59	0.52
1:B:282:GLY:O	1:B:285:ALA:HB2	2.10	0.52
1:A:356:LEU:CD2	1:A:360:ARG:NH2	2.64	0.52
1:B:493:HIS:HD2	1:C:466:HIS:ND1	2.07	0.52
1:A:11:ASP:HA	1:A:65:GLY:O	2.10	0.52
1:A:124:THR:O	1:A:127:ILE:HB	2.10	0.52
1:A:125:GLU:OE1	1:A:125:GLU:O	2.28	0.52
1:C:142:ARG:HG2	1:C:146:LEU:HB2	1.92	0.52
1:B:3:ILE:HD11	1:B:157:GLY:O	2.10	0.52
1:C:28:TYR:HB2	1:C:50:LYS:HB3	1.92	0.52
1:B:11:ASP:C	1:B:13:ALA:H	2.12	0.52
1:C:468:LEU:HD12	1:C:495:GLU:HB3	1.91	0.52
1:B:487:LYS:HG3	1:C:509:LEU:HD21	1.92	0.51
1:C:447:MET:C	1:C:449:SER:H	2.14	0.51
1:A:547:ALA:O	1:A:548:ASP:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLY:C	1:B:69:ILE:HG23	2.30	0.51
1:A:286:ASP:OD1	1:A:286:ASP:N	2.42	0.51
1:C:564:MET:HB3	1:C:565:PRO:CD	2.40	0.51
1:A:589:LEU:O	1:A:592:GLY:N	2.44	0.51
1:A:18:GLU:OE1	1:A:18:GLU:CA	2.57	0.51
1:B:88:HIS:HB2	1:B:124:THR:HG21	1.91	0.51
1:B:259:GLN:O	1:B:262:ALA:CB	2.51	0.51
1:C:33:LEU:HD23	1:C:33:LEU:N	2.25	0.51
1:A:142:ARG:O	1:A:142:ARG:HG2	2.09	0.51
1:B:313:TRP:CE3	1:B:413:LEU:HD12	2.45	0.51
1:B:313:TRP:CZ3	1:B:413:LEU:CD1	2.76	0.51
1:C:547:ALA:CB	1:C:553:PHE:HD2	2.23	0.51
1:B:229:VAL:HG21	1:B:231:ARG:NE	2.17	0.51
1:C:224:LYS:NZ	1:C:225:THR:CG2	2.74	0.51
1:C:318:ALA:C	1:C:320:ILE:N	2.64	0.51
1:B:134:GLU:OE1	1:B:134:GLU:CA	2.56	0.51
1:A:223:ASP:OD1	1:A:224:LYS:N	2.44	0.51
1:C:405:PHE:CD2	1:C:577:THR:HG21	2.46	0.51
1:A:255:GLU:CD	1:A:398:GLY:H	2.14	0.51
1:A:594:ASP:O	1:A:595:VAL:C	2.48	0.51
1:B:53:MET:O	1:B:54:LEU:C	2.47	0.51
1:B:56:GLN:HA	1:B:59:GLU:HB2	1.93	0.51
1:C:204:ILE:CG2	1:C:231:ARG:HB2	2.41	0.51
1:C:28:TYR:HB2	1:C:50:LYS:CB	2.40	0.51
1:B:251:TYR:N	1:B:596:ASP:OD1	2.43	0.51
1:C:423:LYS:HD3	1:C:425:LEU:CG	2.34	0.51
1:B:294:HIS:HA	1:B:321:PRO:HG2	1.93	0.51
1:A:469:PHE:O	1:A:496:ALA:HA	2.11	0.51
1:C:173:ARG:HB2	1:C:178:LEU:CD1	2.40	0.51
1:B:68:GLY:C	1:B:69:ILE:CG2	2.79	0.51
1:A:361:LEU:O	1:A:362:SER:C	2.49	0.51
1:A:288:LEU:O	1:A:289:LEU:C	2.49	0.51
1:B:559:MET:O	1:B:561:ILE:HG12	2.10	0.51
1:B:405:PHE:CD2	1:B:577:THR:HG21	2.46	0.51
1:A:142:ARG:HG3	1:A:213:GLU:HB2	1.91	0.51
1:C:281:LEU:CD1	1:C:285:ALA:HB1	2.41	0.51
1:C:281:LEU:HD21	1:C:389:LEU:CD2	2.39	0.51
1:B:440:LEU:N	1:B:441:PRO:CD	2.73	0.51
1:C:434:VAL:C	1:C:436:GLY:N	2.64	0.51
1:B:417:ALA:O	1:B:420:SER:N	2.44	0.51
1:B:504:HIS:CD2	1:C:300:CYS:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:LYS:C	1:C:489:ILE:N	2.64	0.51
1:C:74:TRP:CH2	1:C:602:ALA:CB	2.94	0.51
1:B:45:LEU:HD21	1:B:57:ALA:CB	2.40	0.51
1:C:308:MET:N	1:C:324:VAL:HG11	2.26	0.51
1:B:90:SER:O	1:B:91:GLU:CB	2.51	0.51
1:A:132:ASN:OD1	1:A:132:ASN:C	2.49	0.51
1:A:143:GLU:O	1:A:147:ARG:HG3	2.11	0.51
1:B:93:ILE:CD1	1:B:93:ILE:N	2.73	0.51
1:A:223:ASP:OD1	1:A:225:THR:N	2.44	0.51
1:B:105:GLU:C	1:B:107:LEU:N	2.64	0.51
1:A:296:GLN:HE21	1:A:297:ILE:N	2.07	0.51
1:B:343:MET:HE2	1:B:362:SER:HB2	1.92	0.51
1:B:472:ARG:NH1	1:B:532:ASN:HD21	2.08	0.51
1:B:600:ASN:CB	1:C:539:ARG:HG3	2.41	0.51
1:A:36:VAL:O	1:A:65:GLY:CA	2.59	0.51
1:B:36:VAL:HG23	1:B:161:MET:SD	2.50	0.51
1:C:158:THR:OG1	1:C:160:ILE:CD1	2.58	0.51
1:C:201:ARG:O	1:C:203:PHE:CE2	2.63	0.51
1:A:29:ASP:O	1:A:49:GLY:N	2.30	0.51
1:B:472:ARG:HH21	1:C:332:TYR:HE2	1.59	0.51
1:C:547:ALA:HB2	1:C:553:PHE:HD2	1.76	0.51
1:B:193:GLN:O	1:B:194:LEU:C	2.48	0.51
1:A:440:LEU:HD22	1:A:574:ILE:HD12	1.93	0.51
1:A:92:HIS:O	1:A:163:SER:OG	2.26	0.51
1:B:606:THR:HG22	3:B:707:HOH:O	2.10	0.51
1:A:486:LEU:CD2	1:A:492:ILE:HG21	2.41	0.51
1:C:530:LYS:HG2	1:C:553:PHE:CE1	2.46	0.51
1:C:553:PHE:HB3	1:C:561:ILE:HD12	1.93	0.51
1:A:411:VAL:O	1:A:414:MET:N	2.44	0.51
1:B:182:LEU:HD11	1:B:204:ILE:CD1	2.41	0.51
1:C:476:TYR:CB	1:C:477:PRO:CD	2.88	0.51
1:C:517:ILE:N	1:C:517:ILE:HD13	2.25	0.51
1:B:276:VAL:HG21	1:B:417:ALA:HB1	1.94	0.50
1:A:396:GLU:CG	1:A:603:LYS:NZ	2.73	0.50
1:A:603:LYS:CG	1:A:604:SER:N	2.71	0.50
1:B:331:ARG:HH11	1:B:354:ASP:HA	1.76	0.50
1:B:179:VAL:HG23	1:B:204:ILE:O	2.11	0.50
1:B:220:ASN:O	1:B:221:ILE:O	2.28	0.50
1:B:371:LEU:HA	1:B:387:LEU:O	2.10	0.50
1:B:447:MET:CE	1:B:564:MET:HE1	2.41	0.50
1:B:523:ASN:HD21	1:B:525:LEU:CB	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:ASN:ND2	1:B:524:GLU:OE2	2.44	0.50
1:C:351:GLU:O	1:C:352:THR:C	2.46	0.50
1:C:489:ILE:HG13	1:C:588:ALA:HB2	1.93	0.50
1:A:179:VAL:HG23	1:A:205:PHE:HA	1.93	0.50
1:C:187:ASN:OD1	1:C:219:VAL:CG2	2.60	0.50
1:A:260:PRO:HG3	1:A:444:ILE:HG22	1.91	0.50
1:A:159:VAL:HG12	1:A:159:VAL:O	2.10	0.50
1:A:296:GLN:NE2	1:A:323:ASP:HB2	2.26	0.50
1:B:302:THR:HG22	1:B:303:SER:N	2.24	0.50
1:B:307:GLY:O	1:B:324:VAL:HG21	2.11	0.50
1:B:453:ARG:HH21	1:B:562:ILE:HA	1.76	0.50
1:C:443:ARG:O	1:C:447:MET:N	2.43	0.50
1:B:333:ARG:HG3	1:B:333:ARG:O	2.11	0.50
1:B:101:ILE:HB	1:B:123:ASP:HB2	1.92	0.50
1:B:20:LEU:HD22	1:B:72:THR:OG1	2.12	0.50
1:B:213:GLU:HG2	1:B:213:GLU:O	2.11	0.50
1:C:4:VAL:HB	1:C:70:ALA:HB3	1.94	0.50
1:B:270:ARG:HD3	1:B:414:MET:HE3	1.91	0.50
1:C:370:SER:OG	1:C:386:ASP:N	2.35	0.50
1:B:103:ASN:OD1	1:B:153:ARG:HB2	2.11	0.50
1:B:311:ARG:C	1:B:313:TRP:N	2.65	0.50
1:B:528:LYS:HD2	1:B:528:LYS:N	2.20	0.50
1:C:127:ILE:O	1:C:128:ALA:C	2.50	0.50
1:B:67:THR:HG22	1:B:68:GLY:N	2.27	0.50
1:C:265:ASN:O	1:C:392:ASN:CB	2.59	0.50
1:C:256:ILE:O	1:C:259:GLN:N	2.45	0.50
1:C:7:ILE:O	1:C:216:ARG:HA	2.12	0.50
1:A:134:GLU:HG3	1:A:148:ALA:HB2	1.93	0.50
1:C:353:ALA:HB2	1:C:606:THR:O	2.12	0.50
1:B:159:VAL:HA	1:B:171:ALA:HA	1.92	0.50
1:B:276:VAL:CG2	1:B:417:ALA:HB1	2.42	0.50
1:B:485:LYS:O	1:B:487:LYS:N	2.44	0.50
1:B:127:ILE:HG12	1:B:152:LEU:HD11	1.93	0.50
1:A:536:VAL:O	1:A:537:ARG:C	2.50	0.50
1:B:146:LEU:CD1	1:B:211:ILE:CD1	2.81	0.50
1:A:266:THR:HG22	1:A:270:ARG:NH1	2.27	0.50
1:A:140:THR:O	1:A:143:GLU:HB2	2.12	0.50
1:A:477:PRO:O	1:A:480:LEU:HB2	2.11	0.50
1:A:47:ARG:CZ	1:A:57:ALA:HB2	2.42	0.50
1:B:557:ASP:OD1	1:B:557:ASP:N	2.43	0.50
1:C:291:LYS:O	1:C:293:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:LEU:HD13	1:B:584:ALA:HA	1.93	0.50
1:B:501:GLU:O	1:B:506:PRO:CD	2.60	0.50
1:B:454:ILE:HD12	1:B:582:LEU:CD1	2.42	0.50
1:C:447:MET:HE1	1:C:575:PHE:O	2.12	0.50
1:B:32:GLY:HA2	1:B:45:LEU:O	2.12	0.50
1:A:533:ILE:HG23	1:A:543:LEU:HD23	1.90	0.50
1:A:348:GLN:HG3	1:A:404:ALA:CB	2.42	0.50
1:C:83:VAL:HG11	1:C:119:VAL:O	2.12	0.50
1:B:158:THR:HG23	1:B:158:THR:O	2.12	0.50
1:B:30:SER:OG	1:B:73:ARG:HB3	2.12	0.50
1:B:359:LEU:CD1	1:B:381:LEU:HD12	2.39	0.50
1:B:524:GLU:CD	1:B:524:GLU:N	2.65	0.50
1:B:523:ASN:O	1:B:526:LEU:HB2	2.12	0.50
1:C:263:ILE:HD11	1:C:406:THR:HG22	1.94	0.50
1:A:190:ALA:HB2	1:A:196:LEU:HD11	1.94	0.50
1:C:158:THR:CG2	1:C:172:ALA:O	2.59	0.50
1:C:181:GLY:O	1:C:182:LEU:HG	2.11	0.50
1:C:82:GLU:CG	1:C:83:VAL:H	2.22	0.50
1:C:330:PHE:HE1	1:C:335:SER:HB3	1.77	0.50
1:A:252:MET:O	1:A:256:ILE:N	2.37	0.50
1:C:74:TRP:HA	1:C:74:TRP:CE3	2.45	0.50
1:A:300:CYS:O	1:A:303:SER:N	2.44	0.50
1:C:565:PRO:HD2	1:C:575:PHE:CE2	2.47	0.49
1:B:94:VAL:O	1:B:95:VAL:HG23	2.12	0.49
1:C:79:GLU:HB3	1:C:81:SER:HG	1.76	0.49
1:B:92:HIS:O	1:B:162:ASP:HA	2.13	0.49
1:B:90:SER:O	1:B:132:ASN:ND2	2.42	0.49
1:B:359:LEU:HD11	1:B:381:LEU:CD1	2.40	0.49
1:C:447:MET:HE1	1:C:578:VAL:HB	1.94	0.49
1:C:525:LEU:O	1:C:528:LYS:HB2	2.12	0.49
1:B:33:LEU:CB	1:B:70:ALA:HB2	2.42	0.49
1:A:567:VAL:HG21	1:A:575:PHE:CG	2.48	0.49
1:A:308:MET:C	1:A:310:SER:N	2.65	0.49
1:B:345:THR:HG21	1:B:359:LEU:HD21	1.94	0.49
1:B:525:LEU:HA	1:B:528:LYS:HD3	1.93	0.49
1:C:263:ILE:HG21	1:C:440:LEU:CD2	2.39	0.49
1:A:103:ASN:C	1:A:106:PRO:HD2	2.32	0.49
1:B:396:GLU:CD	1:B:401:SER:HA	2.33	0.49
1:A:164:ARG:HB2	1:A:165:HIS:ND1	2.27	0.49
1:A:271:ILE:HG22	1:A:271:ILE:O	2.12	0.49
1:C:316:SER:OG	1:C:317:LEU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:HG22	1:A:326:ILE:O	2.12	0.49
1:B:520:ALA:O	1:B:547:ALA:HA	2.12	0.49
1:B:572:ALA:HB3	1:B:573:PRO:HD3	1.94	0.49
1:C:145:VAL:HG11	1:C:170:LEU:CD1	2.41	0.49
1:A:552:GLY:O	1:A:553:PHE:C	2.50	0.49
1:B:90:SER:HB3	1:B:128:ALA:HB1	1.94	0.49
1:A:330:PHE:HD1	1:A:331:ARG:N	2.11	0.49
1:C:433:ILE:O	1:C:436:GLY:N	2.38	0.49
1:A:251:TYR:CG	1:A:397:ILE:HG21	2.47	0.49
1:B:252:MET:O	1:B:256:ILE:HG13	2.13	0.49
1:B:234:ILE:HD12	1:B:235:GLU:N	2.22	0.49
1:B:346:LEU:HD11	1:B:412:LEU:HD11	1.93	0.49
1:A:251:TYR:O	1:A:252:MET:C	2.49	0.49
1:C:259:GLN:N	1:C:260:PRO:HD2	2.28	0.49
1:C:480:LEU:CD2	1:C:496:ALA:HB3	2.40	0.49
1:C:304:TYR:CZ	1:C:308:MET:CE	2.95	0.49
1:C:20:LEU:HD11	1:C:70:ALA:HB1	1.94	0.49
1:B:92:HIS:HD2	1:B:164:ARG:HE	1.59	0.49
1:C:283:PRO:CG	1:C:284:ASN:N	2.76	0.49
1:C:498:ALA:O	1:C:499:ALA:C	2.51	0.49
1:A:33:LEU:O	1:A:33:LEU:CD2	2.51	0.49
1:A:518:VAL:HG11	1:A:533:ILE:HD11	1.94	0.49
1:A:281:LEU:HD21	1:A:389:LEU:HD11	1.94	0.49
1:C:188:PHE:CD2	1:C:200:THR:HG21	2.48	0.49
1:A:417:ALA:HB1	1:A:430:GLU:HG3	1.94	0.49
1:A:374:CYS:SG	1:A:375:ASN:N	2.86	0.49
1:B:515:PRO:O	1:B:516:VAL:CG2	2.60	0.49
1:B:530:LYS:HA	1:B:533:ILE:HD12	1.94	0.49
1:B:406:THR:CA	1:B:409:LEU:HD12	2.16	0.49
1:A:273:HIS:C	1:A:275:GLN:H	2.15	0.49
1:B:180:ILE:HG22	1:B:181:GLY:N	2.26	0.49
1:C:31:ALA:HB2	1:C:51:VAL:CG2	2.40	0.49
1:A:6:ALA:CB	1:A:12:VAL:HB	2.42	0.49
1:A:13:ALA:C	1:A:15:ILE:N	2.66	0.49
1:C:393:ALA:HB2	1:C:407:THR:HG21	1.95	0.49
1:B:91:GLU:CD	1:B:132:ASN:HD21	2.16	0.49
1:A:76:THR:C	1:A:78:GLY:N	2.65	0.49
1:A:401:SER:OG	2:A:700:G6Q:H2	2.13	0.49
1:B:309:VAL:O	1:B:311:ARG:N	2.46	0.49
1:B:499:ALA:O	1:B:501:GLU:N	2.43	0.49
