Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID	:	3H7N
Title	:	Structure of Nup120
Authors	:	Seo, H.S.; Ma, Y.; Debler, E.W.; Blobel, G.; Hoelz, A.
Deposited on	:	2009-04-27
Resolution	:	3.00 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 ⓘ symbol.

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

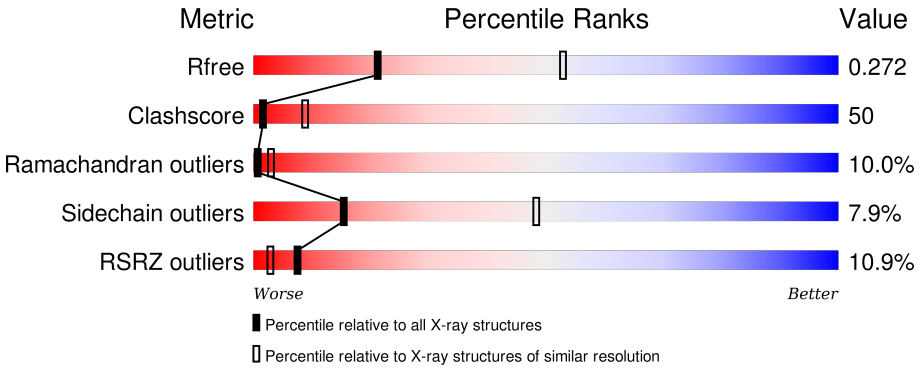
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	729	11% 31% 53% 12% .
1	B	729	10% 31% 53% 12% .
1	C	729	11% 31% 54% 12% .
1	D	729	10% 32% 53% 11% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22992 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 Nucleoporin NUP120.

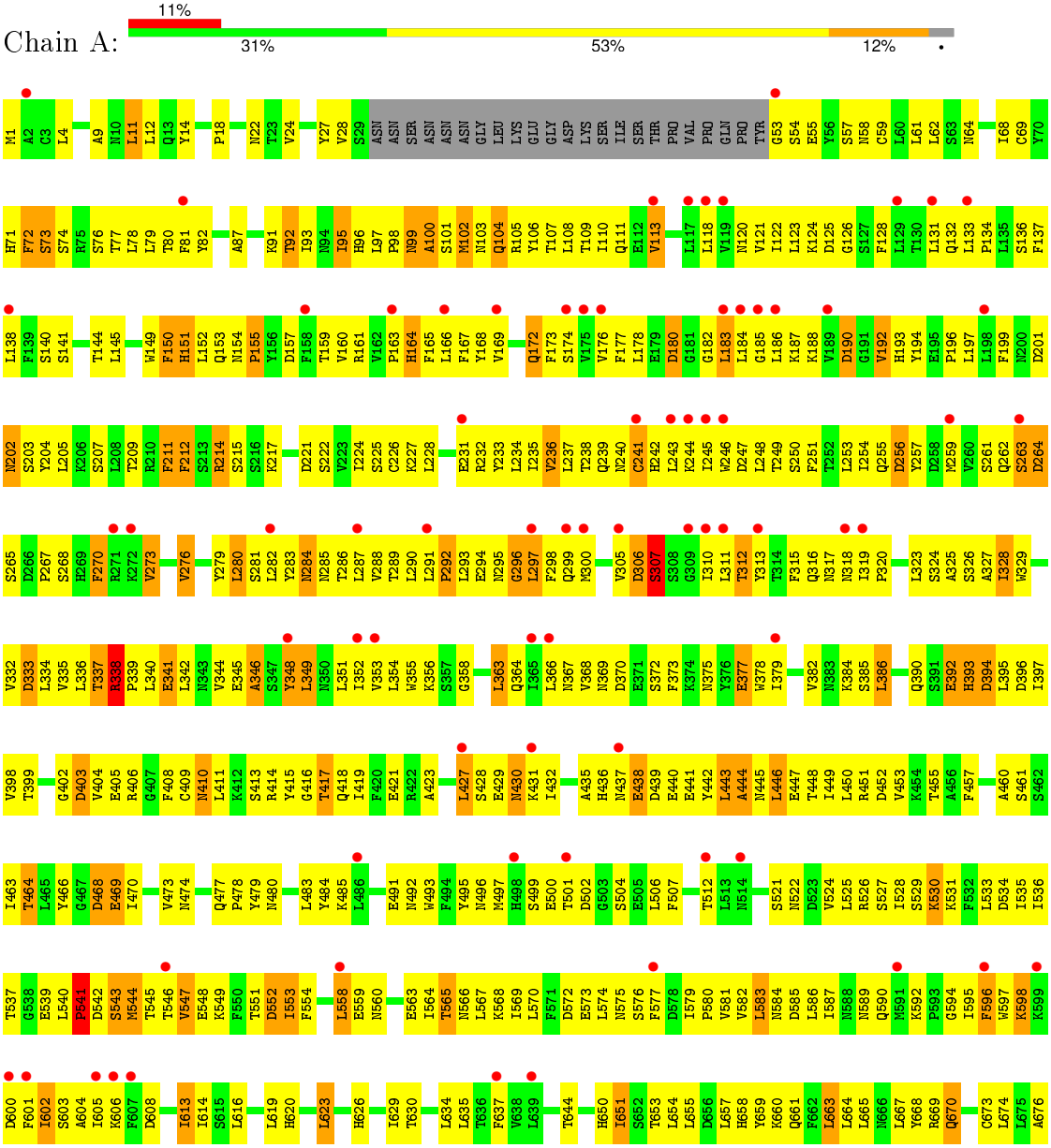
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	0
			5748	3718	913	1099	18			
1	B	706	Total	C	N	O	S	0	0	0
			5748	3718	913	1099	18			
1	C	706	Total	C	N	O	S	0	0	0
			5748	3718	913	1099	18			
1	D	706	Total	C	N	O	S	0	0	0
			5748	3718	913	1099	18			

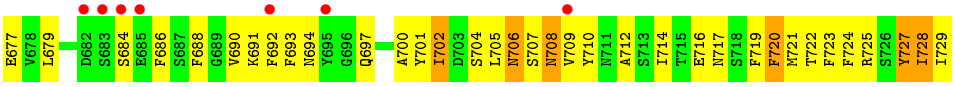
3 Residue-property plots (i)

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: Nucleoporin NUP120

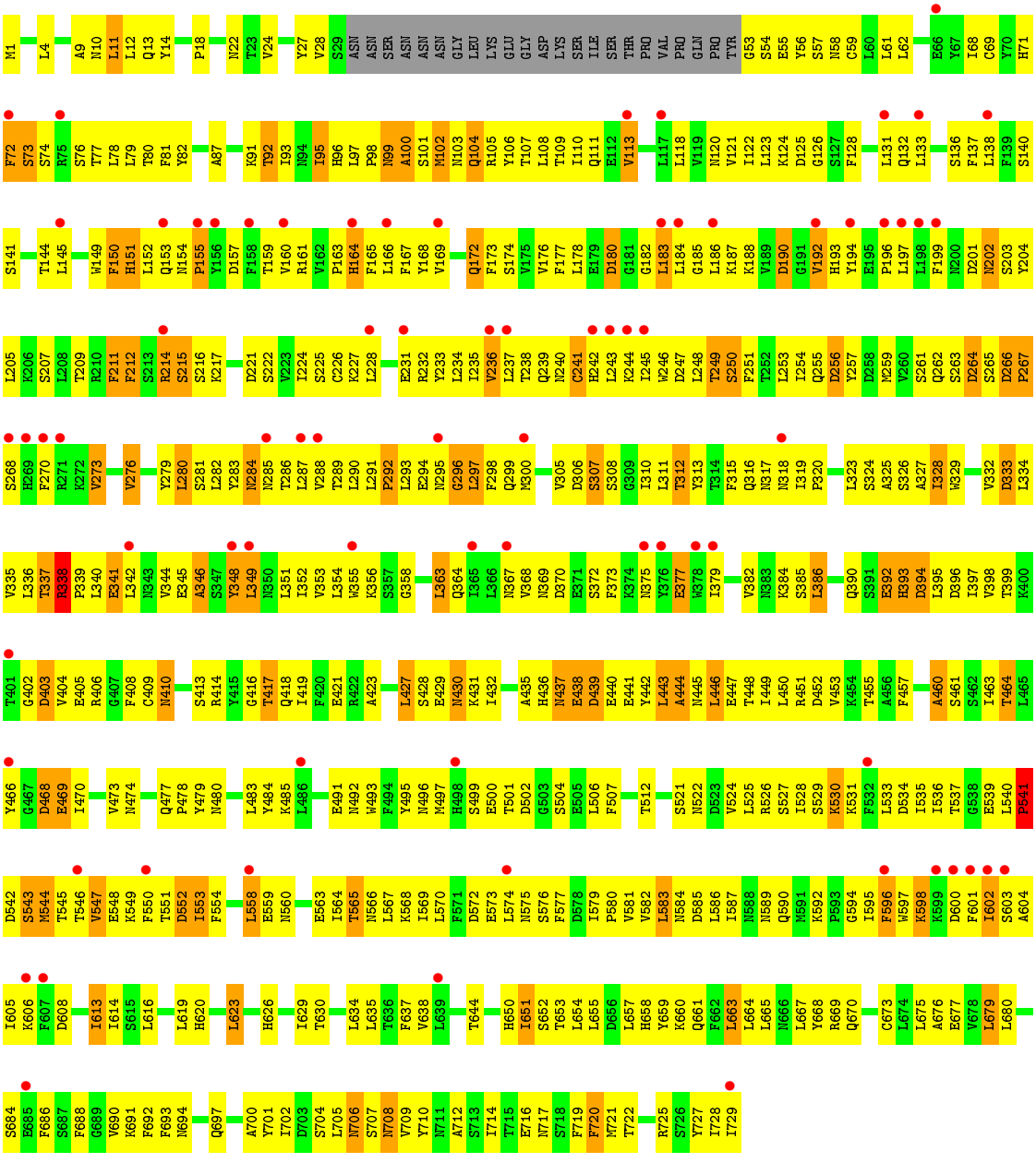
Chain A:





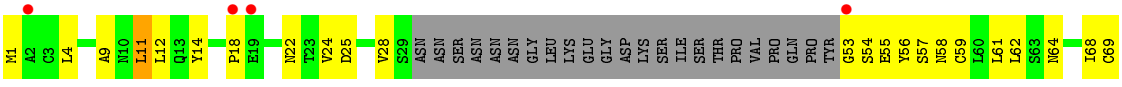
• Molecule 1: Nucleoporin NUP120

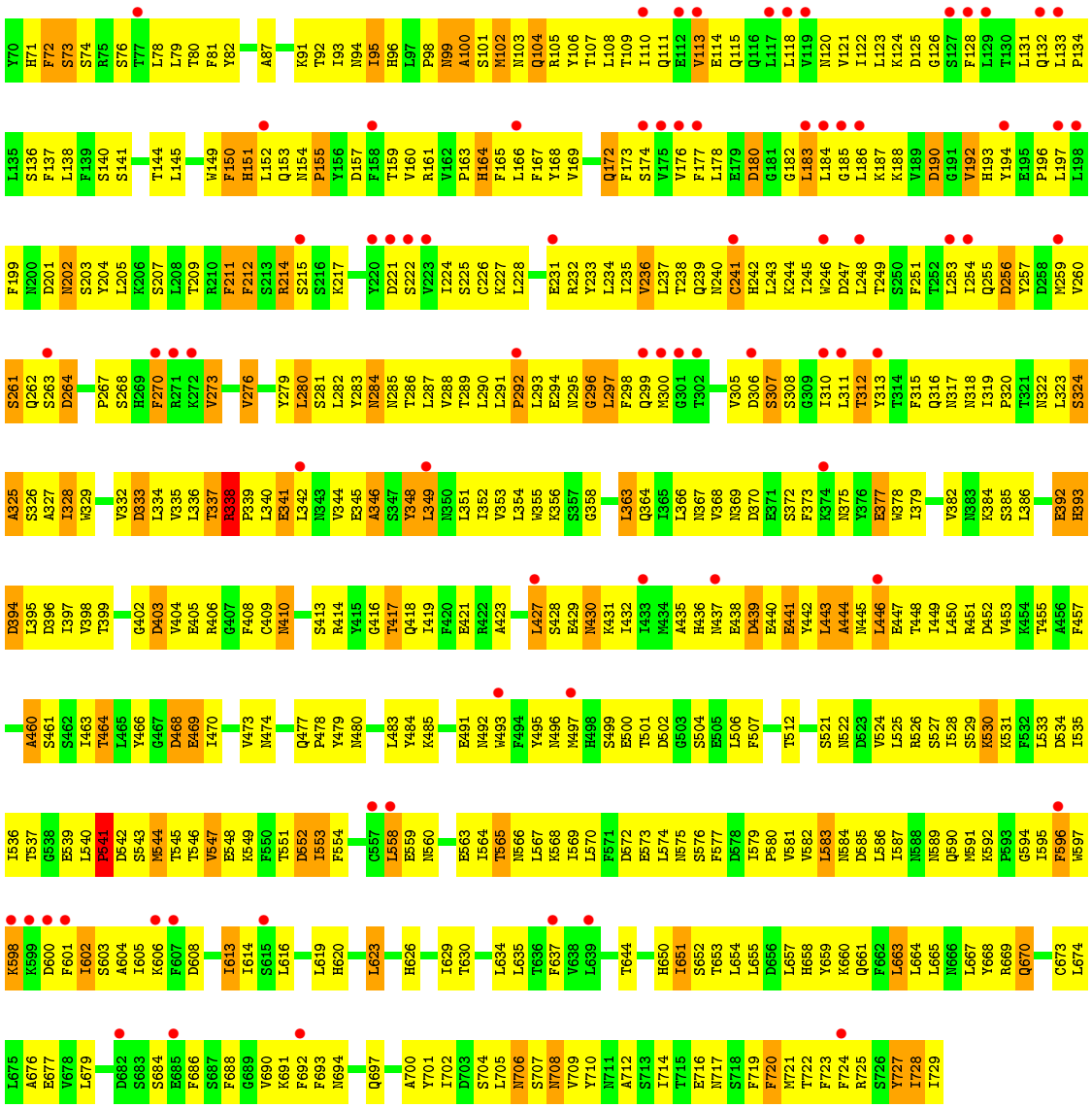
Chain B:



• Molecule 1: Nucleoporin NUP120

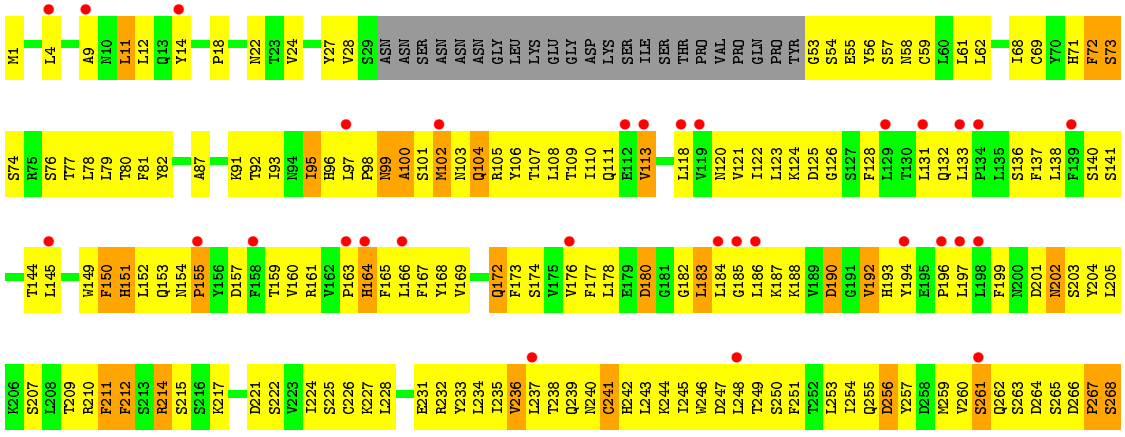
Chain C:

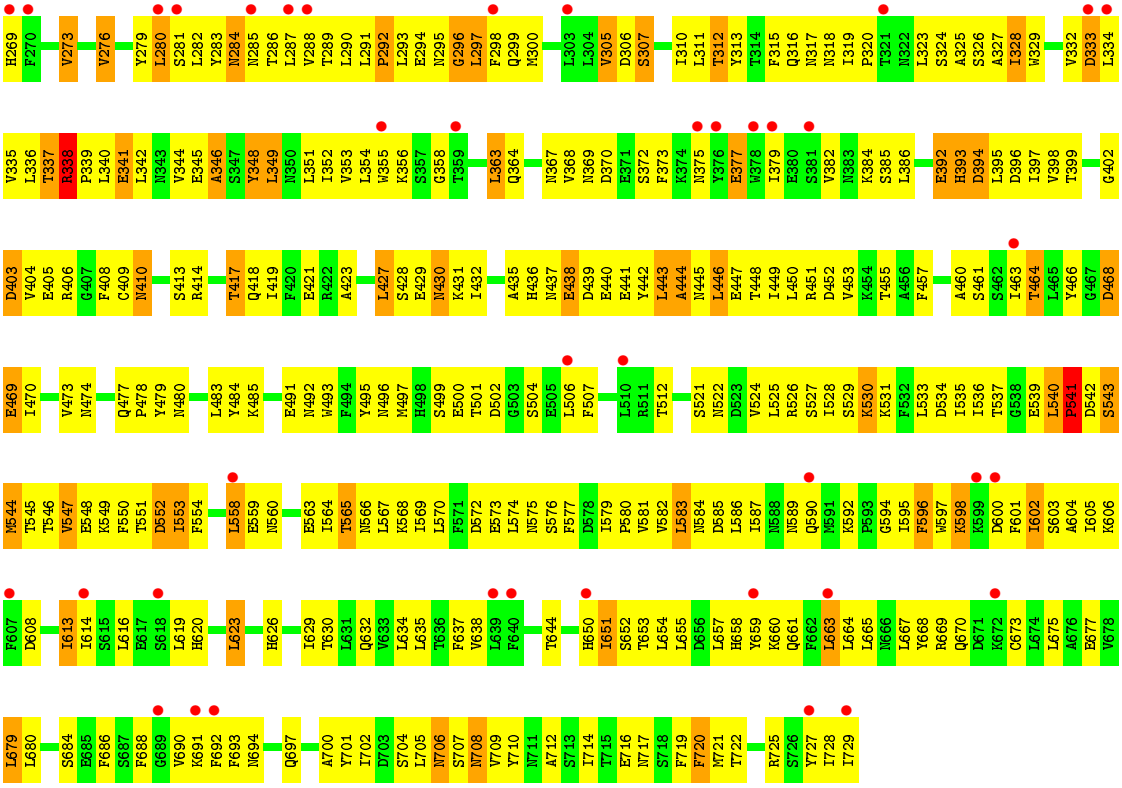




• Molecule 1: Nucleoporin NUP120

Chain D:




H269 F270 V273 V276 Y279 L280 S281 L282 Y283 N284 N285 T286 L287 V288 T289 L290 L291 P292 L293 E294 N295 G296 L297 F298 Q299 N300 L303 L304 V305 D306 S307 I310 L311 T312 Y313 T314 F315 Q316 N317 N318 I319 P320 T321 N322 L323 S324 A325 S326 A327 I328 W329 V332 D333 L334
V335 L336 T337 R338 P339 L340 E341 L342 N343 V344 E345 A346 S347 Y348 L349 N350 L351 I352 V353 L354 W355 K356 S357 G358 T359 L363 Q364 N367 V368 N369 D370 E371 S372 F373 K374 N375 Y376 E377 W378 I379 E380 S381 V382 N383 K384 S385 L386 E392 H393 D394 L395 D396 I397 V398 T399 G402
D403 V404 E405 R406 G407 F408 C409 N410 S413 R414 T417 Q418 I419 F420 E421 R422 A423 L427 S428 E429 N430 K431 I432 A435 H436 N437 E438 D439 E440 E441 Y442 L443 A444 N445 L446 E447 T448 I449 L450 R451 D452 V453 K454 T455 A456 F457 A460 S461 S462 I463 T464 L465 Y466 G467 D468
E469 I470 V473 N474 Q477 P478 Y479 N480 L483 Y484 K485 E491 N492 W493 F494 Y495 N496 M497 H498 S499 E500 T501 D502 G503 S504 E505 L506 F507 L510 R511 T512 S521 N522 D523 V524 L525 R526 S527 I528 S529 K530 K531 F532 L533 D534 I535 I536 T537 G538 E539 L540 F541 D542 S543
M544 T545 T546 V547 E548 K549 F550 T551 D552 I553 F554 L558 E559 N560 E563 I564 T566 N566 L567 K568 I569 L570 F571 D572 E573 L574 N575 S576 F577 D578 I579 P580 V581 V582 L583 N584 D585 L586 I587 N588 N589 Q590 M591 K592 P593 G594 I595 P596 W597 K598 K599 D600 F601 I602 S603 A604 I605 K606
F607 D608 I613 I614 S615 L616 E617 S618 L619 H620 L623 H626 I629 T630 L631 Q632 V633 L634 L635 T636 F637 V638 L639 F640 T644 H650 I651 S652 T653 L654 L655 D656 L657 H658 Y659 K660 Q661 F662 L663 L664 L665 N666 L667 Y668 R669 Q670 D671 K672 C673 L674 L675 A676 E677 V678
L679 L680 S684 E685 F686 S687 F688 G689 V690 K691 F692 F693 N694 Q697 A700 Y701 I702 D703 S704 L705 N706 S707 N708 V709 Y710 N711 A712 S713 I714 T715 E716 N717 S718 F719 F720 M721 T722 R725 S726 Y727 I728 T729

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.99Å 115.72Å 156.08Å 90.06° 89.96° 90.02°	Depositor
Resolution (Å)	50.00 – 3.00 47.47 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 85.3 (47.47-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.255 , 0.274 0.254 , 0.272	Depositor DCC
R_{free} test set	3174 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	93.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 67.2	EDS
Estimated twinning fraction	0.448 for h,-k,-l 0.449 for -h,k,-l 0.447 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 66318 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22992	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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