1:C:346:LEU:CD2	1:C:408:GLN:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:GLN:O	1:C:412:LEU:HG	2.13	0.49
1:A:42:MET:CE	1:A:43:THR:H	2.26	0.49
1:C:531:SER:O	1:C:535:GLU:HG3	2.12	0.49
1:B:185:GLY:O	1:B:186:GLU:CB	2.61	0.49
1:A:551:ALA:CB	1:A:553:PHE:CD1	2.96	0.49
1:B:442:SER:OG	1:B:443:ARG:NH1	2.46	0.49
1:C:344:ILE:N	1:C:344:ILE:HD12	2.28	0.48
1:C:359:LEU:CD2	1:C:381:LEU:CD2	2.91	0.48
1:C:567:VAL:HG11	1:C:575:PHE:CG	2.48	0.48
1:B:332:TYR:HE1	1:C:528:LYS:HZ1	1.58	0.48
1:C:165:HIS:N	1:C:166:PRO:HD3	2.28	0.48
1:B:594:ASP:HB3	1:B:597:GLN:C	2.34	0.48
1:C:16:LEU:O	1:C:20:LEU:HG	2.13	0.48
1:B:371:LEU:CG	1:B:372:ALA:H	2.16	0.48
1:B:415:LEU:CD1	1:B:419:LEU:HD11	2.40	0.48
1:B:433:ILE:HG13	1:B:570:VAL:CG2	2.37	0.48
1:B:502:LEU:O	1:B:506:PRO:CD	2.62	0.48
1:C:308:MET:HB3	1:C:477:PRO:HG3	1.96	0.48
1:B:144:ALA:O	1:B:147:ARG:HB2	2.12	0.48
1:C:460:ASP:O	1:C:461:PHE:HD1	1.96	0.48
1:C:469:PHE:HA	1:C:517:ILE:O	2.13	0.48
1:B:14:GLU:OE2	1:B:15:ILE:HG13	2.13	0.48
1:B:343:MET:CE	1:B:362:SER:HB2	2.43	0.48
1:A:118:PHE:HD2	1:A:125:GLU:OE1	1.96	0.48
1:A:16:LEU:HD11	1:A:68:GLY:CA	2.43	0.48
1:C:17:LEU:HD21	1:C:33:LEU:HD11	1.93	0.48
1:B:501:GLU:O	1:B:506:PRO:HD2	2.12	0.48
1:B:457:LEU:HD23	1:B:562:ILE:HD11	1.95	0.48
1:A:491:TYR:HE1	1:A:599:ARG:HG2	1.78	0.48
1:B:36:VAL:HA	1:B:42:MET:HA	1.95	0.48
1:C:187:ASN:O	1:C:188:PHE:CD1	2.66	0.48
1:C:82:GLU:O	1:C:85:ALA:HB3	2.13	0.48
1:C:469:PHE:CE2	1:C:482:GLY:C	2.86	0.48
1:A:292:VAL:HG21	1:A:342:LEU:CB	2.43	0.48
1:C:540:GLY:O	1:C:541:GLY:O	2.30	0.48
1:B:413:LEU:HD12	1:B:416:VAL:HG21	1.95	0.48
1:B:453:ARG:HH11	1:B:453:ARG:CG	2.27	0.48
1:C:327:ALA:C	1:C:329:GLU:N	2.67	0.48
1:B:45:LEU:HD11	1:B:57:ALA:CB	2.42	0.48
1:B:23:LEU:HD21	1:B:195:ALA:HB2	1.95	0.48
1:C:251:TYR:CD1	1:C:397:ILE:CG2	2.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:HG11	1:C:163:SER:HA	1.94	0.48
1:A:131:VAL:HG11	1:A:160:ILE:HG21	1.94	0.48
1:C:107:LEU:O	1:C:110:GLU:N	2.47	0.48
1:B:509:LEU:C	1:B:510:ILE:HD13	2.34	0.48
1:B:556:SER:C	1:B:558:ASN:H	2.15	0.48
1:A:281:LEU:HD21	1:A:389:LEU:CD1	2.44	0.48
1:A:388:ALA:O	1:A:389:LEU:CD1	2.50	0.48
1:C:31:ALA:HB1	1:C:51:VAL:HG22	1.89	0.48
1:B:162:ASP:C	1:B:164:ARG:N	2.61	0.48
1:B:219:VAL:HG12	1:B:220:ASN:N	2.26	0.48
1:B:440:LEU:N	1:B:441:PRO:HD2	2.29	0.48
1:A:314:PHE:CD1	1:A:416:VAL:HG22	2.49	0.48
1:C:139:GLY:HA3	1:C:143:GLU:HB3	1.96	0.48
1:B:275:GLN:CA	1:B:434:VAL:HG11	2.44	0.48
1:B:276:VAL:HG11	1:B:417:ALA:CB	2.43	0.48
1:B:313:TRP:CH2	1:B:413:LEU:HD13	2.43	0.48
1:A:24:GLU:O	1:A:27:GLY:O	2.32	0.48
1:C:92:HIS:HB2	1:C:163:SER:HB2	1.95	0.48
1:A:567:VAL:HG22	1:A:575:PHE:CZ	2.49	0.48
1:B:4:VAL:HG12	1:B:4:VAL:O	2.13	0.48
1:C:470:LEU:HA	1:C:497:TYR:O	2.14	0.48
1:A:504:HIS:NE2	3:A:707:HOH:O	2.35	0.48
1:B:304:TYR:O	1:B:307:GLY:N	2.47	0.48
1:C:489:ILE:HD11	1:C:584:ALA:O	2.13	0.48
1:A:21:ARG:CG	1:A:51:VAL:HG11	2.39	0.48
1:C:96:VAL:HG23	1:C:159:VAL:HB	1.95	0.48
1:B:169:LEU:O	1:B:170:LEU:HD23	2.11	0.48
1:B:453:ARG:HH11	1:B:453:ARG:HG3	1.78	0.48
1:B:34:ALA:C	1:B:35:VAL:CG1	2.81	0.48
1:C:12:VAL:HG13	1:C:66:GLY:O	2.14	0.48
1:C:480:LEU:HD22	1:C:496:ALA:HB3	1.95	0.48
1:A:523:ASN:ND2	1:A:524:GLU:N	2.62	0.48
1:C:307:GLY:C	1:C:324:VAL:HG21	2.33	0.48
1:A:553:PHE:CD2	1:A:559:MET:HE1	2.39	0.48
1:A:457:LEU:HG	1:A:562:ILE:HD11	1.96	0.48
1:A:578:VAL:N	1:A:579:PRO:CD	2.77	0.48
1:B:197:LEU:N	1:B:198:PRO:CD	2.77	0.48
1:B:196:LEU:HD23	1:B:196:LEU:HA	1.29	0.48
1:B:509:LEU:HD11	1:C:493:HIS:HA	1.95	0.48
1:C:25:TYR:CE1	1:C:603:LYS:HG2	2.49	0.48
1:A:155:ALA:HA	1:A:174:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:GLN:CG	1:C:375:ASN:HB3	2.44	0.48
1:A:348:GLN:O	1:A:375:ASN:HB3	2.13	0.48
1:A:103:ASN:ND2	1:A:103:ASN:H	2.12	0.48
1:A:457:LEU:O	1:A:460:ASP:N	2.42	0.48
1:A:296:GLN:HG2	1:A:367:TYR:OH	2.13	0.47
1:C:453:ARG:O	1:C:457:LEU:HD13	2.13	0.47
1:C:529:LEU:HG	1:C:533:ILE:HD11	1.96	0.47
1:A:16:LEU:HD11	1:A:68:GLY:C	2.34	0.47
1:A:4:VAL:HG21	1:A:19:GLY:HA3	1.95	0.47
1:C:112:LYS:HA	1:C:116:TYR:O	2.14	0.47
1:B:400:ALA:O	1:B:402:THR:HG23	2.14	0.47
1:C:27:GLY:O	1:C:29:ASP:OD1	2.32	0.47
1:A:411:VAL:O	1:A:414:MET:HB2	2.14	0.47
1:A:436:GLY:O	1:A:439:ALA:N	2.47	0.47
1:A:266:THR:CG2	1:A:391:THR:O	2.58	0.47
1:B:396:GLU:OE2	1:B:401:SER:CA	2.58	0.47
1:C:583:LEU:O	1:C:583:LEU:HD12	2.14	0.47
1:A:301:GLY:O	1:A:302:THR:C	2.52	0.47
1:B:307:GLY:C	1:B:324:VAL:HG21	2.34	0.47
1:B:476:TYR:CE1	1:B:498:ALA:HB2	2.49	0.47
1:B:501:GLU:HG2	1:C:326:ILE:HG21	1.96	0.47
1:C:536:VAL:CG2	1:C:537:ARG:N	2.76	0.47
1:B:356:LEU:CD1	1:B:360:ARG:HD2	2.44	0.47
1:B:101:ILE:HB	1:B:104:HIS:HB3	1.97	0.47
1:C:214:ILE:O	1:C:214:ILE:HG22	2.13	0.47
1:B:288:LEU:HD12	1:B:288:LEU:N	2.29	0.47
1:A:559:MET:CG	1:A:559:MET:O	2.61	0.47
1:B:145:VAL:O	1:B:149:ILE:HG12	2.15	0.47
1:B:3:ILE:CG2	1:B:4:VAL:N	2.77	0.47
1:B:3:ILE:HD12	1:B:98:ASN:HB3	1.97	0.47
1:A:52:GLN:CA	1:A:52:GLN:HE21	2.25	0.47
1:C:104:HIS:ND1	1:C:123:ASP:HA	2.28	0.47
1:B:588:ALA:O	1:B:592:GLY:N	2.47	0.47
1:C:413:LEU:O	1:C:416:VAL:CB	2.56	0.47
1:C:572:ALA:O	1:C:576:TYR:HD2	1.97	0.47
1:C:245:LYS:HD2	1:C:251:TYR:CZ	2.49	0.47
1:C:251:TYR:HB3	1:C:397:ILE:HB	1.95	0.47
1:C:216:ARG:HE	1:C:217:ARG:NH1	2.12	0.47
1:A:103:ASN:C	1:A:105:GLU:N	2.68	0.47
1:C:35:VAL:CG2	1:C:43:THR:HB	2.45	0.47
1:C:35:VAL:HG23	1:C:43:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASP:O	1:B:287:GLU:C	2.50	0.47
1:A:551:ALA:HB3	1:A:553:PHE:HD1	1.80	0.47
1:A:223:ASP:CG	1:A:224:LYS:N	2.65	0.47
1:C:460:ASP:O	1:C:461:PHE:CD1	2.68	0.47
1:C:11:ASP:HA	1:C:65:GLY:O	2.14	0.47
1:A:250:HIS:CE1	1:A:595:VAL:HB	2.50	0.47
1:A:231:ARG:O	1:A:232:GLN:O	2.31	0.47
1:A:241:ASP:OD2	1:A:254:LYS:HE3	2.14	0.47
1:C:393:ALA:HB1	1:C:403:LYS:HG3	1.97	0.47
1:A:528:LYS:O	1:A:531:SER:HB3	2.14	0.47
1:C:159:VAL:HA	1:C:171:ALA:CB	2.45	0.47
1:A:145:VAL:C	1:A:147:ARG:N	2.68	0.47
1:A:443:ARG:HG2	1:A:443:ARG:HH11	1.79	0.47
1:C:376:VAL:CG1	1:C:377:PRO:HD2	2.43	0.47
1:C:22:ARG:HG2	1:C:22:ARG:HH11	1.80	0.47
1:B:48:LEU:HD21	1:B:81:SER:CB	2.22	0.47
1:B:94:VAL:C	1:B:95:VAL:HG23	2.34	0.47
1:C:259:GLN:N	1:C:260:PRO:CD	2.78	0.47
1:C:159:VAL:HG12	1:C:159:VAL:O	2.14	0.47
1:A:98:ASN:HB3	1:A:176:SER:OG	2.15	0.47
1:C:306:SER:HB2	1:C:346:LEU:CD1	2.42	0.47
1:C:373:ILE:HD12	1:C:412:LEU:HD23	1.96	0.47
1:C:439:ALA:O	1:C:440:LEU:C	2.53	0.47
1:C:578:VAL:CB	1:C:579:PRO:CD	2.82	0.47
1:B:484:LEU:HA	1:B:484:LEU:HD12	1.63	0.47
1:B:488:GLU:OE1	2:B:701:G6Q:C1	2.61	0.47
1:C:485:LYS:CE	1:C:485:LYS:HA	2.33	0.47
1:A:250:HIS:ND1	1:A:595:VAL:HB	2.30	0.47
1:A:173:ARG:HH21	1:A:208:GLU:HB2	1.80	0.47
1:A:22:ARG:C	1:A:23:LEU:HD23	2.30	0.47
1:B:79:GLU:O	1:B:81:SER:N	2.48	0.47
1:C:142:ARG:CG	1:C:146:LEU:HB2	2.44	0.47
1:B:240:TYR:CD1	1:B:241:ASP:HB2	2.50	0.47
1:C:374:CYS:O	1:C:390:MET:HA	2.15	0.47
1:C:544:TYR:CZ	1:C:560:HIS:HD2	2.31	0.47
1:C:486:LEU:O	1:C:490:SER:OG	2.32	0.47
1:B:78:GLY:H	1:C:538:ALA:CB	2.28	0.47
1:C:576:TYR:O	1:C:577:THR:C	2.53	0.47
1:B:223:ASP:OD1	1:B:227:ALA:HB3	2.15	0.47
1:B:356:LEU:HD11	1:B:360:ARG:CD	2.44	0.47
1:C:526:LEU:O	1:C:527:GLU:C	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ILE:HG22	1:B:257:TYR:N	2.28	0.47
1:C:239:GLN:HG2	1:C:239:GLN:O	2.14	0.47
1:C:557:ASP:O	1:C:560:HIS:HE1	1.98	0.47
1:A:443:ARG:CG	1:A:443:ARG:HH11	2.28	0.47
1:A:48:LEU:HA	1:A:48:LEU:HD12	1.51	0.47
1:C:45:LEU:HD21	1:C:57:ALA:CB	2.44	0.47
1:B:276:VAL:HG21	1:B:418:LYS:H	1.79	0.47
1:B:564:MET:HG3	1:B:576:TYR:CE2	2.50	0.47
1:C:263:ILE:HD11	1:C:406:THR:CG2	2.45	0.47
1:A:245:LYS:HG2	1:A:251:TYR:CZ	2.50	0.47
1:A:534:GLU:CA	1:A:534:GLU:OE1	2.63	0.47
1:C:130:LEU:C	1:C:130:LEU:HD23	2.35	0.47
1:B:337:VAL:O	1:B:338:ARG:O	2.32	0.47
1:C:283:PRO:HG2	1:C:284:ASN:N	2.28	0.47
1:A:358:GLY:O	1:A:359:LEU:C	2.51	0.47
1:B:532:ASN:O	1:B:536:VAL:CG2	2.43	0.47
1:B:331:ARG:HD3	1:B:332:TYR:CE2	2.50	0.47
1:C:69:ILE:CG2	1:C:169:LEU:HD11	2.45	0.47
1:B:179:VAL:CG2	1:B:205:PHE:HA	2.29	0.47
1:B:140:THR:O	1:B:144:ALA:N	2.42	0.47
1:B:28:TYR:CE1	1:B:602:ALA:CB	2.98	0.47
1:A:305:ASN:HD22	1:A:481:GLU:HG2	1.80	0.46
1:B:347:SER:HB3	1:B:381:LEU:HD23	1.97	0.46
1:A:195:ALA:O	1:A:198:PRO:HD2	2.15	0.46
1:B:84:ASN:O	1:B:88:HIS:NE2	2.42	0.46
1:A:103:ASN:N	1:A:103:ASN:HD22	2.11	0.46
1:C:126:VAL:O	1:C:130:LEU:HB2	2.15	0.46
1:C:34:ALA:O	1:C:35:VAL:HG13	2.14	0.46
1:C:32:GLY:CA	1:C:86:HIS:O	2.55	0.46
1:A:502:LEU:HB3	1:A:507:LEU:HB2	1.96	0.46
1:B:475:GLN:HE22	1:B:576:TYR:HB2	1.81	0.46
1:C:381:LEU:C	1:C:383:ARG:N	2.67	0.46
1:C:502:LEU:H	1:C:502:LEU:CD1	2.29	0.46
1:C:571:ILE:HG13	1:C:571:ILE:O	2.15	0.46
1:A:490:SER:O	1:A:491:TYR:HB2	2.14	0.46
1:A:409:LEU:HD13	1:A:574:ILE:HG12	1.98	0.46
1:C:304:TYR:OH	1:C:308:MET:HE1	2.14	0.46
1:A:76:THR:HG22	1:A:77:HIS:N	2.30	0.46
1:C:523:ASN:ND2	1:C:569:GLU:CD	2.69	0.46
1:B:451:ASP:O	1:B:452:LYS:C	2.53	0.46
1:C:223:ASP:OD1	1:C:223:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:GLU:OE1	1:C:493:HIS:NE2	2.46	0.46
1:B:509:LEU:HD23	1:B:509:LEU:O	2.16	0.46
1:B:564:MET:HG3	1:B:576:TYR:HE2	1.80	0.46
1:A:25:TYR:HD1	1:A:25:TYR:C	2.17	0.46
1:A:248:TYR:CB	1:A:254:LYS:HB2	2.46	0.46
1:B:355:THR:O	1:B:356:LEU:C	2.53	0.46
1:C:255:GLU:OE1	1:C:396:GLU:HG2	2.16	0.46
1:A:440:LEU:HD21	1:A:574:ILE:CD1	2.45	0.46
1:B:149:ILE:HB	1:B:150:PRO:HD3	1.97	0.46
1:A:165:HIS:C	1:A:167:ASP:N	2.67	0.46