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	0.48	2/5878 (0.0%)	0.71	3/7981 (0.0%)
1	B	0.46	0/5878	0.71	2/7981 (0.0%)
1	C	0.46	0/5878	0.71	2/7981 (0.0%)
1	D	0.46	0/5878	0.71	3/7981 (0.0%)
All	All	0.47	2/23512 (0.0%)	0.71	10/31924 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	SER	C-O	5.94	1.34	1.23
1	A	306	ASP	CB-CG	5.73	1.63	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	GLY	N-CA-C	-5.81	98.58	113.10
1	D	358	GLY	N-CA-C	-5.73	98.78	113.10
1	C	358	GLY	N-CA-C	-5.72	98.81	113.10
1	A	307	SER	CB-CA-C	5.71	120.95	110.10
1	A	358	GLY	N-CA-C	-5.66	98.95	113.10
1	C	11	LEU	CA-CB-CG	-5.36	102.98	115.30
1	D	11	LEU	CA-CB-CG	-5.20	103.34	115.30
1	B	11	LEU	CA-CB-CG	-5.19	103.37	115.30
1	A	11	LEU	CA-CB-CG	-5.18	103.39	115.30
1	D	305	VAL	CB-CA-C	-5.02	101.87	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5748	0	5657	593	0
1	B	5748	0	5657	564	0
1	C	5748	0	5657	591	0
1	D	5748	0	5657	567	0
All	All	22992	0	22628	2281	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (2281) 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:B:224:ILE:HG12	1:B:273:VAL:HG11	1.23	1.20
1:D:224:ILE:HG12	1:D:273:VAL:HG11	1.23	1.15
1:A:224:ILE:HG12	1:A:273:VAL:HG11	1.24	1.14
1:C:224:ILE:HG12	1:C:273:VAL:HG11	1.22	1.14
1:D:398:VAL:HB	1:D:669:ARG:NH1	1.62	1.14
1:A:398:VAL:HB	1:A:669:ARG:NH1	1.64	1.12
1:C:398:VAL:HB	1:C:669:ARG:NH1	1.64	1.12
1:B:398:VAL:HB	1:B:669:ARG:NH1	1.65	1.11
1:B:153:GLN:HG2	1:B:155:PRO:HD3	1.39	1.04
1:D:153:GLN:HG2	1:D:155:PRO:HD3	1.39	1.04
1:A:153:GLN:HG2	1:A:155:PRO:HD3	1.39	1.03
1:C:153:GLN:HG2	1:C:155:PRO:HD3	1.39	1.03
1:D:293:LEU:HB2	1:D:297:LEU:HG	1.41	1.02
1:B:293:LEU:HB2	1:B:297:LEU:HG	1.41	1.02
1:A:293:LEU:HB2	1:A:297:LEU:HG	1.41	0.99
1:B:338:ARG:HB2	1:B:339:PRO:HD2	1.43	0.99
1:D:160:VAL:HG23	1:D:161:ARG:H	1.25	0.99
1:C:293:LEU:HB2	1:C:297:LEU:HG	1.41	0.99
1:D:338:ARG:HB2	1:D:339:PRO:HD2	1.43	0.99
1:C:338:ARG:HB2	1:C:339:PRO:HD2	1.43	0.98
1:B:160:VAL:HG23	1:B:161:ARG:H	1.26	0.98
1:A:568:LYS:HD2	1:D:210:ARG:HH12	1.24	0.98
1:A:338:ARG:HB2	1:A:339:PRO:HD2	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:PHE:HB2	1:A:697:GLN:HE22	1.28	0.98
1:C:160:VAL:HG23	1:C:161:ARG:H	1.25	0.97
1:C:693:PHE:HB2	1:C:697:GLN:HE22	1.28	0.97
1:A:160:VAL:HG23	1:A:161:ARG:H	1.25	0.97
1:B:693:PHE:HB2	1:B:697:GLN:HE22	1.26	0.96
1:B:306:ASP:OD1	1:B:307:SER:N	1.99	0.95
1:D:693:PHE:HB2	1:D:697:GLN:HE22	1.29	0.95
1:D:227:LYS:HE3	1:D:281:SER:HA	1.50	0.94
1:A:187:LYS:HD3	1:A:197:LEU:HD11	1.50	0.92
1:B:187:LYS:HD3	1:B:197:LEU:HD11	1.51	0.92
1:D:187:LYS:HD3	1:D:197:LEU:HD11	1.51	0.92
1:D:334:LEU:HD13	1:D:351:LEU:HD11	1.52	0.92
1:A:500:GLU:HG2	1:A:501:THR:H	1.36	0.91
1:C:187:LYS:HD3	1:C:197:LEU:HD11	1.51	0.91
1:A:227:LYS:HE3	1:A:281:SER:HA	1.52	0.91
1:C:500:GLU:HG2	1:C:501:THR:H	1.36	0.91
1:B:102:MET:HB3	1:B:107:THR:HG21	1.51	0.90
1:A:605:ILE:HG13	1:A:606:LYS:H	1.36	0.90
1:A:102:MET:HB3	1:A:107:THR:HG21	1.51	0.90
1:C:340:LEU:HD23	1:C:342:LEU:HD21	1.54	0.90
1:B:227:LYS:HE3	1:B:281:SER:HA	1.53	0.90
1:A:334:LEU:HD13	1:A:351:LEU:HD11	1.53	0.90
1:D:102:MET:HB3	1:D:107:THR:HG21	1.51	0.90
1:C:102:MET:HB3	1:C:107:THR:HG21	1.52	0.90
1:C:227:LYS:HE3	1:C:281:SER:HA	1.53	0.90
1:C:605:ILE:HG13	1:C:606:LYS:H	1.37	0.89
1:B:334:LEU:HD13	1:B:351:LEU:HD11	1.55	0.89
1:D:463:ILE:HG22	1:D:464:THR:N	1.87	0.88
1:A:340:LEU:HD23	1:A:342:LEU:HD21	1.56	0.88
1:B:605:ILE:HG13	1:B:606:LYS:H	1.35	0.88
1:B:500:GLU:HG2	1:B:501:THR:H	1.36	0.88
1:B:340:LEU:HD23	1:B:342:LEU:HD21	1.54	0.88
1:C:334:LEU:HD13	1:C:351:LEU:HD11	1.55	0.88
1:B:463:ILE:HG22	1:B:464:THR:N	1.88	0.88
1:D:500:GLU:HG2	1:D:501:THR:H	1.36	0.88
1:A:463:ILE:HG22	1:A:464:THR:N	1.87	0.88
1:C:463:ILE:HG22	1:C:464:THR:N	1.87	0.87
1:C:398:VAL:HB	1:C:669:ARG:HH12	1.40	0.86
1:D:605:ILE:HG13	1:D:606:LYS:H	1.36	0.86
1:C:259:MET:HE1	1:C:262:GLN:HE22	1.40	0.86
1:C:404:VAL:HG11	1:C:438:GLU:HA	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:LEU:HD23	1:D:342:LEU:HD21	1.56	0.85
1:A:398:VAL:HB	1:A:669:ARG:HH12	1.42	0.85
1:A:323:LEU:HD13	1:A:329:TRP:HB2	1.59	0.85
1:B:323:LEU:HD13	1:B:329:TRP:HB2	1.58	0.85
1:D:398:VAL:HB	1:D:669:ARG:HH12	1.39	0.85
1:D:323:LEU:HD13	1:D:329:TRP:HB2	1.59	0.84
1:D:398:VAL:HB	1:D:669:ARG:HH11	1.42	0.84
1:C:323:LEU:HD13	1:C:329:TRP:HB2	1.60	0.84
1:C:239:GLN:HA	1:C:273:VAL:HB	1.59	0.83
1:B:404:VAL:HG11	1:B:438:GLU:HA	1.60	0.83
1:A:122:ILE:HG13	1:A:166:LEU:HD22	1.60	0.83
1:B:239:GLN:HA	1:B:273:VAL:HB	1.58	0.83
1:C:122:ILE:HG13	1:C:166:LEU:HD22	1.61	0.83
1:A:667:LEU:HD22	1:C:723:PHE:CE2	2.13	0.83
1:D:239:GLN:HA	1:D:273:VAL:HB	1.58	0.83
1:B:122:ILE:HG13	1:B:166:LEU:HD22	1.61	0.83
1:B:122:ILE:HD11	1:B:166:LEU:HD13	1.61	0.83
1:D:122:ILE:HD11	1:D:166:LEU:HD13	1.61	0.83
1:C:122:ILE:HD11	1:C:166:LEU:HD13	1.60	0.82
1:D:122:ILE:HG13	1:D:166:LEU:HD22	1.61	0.82
1:A:239:GLN:HA	1:A:273:VAL:HB	1.60	0.82
1:B:398:VAL:HB	1:B:669:ARG:HH11	1.44	0.82
1:A:122:ILE:HD11	1:A:166:LEU:HD13	1.61	0.82
1:D:291:LEU:O	1:D:297:LEU:HB2	1.80	0.82
1:C:398:VAL:HB	1:C:669:ARG:HH11	1.44	0.82
1:D:176:VAL:HG12	1:D:177:PHE:H	1.44	0.81
1:B:291:LEU:O	1:B:297:LEU:HB2	1.80	0.81
1:B:605:ILE:HG13	1:B:606:LYS:N	1.96	0.81
1:D:623:LEU:HD13	1:D:664:LEU:CD2	2.09	0.81
1:B:398:VAL:HB	1:B:669:ARG:HH12	1.42	0.81
1:A:398:VAL:HB	1:A:669:ARG:HH11	1.43	0.81
1:D:605:ILE:HG13	1:D:606:LYS:N	1.97	0.80
1:D:241:CYS:HB3	1:D:259:MET:HB2	1.63	0.80
1:A:623:LEU:HD13	1:A:664:LEU:CD2	2.10	0.80
1:B:176:VAL:HG12	1:B:177:PHE:H	1.45	0.80
1:C:236:VAL:O	1:C:243:LEU:HD12	1.82	0.80
1:B:291:LEU:HD11	1:B:299:GLN:HB2	1.64	0.80
1:A:723:PHE:CE2	1:C:667:LEU:HD22	2.16	0.80
1:C:176:VAL:HG12	1:C:177:PHE:H	1.44	0.80
1:C:291:LEU:HD11	1:C:299:GLN:HB2	1.63	0.80
1:D:291:LEU:HD11	1:D:299:GLN:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASN:H	1:C:107:THR:HG21	1.46	0.80
1:A:176:VAL:HG12	1:A:177:PHE:H	1.44	0.80
1:A:568:LYS:HD2	1:D:210:ARG:NH1	1.97	0.80
1:A:605:ILE:HG13	1:A:606:LYS:N	1.96	0.80
1:C:291:LEU:O	1:C:297:LEU:HB2	1.80	0.80
1:B:103:ASN:H	1:B:107:THR:HG21	1.46	0.80
1:C:623:LEU:HD13	1:C:664:LEU:CD2	2.11	0.79
1:C:605:ILE:HG13	1:C:606:LYS:N	1.97	0.79
1:C:547:VAL:CG2	1:C:644:THR:HG21	2.11	0.79
1:A:317:ASN:ND2	1:A:319:ILE:HG13	1.96	0.79
1:D:236:VAL:O	1:D:243:LEU:HD12	1.82	0.79
1:C:237:LEU:HD12	1:C:238:THR:H	1.47	0.79
1:B:237:LEU:HD12	1:B:238:THR:H	1.47	0.79
1:B:547:VAL:CG2	1:B:644:THR:HG21	2.12	0.79
1:A:291:LEU:HD11	1:A:299:GLN:HB2	1.64	0.79
1:D:103:ASN:H	1:D:107:THR:HG21	1.47	0.79
1:C:55:GLU:OE1	1:C:74:SER:HA	1.83	0.79
1:A:404:VAL:HG11	1:A:438:GLU:HA	1.64	0.79
1:D:317:ASN:ND2	1:D:319:ILE:HG13	1.97	0.79
1:B:623:LEU:HD13	1:B:664:LEU:CD2	2.12	0.79
1:A:103:ASN:H	1:A:107:THR:HG21	1.48	0.78
1:A:237:LEU:HD12	1:A:238:THR:H	1.48	0.78
1:A:236:VAL:O	1:A:243:LEU:HD12	1.84	0.78
1:A:291:LEU:O	1:A:297:LEU:HB2	1.81	0.78
1:A:463:ILE:HG22	1:A:464:THR:H	1.47	0.78
1:D:55:GLU:OE1	1:D:74:SER:HA	1.82	0.78
1:A:547:VAL:CG2	1:A:644:THR:HG21	2.12	0.78
1:D:547:VAL:CG2	1:D:644:THR:HG21	2.12	0.78
1:C:177:PHE:HZ	1:C:234:LEU:HD21	1.49	0.78
1:B:58:ASN:HA	1:B:474:ASN:ND2	1.98	0.78
1:B:55:GLU:OE1	1:B:74:SER:HA	1.83	0.78
1:A:177:PHE:HZ	1:A:234:LEU:HD21	1.49	0.78
1:B:236:VAL:O	1:B:243:LEU:HD12	1.84	0.78
1:A:292:PRO:O	1:A:293:LEU:HD12	1.84	0.78
1:B:237:LEU:HD12	1:B:238:THR:N	1.99	0.78
1:B:546:THR:O	1:B:546:THR:HG22	1.85	0.78
1:B:317:ASN:ND2	1:B:319:ILE:HG13	1.98	0.77
1:C:317:ASN:ND2	1:C:319:ILE:HG13	1.98	0.77
1:B:224:ILE:CG1	1:B:273:VAL:HG11	2.11	0.77
1:D:237:LEU:HD12	1:D:238:THR:H	1.48	0.77
1:D:177:PHE:HZ	1:D:234:LEU:HD21	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LEU:HD12	1:C:238:THR:N	1.99	0.77
1:C:463:ILE:HG22	1:C:464:THR:H	1.48	0.77
1:B:177:PHE:HZ	1:B:234:LEU:HD21	1.49	0.77
1:D:292:PRO:O	1:D:293:LEU:HD12	1.84	0.77
1:B:522:ASN:O	1:B:526:ARG:HG3	1.84	0.77
1:D:224:ILE:CG1	1:D:273:VAL:HG11	2.12	0.77
1:A:55:GLU:OE1	1:A:74:SER:HA	1.85	0.77
1:D:546:THR:O	1:D:546:THR:HG22	1.85	0.77
1:D:237:LEU:HD12	1:D:238:THR:N	2.00	0.77
1:A:237:LEU:HD12	1:A:238:THR:N	2.00	0.77
1:C:292:PRO:O	1:C:293:LEU:HD12	1.86	0.76
1:A:463:ILE:CG2	1:A:464:THR:H	1.99	0.76
1:B:292:PRO:O	1:B:293:LEU:HD12	1.85	0.76
1:A:568:LYS:NZ	1:D:210:ARG:HH22	1.82	0.76
1:B:103:ASN:H	1:B:107:THR:CG2	1.98	0.76
1:B:463:ILE:CG2	1:B:464:THR:H	1.99	0.76
1:A:728:ILE:HD12	1:C:724:PHE:CD1	2.21	0.76
1:C:463:ILE:CG2	1:C:464:THR:H	1.99	0.76
1:D:463:ILE:CG2	1:D:464:THR:H	1.99	0.76
1:A:522:ASN:O	1:A:526:ARG:HG3	1.85	0.76
1:D:160:VAL:HG23	1:D:161:ARG:N	2.01	0.75
1:D:522:ASN:O	1:D:526:ARG:HG3	1.85	0.75
1:D:58:ASN:HA	1:D:474:ASN:ND2	2.01	0.75
1:D:103:ASN:H	1:D:107:THR:CG2	1.99	0.75
1:A:608:ASP:HB2	1:A:691:LYS:NZ	2.02	0.75
1:B:160:VAL:HG23	1:B:161:ARG:N	2.01	0.75
1:A:58:ASN:HA	1:A:474:ASN:ND2	2.02	0.75
1:A:724:PHE:CD1	1:C:728:ILE:HD12	2.22	0.75
1:B:224:ILE:HG12	1:B:273:VAL:CG1	2.12	0.75
1:B:153:GLN:HG2	1:B:155:PRO:CD	2.16	0.74
1:D:259:MET:HA	1:D:262:GLN:NE2	2.03	0.74
1:D:224:ILE:HG12	1:D:273:VAL:CG1	2.13	0.74
1:D:153:GLN:HG2	1:D:155:PRO:CD	2.17	0.74
1:C:160:VAL:HG23	1:C:161:ARG:N	2.01	0.74
1:B:296:GLY:O	1:B:320:PRO:HA	1.86	0.74
1:A:288:VAL:HG22	1:A:336:LEU:HD22	1.69	0.74
1:B:608:ASP:HB2	1:B:691:LYS:NZ	2.02	0.74
1:C:608:ASP:HB2	1:C:691:LYS:NZ	2.03	0.74
1:D:608:ASP:HB2	1:D:691:LYS:NZ	2.01	0.74
1:D:247:ASP:HB2	1:D:254:ILE:CG1	2.18	0.74
1:D:296:GLY:O	1:D:320:PRO:HA	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HG23	1:A:161:ARG:N	2.01	0.74
1:A:103:ASN:H	1:A:107:THR:CG2	1.99	0.74
1:C:103:ASN:H	1:C:107:THR:CG2	1.99	0.74
1:C:522:ASN:O	1:C:526:ARG:HG3	1.87	0.74
1:B:463:ILE:HG22	1:B:464:THR:H	1.48	0.74
1:B:247:ASP:HB2	1:B:254:ILE:CG1	2.17	0.74
1:C:553:ILE:O	1:C:553:ILE:HG22	1.87	0.74
1:A:247:ASP:HB2	1:A:254:ILE:CG1	2.18	0.74
1:A:153:GLN:HG2	1:A:155:PRO:CD	2.17	0.74
1:A:342:LEU:HD13	1:A:379:ILE:HD12	1.70	0.74
1:C:153:GLN:HG2	1:C:155:PRO:CD	2.17	0.74
1:D:288:VAL:HG22	1:D:336:LEU:HD22	1.70	0.73
1:D:463:ILE:HG22	1:D:464:THR:H	1.48	0.73
1:D:500:GLU:HG2	1:D:501:THR:N	2.03	0.73
1:C:568:LYS:HG3	1:C:572:ASP:OD2	1.88	0.73
1:A:296:GLY:O	1:A:320:PRO:HA	1.87	0.73
1:C:296:GLY:O	1:C:320:PRO:HA	1.87	0.73
1:A:608:ASP:HB2	1:A:691:LYS:HZ1	1.53	0.73
1:B:568:LYS:HG3	1:B:572:ASP:OD2	1.88	0.73
1:A:546:THR:O	1:A:546:THR:HG22	1.85	0.73
1:A:297:LEU:HD22	1:A:318:ASN:HD21	1.53	0.73
1:C:288:VAL:HG22	1:C:336:LEU:HD22	1.70	0.73
1:D:235:ILE:H	1:D:235:ILE:HD12	1.51	0.73
1:B:500:GLU:HG2	1:B:501:THR:N	2.03	0.73
1:C:705:LEU:H	1:C:705:LEU:HD12	1.53	0.73
1:C:241:CYS:HB3	1:C:259:MET:HB2	1.71	0.73
1:C:286:THR:HG22	1:C:287:LEU:N	2.03	0.73
1:C:463:ILE:CG2	1:C:464:THR:N	2.51	0.73
1:D:568:LYS:HG3	1:D:572:ASP:OD2	1.89	0.73
1:C:224:ILE:CG1	1:C:273:VAL:HG11	2.11	0.73
1:A:694:ASN:ND2	1:A:697:GLN:HE21	1.87	0.73
1:B:305:VAL:HG12	1:B:311:LEU:HD23	1.69	0.73
1:C:305:VAL:HG12	1:C:311:LEU:HD23	1.68	0.73
1:A:568:LYS:HG3	1:A:572:ASP:OD2	1.89	0.73
1:A:463:ILE:CG2	1:A:464:THR:N	2.51	0.73
1:C:694:ASN:ND2	1:C:697:GLN:HE21	1.86	0.73