1:C:129:HIS:O	1:C:131:VAL:N	2.49	0.46
1:A:326:ILE:HD12	1:A:326:ILE:HA	1.64	0.46
1:C:327:ALA:O	1:C:330:PHE:N	2.38	0.46
1:C:573:PRO:O	1:C:574:ILE:C	2.51	0.46
1:C:36:VAL:HG21	1:C:163:SER:OG	2.16	0.46
1:B:343:MET:O	1:B:371:LEU:N	2.49	0.46
1:B:577:THR:O	1:B:581:GLN:HG3	2.16	0.46
1:C:314:PHE:CD1	1:C:416:VAL:HG22	2.51	0.46
1:C:570:VAL:CG1	1:C:571:ILE:N	2.59	0.46
1:A:599:ARG:CG	1:A:600:ASN:OD1	2.60	0.46
1:B:21:ARG:CG	1:B:21:ARG:NH1	2.61	0.46
1:B:556:SER:O	1:B:558:ASN:N	2.49	0.46
1:C:255:GLU:OE2	1:C:398:GLY:N	2.43	0.46
1:A:267:LEU:CD2	1:A:414:MET:HE3	2.42	0.46
1:B:179:VAL:HG23	1:B:204:ILE:C	2.36	0.46
1:B:178:LEU:HD11	1:B:189:ILE:HD11	1.98	0.46
1:B:5:GLY:HA3	1:B:189:ILE:CG2	2.45	0.46
1:C:361:LEU:O	1:C:365:LEU:HG	2.16	0.46
1:C:567:VAL:HG11	1:C:575:PHE:CE2	2.51	0.46
1:A:597:GLN:HA	1:A:598:PRO:HD2	1.82	0.46
1:A:36:VAL:HG12	1:A:42:MET:CA	2.46	0.46
1:B:316:SER:OG	1:B:317:LEU:N	2.48	0.46
1:C:56:GLN:C	1:C:58:ALA:H	2.18	0.46
1:A:44:ARG:O	1:A:45:LEU:CD1	2.64	0.46
1:C:487:LYS:HD3	1:C:494:ALA:O	2.15	0.46
1:C:443:ARG:NH1	1:C:568:GLU:OE2	2.44	0.46
1:A:124:THR:C	1:A:126:VAL:N	2.69	0.46
1:A:533:ILE:HG23	1:A:543:LEU:HD22	1.97	0.46
1:C:130:LEU:HD11	1:C:152:LEU:HD21	1.98	0.46
1:A:447:MET:HB2	1:A:447:MET:HE2	1.73	0.46
1:C:599:ARG:HG3	1:C:600:ASN:HD22	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:O	1:C:93:ILE:HG22	2.16	0.46
1:B:270:ARG:HA	1:B:277:ASP:HB3	1.98	0.46
1:A:464:LYS:C	1:A:465:HIS:ND1	2.69	0.46
1:A:285:ALA:C	1:A:287:GLU:H	2.18	0.46
1:A:486:LEU:HD21	1:A:492:ILE:HD12	1.98	0.46
1:C:331:ARG:O	1:C:332:TYR:CD1	2.69	0.46
1:C:373:ILE:HD13	1:C:411:VAL:HG11	1.94	0.46
1:B:487:LYS:HG3	1:C:509:LEU:HD11	1.97	0.46
1:A:251:TYR:H	1:A:596:ASP:CG	2.17	0.46
1:A:195:ALA:O	1:A:198:PRO:CD	2.64	0.46
1:A:86:HIS:CE1	1:A:124:THR:HG1	2.33	0.46
1:B:332:TYR:CZ	1:C:528:LYS:NZ	2.69	0.46
1:C:69:ILE:HG13	1:C:96:VAL:CG2	2.46	0.46
1:B:97:HIS:CB	1:B:158:THR:HB	2.42	0.46
1:A:457:LEU:HD21	1:A:562:ILE:HD13	1.97	0.46
1:A:305:ASN:HD22	1:A:481:GLU:CG	2.29	0.46
1:B:306:SER:HA	1:B:405:PHE:HE1	1.81	0.46
1:B:468:LEU:CG	1:B:470:LEU:HD21	2.46	0.46
1:C:359:LEU:HD22	1:C:381:LEU:HD22	1.98	0.46
1:C:498:ALA:O	1:C:500:GLY:N	2.49	0.46
1:A:146:LEU:CD2	1:A:226:GLY:CA	2.89	0.46
1:A:12:VAL:O	1:A:16:LEU:HG	2.16	0.46
1:A:528:LYS:O	1:A:532:ASN:ND2	2.49	0.46
1:B:334:LYS:HD3	1:B:335:SER:N	2.31	0.46
1:B:237:ASN:C	1:B:239:GLN:NE2	2.69	0.46
1:C:178:LEU:O	1:C:206:LEU:HG	2.16	0.46
1:C:525:LEU:O	1:C:526:LEU:C	2.54	0.46
1:B:32:GLY:CA	1:B:54:LEU:CD2	2.94	0.46
1:A:510:ILE:O	1:A:511:ASP:HB3	2.15	0.46
1:C:201:ARG:NH1	1:C:239:GLN:HG3	2.31	0.46
1:B:293:GLU:OE2	1:B:340:ASN:ND2	2.49	0.46
1:A:134:GLU:OE1	1:A:147:ARG:CB	2.64	0.46
1:C:60:GLU:O	1:C:61:HIS:CB	2.58	0.46
1:C:105:GLU:N	1:C:106:PRO:HD2	2.30	0.46
1:B:523:ASN:ND2	1:B:525:LEU:CB	2.79	0.45
1:C:345:THR:HB	1:C:381:LEU:HD13	1.98	0.45
1:C:188:PHE:CE2	1:C:199:VAL:CG2	2.99	0.45
1:B:179:VAL:HG22	1:B:180:ILE:O	2.16	0.45
1:B:337:VAL:CG1	1:B:365:LEU:HD22	2.47	0.45
1:B:5:GLY:HA3	1:B:189:ILE:HG23	1.97	0.45
1:C:356:LEU:O	1:C:357:ALA:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:PHE:HB3	1:C:561:ILE:HD11	1.97	0.45
1:A:118:PHE:HA	1:A:125:GLU:OE2	2.16	0.45
1:A:17:LEU:HD21	1:A:33:LEU:HD12	1.92	0.45
1:A:510:ILE:HD12	1:A:536:VAL:HG12	1.97	0.45
1:C:255:GLU:HA	1:C:403:LYS:HD3	1.98	0.45
1:B:228:GLU:CG	1:B:229:VAL:N	2.78	0.45
1:B:241:ASP:OD2	1:B:254:LYS:HE2	2.15	0.45
1:B:286:ASP:O	1:B:290:SER:OG	2.26	0.45
1:A:476:TYR:CB	1:A:477:PRO:HD3	2.36	0.45
1:B:426:ASP:OD1	1:B:428:SER:HB3	2.15	0.45
1:B:586:HIS:O	1:B:590:ILE:HD11	2.16	0.45
1:A:25:TYR:C	1:A:27:GLY:H	2.19	0.45
1:A:491:TYR:CE1	1:A:599:ARG:CG	2.99	0.45
1:A:121:GLU:O	1:A:122:THR:CB	2.57	0.45
1:B:46:ARG:O	1:B:47:ARG:CG	2.48	0.45
1:A:440:LEU:HD21	1:A:574:ILE:HG21	1.98	0.45
1:A:347:SER:HB2	1:A:381:LEU:HD11	1.98	0.45
1:B:305:ASN:N	1:B:305:ASN:OD1	2.49	0.45
1:B:350:GLY:HA3	1:B:374:CYS:SG	2.57	0.45
1:B:505:GLY:N	1:B:506:PRO:HD2	2.31	0.45
1:B:570:VAL:HG13	1:B:571:ILE:HG23	1.97	0.45
1:A:28:TYR:CE2	1:A:597:GLN:CB	2.99	0.45
1:A:18:GLU:O	1:A:19:GLY:C	2.54	0.45
1:B:259:GLN:N	1:B:260:PRO:CD	2.80	0.45
1:C:454:ILE:HG23	1:C:583:LEU:HB2	1.97	0.45
1:C:583:LEU:HD12	1:C:587:VAL:HG23	1.98	0.45
1:B:440:LEU:HD12	1:B:440:LEU:O	2.17	0.45
1:B:3:ILE:HD11	1:B:98:ASN:CB	2.47	0.45
1:C:104:HIS:CD2	1:C:108:ARG:HB2	2.51	0.45
1:A:448:LEU:C	1:A:450:GLN:N	2.69	0.45
1:C:417:ALA:HB2	1:C:433:ILE:HD12	1.98	0.45
1:C:495:GLU:OE1	1:C:497:TYR:CE2	2.69	0.45
1:B:502:LEU:C	1:B:506:PRO:HD2	2.37	0.45
1:B:515:PRO:HA	1:B:542:GLN:O	2.17	0.45
1:C:27:GLY:C	1:C:29:ASP:N	2.67	0.45
1:A:124:THR:O	1:A:126:VAL:N	2.50	0.45
1:B:118:PHE:HD2	1:B:125:GLU:HG2	1.80	0.45
1:B:130:LEU:HD11	1:B:151:GLN:NE2	2.32	0.45
1:C:18:GLU:CD	1:C:21:ARG:NH1	2.69	0.45
1:B:264:LYS:HD3	1:B:264:LYS:C	2.36	0.45
1:A:294:HIS:ND1	1:A:338:ARG:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:SER:CB	1:A:381:LEU:HD12	2.47	0.45
1:B:515:PRO:C	1:B:516:VAL:HG23	2.36	0.45
1:C:298:LEU:O	1:C:299:ALA:HB2	2.17	0.45
1:C:546:PHE:CE1	1:C:562:ILE:HD12	2.51	0.45
1:A:28:TYR:CE2	1:A:597:GLN:HB2	2.52	0.45
1:C:74:TRP:HA	1:C:74:TRP:HE3	1.81	0.45
1:A:178:LEU:O	1:A:206:LEU:HB2	2.17	0.45
1:A:175:GLY:H	1:A:208:GLU:CD	2.20	0.45
1:A:20:LEU:O	1:A:22:ARG:N	2.50	0.45
1:B:330:PHE:O	1:B:333:ARG:HG3	2.15	0.45
1:B:37:ASP:O	1:B:38:ALA:C	2.54	0.45
1:B:44:ARG:NH1	1:B:88:HIS:HA	2.31	0.45
1:C:259:GLN:O	1:C:260:PRO:C	2.53	0.45
1:C:127:ILE:CG2	1:C:152:LEU:HD13	2.46	0.45
1:A:111:LEU:C	1:A:113:ALA:N	2.66	0.45
1:C:390:MET:N	1:C:390:MET:SD	2.89	0.45
1:B:3:ILE:HG13	1:B:98:ASN:HB2	1.97	0.45
1:C:511:ASP:OD1	1:C:514:MET:HB2	2.17	0.45
1:C:518:VAL:HB	1:C:545:VAL:HG13	1.97	0.45
1:A:42:MET:SD	1:A:94:VAL:HG21	2.57	0.45
1:A:348:GLN:C	1:A:348:GLN:CD	2.76	0.45
1:C:95:VAL:HG11	1:C:127:ILE:CD1	2.46	0.45
1:B:149:ILE:N	1:B:150:PRO:CD	2.79	0.45
1:C:270:ARG:HD3	1:C:414:MET:CE	2.47	0.45
1:B:270:ARG:O	1:B:277:ASP:N	2.44	0.45
1:A:48:LEU:HD13	1:A:48:LEU:N	2.32	0.45
1:A:356:LEU:CD1	1:A:380:SER:HB3	2.47	0.45
1:B:404:ALA:O	1:B:408:GLN:NE2	2.50	0.45
1:A:491:TYR:CD1	1:A:599:ARG:NH1	2.84	0.45
1:A:399:VAL:HG13	1:A:603:LYS:N	2.31	0.45
1:C:29:ASP:OD2	1:C:74:TRP:HE3	2.00	0.45
1:A:421:LYS:O	1:A:422:LEU:C	2.54	0.45
1:B:240:TYR:HE1	1:B:254:LYS:HZ1	1.64	0.45
1:C:371:LEU:HA	1:C:387:LEU:CB	2.40	0.45
1:A:3:ILE:HG23	1:A:3:ILE:HD13	1.37	0.45
1:C:456:ALA:O	1:C:459:GLU:CD	2.55	0.45
1:A:61:HIS:N	1:A:62:PRO:HD3	2.31	0.45
1:A:295:ILE:HG22	1:A:295:ILE:O	2.15	0.45
1:C:211:ILE:HG22	1:C:212:ALA:N	2.32	0.45
1:B:468:LEU:HD11	1:B:470:LEU:CD2	2.46	0.45
1:B:509:LEU:CD1	1:C:493:HIS:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASP:O	1:A:126:VAL:HB	2.17	0.45
1:A:523:ASN:ND2	1:A:524:GLU:H	2.15	0.45
1:B:181:GLY:HA2	1:B:203:PHE:HD1	1.81	0.45
1:A:559:MET:O	1:A:559:MET:HG3	2.16	0.45
1:C:288:LEU:O	1:C:288:LEU:HD12	2.17	0.45
1:B:399:VAL:HG21	1:B:598:PRO:HD2	1.99	0.45
1:B:299:ALA:HB1	1:B:303:SER:HB3	1.99	0.45
1:C:447:MET:O	1:C:448:LEU:C	2.53	0.45
1:B:126:VAL:CG1	1:B:127:ILE:H	2.24	0.45
1:C:255:GLU:HB3	1:C:403:LYS:HD3	1.99	0.45
1:C:131:VAL:C	1:C:133:TRP:N	2.70	0.45
1:C:173:ARG:CG	1:C:178:LEU:HB2	2.47	0.45
1:A:301:GLY:O	1:A:303:SER:N	2.50	0.45
1:B:61:HIS:CD2	1:B:61:HIS:C	2.89	0.45
1:B:569:GLU:OE1	1:B:569:GLU:HA	2.18	0.45
1:B:281:LEU:HD22	1:B:387:LEU:HB3	1.99	0.44
1:B:379:SER:O	1:B:380:SER:C	2.55	0.44
1:C:356:LEU:HD21	1:C:360:ARG:CZ	2.47	0.44
1:C:413:LEU:O	1:C:416:VAL:N	2.50	0.44
1:C:400:ALA:O	1:C:401:SER:C	2.56	0.44
1:B:123:ASP:C	1:B:126:VAL:HG12	2.38	0.44
1:C:42:MET:SD	1:C:94:VAL:HG21	2.57	0.44
1:C:71:HIS:ND1	1:C:72:THR:N	2.64	0.44
1:B:338:ARG:CZ	1:C:321:PRO:HB3	2.47	0.44
1:C:389:LEU:O	1:C:390:MET:O	2.35	0.44
1:A:502:LEU:HD12	1:A:502:LEU:HA	1.70	0.44
1:C:456:ALA:CA	1:C:459:GLU:OE2	2.65	0.44
1:B:588:ALA:HB1	1:B:593:THR:OG1	2.17	0.44
1:C:510:ILE:HD13	1:C:514:MET:HG2	1.99	0.44
1:A:294:HIS:HE2	1:A:323:ASP:CG	2.20	0.44
1:C:405:PHE:HD2	1:C:577:THR:HG21	1.81	0.44
1:B:32:GLY:CA	1:B:46:ARG:HA	2.46	0.44
1:C:67:THR:HG22	1:C:169:LEU:HD23	1.98	0.44
1:B:251:TYR:CD2	1:B:397:ILE:CG2	3.00	0.44
1:B:110:GLU:OE2	1:B:114:ARG:CZ	2.66	0.44
1:A:251:TYR:CG	1:A:397:ILE:CG2	3.01	0.44
1:A:71:HIS:ND1	1:A:86:HIS:CB	2.66	0.44
1:C:254:LYS:O	1:C:256:ILE:N	2.50	0.44
1:C:36:VAL:HG12	1:C:166:PRO:CG	2.48	0.44
1:B:335:SER:O	1:B:337:VAL:N	2.51	0.44
1:C:234:ILE:HD11	1:C:238:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLU:O	1:B:16:LEU:N	2.50	0.44
1:C:178:LEU:HD22	1:C:206:LEU:CD1	2.47	0.44
1:B:327:ALA:O	1:B:328:SER:C	2.54	0.44
1:A:296:GLN:HE22	1:A:323:ASP:HB2	1.83	0.44
1:B:299:ALA:HB3	1:B:304:TYR:HA	2.00	0.44
1:B:372:ALA:HB2	1:B:385:SER:OG	2.18	0.44
1:C:343:MET:HG3	1:C:344:ILE:N	2.32	0.44
1:B:179:VAL:O	1:B:179:VAL:CG1	2.64	0.44
1:C:107:LEU:C	1:C:109:GLU:N	2.70	0.44
1:C:502:LEU:H	1:C:502:LEU:HD12	1.82	0.44
1:B:44:ARG:NH1	1:B:46:ARG:HH21	2.15	0.44
1:C:215:THR:O	1:C:216:ARG:C	2.56	0.44
1:B:260:PRO:HG3	1:B:444:ILE:HG22	2.00	0.44
1:B:421:LYS:O	1:B:422:LEU:C	2.56	0.44
1:B:458:ALA:O	1:B:459:GLU:C	2.53	0.44
1:B:579:PRO:HA	1:B:582:LEU:HD12	1.99	0.44
1:A:585:TYR:CZ	1:A:589:LEU:HD11	2.53	0.44
1:A:409:LEU:O	1:A:410:THR:C	2.56	0.44
1:C:18:GLU:HA	1:C:21:ARG:HD2	2.00	0.44
1:B:252:MET:HE1	1:B:489:ILE:HD13	2.00	0.44
1:C:179:VAL:O	1:C:179:VAL:CG1	2.64	0.44
1:A:567:VAL:CG1	1:A:568:GLU:H	2.22	0.44
1:A:164:ARG:O	1:A:165:HIS:CE1	2.70	0.44