1:C:235:ILE:HD12	1:C:235:ILE:H	1.51	0.73
1:B:293:LEU:HD22	1:B:297:LEU:HD11	1.71	0.73
1:A:553:ILE:HG22	1:A:553:ILE:O	1.88	0.73
1:C:58:ASN:HA	1:C:474:ASN:ND2	2.04	0.73
1:D:553:ILE:O	1:D:553:ILE:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:THR:HG22	1:C:546:THR:O	1.85	0.73
1:B:288:VAL:HG22	1:B:336:LEU:HD22	1.71	0.72
1:C:342:LEU:HD13	1:C:379:ILE:HD12	1.71	0.72
1:B:463:ILE:CG2	1:B:464:THR:N	2.51	0.72
1:A:305:VAL:HG12	1:A:311:LEU:HD23	1.69	0.72
1:A:286:THR:HG22	1:A:287:LEU:N	2.04	0.72
1:D:463:ILE:CG2	1:D:464:THR:N	2.51	0.72
1:B:235:ILE:H	1:B:235:ILE:HD12	1.52	0.72
1:D:342:LEU:CD1	1:D:379:ILE:HD12	2.19	0.72
1:D:247:ASP:OD1	1:D:249:THR:HB	1.89	0.72
1:A:235:ILE:HD12	1:A:235:ILE:H	1.52	0.72
1:D:293:LEU:HD22	1:D:297:LEU:HD11	1.71	0.72
1:A:317:ASN:HD21	1:A:319:ILE:HG13	1.54	0.72
1:D:342:LEU:HD13	1:D:379:ILE:HD12	1.70	0.72
1:C:297:LEU:HD22	1:C:318:ASN:HD21	1.54	0.72
1:A:558:LEU:HD11	1:A:635:LEU:HD11	1.72	0.72
1:B:553:ILE:HG22	1:B:553:ILE:O	1.89	0.72
1:A:254:ILE:HG21	1:A:311:LEU:HB2	1.72	0.72
1:B:342:LEU:CD1	1:B:379:ILE:HD12	2.20	0.72
1:D:558:LEU:HD11	1:D:635:LEU:HD11	1.71	0.71
1:A:224:ILE:CG1	1:A:273:VAL:HG11	2.12	0.71
1:B:694:ASN:ND2	1:B:697:GLN:HE21	1.88	0.71
1:A:500:GLU:HG2	1:A:501:THR:N	2.03	0.71
1:A:705:LEU:H	1:A:705:LEU:HD12	1.55	0.71
1:C:558:LEU:HD11	1:C:635:LEU:HD11	1.72	0.71
1:B:297:LEU:HD22	1:B:318:ASN:HD21	1.53	0.71
1:D:286:THR:HG22	1:D:287:LEU:N	2.04	0.71
1:B:108:LEU:HD23	1:B:109:THR:N	2.05	0.71
1:C:293:LEU:HD22	1:C:297:LEU:HD11	1.72	0.71
1:D:694:ASN:ND2	1:D:697:GLN:HE21	1.89	0.71
1:C:500:GLU:HG2	1:C:501:THR:N	2.04	0.71
1:B:442:TYR:O	1:B:445:ASN:HB2	1.90	0.71
1:C:224:ILE:HG12	1:C:273:VAL:CG1	2.12	0.71
1:A:293:LEU:HD22	1:A:297:LEU:HD11	1.72	0.71
1:C:342:LEU:CD1	1:C:379:ILE:HD12	2.20	0.71
1:A:342:LEU:CD1	1:A:379:ILE:HD12	2.20	0.71
1:B:342:LEU:HD13	1:B:379:ILE:HD12	1.71	0.71
1:D:108:LEU:HD23	1:D:109:THR:N	2.06	0.71
1:A:442:TYR:O	1:A:445:ASN:HB2	1.90	0.71
1:B:286:THR:HG22	1:B:287:LEU:N	2.05	0.70
1:B:608:ASP:HB2	1:B:691:LYS:HZ1	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HD23	1:C:109:THR:N	2.06	0.70
1:D:442:TYR:O	1:D:445:ASN:HB2	1.91	0.70
1:D:297:LEU:HD22	1:D:318:ASN:HD21	1.54	0.70
1:B:705:LEU:HD12	1:B:705:LEU:H	1.56	0.70
1:B:558:LEU:HD11	1:B:635:LEU:HD11	1.72	0.70
1:D:705:LEU:H	1:D:705:LEU:HD12	1.55	0.70
1:C:442:TYR:O	1:C:445:ASN:HB2	1.91	0.70
1:C:247:ASP:HB2	1:C:254:ILE:CG1	2.22	0.70
1:C:201:ASP:OD1	1:C:205:LEU:HG	1.91	0.70
1:B:259:MET:HE1	1:B:262:GLN:HE22	1.55	0.70
1:A:259:MET:HE1	1:A:262:GLN:HE22	1.57	0.70
1:C:254:ILE:HG21	1:C:311:LEU:HB2	1.74	0.70
1:C:521:SER:OG	1:C:524:VAL:HG23	1.92	0.70
1:D:714:ILE:O	1:D:714:ILE:HG13	1.92	0.70
1:A:241:CYS:HB3	1:A:259:MET:HB2	1.74	0.70
1:A:693:PHE:CB	1:A:697:GLN:HE22	2.04	0.70
1:A:201:ASP:OD1	1:A:205:LEU:HG	1.91	0.70
1:A:224:ILE:HG12	1:A:273:VAL:CG1	2.13	0.70
1:B:521:SER:OG	1:B:524:VAL:HG23	1.92	0.70
1:A:108:LEU:HD23	1:A:109:THR:N	2.07	0.70
1:B:201:ASP:OD1	1:B:205:LEU:HG	1.91	0.70
1:D:521:SER:OG	1:D:524:VAL:HG23	1.92	0.69
1:B:693:PHE:CB	1:B:697:GLN:HE22	2.03	0.69
1:C:68:ILE:HD12	1:C:138:LEU:HD13	1.74	0.69
1:D:201:ASP:OD1	1:D:205:LEU:HG	1.91	0.69
1:C:317:ASN:HD21	1:C:319:ILE:HG13	1.56	0.69
1:A:521:SER:OG	1:A:524:VAL:HG23	1.92	0.69
1:B:714:ILE:HG13	1:B:714:ILE:O	1.92	0.69
1:B:226:CYS:SG	1:B:227:LYS:N	2.66	0.69
1:A:701:TYR:O	1:A:705:LEU:HD12	1.93	0.69
1:B:306:ASP:O	1:B:307:SER:OG	2.11	0.69
1:D:154:ASN:N	1:D:155:PRO:HD3	2.07	0.69
1:C:693:PHE:CB	1:C:697:GLN:HE22	2.05	0.69
1:C:701:TYR:O	1:C:704:SER:HB3	1.91	0.69
1:B:154:ASN:N	1:B:155:PRO:HD3	2.07	0.69
1:B:344:VAL:HG12	1:B:345:GLU:N	2.08	0.69
1:C:154:ASN:N	1:C:155:PRO:HD3	2.07	0.69
1:D:317:ASN:HD21	1:D:319:ILE:HG13	1.56	0.69
1:D:176:VAL:HG12	1:D:177:PHE:N	2.08	0.69
1:C:608:ASP:HB2	1:C:691:LYS:HZ1	1.58	0.69
1:A:603:SER:HA	1:A:686:PHE:HD1	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:LEU:HD11	1:B:586:LEU:HB2	1.75	0.69
1:B:136:SER:O	1:B:140:SER:HB3	1.92	0.69
1:A:154:ASN:N	1:A:155:PRO:HD3	2.07	0.68
1:C:310:ILE:O	1:C:310:ILE:HG22	1.92	0.68
1:A:226:CYS:SG	1:A:227:LYS:N	2.65	0.68
1:D:344:VAL:HG12	1:D:345:GLU:N	2.09	0.68
1:D:160:VAL:CG2	1:D:161:ARG:H	2.05	0.68
1:C:603:SER:HA	1:C:686:PHE:HD1	1.59	0.68
1:D:238:THR:OG1	1:D:242:HIS:HB2	1.94	0.68
1:C:176:VAL:HG12	1:C:177:PHE:N	2.08	0.68
1:A:349:LEU:H	1:A:368:VAL:HG22	1.58	0.68
1:C:349:LEU:H	1:C:368:VAL:HG22	1.58	0.68
1:A:136:SER:O	1:A:140:SER:HB3	1.93	0.68
1:C:547:VAL:HG21	1:C:644:THR:HG21	1.74	0.68
1:C:78:LEU:HD12	1:C:79:LEU:H	1.58	0.68
1:B:701:TYR:O	1:B:705:LEU:HD12	1.94	0.68
1:B:603:SER:HA	1:B:686:PHE:HD1	1.59	0.68
1:C:136:SER:O	1:C:140:SER:HB3	1.92	0.68
1:D:78:LEU:HD12	1:D:79:LEU:H	1.57	0.68
1:D:136:SER:O	1:D:140:SER:HB3	1.93	0.68
1:A:68:ILE:HD12	1:A:138:LEU:HD13	1.75	0.68
1:B:238:THR:OG1	1:B:242:HIS:HB2	1.94	0.68
1:B:317:ASN:HD21	1:B:319:ILE:HG13	1.57	0.68
1:B:160:VAL:CG2	1:B:161:ARG:H	2.05	0.68
1:B:176:VAL:HG12	1:B:177:PHE:N	2.09	0.68
1:B:349:LEU:H	1:B:368:VAL:HG22	1.58	0.68
1:D:226:CYS:SG	1:D:227:LYS:N	2.67	0.68
1:A:176:VAL:HG12	1:A:177:PHE:N	2.08	0.68
1:D:506:LEU:HD11	1:D:586:LEU:HB2	1.76	0.68
1:D:603:SER:HA	1:D:686:PHE:HD1	1.59	0.68
1:D:349:LEU:H	1:D:368:VAL:HG22	1.58	0.68
1:B:630:THR:O	1:B:634:LEU:HD12	1.94	0.68
1:C:226:CYS:SG	1:C:227:LYS:N	2.66	0.68
1:A:185:GLY:O	1:A:186:LEU:HD12	1.94	0.68
1:C:404:VAL:HG23	1:C:443:LEU:CD1	2.24	0.67
1:A:238:THR:OG1	1:A:242:HIS:HB2	1.94	0.67
1:C:185:GLY:O	1:C:186:LEU:HD12	1.94	0.67
1:D:368:VAL:O	1:D:368:VAL:HG23	1.94	0.67
1:D:608:ASP:HB2	1:D:691:LYS:HZ1	1.58	0.67
1:D:701:TYR:O	1:D:705:LEU:HD12	1.94	0.67
1:A:338:ARG:HB2	1:A:339:PRO:CD	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:THR:O	1:A:634:LEU:HD12	1.95	0.67
1:C:244:LYS:HB3	1:C:253:LEU:HD11	1.76	0.67
1:D:693:PHE:CB	1:D:697:GLN:HE22	2.05	0.67
1:C:604:ALA:HB1	1:C:691:LYS:HE2	1.75	0.67
1:D:604:ALA:HB1	1:D:691:LYS:HE2	1.75	0.67
1:D:701:TYR:O	1:D:704:SER:HB3	1.94	0.67
1:B:368:VAL:HG23	1:B:368:VAL:O	1.94	0.67
1:D:68:ILE:HD12	1:D:138:LEU:HD13	1.74	0.67
1:C:338:ARG:HB2	1:C:339:PRO:CD	2.22	0.67
1:D:232:ARG:HD3	1:D:247:ASP:OD1	1.95	0.67
1:C:344:VAL:HG12	1:C:345:GLU:N	2.09	0.67
1:B:78:LEU:HD12	1:B:79:LEU:H	1.58	0.67
1:C:238:THR:OG1	1:C:242:HIS:HB2	1.94	0.67
1:A:674:LEU:HD23	1:C:723:PHE:CD1	2.29	0.67
1:A:604:ALA:HB1	1:A:691:LYS:HE2	1.75	0.67
1:B:68:ILE:HD12	1:B:138:LEU:HD13	1.75	0.67
1:D:626:HIS:HB3	1:D:661:GLN:HE21	1.60	0.67
1:A:344:VAL:HG12	1:A:345:GLU:N	2.09	0.67
1:B:604:ALA:HB1	1:B:691:LYS:HE2	1.75	0.67
1:C:701:TYR:O	1:C:705:LEU:HD12	1.95	0.67
1:D:404:VAL:HG11	1:D:438:GLU:HA	1.75	0.67
1:B:701:TYR:O	1:B:704:SER:HB3	1.94	0.67
1:A:626:HIS:HB3	1:A:661:GLN:HE21	1.60	0.67
1:B:626:HIS:HB3	1:B:661:GLN:NE2	2.10	0.67
1:D:241:CYS:O	1:D:259:MET:HG2	1.94	0.67
1:A:506:LEU:HD11	1:A:586:LEU:HB2	1.76	0.67
1:B:232:ARG:HD3	1:B:247:ASP:OD1	1.96	0.67
1:C:232:ARG:HD3	1:C:247:ASP:OD1	1.95	0.67
1:A:701:TYR:O	1:A:704:SER:HB3	1.94	0.67
1:B:547:VAL:HG21	1:B:644:THR:HG21	1.77	0.66
1:A:547:VAL:HG21	1:A:644:THR:HG21	1.76	0.66
1:C:506:LEU:HD11	1:C:586:LEU:HB2	1.76	0.66
1:B:449:ILE:O	1:B:453:VAL:HG23	1.94	0.66
1:A:449:ILE:O	1:A:453:VAL:HG23	1.94	0.66
1:C:541:PRO:HB2	1:C:544:MET:HE2	1.77	0.66
1:A:78:LEU:HD12	1:A:79:LEU:H	1.60	0.66
1:D:185:GLY:O	1:D:186:LEU:HD12	1.94	0.66
1:C:368:VAL:O	1:C:368:VAL:HG23	1.94	0.66
1:A:73:SER:HB3	1:A:78:LEU:H	1.60	0.66
1:B:185:GLY:O	1:B:186:LEU:HD12	1.94	0.66
1:A:232:ARG:HD3	1:A:247:ASP:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:VAL:HG23	1:D:443:LEU:CD1	2.25	0.66
1:A:714:ILE:HG13	1:A:714:ILE:O	1.94	0.66
1:D:547:VAL:HG21	1:D:644:THR:HG21	1.77	0.66
1:B:626:HIS:HB3	1:B:661:GLN:HE21	1.61	0.66
1:C:626:HIS:HB3	1:C:661:GLN:HE21	1.61	0.66
1:C:160:VAL:CG2	1:C:161:ARG:H	2.05	0.66
1:D:259:MET:HA	1:D:262:GLN:HE21	1.61	0.66
1:C:449:ILE:O	1:C:453:VAL:HG23	1.95	0.66
1:B:547:VAL:HG22	1:B:644:THR:HG21	1.77	0.66
1:A:368:VAL:HG23	1:A:368:VAL:O	1.94	0.66
1:A:317:ASN:HD21	1:A:319:ILE:CG1	2.08	0.65
1:C:630:THR:O	1:C:634:LEU:HD12	1.97	0.65
1:A:160:VAL:CG2	1:A:161:ARG:H	2.05	0.65
1:D:317:ASN:HD21	1:D:319:ILE:CG1	2.09	0.65
1:B:338:ARG:HB2	1:B:339:PRO:CD	2.22	0.65
1:C:291:LEU:HB2	1:C:297:LEU:HB3	1.78	0.65
1:D:626:HIS:HB3	1:D:661:GLN:NE2	2.11	0.65
1:C:714:ILE:HG13	1:C:714:ILE:O	1.95	0.65
1:B:291:LEU:HB2	1:B:297:LEU:HB3	1.79	0.65
1:A:291:LEU:HB2	1:A:297:LEU:HB3	1.79	0.65
1:C:725:ARG:O	1:C:729:ILE:HG22	1.95	0.65
1:B:254:ILE:HG21	1:B:311:LEU:HB2	1.79	0.65
1:A:547:VAL:HG22	1:A:644:THR:HG21	1.78	0.65
1:D:547:VAL:HG22	1:D:644:THR:HG21	1.77	0.65
1:C:73:SER:HB3	1:C:78:LEU:H	1.61	0.65
1:A:404:VAL:HG23	1:A:443:LEU:CD1	2.27	0.65
1:D:73:SER:HB3	1:D:78:LEU:H	1.61	0.65
1:C:95:ILE:HD11	1:C:133:LEU:HD11	1.79	0.65
1:D:244:LYS:HB3	1:D:253:LEU:HD11	1.78	0.65
1:B:446:LEU:HD22	1:B:450:LEU:CD1	2.26	0.65
1:B:404:VAL:HG23	1:B:443:LEU:CD1	2.25	0.65
1:B:317:ASN:HD21	1:B:319:ILE:CG1	2.10	0.65
1:C:626:HIS:HB3	1:C:661:GLN:NE2	2.11	0.65
1:B:310:ILE:HG22	1:B:310:ILE:O	1.97	0.65
1:D:291:LEU:HB2	1:D:297:LEU:HB3	1.79	0.64
1:D:449:ILE:O	1:D:453:VAL:HG23	1.96	0.64
1:B:725:ARG:O	1:B:729:ILE:HG22	1.97	0.64
1:A:257:TYR:CE2	1:A:313:TYR:HB3	2.32	0.64
1:D:338:ARG:HB2	1:D:339:PRO:CD	2.23	0.64
1:C:547:VAL:HG22	1:C:644:THR:HG21	1.79	0.64
1:B:73:SER:HB3	1:B:78:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:HIS:HB3	1:A:661:GLN:NE2	2.11	0.64
1:D:341:GLU:C	1:D:342:LEU:HD23	2.18	0.64
1:C:317:ASN:HD21	1:C:319:ILE:CG1	2.10	0.64
1:A:168:TYR:HA	1:A:174:SER:HB2	1.80	0.64
1:B:430:ASN:N	1:B:430:ASN:HD22	1.95	0.64
1:A:721:MET:HE1	1:C:721:MET:HB3	1.79	0.64
1:A:95:ILE:HD11	1:A:133:LEU:HD11	1.80	0.64
1:A:446:LEU:HD22	1:A:450:LEU:CD1	2.27	0.64
1:B:341:GLU:C	1:B:342:LEU:HD23	2.18	0.64
1:D:630:THR:O	1:D:634:LEU:HD12	1.98	0.64
1:B:257:TYR:CE2	1:B:313:TYR:HB3	2.33	0.64
1:C:168:TYR:HA	1:C:174:SER:HB2	1.80	0.64
1:D:725:ARG:O	1:D:729:ILE:HG22	1.98	0.64
1:A:723:PHE:CD1	1:C:674:LEU:HD23	2.32	0.64
1:D:430:ASN:HD22	1:D:430:ASN:N	1.96	0.64
1:A:99:ASN:O	1:A:123:LEU:HD22	1.97	0.63
1:D:99:ASN:O	1:D:123:LEU:HD22	1.97	0.63
1:D:446:LEU:HD22	1:D:450:LEU:CD1	2.28	0.63
1:D:95:ILE:HD11	1:D:133:LEU:HD11	1.80	0.63
1:A:101:SER:HA	1:A:123:LEU:HA	1.80	0.63
1:A:725:ARG:O	1:A:729:ILE:HG22	1.97	0.63
1:B:101:SER:HA	1:B:123:LEU:HA	1.80	0.63
1:D:101:SER:HA	1:D:123:LEU:HA	1.81	0.63
1:A:341:GLU:C	1:A:342:LEU:HD23	2.19	0.63
1:C:430:ASN:N	1:C:430:ASN:HD22	1.95	0.63
1:D:351:LEU:HG	1:D:353:VAL:HG22	1.79	0.63
1:B:168:TYR:HA	1:B:174:SER:HB2	1.80	0.63
1:C:341:GLU:C	1:C:342:LEU:HD23	2.19	0.63
1:A:601:PHE:O	1:A:690:VAL:HG13	1.99	0.63
1:B:397:ILE:HG23	1:B:526:ARG:HG2	1.81	0.63
1:B:247:ASP:HB2	1:B:254:ILE:HG12	1.80	0.62
1:A:244:LYS:HB3	1:A:253:LEU:HD11	1.80	0.62
1:B:297:LEU:HD22	1:B:318:ASN:ND2	2.14	0.62
1:A:430:ASN:HD22	1:A:430:ASN:N	1.96	0.62
1:C:169:VAL:HG23	1:C:174:SER:HA	1.81	0.62
1:B:95:ILE:HD11	1:B:133:LEU:HD11	1.81	0.62
1:D:168:TYR:HA	1:D:174:SER:HB2	1.80	0.62
1:C:132:GLN:NE2	1:C:151:HIS:NE2	2.48	0.62
1:D:297:LEU:HD22	1:D:318:ASN:ND2	2.14	0.62
1:B:99:ASN:O	1:B:123:LEU:HD22	1.98	0.62
1:D:169:VAL:HG23	1:D:174:SER:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:575:ASN:O	1:D:577:PHE:N	2.30	0.62
1:B:417:THR:HG22	1:B:418:GLN:N	2.15	0.62
1:A:541:PRO:HB2	1:A:544:MET:HE2	1.81	0.62
1:A:169:VAL:HG23	1:A:174:SER:HA	1.81	0.62
1:D:132:GLN:NE2	1:D:151:HIS:NE2	2.48	0.62
1:A:581:VAL:O	1:A:584:ASN:N	2.31	0.62
1:C:291:LEU:HB2	1:C:297:LEU:CB	2.30	0.62
1:C:601:PHE:O	1:C:690:VAL:HG13	2.00	0.62
1:A:436:HIS:CD2	1:A:438:GLU:HB2	2.35	0.62
1:A:397:ILE:HG23	1:A:526:ARG:HG2	1.82	0.62
1:B:601:PHE:O	1:B:690:VAL:HG13	2.00	0.62
1:A:190:ASP:OD1	1:A:193:HIS:HB2	2.00	0.62
1:A:297:LEU:HD22	1:A:318:ASN:ND2	2.14	0.62
1:C:351:LEU:HG	1:C:353:VAL:HG22	1.80	0.62
1:C:446:LEU:HD22	1:C:450:LEU:CD1	2.30	0.62
1:B:132:GLN:NE2	1:B:151:HIS:NE2	2.48	0.62
1:D:190:ASP:OD1	1:D:193:HIS:HB2	2.00	0.61
1:C:581:VAL:O	1:C:584:ASN:N	2.31	0.61
1:A:637:PHE:HD2	1:A:651:ILE:HD11	1.65	0.61
1:C:99:ASN:O	1:C:123:LEU:HD22	1.99	0.61
1:A:545:THR:C	1:A:547:VAL:H	2.02	0.61
1:A:132:GLN:NE2	1:A:151:HIS:NE2	2.49	0.61
1:A:291:LEU:HB2	1:A:297:LEU:CB	2.31	0.61
1:C:690:VAL:HG12	1:C:691:LYS:N	2.15	0.61
1:D:601:PHE:O	1:D:690:VAL:HG13	2.00	0.61
1:A:579:ILE:HB	1:A:580:PRO:HD3	1.82	0.61
1:B:579:ILE:HB	1:B:580:PRO:HD3	1.82	0.61
1:C:297:LEU:HD22	1:C:318:ASN:ND2	2.15	0.61
1:C:101:SER:HA	1:C:123:LEU:HA	1.82	0.61
1:B:545:THR:C	1:B:547:VAL:H	2.03	0.61
1:D:305:VAL:HG23	1:D:306:ASP:N	2.14	0.61
1:B:351:LEU:HG	1:B:353:VAL:HG22	1.81	0.61
1:B:101:SER:HB2	1:B:107:THR:OG1	2.00	0.61
1:D:101:SER:HB2	1:D:107:THR:OG1	2.00	0.61
1:A:721:MET:HB3	1:C:721:MET:HE1	1.81	0.61
1:B:217:LYS:O	1:B:217:LYS:HG3	2.00	0.61
1:D:217:LYS:O	1:D:217:LYS:HG3	2.00	0.61
1:A:351:LEU:HG	1:A:353:VAL:HG22	1.81	0.61
1:A:101:SER:HB2	1:A:107:THR:OG1	2.01	0.61
1:C:545:THR:OG1	1:C:548:GLU:HG3	2.01	0.61
1:A:427:LEU:HD12	1:A:442:TYR:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:THR:C	1:D:547:VAL:H	2.03	0.61
1:D:417:THR:HG22	1:D:418:GLN:N	2.16	0.61
1:C:101:SER:HB2	1:C:107:THR:OG1	2.01	0.61
1:D:579:ILE:HB	1:D:580:PRO:HD3	1.83	0.61
1:D:398:VAL:CB	1:D:669:ARG:HH12	2.13	0.61
1:B:190:ASP:OD1	1:B:193:HIS:HB2	2.01	0.61
1:B:690:VAL:HG12	1:B:691:LYS:N	2.15	0.61
1:B:293:LEU:HD22	1:B:297:LEU:HD21	1.83	0.60
1:B:169:VAL:HG23	1:B:174:SER:HA	1.82	0.60
1:A:217:LYS:O	1:A:217:LYS:HG3	2.00	0.60
1:C:291:LEU:HD11	1:C:299:GLN:CB	2.31	0.60
1:B:334:LEU:HD12	1:B:335:VAL:N	2.17	0.60
1:D:545:THR:OG1	1:D:548:GLU:HG3	2.01	0.60
1:D:397:ILE:HG23	1:D:526:ARG:HG2	1.83	0.60
1:A:690:VAL:HG12	1:A:691:LYS:N	2.16	0.60
1:C:217:LYS:O	1:C:217:LYS:HG3	2.00	0.60
1:C:190:ASP:OD1	1:C:193:HIS:HB2	2.01	0.60
1:D:293:LEU:HD22	1:D:297:LEU:HD21	1.83	0.60
1:B:291:LEU:HB2	1:B:297:LEU:CB	2.31	0.60
1:D:690:VAL:HG12	1:D:691:LYS:N	2.15	0.60
1:C:545:THR:C	1:C:547:VAL:H	2.03	0.60
1:A:545:THR:OG1	1:A:548:GLU:HG3	2.02	0.60
1:D:241:CYS:O	1:D:259:MET:CG	2.49	0.60
1:C:530:LYS:HE2	1:C:530:LYS:HA	1.84	0.60
1:B:539:GLU:O	1:B:541:PRO:HD3	2.01	0.60
1:C:167:PHE:CD2	1:C:168:TYR:N	2.69	0.60
1:C:579:ILE:HB	1:C:580:PRO:HD3	1.84	0.60
1:B:581:VAL:O	1:B:584:ASN:N	2.30	0.60
1:D:291:LEU:HB2	1:D:297:LEU:CB	2.31	0.60
1:D:427:LEU:HD12	1:D:442:TYR:CE2	2.36	0.60
1:C:332:VAL:HB	1:C:354:LEU:HD23	1.84	0.60
1:C:293:LEU:HD22	1:C:297:LEU:HD21	1.83	0.60
1:A:167:PHE:CD2	1:A:168:TYR:N	2.69	0.60
1:D:719:PHE:O	1:D:721:MET:N	2.35	0.60
1:B:332:VAL:HB	1:B:354:LEU:HD23	1.84	0.60
1:B:637:PHE:HD2	1:B:651:ILE:HD11	1.67	0.60
1:D:310:ILE:O	1:D:310:ILE:HG22	2.00	0.60
1:C:570:LEU:O	1:C:574:LEU:HB2	2.02	0.60
1:C:443:LEU:O	1:C:445:ASN:N	2.35	0.59
1:A:539:GLU:O	1:A:541:PRO:HD3	2.01	0.59
1:D:165:PHE:HD2	1:D:177:PHE:CD2	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:GLU:O	1:C:541:PRO:HD3	2.02	0.59
1:C:693:PHE:H	1:C:697:GLN:NE2	2.00	0.59
1:A:530:LYS:HA	1:A:530:LYS:HE2	1.85	0.59
1:B:165:PHE:HD2	1:B:177:PHE:CD2	2.20	0.59
1:A:721:MET:HB3	1:C:721:MET:CE	2.32	0.59
1:A:719:PHE:O	1:A:721:MET:N	2.35	0.59
1:D:581:VAL:O	1:D:584:ASN:N	2.31	0.59
1:D:539:GLU:O	1:D:541:PRO:HD3	2.02	0.59
1:B:241:CYS:HB3	1:B:259:MET:HB2	1.85	0.59
1:C:165:PHE:HD2	1:C:177:PHE:CD2	2.19	0.59
1:D:291:LEU:HD11	1:D:299:GLN:CB	2.31	0.59
1:A:291:LEU:HD11	1:A:299:GLN:CB	2.32	0.59
1:B:693:PHE:H	1:B:697:GLN:NE2	2.00	0.59
1:C:404:VAL:HG23	1:C:443:LEU:HD12	1.84	0.59
1:D:183:LEU:HD21	1:D:246:TRP:CZ2	2.38	0.59
1:B:545:THR:OG1	1:B:548:GLU:HG3	2.02	0.59
1:A:443:LEU:O	1:A:445:ASN:N	2.35	0.59
1:D:257:TYR:CE2	1:D:313:TYR:HB3	2.37	0.59
1:C:533:LEU:HD13	1:C:729:ILE:HD11	1.84	0.59
1:B:575:ASN:O	1:B:577:PHE:N	2.32	0.59
1:D:443:LEU:O	1:D:445:ASN:N	2.35	0.59
1:D:332:VAL:HB	1:D:354:LEU:HD23	1.85	0.59
1:A:293:LEU:HD22	1:A:297:LEU:HD21	1.84	0.59
1:D:637:PHE:HD2	1:D:651:ILE:HD11	1.68	0.59
1:D:512:THR:HG22	1:D:573:GLU:OE2	2.03	0.59
1:B:244:LYS:HB3	1:B:253:LEU:HD11	1.85	0.59
1:C:398:VAL:CB	1:C:669:ARG:HH12	2.14	0.59
1:D:297:LEU:HD13	1:D:318:ASN:HD21	1.68	0.59
1:B:291:LEU:CD1	1:B:299:GLN:HB2	2.33	0.59
1:C:492:ASN:O	1:C:496:ASN:HB2	2.02	0.59
1:D:492:ASN:O	1:D:496:ASN:HB2	2.02	0.59
1:D:291:LEU:CD1	1:D:299:GLN:HB2	2.33	0.59
1:D:293:LEU:CB	1:D:297:LEU:HG	2.27	0.59
1:D:693:PHE:H	1:D:697:GLN:NE2	2.00	0.59
1:B:443:LEU:O	1:B:445:ASN:N	2.36	0.59
1:C:244:LYS:HE2	1:C:256:ASP:OD1	2.02	0.59
1:B:291:LEU:HD11	1:B:299:GLN:CB	2.31	0.59
1:A:568:LYS:HZ2	1:D:210:ARG:HH22	1.51	0.59
1:A:533:LEU:HD13	1:A:729:ILE:HD11	1.85	0.59
1:C:247:ASP:HB2	1:C:254:ILE:HG12	1.84	0.59
1:C:332:VAL:O	1:C:333:ASP:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:HB	1:A:354:LEU:HD23	1.85	0.59
1:C:244:LYS:HB3	1:C:253:LEU:CD1	2.33	0.59
1:C:154:ASN:H	1:C:155:PRO:HD3	1.68	0.59
1:C:427:LEU:HD12	1:C:442:TYR:CE2	2.38	0.59
1:A:165:PHE:HD2	1:A:177:PHE:CD2	2.20	0.59
1:B:108:LEU:HD23	1:B:108:LEU:C	2.24	0.59
1:C:719:PHE:O	1:C:721:MET:N	2.36	0.59
1:B:224:ILE:HA	1:B:276:VAL:HG13	1.85	0.58
1:B:183:LEU:HD21	1:B:246:TRP:CZ2	2.38	0.58
1:B:719:PHE:O	1:B:721:MET:N	2.36	0.58
1:C:457:PHE:CD1	1:C:477:GLN:HG2	2.38	0.58
1:D:397:ILE:O	1:D:397:ILE:HG22	2.04	0.58
1:B:530:LYS:HA	1:B:530:LYS:HE2	1.84	0.58
1:D:167:PHE:CD2	1:D:168:TYR:N	2.69	0.58
1:D:247:ASP:HB2	1:D:254:ILE:HG13	1.85	0.58
1:C:596:PHE:C	1:C:598:LYS:H	2.07	0.58
1:A:154:ASN:H	1:A:155:PRO:HD3	1.69	0.58
1:D:334:LEU:HD12	1:D:335:VAL:N	2.19	0.58
1:B:167:PHE:CD2	1:B:168:TYR:N	2.69	0.58
1:D:332:VAL:O	1:D:333:ASP:HB2	2.03	0.58
1:A:332:VAL:O	1:A:333:ASP:HB2	2.04	0.58
1:D:292:PRO:C	1:D:293:LEU:HD12	2.23	0.58
1:B:297:LEU:HD13	1:B:318:ASN:HD21	1.69	0.58
1:A:693:PHE:H	1:A:697:GLN:NE2	2.01	0.58
1:A:694:ASN:ND2	1:A:697:GLN:NE2	2.50	0.58
1:B:570:LEU:O	1:B:574:LEU:HB2	2.03	0.58
1:D:255:GLN:O	1:D:256:ASP:HB2	2.03	0.58
1:A:241:CYS:O	1:A:259:MET:HG2	2.02	0.58
1:C:180:ASP:OD2	1:C:180:ASP:N	2.34	0.58
1:C:293:LEU:HD13	1:C:297:LEU:CD1	2.34	0.58
1:B:501:THR:O	1:B:502:ASP:HB2	2.03	0.58
1:B:427:LEU:HD12	1:B:442:TYR:CE2	2.38	0.58
1:D:232:ARG:HG2	1:D:248:LEU:H	1.69	0.58
1:A:247:ASP:HB2	1:A:254:ILE:HG12	1.85	0.58
1:D:404:VAL:HG23	1:D:443:LEU:HD12	1.84	0.58
1:D:211:PHE:CD1	1:D:212:PHE:N	2.72	0.58
1:A:596:PHE:C	1:A:598:LYS:H	2.07	0.58
1:D:694:ASN:ND2	1:D:697:GLN:NE2	2.52	0.58
1:C:417:THR:HG22	1:C:418:GLN:N	2.17	0.58
1:A:492:ASN:O	1:A:496:ASN:HB2	2.04	0.58
1:B:492:ASN:O	1:B:496:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:CYS:O	1:C:259:MET:HG2	2.03	0.58
1:A:152:LEU:O	1:A:153:GLN:HB2	2.04	0.58
1:C:152:LEU:O	1:C:153:GLN:HB2	2.04	0.58
1:B:694:ASN:ND2	1:B:697:GLN:NE2	2.52	0.58
1:A:180:ASP:OD2	1:A:180:ASP:N	2.35	0.58
1:B:397:ILE:HG22	1:B:397:ILE:O	2.04	0.58
1:D:254:ILE:HG21	1:D:311:LEU:HB2	1.85	0.58
1:D:530:LYS:HA	1:D:530:LYS:HE2	1.84	0.58
1:B:332:VAL:O	1:B:333:ASP:HB2	2.03	0.58
1:B:292:PRO:C	1:B:293:LEU:HD12	2.23	0.58
1:C:694:ASN:ND2	1:C:697:GLN:NE2	2.50	0.58
1:D:533:LEU:HD13	1:D:729:ILE:HD11	1.85	0.58
1:B:398:VAL:CB	1:B:669:ARG:HH12	2.16	0.57
1:C:297:LEU:HD13	1:C:318:ASN:HD21	1.68	0.57
1:D:501:THR:O	1:D:502:ASP:HB2	2.04	0.57
1:C:637:PHE:HD2	1:C:651:ILE:HD11	1.69	0.57
1:C:183:LEU:HD21	1:C:246:TRP:CZ2	2.39	0.57
1:C:183:LEU:HD12	1:C:199:PHE:CE1	2.39	0.57
1:A:398:VAL:CB	1:A:669:ARG:HH12	2.15	0.57
1:A:334:LEU:HD12	1:A:335:VAL:N	2.19	0.57
1:D:180:ASP:N	1:D:180:ASP:OD2	2.34	0.57
1:A:446:LEU:HD22	1:A:450:LEU:HD11	1.85	0.57
1:B:541:PRO:HB2	1:B:544:MET:HE2	1.86	0.57
1:D:457:PHE:CD1	1:D:477:GLN:HG2	2.40	0.57
1:A:417:THR:HG22	1:A:418:GLN:N	2.18	0.57
1:C:501:THR:O	1:C:502:ASP:HB2	2.04	0.57
1:C:122:ILE:CD1	1:C:166:LEU:HD13	2.32	0.57
1:A:403:ASP:OD2	1:A:404:VAL:N	2.34	0.57
1:D:58:ASN:OD1	1:D:59:CYS:N	2.37	0.57
1:B:596:PHE:C	1:B:598:LYS:H	2.07	0.57
1:D:473:VAL:HG21	1:D:484:TYR:HE2	1.68	0.57
1:C:211:PHE:CD1	1:C:212:PHE:N	2.72	0.57
1:B:512:THR:HG22	1:B:573:GLU:OE2	2.04	0.57
1:A:244:LYS:HB3	1:A:253:LEU:CD1	2.34	0.57
1:C:403:ASP:OD2	1:C:404:VAL:N	2.34	0.57
1:B:446:LEU:HD22	1:B:450:LEU:HD11	1.85	0.57
1:A:704:SER:O	1:A:707:SER:HB2	2.04	0.57
1:D:446:LEU:HD22	1:D:450:LEU:HD11	1.85	0.57
1:B:533:LEU:HD13	1:B:729:ILE:HD11	1.85	0.57
1:A:211:PHE:CD1	1:A:212:PHE:N	2.73	0.57
1:D:596:PHE:C	1:D:598:LYS:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PHE:CD1	1:B:212:PHE:N	2.73	0.57
1:B:255:GLN:O	1:B:256:ASP:HB2	2.04	0.57
1:A:188:LYS:HA	1:A:193:HIS:O	2.05	0.57
1:C:334:LEU:HD12	1:C:335:VAL:N	2.19	0.57
1:A:501:THR:O	1:A:502:ASP:HB2	2.04	0.57
1:B:180:ASP:N	1:B:180:ASP:OD2	2.34	0.57
1:A:183:LEU:HD21	1:A:246:TRP:CZ2	2.39	0.57
1:A:404:VAL:HG23	1:A:443:LEU:HD12	1.86	0.57
1:B:344:VAL:HG12	1:B:345:GLU:H	1.69	0.57
1:D:224:ILE:HA	1:D:276:VAL:HG13	1.86	0.57
1:B:152:LEU:O	1:B:153:GLN:HB2	2.03	0.57
1:A:293:LEU:HD13	1:A:297:LEU:CD1	2.35	0.57
1:C:397:ILE:HG23	1:C:526:ARG:HG2	1.87	0.57
1:D:108:LEU:C	1:D:108:LEU:HD23	2.25	0.57
1:D:78:LEU:HD12	1:D:79:LEU:N	2.20	0.57
1:B:293:LEU:HD13	1:B:297:LEU:CD1	2.35	0.57
1:A:183:LEU:HD12	1:A:199:PHE:CE1	2.40	0.57
1:A:545:THR:O	1:A:547:VAL:N	2.33	0.57
1:D:545:THR:O	1:D:547:VAL:N	2.33	0.57
1:D:403:ASP:CG	1:D:404:VAL:H	2.08	0.57
1:D:658:HIS:HA	1:D:661:GLN:OE1	2.05	0.57
1:A:570:LEU:O	1:A:574:LEU:HB2	2.05	0.57
1:C:384:LYS:NZ	1:C:392:GLU:OE2	2.36	0.57
1:B:188:LYS:HA	1:B:193:HIS:O	2.05	0.57
1:D:317:ASN:OD1	1:D:318:ASN:N	2.38	0.57
1:B:545:THR:O	1:B:547:VAL:N	2.33	0.57
1:B:58:ASN:OD1	1:B:59:CYS:N	2.37	0.57
1:A:721:MET:CE	1:C:721:MET:HB3	2.34	0.57
1:D:211:PHE:CG	1:D:212:PHE:N	2.72	0.57
1:B:163:PRO:HA	1:B:178:LEU:HA	1.87	0.57
1:C:257:TYR:CE2	1:C:313:TYR:HB3	2.40	0.57
1:C:188:LYS:HA	1:C:193:HIS:O	2.05	0.57
1:C:292:PRO:C	1:C:293:LEU:HD12	2.24	0.57
1:A:122:ILE:CD1	1:A:166:LEU:HD13	2.33	0.57
1:C:716:GLU:HG2	1:C:722:THR:HA	1.87	0.57
1:A:255:GLN:O	1:A:256:ASP:HB2	2.03	0.57
1:C:446:LEU:HD22	1:C:450:LEU:HD11	1.87	0.57
1:B:404:VAL:HG23	1:B:443:LEU:HD12	1.86	0.57
1:C:658:HIS:HA	1:C:661:GLN:OE1	2.04	0.57
1:B:211:PHE:CG	1:B:212:PHE:N	2.72	0.57
1:D:293:LEU:HD13	1:D:297:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PRO:C	1:A:293:LEU:HD12	2.24	0.56