1:B:281:LEU:CD1	1:B:387:LEU:CD1	2.63	0.44
1:B:391:THR:O	1:B:393:ALA:N	2.49	0.44
1:B:447:MET:HE3	1:B:564:MET:HE1	1.95	0.44
1:A:88:HIS:CD2	1:A:124:THR:HG21	2.52	0.44
1:A:212:ALA:HB2	1:A:221:ILE:HG13	2.00	0.44
1:A:440:LEU:HB3	1:A:441:PRO:CD	2.42	0.44
1:A:292:VAL:HG23	1:A:368:LEU:HD12	2.00	0.44
1:A:352:THR:HG22	1:A:353:ALA:N	2.33	0.44
1:B:490:SER:O	1:B:491:TYR:HB2	2.17	0.44
1:A:12:VAL:HG13	1:A:66:GLY:HA2	2.00	0.44
1:B:42:MET:O	1:B:43:THR:OG1	2.30	0.44
1:C:36:VAL:CG1	1:C:166:PRO:HG3	2.46	0.44
1:C:557:ASP:OD1	1:C:557:ASP:N	2.37	0.44
1:A:530:LYS:C	1:A:530:LYS:HD2	2.38	0.44
1:B:412:LEU:HA	1:B:412:LEU:HD23	1.80	0.44
1:B:491:TYR:CD1	1:B:491:TYR:N	2.81	0.44
1:C:351:GLU:HG2	1:C:380:SER:CB	2.44	0.44
1:A:241:ASP:O	1:A:242:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ALA:O	1:A:88:HIS:CE1	2.71	0.44
1:C:251:TYR:O	1:C:255:GLU:HG3	2.17	0.44
1:C:12:VAL:O	1:C:15:ILE:N	2.51	0.44
1:C:127:ILE:CG2	1:C:152:LEU:CD1	2.92	0.44
1:C:278:LEU:CD2	1:C:414:MET:HE3	2.48	0.44
1:A:89:VAL:CG2	1:A:89:VAL:O	2.65	0.44
1:B:433:ILE:O	1:B:437:LEU:HG	2.18	0.43
1:B:480:LEU:HD23	1:B:496:ALA:HB3	1.99	0.43
1:B:485:LYS:C	1:B:487:LYS:N	2.69	0.43
1:A:250:HIS:HB3	1:A:596:ASP:CG	2.36	0.43
1:A:34:ALA:HB1	1:A:42:MET:HE1	2.00	0.43
1:B:354:ASP:O	1:B:355:THR:C	2.51	0.43
1:B:34:ALA:HB2	1:B:87:PRO:CG	2.34	0.43
1:A:199:VAL:CG2	1:A:200:THR:N	2.64	0.43
1:B:179:VAL:HG23	1:B:205:PHE:N	2.33	0.43
1:B:202:ARG:O	1:B:203:PHE:CD1	2.71	0.43
1:B:294:HIS:CD2	1:B:338:ARG:HG2	2.53	0.43
1:A:136:LYS:CB	1:A:137:GLN:NE2	2.79	0.43
1:A:476:TYR:CD1	1:A:476:TYR:C	2.87	0.43
1:C:107:LEU:N	1:C:107:LEU:HD12	2.32	0.43
1:B:308:MET:HB2	1:B:477:PRO:HB3	2.00	0.43
1:B:348:GLN:OE1	1:B:348:GLN:C	2.57	0.43
1:B:580:LEU:O	1:B:581:GLN:C	2.55	0.43
1:B:600:ASN:HA	1:C:539:ARG:CZ	2.48	0.43
1:C:565:PRO:C	1:C:566:HIS:O	2.55	0.43
1:A:589:LEU:O	1:A:590:ILE:C	2.57	0.43
1:A:178:LEU:HD22	1:A:189:ILE:HD11	1.99	0.43
1:B:124:THR:HG22	1:B:125:GLU:N	2.32	0.43
1:C:259:GLN:CG	1:C:403:LYS:HA	2.48	0.43
1:C:3:ILE:HG22	1:C:4:VAL:N	2.33	0.43
1:C:98:ASN:HD21	1:C:176:SER:HG	1.64	0.43
1:A:35:VAL:HG21	3:A:702:HOH:O	2.19	0.43
1:B:507:LEU:HD12	1:B:507:LEU:O	2.17	0.43
1:B:453:ARG:NH2	1:B:563:GLU:H	2.15	0.43
1:B:567:VAL:HG11	1:B:575:PHE:CE1	2.53	0.43
1:C:373:ILE:HD11	1:C:411:VAL:HG12	1.95	0.43
1:A:253:GLN:HB2	1:A:585:TYR:CE2	2.53	0.43
1:A:239:GLN:C	1:A:241:ASP:N	2.72	0.43
1:A:36:VAL:O	1:A:65:GLY:HA2	2.18	0.43
1:B:20:LEU:HA	1:B:20:LEU:HD23	1.65	0.43
1:C:505:GLY:O	1:C:508:ALA:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:HIS:C	1:C:131:VAL:N	2.72	0.43
1:B:8:ALA:O	1:B:216:ARG:HB2	2.18	0.43
1:A:48:LEU:HD11	1:A:81:SER:C	2.39	0.43
1:B:405:PHE:HD2	1:B:577:THR:HG21	1.83	0.43
1:A:36:VAL:O	1:A:65:GLY:HA3	2.18	0.43
1:A:344:ILE:HG12	1:A:371:LEU:HB3	2.00	0.43
1:C:255:GLU:CB	1:C:403:LYS:HD3	2.48	0.43
1:B:3:ILE:C	1:B:4:VAL:CG2	2.87	0.43
1:B:397:ILE:HA	1:B:397:ILE:HD13	1.67	0.43
1:C:463:ASP:OD1	1:C:464:LYS:N	2.51	0.43
1:B:470:LEU:N	1:B:470:LEU:HD23	2.33	0.43
1:C:467:ALA:N	1:C:493:HIS:O	2.51	0.43
1:A:173:ARG:NH2	1:A:208:GLU:HB2	2.33	0.43
1:A:239:GLN:OE1	1:A:240:TYR:N	2.52	0.43
1:C:86:HIS:NE2	1:C:97:HIS:CE1	2.87	0.43
1:C:135:LEU:CD1	1:C:164:ARG:HH22	2.20	0.43
1:B:220:ASN:O	1:B:221:ILE:C	2.57	0.43
1:A:132:ASN:OD1	1:A:133:TRP:N	2.52	0.43
1:A:330:PHE:CD1	1:A:331:ARG:N	2.86	0.43
1:B:606:THR:HG22	1:B:606:THR:O	2.19	0.43
1:B:483:ALA:O	1:B:487:LYS:CB	2.62	0.43
1:B:487:LYS:HE2	1:B:494:ALA:O	2.19	0.43
1:B:549:GLN:C	1:B:551:ALA:H	2.22	0.43
1:B:553:PHE:HD2	1:B:559:MET:CE	2.31	0.43
1:B:578:VAL:O	1:B:582:LEU:HG	2.19	0.43
1:C:306:SER:N	1:C:405:PHE:HE1	2.17	0.43
1:C:576:TYR:C	1:C:579:PRO:HD2	2.39	0.43
1:A:491:TYR:CD2	1:A:599:ARG:NH1	2.86	0.43
1:A:211:ILE:O	1:A:212:ALA:C	2.57	0.43
1:C:187:ASN:OD1	1:C:219:VAL:HG21	2.18	0.43
1:A:437:LEU:C	1:A:439:ALA:N	2.71	0.43
1:A:111:LEU:O	1:A:113:ALA:CA	2.65	0.43
1:C:203:PHE:O	1:C:233:ASP:HB2	2.17	0.43
1:B:267:LEU:HB3	1:B:414:MET:SD	2.59	0.43
1:B:283:PRO:C	1:B:285:ALA:N	2.71	0.43
1:C:258:GLU:O	1:C:262:ALA:HB2	2.19	0.43
1:B:412:LEU:O	1:B:416:VAL:HG23	2.19	0.43
1:B:468:LEU:CD1	1:B:470:LEU:HD21	2.49	0.43
1:B:504:HIS:CE1	1:C:300:CYS:CB	3.01	0.43
1:C:405:PHE:CZ	1:C:409:LEU:HD11	2.54	0.43
1:C:571:ILE:HB	1:C:574:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:ALA:HB1	1:C:593:THR:HG23	2.00	0.43
1:A:251:TYR:CD2	1:A:397:ILE:HG21	2.53	0.43
1:A:413:LEU:HD12	1:A:413:LEU:HA	1.84	0.43
1:C:259:GLN:HG2	1:C:403:LYS:HA	2.01	0.43
1:A:149:ILE:C	1:A:151:GLN:H	2.22	0.43
1:B:237:ASN:HA	1:B:239:GLN:HE22	1.82	0.43
1:A:300:CYS:O	1:A:301:GLY:C	2.57	0.43
1:A:401:SER:H	2:A:700:G6Q:H2	1.84	0.43
1:B:476:TYR:HB3	1:B:477:PRO:CD	2.44	0.43
1:B:578:VAL:H	1:B:578:VAL:HG23	1.53	0.43
1:B:180:ILE:CD1	1:B:206:LEU:HD21	2.49	0.43
1:C:289:LEU:O	1:C:422:LEU:CD2	2.65	0.43
1:C:353:ALA:HB2	1:C:606:THR:C	2.39	0.43
1:B:249:ARG:O	1:B:249:ARG:CG	2.65	0.43
1:B:553:PHE:CD2	1:B:559:MET:CE	3.02	0.43
1:C:447:MET:HE3	1:C:578:VAL:CG1	2.49	0.43
1:A:196:LEU:C	1:A:198:PRO:CD	2.83	0.43
1:B:555:SER:C	1:B:556:SER:HG	2.22	0.43
1:B:258:GLU:O	1:B:262:ALA:HB2	2.19	0.43
1:C:197:LEU:HD23	1:C:203:PHE:CZ	2.51	0.43
1:B:219:VAL:C	1:B:220:ASN:OD1	2.58	0.43
1:C:270:ARG:HD3	1:C:414:MET:HE1	2.01	0.43
1:B:267:LEU:O	1:B:270:ARG:HB2	2.19	0.43
1:B:283:PRO:O	1:B:285:ALA:N	2.52	0.43
1:B:519:VAL:HG11	1:B:576:TYR:HB3	2.01	0.43
1:C:485:LYS:N	1:C:485:LYS:HE3	2.34	0.43
1:A:122:THR:HG23	1:A:125:GLU:CB	2.49	0.43
1:B:356:LEU:CD1	1:B:360:ARG:CD	2.96	0.43
1:B:312:TYR:O	1:B:316:SER:HB3	2.19	0.43
1:C:83:VAL:HG12	1:C:120:SER:OG	2.19	0.43
1:A:457:LEU:O	1:A:459:GLU:N	2.52	0.43
1:C:298:LEU:HG	1:C:343:MET:SD	2.59	0.42
1:C:356:LEU:HD13	1:C:380:SER:HB3	2.00	0.42
1:A:251:TYR:N	1:A:596:ASP:OD2	2.42	0.42
1:A:178:LEU:HA	1:A:190:ALA:O	2.19	0.42
1:A:529:LEU:C	1:A:531:SER:N	2.71	0.42
1:B:294:HIS:HE1	1:B:296:GLN:HB2	1.84	0.42
1:B:458:ALA:C	1:B:460:ASP:N	2.70	0.42
1:B:169:LEU:HD23	1:B:169:LEU:HA	1.70	0.42
1:B:170:LEU:HA	1:B:212:ALA:O	2.19	0.42
1:C:63:LEU:N	1:C:63:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:CD1	1:B:235:GLU:N	2.80	0.42
1:A:377:PRO:O	1:A:378:GLY:C	2.58	0.42
1:B:478:ILE:HG13	1:B:573:PRO:HA	2.00	0.42
1:A:585:TYR:CE1	1:A:595:VAL:HG11	2.54	0.42
1:A:510:ILE:HD11	1:A:536:VAL:HG12	1.97	0.42
1:C:88:HIS:NE2	1:C:124:THR:HB	2.34	0.42
1:B:294:HIS:O	1:B:342:LEU:N	2.46	0.42
1:C:320:ILE:HA	1:C:321:PRO:HD3	1.89	0.42
1:A:141:LEU:O	1:A:143:GLU:N	2.51	0.42
1:C:89:VAL:O	1:C:129:HIS:NE2	2.53	0.42
1:C:131:VAL:O	1:C:133:TRP:N	2.53	0.42
1:C:281:LEU:HD12	1:C:285:ALA:HB1	2.00	0.42
1:B:443:ARG:O	1:B:446:GLN:HB3	2.19	0.42
1:C:178:LEU:HD22	1:C:206:LEU:HD12	2.01	0.42
1:B:583:LEU:HD12	1:B:587:VAL:HG23	1.99	0.42
1:C:453:ARG:NH1	1:C:563:GLU:O	2.52	0.42
1:C:546:PHE:CE2	1:C:579:PRO:HB2	2.53	0.42
1:A:598:PRO:HG3	1:A:601:LEU:HD12	2.00	0.42
1:C:585:TYR:CZ	1:C:589:LEU:HD11	2.54	0.42
1:C:73:ARG:HG2	1:C:74:TRP:H	1.83	0.42
1:A:42:MET:HE3	1:A:43:THR:H	1.84	0.42
1:A:412:LEU:O	1:A:413:LEU:C	2.56	0.42
1:A:388:ALA:C	1:A:389:LEU:CD1	2.86	0.42
1:C:251:TYR:CD1	1:C:397:ILE:CB	3.02	0.42
1:C:348:GLN:HB3	1:C:348:GLN:HE21	1.49	0.42
1:B:293:GLU:HG3	1:B:340:ASN:HB2	2.02	0.42
1:B:90:SER:O	1:B:90:SER:OG	2.36	0.42
1:A:139:GLY:HA2	1:A:143:GLU:OE1	2.20	0.42
1:A:14:GLU:CG	1:A:14:GLU:O	2.63	0.42
1:B:513:ASP:O	1:B:514:MET:CB	2.61	0.42
1:B:5:GLY:O	1:B:6:ALA:HB2	2.20	0.42
1:A:538:ALA:C	1:A:539:ARG:HG2	2.39	0.42
1:C:429:ILE:O	1:C:430:GLU:C	2.57	0.42
1:C:302:THR:HG22	1:C:302:THR:O	2.18	0.42
1:A:463:ASP:N	1:A:463:ASP:OD1	2.51	0.42
1:A:360:ARG:O	1:A:363:LYS:HB2	2.19	0.42
1:A:305:ASN:HD22	1:A:481:GLU:HA	1.84	0.42
1:B:46:ARG:HG2	1:B:46:ARG:H	1.59	0.42
1:B:193:GLN:C	1:B:195:ALA:H	2.23	0.42
1:C:234:ILE:HD12	1:C:235:GLU:CA	2.48	0.42
1:A:506:PRO:C	1:A:508:ALA:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ARG:N	1:A:338:ARG:CD	2.81	0.42
1:B:266:THR:CG2	1:B:411:VAL:HG23	2.50	0.42
1:B:343:MET:HB3	1:B:370:SER:CA	2.49	0.42
1:C:381:LEU:O	1:C:383:ARG:N	2.53	0.42
1:C:348:GLN:O	1:C:348:GLN:NE2	2.52	0.42
1:C:127:ILE:HA	1:C:130:LEU:CB	2.50	0.42
1:B:218:SER:OG	1:B:219:VAL:N	2.51	0.42
1:A:148:ALA:O	1:A:149:ILE:C	2.57	0.42
1:C:90:SER:OG	1:C:129:HIS:CG	2.73	0.42
1:C:234:ILE:HD12	1:C:234:ILE:C	2.40	0.42
1:C:426:ASP:OD1	1:C:428:SER:OG	2.33	0.42
1:B:374:CYS:SG	1:B:375:ASN:N	2.92	0.42
1:B:523:ASN:C	1:B:525:LEU:H	2.22	0.42
1:A:266:THR:HG22	1:A:270:ARG:HH12	1.84	0.42
1:A:529:LEU:CA	1:A:532:ASN:ND2	2.79	0.42
1:C:224:LYS:CE	1:C:225:THR:HG23	2.48	0.42
1:B:238:LEU:HD23	1:B:242:ALA:HA	2.01	0.42
1:B:246:GLY:O	1:B:248:TYR:N	2.53	0.42
1:C:89:VAL:O	1:C:129:HIS:CE1	2.72	0.42
1:C:583:LEU:CD1	1:C:587:VAL:HG23	2.50	0.42
1:A:554:VAL:HG12	1:A:555:SER:O	2.20	0.42
1:B:464:LYS:C	1:B:465:HIS:ND1	2.73	0.42
1:A:356:LEU:HD13	1:A:380:SER:HB3	2.01	0.42
1:B:453:ARG:NH1	1:B:453:ARG:CG	2.81	0.42
1:C:409:LEU:O	1:C:412:LEU:N	2.53	0.42
1:A:237:ASN:O	1:A:239:GLN:OE1	2.38	0.42
1:A:248:TYR:CD2	1:A:254:LYS:CG	3.03	0.42
1:B:83:VAL:O	1:B:88:HIS:HE1	2.02	0.42
1:A:421:LYS:C	1:A:423:LYS:N	2.73	0.42
1:A:105:GLU:C	1:A:107:LEU:N	2.73	0.42
1:C:476:TYR:O	1:C:479:ALA:CB	2.66	0.42
1:C:135:LEU:C	1:C:137:GLN:H	2.23	0.42
1:C:486:LEU:HD11	1:C:587:VAL:HG11	2.02	0.42
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.84	0.42
1:A:3:ILE:HD12	1:A:3:ILE:HG21	1.53	0.42
1:B:376:VAL:O	1:B:379:SER:OG	2.19	0.42