1:A:297:LEU:HD13	1:A:318:ASN:HD21	1.70	0.56
1:C:291:LEU:CD1	1:C:299:GLN:HB2	2.33	0.56
1:C:704:SER:O	1:C:707:SER:HB2	2.05	0.56
1:D:558:LEU:HD11	1:D:635:LEU:CD1	2.35	0.56
1:B:457:PHE:CD1	1:B:477:GLN:HG2	2.41	0.56
1:C:473:VAL:HG21	1:C:484:TYR:HE2	1.70	0.56
1:D:152:LEU:O	1:D:153:GLN:HB2	2.04	0.56
1:D:188:LYS:HA	1:D:193:HIS:O	2.06	0.56
1:A:291:LEU:CD1	1:A:299:GLN:HB2	2.33	0.56
1:C:545:THR:O	1:C:547:VAL:N	2.33	0.56
1:D:704:SER:O	1:D:707:SER:HB2	2.05	0.56
1:A:658:HIS:HA	1:A:661:GLN:OE1	2.05	0.56
1:A:716:GLU:HG2	1:A:722:THR:HA	1.87	0.56
1:B:716:GLU:HG2	1:B:722:THR:HA	1.87	0.56
1:A:473:VAL:HG21	1:A:484:TYR:HE2	1.70	0.56
1:C:255:GLN:O	1:C:256:ASP:HB2	2.03	0.56
1:C:224:ILE:HA	1:C:276:VAL:HG13	1.86	0.56
1:C:286:THR:HG22	1:C:287:LEU:H	1.70	0.56
1:D:183:LEU:HD12	1:D:199:PHE:CE1	2.39	0.56
1:B:183:LEU:HD12	1:B:199:PHE:CE1	2.39	0.56
1:C:58:ASN:OD1	1:C:59:CYS:N	2.38	0.56
1:B:558:LEU:HD11	1:B:635:LEU:CD1	2.36	0.56
1:D:344:VAL:HG12	1:D:345:GLU:H	1.70	0.56
1:B:78:LEU:HD12	1:B:79:LEU:N	2.20	0.56
1:A:344:VAL:HG12	1:A:345:GLU:H	1.70	0.56
1:C:211:PHE:CG	1:C:212:PHE:N	2.72	0.56
1:D:163:PRO:HA	1:D:178:LEU:HA	1.87	0.56
1:B:473:VAL:HG21	1:B:484:TYR:HE2	1.69	0.56
1:C:344:VAL:HG12	1:C:345:GLU:H	1.70	0.56
1:B:658:HIS:HA	1:B:661:GLN:OE1	2.06	0.56
1:D:570:LEU:O	1:D:574:LEU:HB2	2.04	0.56
1:A:393:HIS:O	1:A:395:LEU:HG	2.04	0.56
1:A:634:LEU:CD2	1:A:655:LEU:HD23	2.36	0.56
1:D:716:GLU:HG2	1:D:722:THR:HA	1.88	0.56
1:A:211:PHE:CG	1:A:212:PHE:N	2.72	0.56
1:A:457:PHE:CD1	1:A:477:GLN:HG2	2.40	0.56
1:C:108:LEU:C	1:C:108:LEU:HD23	2.25	0.56
1:A:575:ASN:O	1:A:577:PHE:N	2.31	0.56
1:A:286:THR:HG22	1:A:287:LEU:H	1.70	0.56
1:B:650:HIS:O	1:B:653:THR:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LYS:NZ	1:B:392:GLU:OE2	2.37	0.56
1:A:512:THR:HG22	1:A:573:GLU:OE2	2.04	0.56
1:C:512:THR:HG22	1:C:573:GLU:OE2	2.04	0.56
1:B:405:GLU:OE2	1:B:437:ASN:ND2	2.39	0.56
1:C:575:ASN:O	1:C:577:PHE:N	2.31	0.56
1:B:18:PRO:HG3	1:B:421:GLU:OE1	2.06	0.56
1:B:289:THR:O	1:B:298:PHE:HA	2.06	0.56
1:D:244:LYS:HB3	1:D:253:LEU:CD1	2.36	0.56
1:B:101:SER:HB2	1:B:107:THR:HG1	1.71	0.56
1:A:405:GLU:OE2	1:A:437:ASN:ND2	2.39	0.56
1:A:397:ILE:HG22	1:A:397:ILE:O	2.05	0.56
1:B:332:VAL:HG22	1:B:356:LYS:HB2	1.88	0.56
1:B:403:ASP:CG	1:B:404:VAL:H	2.09	0.55
1:C:634:LEU:CD2	1:C:655:LEU:HD23	2.37	0.55
1:C:332:VAL:HG22	1:C:356:LYS:HB2	1.87	0.55
1:D:541:PRO:HB2	1:D:544:MET:HE2	1.88	0.55
1:D:384:LYS:NZ	1:D:392:GLU:OE2	2.38	0.55
1:B:704:SER:O	1:B:707:SER:HB2	2.06	0.55
1:D:650:HIS:O	1:D:653:THR:N	2.35	0.55
1:B:11:LEU:HB3	1:B:87:ALA:CB	2.37	0.55
1:D:332:VAL:HG22	1:D:356:LYS:HB2	1.89	0.55
1:B:149:TRP:CE3	1:B:150:PHE:HB3	2.41	0.55
1:D:552:ASP:C	1:D:554:PHE:H	2.10	0.55
1:C:397:ILE:HG22	1:C:397:ILE:O	2.05	0.55
1:C:113:VAL:HG23	1:C:118:LEU:HB2	1.87	0.55
1:A:558:LEU:HD11	1:A:635:LEU:CD1	2.36	0.55
1:C:558:LEU:HD11	1:C:635:LEU:CD1	2.36	0.55
1:D:419:ILE:HG12	1:D:457:PHE:CD2	2.41	0.55
1:B:293:LEU:CB	1:B:297:LEU:HG	2.27	0.55
1:C:289:THR:O	1:C:298:PHE:HA	2.06	0.55
1:A:724:PHE:HE1	1:C:667:LEU:HD21	1.70	0.55
1:C:11:LEU:HB3	1:C:87:ALA:CB	2.37	0.55
1:A:403:ASP:CG	1:A:404:VAL:H	2.09	0.55
1:A:108:LEU:C	1:A:108:LEU:HD23	2.26	0.55
1:D:634:LEU:CD2	1:D:655:LEU:HD23	2.36	0.55
1:A:149:TRP:CE3	1:A:150:PHE:HB3	2.42	0.55
1:D:149:TRP:CE3	1:D:150:PHE:HB3	2.42	0.55
1:C:149:TRP:CE3	1:C:150:PHE:HB3	2.42	0.55
1:A:293:LEU:CB	1:A:297:LEU:HG	2.27	0.55
1:C:450:LEU:O	1:C:451:ARG:C	2.44	0.55
1:D:403:ASP:OD2	1:D:404:VAL:N	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:HB2	1:A:78:LEU:HB3	1.89	0.55
1:D:393:HIS:O	1:D:395:LEU:HG	2.06	0.55
1:B:552:ASP:C	1:B:554:PHE:H	2.10	0.55
1:B:113:VAL:HG23	1:B:118:LEU:HB2	1.88	0.55
1:D:239:GLN:O	1:D:273:VAL:HG23	2.07	0.55
1:A:224:ILE:HA	1:A:276:VAL:HG13	1.88	0.55
1:A:163:PRO:HA	1:A:178:LEU:HA	1.87	0.55
1:B:403:ASP:HB3	1:B:406:ARG:HB3	1.89	0.55
1:C:428:SER:O	1:C:431:LYS:N	2.39	0.55
1:D:154:ASN:H	1:D:155:PRO:HD3	1.69	0.55
1:B:286:THR:HG22	1:B:287:LEU:H	1.71	0.55
1:C:404:VAL:HG23	1:C:443:LEU:HD11	1.87	0.55
1:A:674:LEU:HD23	1:C:723:PHE:CE1	2.42	0.55
1:A:289:THR:O	1:A:298:PHE:HA	2.07	0.55
1:C:163:PRO:HA	1:C:178:LEU:HA	1.87	0.55
1:A:241:CYS:O	1:A:259:MET:CG	2.55	0.54
1:C:293:LEU:CB	1:C:297:LEU:HG	2.27	0.54
1:C:11:LEU:HD12	1:C:479:TYR:HA	1.89	0.54
1:C:71:HIS:CE1	1:C:478:PRO:CA	2.90	0.54
1:A:545:THR:C	1:A:547:VAL:N	2.60	0.54
1:B:71:HIS:CE1	1:B:478:PRO:CA	2.90	0.54
1:A:332:VAL:HG22	1:A:356:LYS:HB2	1.88	0.54
1:A:243:LEU:HB3	1:A:259:MET:HE3	1.88	0.54
1:B:122:ILE:CD1	1:B:166:LEU:HD13	2.33	0.54
1:D:122:ILE:CD1	1:D:166:LEU:HD13	2.33	0.54
1:A:58:ASN:OD1	1:A:59:CYS:N	2.40	0.54
1:D:404:VAL:HG13	1:D:405:GLU:N	2.23	0.54
1:D:113:VAL:HG23	1:D:118:LEU:HB2	1.88	0.54
1:A:113:VAL:HG23	1:A:118:LEU:HB2	1.88	0.54
1:B:154:ASN:H	1:B:155:PRO:HD3	1.69	0.54
1:B:546:THR:O	1:B:546:THR:CG2	2.54	0.54
1:D:247:ASP:HB2	1:D:254:ILE:HG12	1.90	0.54
1:C:286:THR:CG2	1:C:287:LEU:N	2.71	0.54
1:C:403:ASP:CG	1:C:404:VAL:H	2.09	0.54
1:C:73:SER:HB2	1:C:78:LEU:HB3	1.89	0.54
1:C:78:LEU:HD12	1:C:79:LEU:N	2.20	0.54
1:A:403:ASP:HB3	1:A:406:ARG:HB3	1.89	0.54
1:B:634:LEU:CD2	1:B:655:LEU:HD23	2.36	0.54
1:C:457:PHE:CE1	1:C:477:GLN:HG2	2.43	0.54
1:D:211:PHE:CE1	1:D:212:PHE:HB2	2.42	0.54
1:C:393:HIS:O	1:C:395:LEU:HG	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:VAL:HG13	1:B:405:GLU:N	2.23	0.54
1:D:719:PHE:C	1:D:721:MET:N	2.60	0.54
1:C:28:VAL:HB	1:C:98:PRO:HD3	1.90	0.54
1:A:428:SER:O	1:A:431:LYS:N	2.40	0.54
1:D:11:LEU:HB3	1:D:87:ALA:CB	2.38	0.54
1:D:224:ILE:HG22	1:D:276:VAL:HA	1.89	0.54
1:D:286:THR:HG22	1:D:287:LEU:H	1.70	0.54
1:C:404:VAL:HG13	1:C:405:GLU:N	2.23	0.54
1:A:723:PHE:CE1	1:C:674:LEU:HD23	2.42	0.54
1:C:545:THR:C	1:C:547:VAL:N	2.61	0.54
1:C:54:SER:HB2	1:C:74:SER:OG	2.08	0.54
1:A:404:VAL:HG13	1:A:405:GLU:N	2.23	0.54
1:B:527:SER:O	1:B:530:LYS:HB3	2.08	0.54
1:C:551:THR:O	1:C:554:PHE:HB3	2.08	0.54
1:D:257:TYR:CZ	1:D:313:TYR:HB3	2.43	0.54
1:D:289:THR:O	1:D:298:PHE:HA	2.08	0.54
1:D:286:THR:CG2	1:D:287:LEU:N	2.71	0.54
1:B:403:ASP:OD2	1:B:404:VAL:N	2.34	0.54
1:A:54:SER:HB2	1:A:74:SER:OG	2.08	0.54
1:D:73:SER:HB2	1:D:78:LEU:HB3	1.89	0.54
1:B:551:THR:O	1:B:554:PHE:HB3	2.08	0.54
1:A:384:LYS:NZ	1:A:392:GLU:OE2	2.39	0.54
1:B:404:VAL:HG23	1:B:443:LEU:HD11	1.88	0.54
1:B:604:ALA:HB2	1:B:691:LYS:HG2	1.90	0.54
1:C:521:SER:O	1:C:524:VAL:HB	2.08	0.54
1:C:527:SER:O	1:C:530:LYS:HB3	2.08	0.54
1:A:286:THR:CG2	1:A:287:LEU:N	2.71	0.54
1:D:546:THR:O	1:D:546:THR:CG2	2.54	0.54
1:D:71:HIS:CE1	1:D:478:PRO:CA	2.91	0.54
1:C:211:PHE:CE1	1:C:212:PHE:HB2	2.43	0.54
1:A:211:PHE:CE1	1:A:212:PHE:HB2	2.43	0.54
1:B:28:VAL:HB	1:B:98:PRO:HD3	1.90	0.54
1:A:551:THR:O	1:A:554:PHE:HB3	2.08	0.54
1:C:224:ILE:HG22	1:C:276:VAL:HA	1.90	0.54
1:D:604:ALA:HB2	1:D:691:LYS:HG2	1.90	0.54
1:D:403:ASP:HB3	1:D:406:ARG:HB3	1.90	0.54
1:B:719:PHE:C	1:B:721:MET:N	2.61	0.54
1:A:419:ILE:HG12	1:A:457:PHE:CD2	2.43	0.53
1:D:28:VAL:HB	1:D:98:PRO:HD3	1.90	0.53
1:B:393:HIS:O	1:B:395:LEU:HG	2.07	0.53
1:C:286:THR:HG22	1:C:287:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:ALA:HB2	1:C:691:LYS:HG2	1.89	0.53
1:A:552:ASP:C	1:A:554:PHE:H	2.10	0.53
1:C:601:PHE:O	1:C:602:ILE:HB	2.09	0.53
1:A:172:GLN:H	1:A:172:GLN:CD	2.11	0.53
1:B:286:THR:CG2	1:B:287:LEU:N	2.72	0.53
1:A:500:GLU:CG	1:A:501:THR:H	2.15	0.53
1:A:427:LEU:HD12	1:A:442:TYR:HE2	1.74	0.53
1:A:604:ALA:HB2	1:A:691:LYS:HG2	1.90	0.53
1:B:109:THR:HG23	1:B:120:ASN:HD22	1.74	0.53
1:B:73:SER:HB2	1:B:78:LEU:HB3	1.90	0.53
1:A:78:LEU:HD12	1:A:79:LEU:N	2.21	0.53
1:D:527:SER:O	1:D:530:LYS:HB3	2.09	0.53
1:C:419:ILE:HG12	1:C:457:PHE:CD2	2.43	0.53
1:B:211:PHE:CE1	1:B:212:PHE:HB2	2.43	0.53
1:D:414:ARG:O	1:D:414:ARG:HG2	2.07	0.53
1:B:239:GLN:O	1:B:273:VAL:HG23	2.09	0.53
1:A:286:THR:HG22	1:A:287:LEU:O	2.08	0.53
1:A:670:GLN:HG3	1:C:727:TYR:OH	2.07	0.53
1:A:173:PHE:HD1	1:A:186:LEU:O	1.92	0.53
1:B:54:SER:HB2	1:B:74:SER:OG	2.08	0.53
1:A:601:PHE:N	1:A:601:PHE:CD1	2.77	0.53
1:D:109:THR:HG23	1:D:120:ASN:HD22	1.74	0.53
1:D:450:LEU:O	1:D:451:ARG:C	2.44	0.53
1:D:707:SER:O	1:D:709:VAL:N	2.41	0.53
1:A:349:LEU:H	1:A:368:VAL:CG2	2.20	0.53
1:B:419:ILE:HG12	1:B:457:PHE:CD2	2.44	0.53
1:D:551:THR:O	1:D:554:PHE:HB3	2.09	0.53
1:A:297:LEU:CD2	1:A:318:ASN:HD21	2.21	0.53
1:D:286:THR:HG22	1:D:287:LEU:O	2.08	0.53
1:A:71:HIS:CE1	1:A:478:PRO:CA	2.91	0.53
1:A:28:VAL:HB	1:A:98:PRO:HD3	1.91	0.53
1:C:552:ASP:C	1:C:554:PHE:H	2.11	0.53
1:D:259:MET:HE1	1:D:262:GLN:HE22	1.74	0.53
1:C:241:CYS:O	1:C:259:MET:CG	2.56	0.53
1:A:188:LYS:HB2	1:A:194:TYR:CE1	2.44	0.53
1:C:403:ASP:HB3	1:C:406:ARG:HB3	1.91	0.53
1:B:545:THR:C	1:B:547:VAL:N	2.60	0.53
1:A:546:THR:O	1:A:546:THR:CG2	2.54	0.53
1:A:521:SER:O	1:A:524:VAL:HB	2.09	0.53
1:B:663:LEU:O	1:B:667:LEU:HG	2.09	0.53
1:A:457:PHE:CE1	1:A:477:GLN:HG2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PHE:O	1:C:73:SER:C	2.46	0.53
1:A:450:LEU:O	1:A:451:ARG:C	2.46	0.53
1:A:254:ILE:CG2	1:A:311:LEU:HB2	2.39	0.53
1:A:11:LEU:HB3	1:A:87:ALA:CB	2.39	0.53
1:B:232:ARG:HG2	1:B:248:LEU:H	1.75	0.53
1:C:601:PHE:CD1	1:C:601:PHE:N	2.77	0.53
1:D:601:PHE:O	1:D:602:ILE:HB	2.09	0.53
1:C:707:SER:O	1:C:709:VAL:N	2.42	0.53
1:C:546:THR:CG2	1:C:546:THR:O	2.55	0.53
1:D:349:LEU:H	1:D:368:VAL:CG2	2.20	0.53
1:B:111:GLN:HG3	1:B:168:TYR:CD2	2.44	0.53
1:D:483:LEU:HD13	1:D:614:ILE:HD12	1.91	0.53
1:A:239:GLN:O	1:A:273:VAL:HG23	2.09	0.52
1:A:293:LEU:HB2	1:A:297:LEU:CG	2.27	0.52
1:C:101:SER:HB2	1:C:107:THR:HG1	1.73	0.52
1:A:601:PHE:O	1:A:602:ILE:HB	2.09	0.52
1:A:707:SER:O	1:A:709:VAL:N	2.42	0.52
1:D:404:VAL:HG23	1:D:443:LEU:HD11	1.89	0.52
1:B:11:LEU:HD12	1:B:479:TYR:HA	1.90	0.52
1:B:92:THR:HG21	1:B:479:TYR:OH	2.09	0.52
1:D:111:GLN:HG3	1:D:168:TYR:CD2	2.44	0.52
1:C:414:ARG:O	1:C:414:ARG:HG2	2.08	0.52
1:D:172:GLN:CD	1:D:172:GLN:H	2.12	0.52
1:B:297:LEU:CD2	1:B:318:ASN:HD21	2.22	0.52
1:C:293:LEU:HB2	1:C:297:LEU:CG	2.28	0.52
1:B:450:LEU:O	1:B:451:ARG:C	2.44	0.52
1:D:184:LEU:HG	1:D:185:GLY:H	1.73	0.52
1:B:601:PHE:O	1:B:602:ILE:HB	2.09	0.52
1:B:14:TYR:HB3	1:B:673:CYS:HB2	1.90	0.52
1:A:224:ILE:HG22	1:A:276:VAL:HA	1.92	0.52
1:C:239:GLN:O	1:C:273:VAL:HG23	2.09	0.52
1:C:500:GLU:CG	1:C:501:THR:H	2.16	0.52
1:A:404:VAL:HG23	1:A:443:LEU:HD11	1.90	0.52
1:D:72:PHE:O	1:D:73:SER:C	2.45	0.52
1:B:349:LEU:H	1:B:368:VAL:CG2	2.20	0.52
1:A:634:LEU:HD21	1:A:655:LEU:HD23	1.92	0.52
1:A:14:TYR:HB3	1:A:673:CYS:HB2	1.91	0.52
1:B:286:THR:HG22	1:B:287:LEU:O	2.09	0.52
1:C:317:ASN:OD1	1:C:318:ASN:N	2.38	0.52
1:B:184:LEU:HG	1:B:185:GLY:H	1.74	0.52
1:D:545:THR:C	1:D:547:VAL:N	2.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:LEU:HD12	1:D:442:TYR:HE2	1.74	0.52
1:B:73:SER:N	1:B:78:LEU:O	2.42	0.52
1:D:428:SER:O	1:D:431:LYS:N	2.38	0.52
1:B:224:ILE:HG22	1:B:276:VAL:HA	1.90	0.52
1:D:237:LEU:HD11	1:D:241:CYS:HA	1.91	0.52
1:C:173:PHE:HD1	1:C:186:LEU:O	1.93	0.52
1:B:317:ASN:OD1	1:B:318:ASN:N	2.38	0.52
1:C:663:LEU:CD1	1:C:729:ILE:HD12	2.40	0.52
1:A:623:LEU:HD13	1:A:664:LEU:HD22	1.91	0.52
1:D:54:SER:HB2	1:D:74:SER:OG	2.09	0.52
1:B:601:PHE:CD1	1:B:601:PHE:N	2.77	0.52
1:C:201:ASP:O	1:C:203:SER:N	2.42	0.52
1:A:201:ASP:O	1:A:203:SER:N	2.42	0.52
1:A:536:ILE:HD11	1:A:655:LEU:HB3	1.90	0.52
1:A:72:PHE:O	1:A:73:SER:C	2.46	0.52
1:B:457:PHE:CE1	1:B:477:GLN:HG2	2.44	0.52
1:C:259:MET:HE1	1:C:262:GLN:NE2	2.17	0.52
1:A:317:ASN:OD1	1:A:318:ASN:N	2.38	0.52
1:A:104:GLN:O	1:A:106:TYR:N	2.43	0.52
1:C:623:LEU:HD13	1:C:664:LEU:HD22	1.91	0.52
1:A:650:HIS:O	1:A:653:THR:N	2.35	0.52
1:B:541:PRO:HB2	1:B:544:MET:CE	2.40	0.52
1:D:457:PHE:CE1	1:D:477:GLN:HG2	2.44	0.52
1:A:257:TYR:CZ	1:A:313:TYR:HB3	2.45	0.52
1:A:172:GLN:N	1:A:172:GLN:NE2	2.58	0.52
1:D:201:ASP:O	1:D:203:SER:N	2.42	0.52
1:B:506:LEU:HA	1:B:582:VAL:CG1	2.40	0.52
1:C:349:LEU:H	1:C:368:VAL:CG2	2.21	0.52
1:D:73:SER:N	1:D:78:LEU:O	2.42	0.52
1:B:72:PHE:O	1:B:73:SER:C	2.46	0.52
1:C:536:ILE:HD12	1:C:659:TYR:HB2	1.91	0.52
1:D:297:LEU:CD2	1:D:318:ASN:HD21	2.22	0.52
1:B:521:SER:O	1:B:524:VAL:HB	2.09	0.52
1:C:650:HIS:O	1:C:653:THR:N	2.35	0.52
1:D:225:SER:OG	1:D:279:TYR:HB2	2.10	0.52
1:C:317:ASN:HB3	1:C:373:PHE:HB3	1.92	0.52
1:D:173:PHE:HD1	1:D:186:LEU:O	1.92	0.52
1:D:601:PHE:N	1:D:601:PHE:CD1	2.77	0.52
1:D:405:GLU:OE2	1:D:437:ASN:ND2	2.42	0.52
1:B:368:VAL:CG2	1:B:368:VAL:O	2.57	0.52
1:D:368:VAL:O	1:D:368:VAL:CG2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:GLU:HG2	1:C:722:THR:N	2.25	0.52
1:C:14:TYR:HB3	1:C:673:CYS:HB2	1.91	0.52
1:B:237:LEU:HD11	1:B:241:CYS:HA	1.92	0.52
1:B:104:GLN:C	1:B:106:TYR:H	2.13	0.52
1:A:104:GLN:C	1:A:106:TYR:H	2.13	0.52
1:C:663:LEU:O	1:C:667:LEU:HG	2.09	0.52
1:D:708:ASN:O	1:D:712:ALA:HB2	2.09	0.52
1:B:201:ASP:O	1:B:203:SER:N	2.43	0.52
1:D:393:HIS:O	1:D:394:ASP:C	2.48	0.52
1:C:410:ASN:O	1:C:413:SER:N	2.42	0.52
1:B:172:GLN:CD	1:B:172:GLN:H	2.13	0.51
1:C:297:LEU:CD2	1:C:318:ASN:HD21	2.23	0.51
1:C:111:GLN:HG3	1:C:168:TYR:CD2	2.45	0.51
1:B:650:HIS:O	1:B:651:ILE:C	2.48	0.51
1:D:332:VAL:CG2	1:D:356:LYS:HB2	2.40	0.51
1:D:11:LEU:HD12	1:D:479:TYR:HA	1.91	0.51
1:C:237:LEU:HD11	1:C:241:CYS:HA	1.91	0.51
1:C:283:TYR:CG	1:C:284:ASN:N	2.78	0.51
1:A:564:ILE:HG21	1:D:203:SER:HB2	1.93	0.51
1:B:634:LEU:HD21	1:B:655:LEU:HD23	1.92	0.51
1:B:188:LYS:HB2	1:B:194:TYR:CE1	2.45	0.51
1:A:184:LEU:HG	1:A:185:GLY:H	1.74	0.51
1:C:92:THR:HG21	1:C:479:TYR:OH	2.11	0.51
1:A:11:LEU:HD12	1:A:479:TYR:HA	1.92	0.51
1:B:663:LEU:CD1	1:B:729:ILE:HD12	2.40	0.51
1:D:536:ILE:HD11	1:D:655:LEU:HB3	1.91	0.51
1:B:483:LEU:HD13	1:B:614:ILE:HD12	1.92	0.51
1:D:214:ARG:HG2	1:D:214:ARG:O	2.11	0.51
1:C:184:LEU:HG	1:C:185:GLY:H	1.74	0.51
1:C:188:LYS:HB2	1:C:194:TYR:CE1	2.46	0.51
1:D:104:GLN:C	1:D:106:TYR:H	2.14	0.51
1:A:663:LEU:CD1	1:A:729:ILE:HD12	2.40	0.51
1:B:214:ARG:O	1:B:214:ARG:HG2	2.11	0.51
1:B:414:ARG:HG2	1:B:414:ARG:O	2.10	0.51
1:D:188:LYS:HB2	1:D:194:TYR:CE1	2.45	0.51
1:A:568:LYS:CD	1:D:210:ARG:HH22	2.23	0.51
1:C:104:GLN:O	1:C:106:TYR:N	2.44	0.51
1:B:690:VAL:CG1	1:B:691:LYS:N	2.74	0.51
1:D:506:LEU:HA	1:D:582:VAL:CG1	2.41	0.51
1:A:111:GLN:HG3	1:A:168:TYR:CD2	2.45	0.51
1:D:18:PRO:HG3	1:D:421:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:O	1:C:214:ARG:HG2	2.10	0.51
1:C:172:GLN:H	1:C:172:GLN:CD	2.14	0.51
1:A:317:ASN:HB3	1:A:373:PHE:HB3	1.93	0.51
1:D:232:ARG:NH1	1:D:233:TYR:OH	2.44	0.51
1:C:232:ARG:NH1	1:C:233:TYR:OH	2.44	0.51
1:B:707:SER:O	1:B:709:VAL:N	2.43	0.51
1:C:368:VAL:CG2	1:C:368:VAL:O	2.57	0.51
1:A:719:PHE:C	1:A:721:MET:N	2.60	0.51
1:D:634:LEU:HD21	1:D:655:LEU:HD23	1.92	0.51
1:A:1:MET:O	1:A:1:MET:HG2	2.10	0.51
1:B:244:LYS:HB3	1:B:253:LEU:CD1	2.41	0.51
1:B:257:TYR:CZ	1:B:313:TYR:HB3	2.46	0.51
1:A:237:LEU:HD11	1:A:241:CYS:HA	1.92	0.51
1:B:290:LEU:O	1:B:291:LEU:HD23	2.10	0.51
1:A:667:LEU:HD21	1:C:724:PHE:HE1	1.74	0.51
1:B:173:PHE:HD1	1:B:186:LEU:O	1.93	0.51
1:A:410:ASN:O	1:A:413:SER:N	2.43	0.51
1:B:104:GLN:O	1:B:106:TYR:N	2.43	0.51
1:D:104:GLN:O	1:D:106:TYR:N	2.43	0.51
1:A:527:SER:O	1:A:530:LYS:HB3	2.11	0.51
1:D:690:VAL:CG1	1:D:691:LYS:N	2.74	0.51
1:D:247:ASP:HB3	1:D:250:SER:HB2	1.92	0.51
1:B:708:ASN:O	1:B:712:ALA:HB2	2.10	0.51
1:D:650:HIS:O	1:D:651:ILE:C	2.49	0.51
1:B:393:HIS:O	1:B:394:ASP:C	2.49	0.51
1:D:69:CYS:HB2	1:D:82:TYR:CE1	2.46	0.51
1:A:483:LEU:HD13	1:A:614:ILE:HD12	1.91	0.51
1:A:214:ARG:O	1:A:214:ARG:HG2	2.11	0.51
1:D:1:MET:HG2	1:D:1:MET:O	2.11	0.51
1:D:317:ASN:HB3	1:D:373:PHE:HB3	1.92	0.51
1:A:283:TYR:CG	1:A:284:ASN:N	2.79	0.51
1:B:232:ARG:NH1	1:B:233:TYR:OH	2.44	0.51
1:A:443:LEU:C	1:A:445:ASN:N	2.64	0.51
1:C:399:THR:O	1:C:526:ARG:NH2	2.44	0.51
1:A:311:LEU:O	1:A:312:THR:HG23	2.11	0.51
1:D:536:ILE:HD11	1:D:655:LEU:C	2.32	0.51
1:D:663:LEU:O	1:D:667:LEU:HG	2.11	0.51
1:C:332:VAL:CG2	1:C:356:LYS:HB2	2.40	0.51
1:B:716:GLU:HG2	1:B:722:THR:N	2.26	0.51
1:D:9:ALA:CB	1:D:613:ILE:HD11	2.41	0.51
1:D:317:ASN:ND2	1:D:319:ILE:CG1	2.70	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:LEU:C	1:C:445:ASN:N	2.64	0.51
1:C:553:ILE:O	1:C:553:ILE:CG2	2.59	0.51
1:A:232:ARG:NH1	1:A:233:TYR:OH	2.44	0.51
1:D:521:SER:O	1:D:524:VAL:HB	2.11	0.51
1:A:368:VAL:CG2	1:A:368:VAL:O	2.58	0.51
1:A:506:LEU:HA	1:A:582:VAL:CG1	2.40	0.51
1:D:541:PRO:HB2	1:D:544:MET:CE	2.41	0.51
1:B:317:ASN:HB3	1:B:373:PHE:HB3	1.92	0.50
1:C:290:LEU:O	1:C:291:LEU:HD23	2.11	0.50
1:B:311:LEU:O	1:B:312:THR:HG23	2.11	0.50
1:D:604:ALA:O	1:D:688:PHE:HB2	2.11	0.50
1:D:92:THR:HG21	1:D:479:TYR:OH	2.11	0.50
1:D:9:ALA:HB1	1:D:613:ILE:HD11	1.92	0.50
1:A:620:HIS:CD2	1:A:668:TYR:CD2	2.99	0.50
1:B:280:LEU:HD12	1:B:280:LEU:O	2.12	0.50
1:B:335:VAL:CG1	1:B:352:ILE:HB	2.42	0.50
1:C:104:GLN:C	1:C:106:TYR:H	2.14	0.50
1:A:727:TYR:OH	1:C:670:GLN:HG3	2.09	0.50
1:A:724:PHE:HB3	1:C:724:PHE:HB3	1.92	0.50
1:D:623:LEU:HD13	1:D:664:LEU:HD22	1.91	0.50
1:C:690:VAL:CG1	1:C:691:LYS:N	2.74	0.50
1:C:708:ASN:O	1:C:712:ALA:HB2	2.10	0.50
1:A:109:THR:HG23	1:A:120:ASN:HD22	1.75	0.50
1:C:719:PHE:C	1:C:721:MET:N	2.61	0.50
1:A:332:VAL:CG2	1:A:356:LYS:HB2	2.41	0.50
1:A:249:THR:O	1:A:249:THR:HG22	2.11	0.50
1:B:287:LEU:HG	1:B:288:VAL:N	2.26	0.50
1:D:500:GLU:CG	1:D:501:THR:H	2.15	0.50
1:D:575:ASN:C	1:D:577:PHE:H	2.14	0.50
1:A:708:ASN:O	1:A:712:ALA:HB2	2.10	0.50
1:D:707:SER:O	1:D:708:ASN:C	2.50	0.50
1:B:536:ILE:HD11	1:B:655:LEU:HB3	1.92	0.50
1:D:663:LEU:CD1	1:D:729:ILE:HD12	2.41	0.50
1:B:370:ASP:OD1	1:B:372:SER:HB3	2.11	0.50
1:B:221:ASP:O	1:B:238:THR:HB	2.12	0.50
1:B:239:GLN:HG2	1:B:273:VAL:O	2.11	0.50
1:B:192:VAL:O	1:B:192:VAL:HG12	2.11	0.50
1:D:172:GLN:NE2	1:D:172:GLN:N	2.60	0.50
1:B:55:GLU:OE1	1:B:74:SER:CA	2.59	0.50
1:C:719:PHE:O	1:C:720:PHE:C	2.50	0.50
1:A:541:PRO:HB2	1:A:544:MET:CE	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:VAL:CG2	1:B:356:LYS:HB2	2.41	0.50
1:A:69:CYS:HB2	1:A:82:TYR:CE1	2.47	0.50
1:D:370:ASP:OD1	1:D:372:SER:HB3	2.11	0.50
1:B:317:ASN:ND2	1:B:319:ILE:CG1	2.71	0.50
1:C:284:ASN:HB3	1:C:285:ASN:OD1	2.11	0.50
1:B:342:LEU:HD12	1:B:379:ILE:HD12	1.94	0.50
1:A:528:ILE:O	1:A:529:SER:C	2.50	0.50
1:B:604:ALA:O	1:B:688:PHE:HB2	2.12	0.50
1:C:109:THR:HG23	1:C:120:ASN:HD22	1.76	0.50
1:B:225:SER:OG	1:B:279:TYR:HB2	2.12	0.50
1:C:306:ASP:OD1	1:C:307:SER:N	2.44	0.50
1:B:428:SER:O	1:B:431:LYS:N	2.40	0.50
1:D:224:ILE:CG2	1:D:276:VAL:HA	2.41	0.50
1:B:500:GLU:CG	1:B:501:THR:H	2.15	0.50
1:C:427:LEU:HD12	1:C:442:TYR:HE2	1.77	0.50
1:C:311:LEU:O	1:C:312:THR:HG23	2.12	0.50
1:B:349:LEU:N	1:B:368:VAL:HG22	2.26	0.50
1:D:657:LEU:O	1:D:658:HIS:C	2.50	0.50
1:C:634:LEU:HD21	1:C:655:LEU:HD23	1.94	0.50
1:A:393:HIS:O	1:A:394:ASP:C	2.49	0.50
1:B:493:TRP:CD1	1:B:507:PHE:HD1	2.29	0.50
1:D:221:ASP:O	1:D:238:THR:HB	2.12	0.50
1:D:290:LEU:O	1:D:291:LEU:HD23	2.11	0.50
1:A:323:LEU:HD11	1:A:355:TRP:CD2	2.47	0.50
1:A:663:LEU:O	1:A:667:LEU:HG	2.11	0.50
1:A:247:ASP:HB2	1:A:254:ILE:HG13	1.94	0.50
1:D:349:LEU:N	1:D:368:VAL:HG22	2.26	0.50
1:B:536:ILE:HD11	1:B:655:LEU:C	2.32	0.50
1:A:536:ILE:HD11	1:A:655:LEU:C	2.32	0.50
1:C:344:VAL:CG1	1:C:345:GLU:N	2.74	0.50
1:D:95:ILE:HD13	1:D:131:LEU:HD13	1.93	0.50
1:C:528:ILE:O	1:C:529:SER:C	2.50	0.50
1:C:18:PRO:HG3	1:C:421:GLU:OE1	2.12	0.50
1:B:410:ASN:O	1:B:413:SER:N	2.43	0.50
1:C:225:SER:OG	1:C:279:TYR:HB2	2.12	0.50
1:A:414:ARG:O	1:A:414:ARG:HG2	2.11	0.50
1:C:57:SER:HB2	1:C:71:HIS:CD2	2.47	0.50
1:D:525:LEU:O	1:D:526:ARG:C	2.49	0.50
1:A:604:ALA:O	1:A:688:PHE:HB2	2.12	0.50
1:C:396:ASP:OD1	1:C:396:ASP:C	2.50	0.50
1:C:575:ASN:C	1:C:577:PHE:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ILE:CG2	1:A:553:ILE:O	2.60	0.50
1:D:404:VAL:O	1:D:408:PHE:HB2	2.12	0.50
1:B:11:LEU:HB3	1:B:87:ALA:HB3	1.94	0.50
1:C:506:LEU:HA	1:C:582:VAL:CG1	2.41	0.50
1:A:225:SER:OG	1:A:279:TYR:HB2	2.12	0.50
1:C:1:MET:HG2	1:C:1:MET:O	2.12	0.50
1:A:396:ASP:OD1	1:A:396:ASP:C	2.50	0.50
1:A:290:LEU:O	1:A:291:LEU:HD23	2.12	0.49
1:D:176:VAL:CG1	1:D:177:PHE:H	2.21	0.49
1:B:575:ASN:C	1:B:577:PHE:H	2.14	0.49
1:D:11:LEU:HB3	1:D:87:ALA:HB3	1.94	0.49
1:D:236:VAL:HG23	1:D:244:LYS:HB2	1.95	0.49
1:D:262:GLN:OE1	1:D:315:PHE:HB2	2.12	0.49
1:C:287:LEU:HG	1:C:288:VAL:N	2.26	0.49
1:A:575:ASN:C	1:A:577:PHE:H	2.14	0.49
1:A:287:LEU:HG	1:A:288:VAL:N	2.27	0.49
1:B:140:SER:OG	1:B:141:SER:N	2.43	0.49
1:C:95:ILE:CD1	1:C:133:LEU:HD11	2.41	0.49
1:C:69:CYS:HB2	1:C:82:TYR:CE1	2.47	0.49
1:B:69:CYS:HB2	1:B:82:TYR:CE1	2.47	0.49
1:D:192:VAL:HG12	1:D:192:VAL:O	2.12	0.49
1:C:172:GLN:NE2	1:C:172:GLN:N	2.61	0.49
1:C:707:SER:O	1:C:708:ASN:C	2.50	0.49
1:A:73:SER:N	1:A:78:LEU:O	2.41	0.49
1:D:716:GLU:HG2	1:D:722:THR:N	2.28	0.49
1:D:280:LEU:HD12	1:D:280:LEU:O	2.13	0.49
1:B:224:ILE:CG2	1:B:276:VAL:HA	2.43	0.49
1:D:287:LEU:HG	1:D:288:VAL:N	2.27	0.49
1:A:568:LYS:NZ	1:D:210:ARG:NH2	2.57	0.49
1:B:404:VAL:O	1:B:408:PHE:HB2	2.13	0.49
1:B:58:ASN:HA	1:B:474:ASN:HD22	1.75	0.49
1:B:399:THR:O	1:B:526:ARG:NH2	2.45	0.49
1:B:95:ILE:HD13	1:B:131:LEU:HD13	1.93	0.49
1:D:719:PHE:O	1:D:720:PHE:C	2.50	0.49
1:C:9:ALA:CB	1:C:613:ILE:HD11	2.42	0.49
1:A:207:SER:C	1:A:209:THR:H	2.15	0.49
1:C:176:VAL:CG1	1:C:177:PHE:H	2.21	0.49
1:C:221:ASP:O	1:C:238:THR:HB	2.12	0.49
1:C:404:VAL:O	1:C:408:PHE:HB2	2.12	0.49
1:B:344:VAL:CG1	1:B:345:GLU:N	2.73	0.49
1:B:71:HIS:O	1:B:79:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:CG1	1:A:345:GLU:N	2.75	0.49
1:C:536:ILE:HD11	1:C:655:LEU:HB3	1.93	0.49
1:C:393:HIS:O	1:C:394:ASP:C	2.50	0.49
1:C:14:TYR:CE2	1:C:613:ILE:HG22	2.47	0.49
1:D:396:ASP:C	1:D:396:ASP:OD1	2.50	0.49
1:C:236:VAL:HG23	1:C:244:LYS:HB2	1.94	0.49
1:D:283:TYR:CG	1:D:284:ASN:N	2.79	0.49
1:C:335:VAL:CG1	1:C:352:ILE:HB	2.43	0.49
1:A:335:VAL:CG1	1:A:352:ILE:HB	2.43	0.49
1:A:80:THR:HG22	1:A:81:PHE:N	2.27	0.49
1:B:57:SER:HB2	1:B:71:HIS:CD2	2.47	0.49
1:A:716:GLU:HG2	1:A:722:THR:N	2.27	0.49
1:B:207:SER:C	1:B:209:THR:H	2.15	0.49
1:C:4:LEU:HA	1:C:485:LYS:O	2.12	0.49
1:B:172:GLN:N	1:B:172:GLN:NE2	2.61	0.49
1:C:192:VAL:O	1:C:192:VAL:HG12	2.12	0.49
1:D:335:VAL:CG1	1:D:352:ILE:HB	2.43	0.49