1:B:507:LEU:HD12	1:B:510:ILE:CG1	2.26	0.42
1:C:533:ILE:CG2	1:C:559:MET:CE	2.98	0.42
1:A:266:THR:HA	1:A:392:ASN:ND2	2.34	0.42
1:C:79:GLU:N	1:C:80:PRO:CD	2.83	0.42
1:B:286:ASP:HB3	1:B:422:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:HIS:H	1:C:62:PRO:CD	2.27	0.42
1:A:505:GLY:C	1:A:507:LEU:N	2.72	0.42
1:A:565:PRO:O	1:A:566:HIS:C	2.58	0.42
1:C:532:ASN:HD22	1:C:532:ASN:N	2.06	0.42
1:A:86:HIS:CE1	1:A:124:THR:OG1	2.73	0.42
1:B:33:LEU:HB3	1:B:70:ALA:HB2	2.01	0.42
1:B:555:SER:C	1:B:556:SER:OG	2.58	0.42
1:B:205:PHE:CD1	1:B:205:PHE:N	2.88	0.42
1:C:18:GLU:OE2	1:C:21:ARG:CZ	2.68	0.42
1:B:425:LEU:HG	1:B:426:ASP:N	2.35	0.42
1:C:523:ASN:OD1	1:C:569:GLU:OE2	2.36	0.42
1:B:61:HIS:O	1:B:61:HIS:CG	2.70	0.42
1:B:450:GLN:O	1:B:454:ILE:HG13	2.20	0.42
1:B:308:MET:CB	1:B:477:PRO:HB3	2.50	0.42
1:B:433:ILE:CG1	1:B:570:VAL:CG2	2.97	0.42
1:C:330:PHE:C	1:C:332:TYR:N	2.73	0.42
1:C:379:SER:O	1:C:380:SER:C	2.58	0.42
1:C:408:GLN:O	1:C:409:LEU:C	2.58	0.42
1:A:599:ARG:C	1:A:601:LEU:H	2.23	0.42
1:A:36:VAL:CG1	1:A:42:MET:CA	2.84	0.42
1:B:356:LEU:HD12	1:B:360:ARG:HD2	2.01	0.42
1:A:80:PRO:HB2	1:A:83:VAL:HB	2.02	0.42
1:A:306:SER:O	1:A:307:GLY:C	2.57	0.41
1:B:297:ILE:CD1	1:B:324:VAL:HG22	2.44	0.41
1:C:530:LYS:HA	1:C:533:ILE:HD12	2.02	0.41
1:C:250:HIS:NE2	1:C:589:LEU:HD21	2.35	0.41
1:B:20:LEU:HD11	1:B:70:ALA:HB1	2.02	0.41
1:A:375:ASN:CG	1:A:393:ALA:HB3	2.39	0.41
1:A:133:TRP:CE3	1:A:134:GLU:OE2	2.73	0.41
1:C:93:ILE:HG21	1:C:131:VAL:CB	2.49	0.41
1:C:386:ASP:C	1:C:387:LEU:HG	2.40	0.41
1:A:32:GLY:CA	1:A:54:LEU:HD21	2.48	0.41
1:B:255:GLU:O	1:B:403:LYS:HB3	2.21	0.41
1:B:408:GLN:O	1:B:412:LEU:HB2	2.20	0.41
1:B:468:LEU:HD21	1:B:470:LEU:HD21	2.02	0.41
1:B:483:ALA:HB1	1:B:494:ALA:O	2.20	0.41
1:C:300:CYS:O	1:C:303:SER:HB2	2.19	0.41
1:C:502:LEU:CD1	1:C:502:LEU:N	2.82	0.41
1:A:74:TRP:CZ2	1:A:601:LEU:HA	2.55	0.41
1:B:22:ARG:HG2	1:B:194:LEU:CD2	2.50	0.41
1:A:529:LEU:C	1:A:532:ASN:ND2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:MET:CE	1:C:185:GLY:N	2.82	0.41
1:C:224:LYS:HZ2	1:C:225:THR:CG2	2.31	0.41
1:C:111:LEU:HB2	1:C:118:PHE:HE1	1.85	0.41
1:A:32:GLY:HA3	1:A:45:LEU:O	2.20	0.41
1:B:326:ILE:HG23	1:C:501:GLU:OE2	2.20	0.41
1:B:306:SER:OG	1:B:307:GLY:N	2.53	0.41
1:B:276:VAL:CG2	1:B:417:ALA:CB	2.93	0.41
1:B:34:ALA:HA	1:B:43:THR:O	2.20	0.41
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.84	0.41
1:C:95:VAL:HG13	1:C:96:VAL:H	1.85	0.41
1:C:111:LEU:CD1	1:C:116:TYR:CD2	2.91	0.41
1:A:100:ILE:CD1	1:A:607:VAL:CA	2.95	0.41
1:A:324:VAL:CG1	1:A:324:VAL:O	2.64	0.41
1:C:489:ILE:HD11	1:C:584:ALA:C	2.40	0.41
1:C:565:PRO:HD2	1:C:575:PHE:HE2	1.84	0.41
1:A:67:THR:HG22	1:A:161:MET:SD	2.60	0.41
1:C:525:LEU:O	1:C:528:LYS:N	2.53	0.41
1:A:276:VAL:CG1	1:A:276:VAL:O	2.68	0.41
1:B:503:LYS:HE2	1:C:601:LEU:HD23	2.03	0.41
1:A:224:LYS:HE2	1:A:224:LYS:HB3	1.80	0.41
1:B:237:ASN:CA	1:B:239:GLN:HE22	2.33	0.41
1:A:45:LEU:CD2	1:A:57:ALA:O	2.68	0.41
1:A:353:ALA:HB2	1:A:607:VAL:O	2.20	0.41
1:B:309:VAL:CG2	1:B:477:PRO:HB2	2.50	0.41
1:B:576:TYR:C	1:B:579:PRO:HD2	2.41	0.41
1:C:359:LEU:CD2	1:C:381:LEU:HD22	2.50	0.41
1:C:27:GLY:H	1:C:602:ALA:HB1	1.86	0.41
1:A:231:ARG:C	1:A:232:GLN:O	2.58	0.41
1:B:118:PHE:CD1	1:B:118:PHE:N	2.88	0.41
1:A:574:ILE:HG21	1:A:574:ILE:HD13	1.74	0.41
1:A:527:GLU:O	1:A:528:LYS:C	2.58	0.41
1:C:71:HIS:HD2	1:C:96:VAL:CB	2.34	0.41
1:B:180:ILE:HG13	1:B:206:LEU:HD21	2.02	0.41
1:A:567:VAL:CG1	1:A:568:GLU:N	2.66	0.41
1:A:131:VAL:CG2	1:A:145:VAL:HG22	2.50	0.41
1:A:548:ASP:OD1	1:A:549:GLN:N	2.53	0.41
1:C:105:GLU:O	1:C:108:ARG:HB3	2.20	0.41
1:A:48:LEU:CD1	1:A:48:LEU:N	2.78	0.41
1:A:312:TYR:CE2	1:A:473:GLY:O	2.72	0.41
1:B:119:VAL:HG23	1:B:119:VAL:O	2.18	0.41
1:B:527:GLU:O	1:B:528:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:PHE:HD2	1:B:561:ILE:CD1	2.33	0.41
1:A:251:TYR:CD1	1:A:397:ILE:HG21	2.55	0.41
1:C:145:VAL:O	1:C:147:ARG:N	2.53	0.41
1:A:128:ALA:O	1:A:129:HIS:C	2.54	0.41
1:C:173:ARG:HE	1:C:177:PRO:HA	1.85	0.41
1:B:105:GLU:HB3	1:B:106:PRO:CD	2.48	0.41
1:A:497:TYR:CZ	1:A:506:PRO:HB3	2.56	0.41
1:A:307:GLY:C	1:A:324:VAL:HG11	2.41	0.41
1:B:313:TRP:HZ2	1:B:573:PRO:CG	2.34	0.41
1:B:549:GLN:C	1:B:551:ALA:N	2.74	0.41
1:B:600:ASN:HA	1:C:539:ARG:NE	2.35	0.41
1:A:28:TYR:CE1	1:A:602:ALA:HA	2.53	0.41
1:C:399:VAL:HG11	1:C:602:ALA:O	2.18	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.44	0.41
1:A:247:ILE:HD13	1:A:248:TYR:CD2	2.56	0.41
1:A:535:GLU:O	1:A:536:VAL:C	2.56	0.41
1:A:276:VAL:HG13	1:A:276:VAL:O	2.19	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.78	0.41
1:A:525:LEU:O	1:A:526:LEU:C	2.59	0.41
1:C:169:LEU:HA	1:C:169:LEU:HD13	1.87	0.41
1:C:192:ASP:OD2	1:C:194:LEU:HB2	2.21	0.41
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.58	0.41
1:C:61:HIS:O	1:C:63:LEU:HD22	2.20	0.41
1:A:457:LEU:O	1:A:458:ALA:C	2.57	0.41
1:A:282:GLY:HA2	1:A:283:PRO:HD2	1.85	0.41
1:A:467:ALA:O	1:A:494:ALA:HA	2.20	0.41
1:A:356:LEU:HA	1:A:381:LEU:CD2	2.48	0.41
1:B:520:ALA:HA	1:B:521:PRO:HD3	1.79	0.41
1:C:466:HIS:HA	1:C:493:HIS:O	2.21	0.41
1:C:576:TYR:C	1:C:578:VAL:N	2.69	0.41
1:A:16:LEU:HB3	1:A:70:ALA:HB2	2.02	0.41
1:B:325:GLU:OE2	1:B:333:ARG:NH2	2.51	0.41
1:C:472:ARG:O	1:C:475:GLN:HB2	2.20	0.41
1:B:146:LEU:HA	1:B:146:LEU:HD12	1.83	0.41
1:C:165:HIS:N	1:C:166:PRO:CD	2.83	0.41
1:A:104:HIS:O	1:A:104:HIS:CG	2.74	0.41
1:A:107:LEU:C	1:A:109:GLU:N	2.74	0.41
1:B:234:ILE:CG1	1:B:235:GLU:H	2.29	0.41
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.89	0.41
1:B:103:ASN:C	1:B:105:GLU:H	2.22	0.41
1:B:281:LEU:CD2	1:B:387:LEU:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:TYR:CD2	1:B:599:ARG:CZ	3.04	0.41
1:B:599:ARG:O	1:B:600:ASN:HB2	2.21	0.41
1:C:447:MET:CE	1:C:578:VAL:HB	2.51	0.41
1:B:371:LEU:O	1:B:372:ALA:HB2	2.21	0.41
1:B:454:ILE:CD1	1:B:582:LEU:HD12	2.48	0.41
1:C:263:ILE:O	1:C:266:THR:CB	2.63	0.41
1:C:437:LEU:O	1:C:440:LEU:CB	2.69	0.41
1:A:74:TRP:CZ3	1:A:602:ALA:O	2.74	0.41
1:B:537:ARG:CZ	1:B:558:ASN:HD21	2.28	0.41
1:A:499:ALA:HB1	1:A:532:ASN:OD1	2.20	0.41
1:C:166:PRO:O	1:C:167:ASP:C	2.59	0.41
1:C:127:ILE:HA	1:C:130:LEU:HB3	2.03	0.41
1:B:7:ILE:HD13	1:B:215:THR:HA	2.02	0.41
1:B:234:ILE:H	1:B:234:ILE:HG23	1.63	0.41
1:B:271:ILE:HG22	1:B:271:ILE:O	2.20	0.41
1:B:452:LYS:HA	1:B:452:LYS:HD3	1.81	0.41
1:C:514:MET:HB2	1:C:514:MET:HE3	1.85	0.41
1:C:421:LYS:HB3	1:C:421:LYS:HE3	1.64	0.41
1:B:390:MET:CE	1:B:390:MET:HA	2.51	0.41
1:C:528:LYS:O	1:C:531:SER:N	2.52	0.41
1:B:130:LEU:HD11	1:B:151:GLN:HE22	1.85	0.41
1:A:440:LEU:HD21	1:A:574:ILE:HD12	2.03	0.41
1:C:7:ILE:HD13	1:C:168:THR:O	2.20	0.41
1:B:7:ILE:H	1:B:7:ILE:HG22	1.50	0.41
1:B:267:LEU:CB	1:B:414:MET:SD	3.09	0.41
1:A:454:ILE:HD12	1:A:582:LEU:HD12	2.03	0.41
1:A:457:LEU:CD2	1:A:562:ILE:HD13	2.52	0.41
1:C:45:LEU:CD2	1:C:57:ALA:O	2.69	0.41
1:B:359:LEU:O	1:B:363:LYS:HG2	2.22	0.40
1:B:480:LEU:O	1:B:483:ALA:N	2.54	0.40
1:B:504:HIS:NE2	1:C:300:CYS:SG	2.95	0.40
1:B:600:ASN:O	1:C:507:LEU:HD23	2.21	0.40
1:B:487:LYS:CD	1:C:509:LEU:HD11	2.50	0.40
1:A:440:LEU:CD2	1:A:574:ILE:CD1	2.99	0.40
1:A:102:GLU:C	1:A:104:HIS:N	2.72	0.40
1:A:457:LEU:HD21	1:A:562:ILE:CD1	2.51	0.40
1:C:173:ARG:HD3	1:C:207:GLU:O	2.21	0.40
1:B:8:ALA:O	1:B:9:GLN:HB2	2.20	0.40
1:A:359:LEU:HD11	1:A:370:SER:HB3	2.03	0.40
1:B:554:VAL:HG23	1:B:554:VAL:O	2.20	0.40
1:A:26:ARG:HH11	1:A:26:ARG:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LEU:CD2	1:C:54:LEU:HD21	2.52	0.40
1:C:230:LYS:C	1:C:231:ARG:HD3	2.37	0.40
1:B:601:LEU:O	1:B:602:ALA:HB2	2.22	0.40
1:C:55:ALA:O	1:C:58:ALA:HB3	2.20	0.40
1:C:28:TYR:CD2	1:C:50:LYS:HD3	2.56	0.40
1:B:159:VAL:HG22	1:B:171:ALA:CB	2.49	0.40
1:B:109:GLU:O	1:B:110:GLU:C	2.59	0.40
1:B:504:HIS:CE1	1:C:300:CYS:HB3	2.56	0.40
1:C:314:PHE:CE1	1:C:416:VAL:CG2	3.03	0.40
1:C:480:LEU:O	1:C:483:ALA:N	2.53	0.40
1:C:184:MET:CA	1:C:184:MET:HE2	2.50	0.40
1:C:96:VAL:CG2	1:C:159:VAL:HB	2.52	0.40
1:C:222:PHE:HA	1:C:228:GLU:HA	2.03	0.40
1:C:102:GLU:O	1:C:104:HIS:N	2.48	0.40
1:B:116:TYR:HE2	1:B:133:TRP:HB2	1.86	0.40
1:B:390:MET:HE2	1:B:390:MET:HA	2.02	0.40
1:A:305:ASN:O	1:A:308:MET:N	2.54	0.40
1:B:507:LEU:O	1:B:509:LEU:N	2.54	0.40
1:C:331:ARG:HD2	1:C:354:ASP:HA	2.02	0.40
1:C:547:ALA:O	1:C:549:GLN:N	2.53	0.40
1:C:553:PHE:CB	1:C:561:ILE:HD12	2.50	0.40
1:A:34:ALA:HB1	1:A:42:MET:CE	2.51	0.40
1:A:267:LEU:HD22	1:A:414:MET:HE2	2.02	0.40
1:C:480:LEU:O	1:C:483:ALA:HB3	2.22	0.40
1:A:402:THR:OG1	1:A:403:LYS:N	2.54	0.40
1:C:86:HIS:CD2	1:C:88:HIS:NE2	2.89	0.40
1:B:24:GLU:CD	1:B:597:GLN:NE2	2.70	0.40
1:B:320:ILE:HA	1:B:321:PRO:HD2	1.93	0.40
1:B:458:ALA:C	1:B:460:ASP:H	2.25	0.40
1:A:149:ILE:HB	1:A:150:PRO:CD	2.44	0.40
1:B:4:VAL:O	1:B:16:LEU:HD21	2.21	0.40
1:B:105:GLU:N	1:B:106:PRO:HD2	2.34	0.40
1:B:572:ALA:CB	1:B:573:PRO:CD	2.91	0.40
1:A:601:LEU:O	1:A:602:ALA:HB2	2.22	0.40
1:C:252:MET:O	1:C:253:GLN:C	2.59	0.40
1:A:197:LEU:HA	1:A:197:LEU:HD22	1.51	0.40
1:A:22:ARG:O	1:A:194:LEU:HD23	2.22	0.40
1:B:48:LEU:CD1	1:B:82:GLU:HB2	2.51	0.40
1:C:407:THR:HG23	1:C:407:THR:H	1.63	0.40
1:C:6:ALA:CB	1:C:12:VAL:HG11	2.47	0.40
1:A:417:ALA:HA	1:A:420:SER:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HA	1:C:171:ALA:CA	2.49	0.40
1:A:133:TRP:HZ3	1:A:134:GLU:OE2	2.02	0.40
1:C:580:LEU:O	1:C:583:LEU:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LYS:NZ	1:A:497:TYR:OH[2_555]	2.05	0.15

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	606/608 (100%)	417 (69%)	128 (21%)	61 (10%)	1	4
1	B	606/608 (100%)	423 (70%)	113 (19%)	70 (12%)	0	2
1	C	606/608 (100%)	374 (62%)	164 (27%)	68 (11%)	0	3
All	All	1818/1824 (100%)	1214 (67%)	405 (22%)	199 (11%)	0	3

All (199) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	71	HIS
1	A	77	HIS
1	A	103	ASN
1	A	111	LEU
1	A	112	LYS
1	A	125	GLU
1	A	128	ALA
1	A	129	HIS

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Mol	Chain	Res	Type
1	A	199	VAL
1	A	212	ALA
1	A	238	LEU
1	A	240	TYR
1	A	273	HIS
1	A	280	GLU
1	A	283	PRO
1	A	424	GLY
1	A	485	LYS
1	A	541	GLY
1	A	600	ASN
1	A	603	LYS
1	A	604	SER
1	A	607	VAL
1	B	4	VAL
1	B	9	GLN
1	B	13	ALA
1	B	81	SER
1	B	91	GLU
1	B	119	VAL
1	B	123	ASP
1	B	163	SER
1	B	186	GLU
1	B	221	ILE
1	B	234	ILE
1	B	236	SER
1	B	285	ALA
1	B	312	TYR
1	B	330	PHE
1	B	338	ARG
1	B	414	MET
1	B	417	ALA
1	B	459	GLU
1	B	485	LYS
1	B	493	HIS
1	B	499	ALA
1	B	603	LYS
1	C	7	ILE
1	C	28	TYR
1	C	61	HIS
1	C	64	HIS
1	C	81	SER

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Mol	Chain	Res	Type
1	C	227	ALA
1	C	328	SER
1	C	331	ARG
1	C	349	SER
1	C	488	GLU
1	C	499	ALA
1	C	541	GLY
1	C	550	ASP
1	C	595	VAL
1	A	104	HIS
1	A	108	ARG
1	A	142	ARG
1	A	146	LEU
1	A	193	GLN
1	A	232	GLN
1	A	274	GLY
1	A	282	GLY
1	A	309	VAL
1	A	385	SER
1	A	438	GLN
1	A	449	SER
1	B	38	ALA
1	B	45	LEU
1	B	113	ALA
1	B	241	ASP
1	B	284	ASN
1	B	310	SER
1	B	336	ALA
1	B	353	ALA
1	B	366	GLY
1	B	368	LEU
1	B	386	ASP
1	B	418	LYS
1	B	512	ALA
1	B	516	VAL
1	B	595	VAL
1	C	13	ALA
1	C	51	VAL
1	C	78	GLY
1	C	82	GLU
1	C	108	ARG
1	C	130	LEU

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Mol	Chain	Res	Type
1	C	138	GLY
1	C	141	LEU
1	C	146	LEU
1	C	169	LEU
1	C	187	ASN
1	C	233	ASP
1	C	283	PRO
1	C	367	TYR
1	C	368	LEU
1	C	370	SER
1	C	390	MET
1	C	448	LEU
1	C	461	PHE
1	C	507	LEU
1	C	523	ASN
1	C	549	GLN
1	C	566	HIS
1	C	600	ASN
1	A	14	GLU
1	A	105	GLU
1	A	121	GLU
1	A	196	LEU
1	A	284	ASN
1	A	286	ASP
1	A	425	LEU
1	A	439	ALA
1	A	568	GLU
1	A	594	ASP
1	A	602	ALA
1	B	95	VAL
1	B	114	ARG
1	B	175	GLY
1	B	247	ILE
1	B	372	ALA
1	B	380	SER
1	B	508	ALA
1	B	557	ASP
1	C	37	ASP
1	C	66	GLY
1	C	103	ASN
1	C	299	ALA
1	C	319	GLY

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Mol	Chain	Res	Type
1	C	378	GLY
1	C	429	ILE
1	C	548	ASP
1	C	598	PRO
1	A	80	PRO
1	A	308	MET
1	A	548	ASP
1	B	6	ALA
1	B	43	THR
1	B	167	ASP
1	B	194	LEU
1	B	246	GLY
1	B	273	HIS
1	B	356	LEU
1	B	405	PHE
1	B	500	GLY
1	C	75	ALA
1	C	91	GLU
1	C	132	ASN
1	C	174	SER
1	C	195	ALA
1	C	280	GLU
1	C	383	ARG
1	C	459	GLU
1	C	551	ALA
1	A	102	GLU
1	A	122	THR
1	A	150	PRO
1	A	166	PRO
1	A	245	LYS
1	A	301	GLY
1	A	386	ASP
1	A	511	ASP
1	B	34	ALA
1	B	306	SER
1	B	331	ARG
1	B	355	THR
1	B	392	ASN
1	B	514	MET
1	B	521	PRO
1	B	523	ASN
1	C	106	PRO

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Mol	Chain	Res	Type
1	C	216	ARG
1	C	260	PRO
1	C	442	SER
1	A	410	THR
1	B	105	GLU
1	B	410	THR
1	C	80	PRO
1	C	197	LEU
1	C	433	ILE
1	A	139	GLY
1	B	12	VAL
1	C	219	VAL
1	B	32	GLY
1	B	36	VAL
1	C	573	PRO
1	B	40	GLY
1	B	260	PRO
1	C	183	GLY
1	C	229	VAL
1	C	398	GLY
1	A	115	GLY
1	A	378	GLY

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	500/500 (100%)	393 (79%)	107 (21%)	1 5
1	B	500/500 (100%)	422 (84%)	78 (16%)	3 14
1	C	500/500 (100%)	433 (87%)	67 (13%)	5 20
All	All	1500/1500 (100%)	1248 (83%)	252 (17%)	2 11

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	3	ILE
1	A	25	TYR
1	A	26	ARG
1	A	30	SER
1	A	33	LEU
1	A	35	VAL
1	A	36	VAL
1	A	42	MET
1	A	44	ARG
1	A	46	ARG
1	A	48	LEU
1	A	51	VAL
1	A	52	GLN
1	A	97	HIS
1	A	102	GLU
1	A	103	ASN
1	A	114	ARG
1	A	125	GLU
1	A	131	VAL
1	A	132	ASN
1	A	140	THR
1	A	146	LEU
1	A	161	MET
1	A	163	SER
1	A	170	LEU
1	A	180	ILE
1	A	189	ILE
1	A	194	LEU
1	A	197	LEU
1	A	202	ARG
1	A	211	ILE
1	A	221	ILE
1	A	223	ASP
1	A	224	LYS
1	A	233	ASP
1	A	235	GLU
1	A	239	GLN
1	A	240	TYR
1	A	247	ILE
1	A	259	GLN
1	A	266	THR
1	A	268	THR

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Mol	Chain	Res	Type
1	A	273	HIS
1	A	279	SER
1	A	288	LEU
1	A	290	SER
1	A	296	GLN
1	A	303	SER
1	A	326	ILE
1	A	333	ARG
1	A	337	VAL
1	A	341	SER
1	A	346	LEU
1	A	347	SER
1	A	348	GLN
1	A	349	SER
1	A	351	GLU
1	A	359	LEU
1	A	361	LEU
1	A	362	SER
1	A	368	LEU
1	A	370	SER
1	A	371	LEU
1	A	376	VAL
1	A	379	SER
1	A	380	SER
1	A	383	ARG
1	A	390	MET
1	A	391	THR
1	A	395	THR
1	A	397	ILE
1	A	401	SER
1	A	403	LYS
1	A	420	SER
1	A	422	LEU
1	A	428	SER
1	A	433	ILE
1	A	441	PRO
1	A	442	SER
1	A	443	ARG
1	A	457	LEU
1	A	464	LYS
1	A	465	HIS
1	A	468	LEU

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Mol	Chain	Res	Type
1	A	476	TYR
1	A	481	GLU
1	A	492	ILE
1	A	502	LEU
1	A	503	LYS
1	A	511	ASP
1	A	518	VAL
1	A	519	VAL
1	A	523	ASN
1	A	525	LEU
1	A	528	LYS
1	A	530	LYS
1	A	532	ASN
1	A	534	GLU
1	A	555	SER
1	A	556	SER
1	A	558	ASN
1	A	559	MET
1	A	561	ILE
1	A	570	VAL
1	A	599	ARG
1	A	600	ASN
1	B	14	GLU
1	B	21	ARG
1	B	33	LEU
1	B	35	VAL
1	B	37	ASP
1	B	46	ARG
1	B	53	MET
1	B	59	GLU
1	B	63	LEU
1	B	72	THR
1	B	86	HIS
1	B	93	ILE
1	B	120	SER
1	B	124	THR
1	B	135	LEU
1	B	143	GLU
1	B	152	LEU
1	B	158	THR
1	B	161	MET
1	B	163	SER

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Mol	Chain	Res	Type
1	B	170	LEU
1	B	174	SER
1	B	178	LEU
1	B	184	MET
1	B	186	GLU
1	B	187	ASN
1	B	206	LEU
1	B	208	GLU
1	B	210	ASP
1	B	215	THR
1	B	218	SER
1	B	221	ILE
1	B	223	ASP
1	B	225	THR
1	B	232	GLN
1	B	233	ASP
1	B	234	ILE
1	B	239	GLN
1	B	245	LYS
1	B	248	TYR
1	B	252	MET
1	B	257	TYR
1	B	259	GLN
1	B	267	LEU
1	B	273	HIS
1	B	302	THR
1	B	303	SER
1	B	306	SER
1	B	316	SER
1	B	334	LYS
1	B	348	GLN
1	B	362	SER
1	B	385	SER
1	B	395	THR
1	B	423	LYS
1	B	428	SER
1	B	429	ILE
1	B	440	LEU
1	B	442	SER
1	B	447	MET
1	B	453	ARG
1	B	454	ILE

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Mol	Chain	Res	Type
1	B	503	LYS
1	B	509	LEU
1	B	513	ASP
1	B	514	MET
1	B	523	ASN
1	B	524	GLU
1	B	526	LEU
1	B	528	LYS
1	B	536	VAL
1	B	548	ASP
1	B	556	SER
1	B	568	GLU
1	B	571	ILE
1	B	591	LYS
1	B	594	ASP
1	B	607	VAL
1	C	10	ARG
1	C	15	ILE
1	C	21	ARG
1	C	33	LEU
1	C	35	VAL
1	C	47	ARG
1	C	63	LEU
1	C	69	ILE
1	C	74	TRP
1	C	79	GLU
1	C	90	SER
1	C	118	PHE
1	C	120	SER
1	C	158	THR
1	C	163	SER
1	C	169	LEU
1	C	176	SER
1	C	178	LEU
1	C	184	MET
1	C	186	GLU
1	C	187	ASN
1	C	191	SER
1	C	194	LEU
1	C	196	LEU
1	C	200	THR
1	C	217	ARG

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Mol	Chain	Res	Type
1	C	222	PHE
1	C	224	LYS
1	C	230	LYS
1	C	234	ILE
1	C	238	LEU
1	C	247	ILE
1	C	272	SER
1	C	306	SER
1	C	322	CYS
1	C	328	SER
1	C	333	ARG
1	C	334	LYS
1	C	338	ARG
1	C	348	GLN
1	C	349	SER
1	C	368	LEU
1	C	390	MET
1	C	402	THR
1	C	421	LYS
1	C	452	LYS
1	C	457	LEU
1	C	461	PHE
1	C	462	SER
1	C	485	LYS
1	C	490	SER
1	C	497	TYR
1	C	518	VAL
1	C	523	ASN
1	C	524	GLU
1	C	527	GLU
1	C	528	LYS
1	C	531	SER
1	C	532	ASN
1	C	534	GLU
1	C	539	ARG
1	C	545	VAL
1	C	557	ASP
1	C	590	ILE
1	C	591	LYS
1	C	593	THR
1	C	604	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	56	GLN
1	A	84	ASN
1	A	88	HIS
1	A	103	ASN
1	A	137	GLN
1	A	151	GLN
1	A	265	ASN
1	A	296	GLN
1	A	305	ASN
1	A	392	ASN
1	A	435	HIS
1	A	438	GLN
1	A	523	ASN
1	A	532	ASN
1	A	549	GLN
1	B	61	HIS
1	B	64	HIS
1	B	86	HIS
1	B	137	GLN
1	B	151	GLN
1	B	165	HIS
1	B	187	ASN
1	B	239	GLN
1	B	250	HIS
1	B	296	GLN
1	B	375	ASN
1	B	438	GLN
1	B	466	HIS
1	B	475	GLN
1	B	493	HIS
1	B	523	ASN
1	B	532	ASN
1	B	558	ASN
1	B	600	ASN
1	C	98	ASN
1	C	137	GLN
1	C	193	GLN
1	C	239	GLN
1	C	250	HIS
1	C	265	ASN
1	C	340	ASN

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Mol	Chain	Res	Type
1	C	348	GLN
1	C	375	ASN
1	C	438	GLN
1	C	465	HIS
1	C	523	ASN
1	C	560	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	G6Q	A	700	-	15,15,15	2.13	6 (40%)	18,21,21	2.85	11 (61%)
2	G6Q	B	701	1	15,15,15	1.38	3 (20%)	18,21,21	2.05	5 (27%)

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
2	G6Q	A	700	-	-	0/18/20/20	0/0/0/0
2	G6Q	B	701	1	-	0/18/20/20	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	G6Q	O5-C5	-3.19	1.36	1.43
2	A	700	G6Q	P-O2P	-2.96	1.44	1.54
2	B	701	G6Q	C3-C2	-2.63	1.48	1.53
2	B	701	G6Q	O4-C4	-2.44	1.37	1.43
2	A	700	G6Q	C3-C2	-2.33	1.49	1.53
2	A	700	G6Q	C6-C5	-2.14	1.48	1.51
2	A	700	G6Q	P-O3P	-2.12	1.47	1.54
2	B	701	G6Q	C2-C1	2.19	1.54	1.50
2	A	700	G6Q	C2-C1	4.59	1.58	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	G6Q	C3-C2-C1	-4.79	104.62	111.68
2	B	701	G6Q	O1-C1-C2	-4.56	112.30	125.60
2	A	700	G6Q	O1-C1-C2	-4.45	112.63	125.60
2	A	700	G6Q	O2-C2-C1	-4.26	100.05	110.22
2	A	700	G6Q	O3P-P-O1P	-4.12	97.30	110.58
2	B	701	G6Q	O2-C2-C1	-3.97	100.73	110.22
2	A	700	G6Q	O3-C3-C4	-3.07	102.08	109.45
2	B	701	G6Q	O3-C3-C4	-2.47	103.53	109.45
2	A	700	G6Q	O6-P-O1P	2.09	112.47	107.14
2	B	701	G6Q	O6-P-O1P	2.14	112.60	107.14
2	A	700	G6Q	O4-C4-C3	2.22	114.77	109.45
2	A	700	G6Q	O3P-P-O6	2.26	113.08	106.56
2	A	700	G6Q	C4-C3-C2	3.01	118.82	113.57
2	B	701	G6Q	O4-C4-C3	3.17	117.06	109.45
2	A	700	G6Q	O3P-P-O2P	3.56	120.94	107.38
2	A	700	G6Q	O5-C5-C4	3.95	118.95	109.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	G6Q	4	0
2	B	701	G6Q	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	608/608 (100%)	-0.72	6 (0%) 84 69	9, 38, 101, 133	0
1	B	608/608 (100%)	-0.51	6 (0%) 84 69	19, 78, 125, 138	0
1	C	608/608 (100%)	0.08	32 (5%) 30 13	44, 113, 137, 151	0
All	All	1824/1824 (100%)	-0.38	44 (2%) 62 39	9, 79, 131, 151	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	8.8
1	C	89	VAL	5.7
1	C	81	SER	5.7
1	B	240	TYR	4.9
1	A	85	ALA	4.7
1	B	522	ASN	4.7
1	C	84	ASN	4.6
1	C	83	VAL	3.4
1	C	237	ASN	3.2
1	C	82	GLU	3.2
1	C	105	GLU	3.2
1	C	41	HIS	3.0
1	C	117	THR	3.0
1	A	81	SER	2.9
1	C	138	GLY	2.9
1	C	80	PRO	2.9
1	C	88	HIS	2.9
1	C	229	VAL	2.9
1	C	78	GLY	2.7
1	C	248	TYR	2.6
1	C	62	PRO	2.6
1	C	225	THR	2.6
1	C	240	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	88	HIS	2.5
1	C	351	GLU	2.5
1	C	74	TRP	2.5
1	C	38	ALA	2.5
1	B	80	PRO	2.4
1	C	230	LYS	2.4
1	B	340	ASN	2.4
1	C	85	ALA	2.4
1	A	83	VAL	2.4
1	C	522	ASN	2.4
1	C	61	HIS	2.3
1	C	435	HIS	2.3
1	C	347	SER	2.3
1	B	272	SER	2.3
1	C	100	ILE	2.2
1	C	235	GLU	2.1
1	C	236	SER	2.1
1	C	287	GLU	2.1
1	B	271	ILE	2.1
1	A	80	PRO	2.0
1	C	159	VAL	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
2	G6Q	B	701	16/16	0.94	0.17	0.78	62,73,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	G6Q	A	700	16/16	0.96	0.13	0.38	25,31,35,36	0

6.5 Other polymers (i)

There are no such residues in this entry.