1:B:187:LYS:HD3	1:B:197:LEU:CD1	2.34	0.49
1:A:176:VAL:CG1	1:A:177:PHE:H	2.21	0.49
1:D:311:LEU:O	1:D:312:THR:HG23	2.12	0.49
1:C:95:ILE:HD13	1:C:131:LEU:HD13	1.93	0.49
1:A:95:ILE:HD13	1:A:131:LEU:HD13	1.93	0.49
1:D:410:ASN:O	1:D:413:SER:N	2.43	0.49
1:A:221:ASP:O	1:A:238:THR:HB	2.12	0.49
1:A:284:ASN:HB3	1:A:285:ASN:OD1	2.12	0.49
1:C:693:PHE:N	1:C:697:GLN:NE2	2.60	0.49
1:C:604:ALA:O	1:C:688:PHE:HB2	2.13	0.49
1:A:707:SER:O	1:A:708:ASN:C	2.51	0.49
1:D:57:SER:HB2	1:D:71:HIS:CD2	2.47	0.49
1:A:719:PHE:O	1:A:720:PHE:C	2.51	0.49
1:C:9:ALA:HB1	1:C:613:ILE:HD11	1.93	0.49
1:C:207:SER:C	1:C:209:THR:H	2.16	0.49
1:B:1:MET:O	1:B:1:MET:HG2	2.12	0.49
1:A:236:VAL:HG23	1:A:244:LYS:HB2	1.95	0.49
1:B:283:TYR:CG	1:B:284:ASN:N	2.79	0.49
1:B:693:PHE:N	1:B:697:GLN:NE2	2.60	0.49
1:B:176:VAL:CG1	1:B:177:PHE:H	2.22	0.49
1:A:404:VAL:O	1:A:408:PHE:HB2	2.12	0.49
1:C:140:SER:OG	1:C:141:SER:N	2.43	0.49
1:D:71:HIS:O	1:D:79:LEU:HD12	2.12	0.49
1:C:541:PRO:HB2	1:C:544:MET:CE	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:HG3	1:A:421:GLU:OE1	2.13	0.49
1:C:587:ILE:O	1:C:592:LYS:HB2	2.13	0.49
1:A:690:VAL:CG1	1:A:691:LYS:N	2.75	0.49
1:C:201:ASP:O	1:C:204:TYR:N	2.46	0.49
1:D:344:VAL:CG1	1:D:345:GLU:N	2.74	0.49
1:B:80:THR:HG22	1:B:81:PHE:N	2.27	0.49
1:A:71:HIS:O	1:A:79:LEU:HD12	2.12	0.49
1:C:536:ILE:HD11	1:C:655:LEU:C	2.33	0.49
1:C:716:GLU:HG2	1:C:722:THR:CA	2.43	0.49
1:A:95:ILE:CD1	1:A:133:LEU:HD11	2.43	0.49
1:C:650:HIS:O	1:C:651:ILE:C	2.50	0.49
1:D:14:TYR:HB3	1:D:673:CYS:HB2	1.94	0.49
1:B:587:ILE:O	1:B:592:LYS:HB2	2.12	0.49
1:A:4:LEU:HA	1:A:485:LYS:O	2.12	0.49
1:B:236:VAL:HG23	1:B:244:LYS:HB2	1.95	0.48
1:A:192:VAL:HG12	1:A:192:VAL:O	2.12	0.48
1:D:336:LEU:C	1:D:337:THR:HG22	2.33	0.48
1:C:335:VAL:HG22	1:C:337:THR:HG22	1.95	0.48
1:B:427:LEU:HD12	1:B:442:TYR:HE2	1.77	0.48
1:B:525:LEU:O	1:B:526:ARG:C	2.50	0.48
1:B:707:SER:O	1:B:708:ASN:C	2.51	0.48
1:A:140:SER:OG	1:A:141:SER:N	2.44	0.48
1:B:536:ILE:HD12	1:B:659:TYR:HB2	1.93	0.48
1:A:657:LEU:O	1:A:658:HIS:C	2.52	0.48
1:A:57:SER:HB2	1:A:71:HIS:CD2	2.48	0.48
1:D:18:PRO:HB3	1:D:417:THR:CG2	2.43	0.48
1:D:566:ASN:HA	1:D:569:ILE:HD12	1.94	0.48
1:D:587:ILE:O	1:D:592:LYS:HB2	2.12	0.48
1:C:363:LEU:HG	1:C:364:GLN:N	2.28	0.48
1:C:224:ILE:CG2	1:C:276:VAL:HA	2.42	0.48
1:A:335:VAL:HG22	1:A:337:THR:HG22	1.96	0.48
1:D:187:LYS:HD3	1:D:197:LEU:CD1	2.34	0.48
1:A:92:THR:HG21	1:A:479:TYR:OH	2.13	0.48
1:B:382:VAL:HG21	1:B:495:TYR:CD1	2.48	0.48
1:C:566:ASN:HA	1:C:569:ILE:HD12	1.95	0.48
1:C:493:TRP:CD1	1:C:507:PHE:HD1	2.31	0.48
1:D:493:TRP:CD1	1:D:507:PHE:HD1	2.31	0.48
1:C:405:GLU:OE2	1:C:437:ASN:ND2	2.47	0.48
1:B:323:LEU:HD11	1:B:355:TRP:CD2	2.48	0.48
1:B:180:ASP:C	1:B:182:GLY:H	2.17	0.48
1:B:247:ASP:HB2	1:B:254:ILE:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:O	1:C:79:LEU:HD12	2.12	0.48
1:D:201:ASP:O	1:D:204:TYR:N	2.46	0.48
1:A:448:THR:O	1:A:452:ASP:OD2	2.31	0.48
1:A:370:ASP:OD1	1:A:372:SER:HB3	2.12	0.48
1:B:101:SER:HB3	1:B:121:VAL:HG13	1.94	0.48
1:A:101:SER:HB3	1:A:121:VAL:CG1	2.44	0.48
1:A:101:SER:HB3	1:A:121:VAL:HG13	1.94	0.48
1:B:403:ASP:HB3	1:B:406:ARG:CB	2.43	0.48
1:C:71:HIS:HE1	1:C:478:PRO:N	2.11	0.48
1:B:201:ASP:O	1:B:204:TYR:N	2.46	0.48
1:C:657:LEU:O	1:C:658:HIS:C	2.52	0.48
1:A:650:HIS:O	1:A:651:ILE:C	2.50	0.48
1:A:566:ASN:HA	1:A:569:ILE:HD12	1.95	0.48
1:D:101:SER:HB3	1:D:121:VAL:HG13	1.94	0.48
1:C:533:LEU:HD13	1:C:729:ILE:CD1	2.44	0.48
1:A:201:ASP:O	1:A:204:TYR:N	2.46	0.48
1:C:80:THR:HG22	1:C:81:PHE:N	2.28	0.48
1:D:207:SER:C	1:D:209:THR:H	2.16	0.48
1:C:263:SER:O	1:C:264:ASP:C	2.51	0.48
1:B:101:SER:HB3	1:B:121:VAL:CG1	2.44	0.48
1:D:101:SER:HB3	1:D:121:VAL:CG1	2.44	0.48
1:A:533:LEU:HD13	1:A:729:ILE:CD1	2.44	0.48
1:B:254:ILE:CG2	1:B:311:LEU:HB2	2.44	0.48
1:D:533:LEU:HD13	1:D:729:ILE:CD1	2.44	0.48
1:A:263:SER:O	1:A:264:ASP:C	2.51	0.48
1:A:363:LEU:HG	1:A:364:GLN:N	2.29	0.48
1:C:483:LEU:HD13	1:C:614:ILE:HD12	1.94	0.48
1:A:587:ILE:O	1:A:592:LYS:HB2	2.13	0.48
1:B:293:LEU:HB2	1:B:297:LEU:CG	2.27	0.48
1:C:101:SER:HB3	1:C:121:VAL:CG1	2.44	0.48
1:B:232:ARG:HD2	1:B:233:TYR:CE1	2.49	0.48
1:C:11:LEU:HB3	1:C:87:ALA:HB3	1.94	0.48
1:B:623:LEU:HD13	1:B:664:LEU:HD22	1.93	0.48
1:B:506:LEU:HA	1:B:582:VAL:HG13	1.94	0.48
1:D:80:THR:HG22	1:D:81:PHE:N	2.27	0.48
1:B:657:LEU:O	1:B:658:HIS:C	2.52	0.48
1:B:263:SER:O	1:B:264:ASP:C	2.51	0.48
1:B:335:VAL:HG22	1:B:337:THR:HG22	1.96	0.48
1:D:283:TYR:O	1:D:284:ASN:O	2.32	0.48
1:A:693:PHE:N	1:A:697:GLN:NE2	2.61	0.48
1:B:249:THR:O	1:B:249:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ILE:HD12	1:A:659:TYR:HB2	1.95	0.48
1:C:370:ASP:OD1	1:C:372:SER:HB3	2.13	0.48
1:A:317:ASN:CG	1:A:318:ASN:N	2.67	0.48
1:D:335:VAL:HG22	1:D:337:THR:HG22	1.96	0.48
1:D:693:PHE:N	1:D:697:GLN:NE2	2.60	0.48
1:D:232:ARG:HD2	1:D:233:TYR:CE1	2.49	0.48
1:C:28:VAL:HG23	1:C:96:HIS:O	2.14	0.48
1:A:493:TRP:CD1	1:A:507:PHE:HD1	2.31	0.48
1:D:239:GLN:HG2	1:D:273:VAL:O	2.13	0.48
1:C:253:LEU:HG	1:C:255:GLN:O	2.14	0.48
1:B:336:LEU:C	1:B:337:THR:HG22	2.34	0.48
1:D:619:LEU:HD11	1:D:623:LEU:HD11	1.96	0.48
1:B:71:HIS:HE1	1:B:478:PRO:N	2.11	0.48
1:D:585:ASP:OD1	1:D:589:ASN:HB2	2.14	0.48
1:D:293:LEU:HB2	1:D:297:LEU:CG	2.28	0.47
1:C:101:SER:HB3	1:C:121:VAL:HG13	1.95	0.47
1:D:180:ASP:C	1:D:182:GLY:H	2.18	0.47
1:C:55:GLU:OE1	1:C:74:SER:CA	2.60	0.47
1:D:140:SER:OG	1:D:141:SER:N	2.44	0.47
1:A:9:ALA:CB	1:A:613:ILE:HD11	2.43	0.47
1:C:157:ASP:OD2	1:C:159:THR:HB	2.14	0.47
1:D:157:ASP:OD2	1:D:159:THR:HB	2.14	0.47
1:B:585:ASP:OD1	1:B:589:ASN:HB2	2.14	0.47
1:D:243:LEU:HB3	1:D:259:MET:HE3	1.95	0.47
1:D:323:LEU:HD11	1:D:355:TRP:CD2	2.49	0.47
1:C:73:SER:N	1:C:78:LEU:O	2.42	0.47
1:B:349:LEU:HB2	1:B:368:VAL:HG21	1.97	0.47
1:B:528:ILE:O	1:B:529:SER:C	2.50	0.47
1:D:536:ILE:HD12	1:D:659:TYR:HB2	1.95	0.47
1:D:18:PRO:N	1:D:417:THR:HG21	2.29	0.47
1:A:28:VAL:HG23	1:A:96:HIS:O	2.14	0.47
1:C:307:SER:O	1:C:308:SER:C	2.50	0.47
1:D:317:ASN:CG	1:D:318:ASN:N	2.67	0.47
1:C:317:ASN:CG	1:C:318:ASN:N	2.68	0.47
1:D:284:ASN:HB3	1:D:285:ASN:OD1	2.13	0.47
1:D:101:SER:HB2	1:D:107:THR:HG1	1.79	0.47
1:C:71:HIS:CE1	1:C:478:PRO:HA	2.50	0.47
1:A:716:GLU:HG2	1:A:722:THR:CA	2.44	0.47
1:D:579:ILE:O	1:D:583:LEU:HB2	2.14	0.47
1:D:491:GLU:O	1:D:495:TYR:HD2	1.96	0.47
1:B:28:VAL:HG23	1:B:96:HIS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG21	1:A:495:TYR:CD1	2.49	0.47
1:A:9:ALA:HB1	1:A:613:ILE:HD11	1.95	0.47
1:B:253:LEU:HG	1:B:255:GLN:O	2.14	0.47
1:B:443:LEU:C	1:B:445:ASN:N	2.65	0.47
1:A:723:PHE:CD2	1:C:667:LEU:HD13	2.49	0.47
1:A:506:LEU:HA	1:A:582:VAL:HG13	1.95	0.47
1:D:629:ILE:O	1:D:630:THR:C	2.52	0.47
1:B:579:ILE:O	1:B:583:LEU:HB2	2.14	0.47
1:B:719:PHE:O	1:B:720:PHE:C	2.52	0.47
1:B:9:ALA:HB1	1:B:613:ILE:HD11	1.95	0.47
1:A:326:SER:OG	1:A:328:ILE:HG13	2.13	0.47
1:A:157:ASP:OD2	1:A:159:THR:HB	2.15	0.47
1:B:224:ILE:HD11	1:B:237:LEU:HG	1.97	0.47
1:B:284:ASN:HB3	1:B:285:ASN:OD1	2.13	0.47
1:C:323:LEU:HD11	1:C:355:TRP:CD2	2.49	0.47
1:B:619:LEU:HD11	1:B:623:LEU:HD11	1.97	0.47
1:A:525:LEU:O	1:A:526:ARG:C	2.52	0.47
1:A:232:ARG:HG2	1:A:248:LEU:H	1.80	0.47
1:D:443:LEU:C	1:D:445:ASN:N	2.65	0.47
1:D:349:LEU:HB2	1:D:368:VAL:HG21	1.97	0.47
1:C:579:ILE:O	1:C:583:LEU:HB2	2.14	0.47
1:D:224:ILE:HD11	1:D:237:LEU:HG	1.97	0.47
1:D:244:LYS:HE2	1:D:256:ASP:OD1	2.14	0.47
1:C:185:GLY:C	1:C:186:LEU:HD12	2.35	0.47
1:C:180:ASP:C	1:C:182:GLY:H	2.17	0.47
1:B:283:TYR:O	1:B:284:ASN:O	2.33	0.47
1:A:336:LEU:C	1:A:337:THR:HG22	2.34	0.47
1:C:342:LEU:HD12	1:C:379:ILE:HD12	1.94	0.47
1:A:180:ASP:C	1:A:182:GLY:H	2.17	0.47
1:B:71:HIS:CE1	1:B:478:PRO:HA	2.49	0.47
1:C:344:VAL:CG1	1:C:345:GLU:H	2.28	0.47
1:B:533:LEU:HD13	1:B:729:ILE:CD1	2.45	0.47
1:D:95:ILE:CD1	1:D:133:LEU:HD11	2.43	0.47
1:B:566:ASN:HA	1:B:569:ILE:HD12	1.96	0.47
1:A:569:ILE:HG22	1:A:573:GLU:OE1	2.15	0.47
1:A:150:PHE:CD1	1:A:150:PHE:C	2.88	0.47
1:B:9:ALA:CB	1:B:613:ILE:HD11	2.45	0.47
1:B:124:LYS:O	1:B:126:GLY:N	2.48	0.47
1:D:4:LEU:HA	1:D:485:LYS:O	2.14	0.47
1:B:396:ASP:C	1:B:396:ASP:OD1	2.52	0.47
1:A:239:GLN:HG2	1:A:273:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HG	1:A:255:GLN:O	2.15	0.47
1:A:342:LEU:HD12	1:A:379:ILE:HD12	1.94	0.47
1:D:245:ILE:HG21	1:D:311:LEU:CD2	2.45	0.47
1:A:71:HIS:CE1	1:A:478:PRO:HA	2.50	0.47
1:D:534:ASP:HA	1:D:537:THR:OG1	2.15	0.47
1:B:18:PRO:HB3	1:B:417:THR:CG2	2.45	0.47
1:A:579:ILE:O	1:A:583:LEU:HB2	2.15	0.47
1:B:569:ILE:HG22	1:B:573:GLU:OE1	2.15	0.47
1:B:241:CYS:O	1:B:259:MET:HG2	2.14	0.47
1:A:236:VAL:HB	1:A:237:LEU:H	1.62	0.47
1:A:224:ILE:HD11	1:A:237:LEU:HG	1.96	0.47
1:C:239:GLN:HG2	1:C:273:VAL:O	2.14	0.47
1:A:185:GLY:C	1:A:186:LEU:HD12	2.36	0.47
1:A:403:ASP:HB3	1:A:406:ARG:CB	2.44	0.47
1:D:506:LEU:HA	1:D:582:VAL:HG13	1.95	0.47
1:D:528:ILE:O	1:D:529:SER:C	2.51	0.47
1:D:150:PHE:CD1	1:D:150:PHE:C	2.89	0.47
1:D:124:LYS:O	1:D:126:GLY:N	2.48	0.47
1:B:363:LEU:HG	1:B:364:GLN:N	2.29	0.47
1:D:448:THR:O	1:D:452:ASP:OD2	2.33	0.47
1:A:585:ASP:OD1	1:A:589:ASN:HB2	2.14	0.47
1:C:563:GLU:HB3	1:C:565:THR:CG2	2.45	0.47
1:A:224:ILE:CG2	1:A:276:VAL:HA	2.44	0.47
1:C:236:VAL:HB	1:C:237:LEU:H	1.61	0.47
1:C:124:LYS:O	1:C:126:GLY:N	2.48	0.47
1:C:445:ASN:O	1:C:446:LEU:C	2.53	0.47
1:D:399:THR:O	1:D:526:ARG:NH2	2.48	0.47
1:D:403:ASP:HB3	1:D:406:ARG:CB	2.45	0.47
1:B:506:LEU:CD1	1:B:582:VAL:HG12	2.44	0.47
1:C:506:LEU:HA	1:C:582:VAL:HG13	1.96	0.47
1:B:716:GLU:HG2	1:B:722:THR:CA	2.44	0.47
1:B:150:PHE:C	1:B:150:PHE:CD1	2.89	0.47
1:C:113:VAL:CG2	1:C:118:LEU:HB2	2.45	0.47
1:D:253:LEU:HG	1:D:255:GLN:O	2.15	0.46
1:B:317:ASN:CG	1:B:318:ASN:N	2.68	0.46
1:C:336:LEU:C	1:C:337:THR:HG22	2.35	0.46
1:B:185:GLY:C	1:B:186:LEU:HD12	2.35	0.46
1:D:55:GLU:OE1	1:D:74:SER:CA	2.58	0.46
1:A:55:GLU:OE1	1:A:74:SER:CA	2.60	0.46
1:A:399:THR:O	1:A:526:ARG:NH2	2.48	0.46
1:B:344:VAL:CG1	1:B:345:GLU:H	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HB3	1:A:87:ALA:HB3	1.95	0.46
1:D:28:VAL:HG23	1:D:96:HIS:O	2.15	0.46
1:B:157:ASP:OD2	1:B:159:THR:HB	2.15	0.46
1:C:326:SER:OG	1:C:328:ILE:HG13	2.14	0.46
1:A:563:GLU:HB3	1:A:565:THR:CG2	2.45	0.46
1:C:68:ILE:HD11	1:C:81:PHE:HD1	1.80	0.46
1:A:349:LEU:N	1:A:368:VAL:HG22	2.26	0.46
1:D:71:HIS:CE1	1:D:478:PRO:HA	2.50	0.46
1:B:95:ILE:CD1	1:B:133:LEU:HD11	2.43	0.46
1:C:585:ASP:OD1	1:C:589:ASN:HB2	2.14	0.46
1:C:172:GLN:HA	1:C:188:LYS:HB3	1.97	0.46
1:D:71:HIS:HE1	1:D:478:PRO:N	2.13	0.46
1:A:344:VAL:CG1	1:A:345:GLU:H	2.29	0.46
1:D:716:GLU:HG2	1:D:722:THR:CA	2.44	0.46
1:D:496:ASN:HA	1:D:499:SER:HB3	1.97	0.46
1:C:150:PHE:C	1:C:150:PHE:CD1	2.89	0.46
1:D:563:GLU:HB3	1:D:565:THR:CG2	2.45	0.46
1:D:326:SER:OG	1:D:328:ILE:HG13	2.15	0.46
1:B:563:GLU:HB3	1:B:565:THR:CG2	2.45	0.46
1:D:243:LEU:HB3	1:D:259:MET:CE	2.45	0.46
1:A:255:GLN:OE1	1:A:257:TYR:CE2	2.69	0.46
1:C:351:LEU:HG	1:C:353:VAL:CG2	2.44	0.46
1:D:250:SER:O	1:D:251:PHE:HB2	2.15	0.46
1:C:349:LEU:N	1:C:368:VAL:HG22	2.26	0.46
1:B:113:VAL:CG2	1:B:118:LEU:HB2	2.46	0.46
1:D:14:TYR:CE2	1:D:613:ILE:HG22	2.50	0.46
1:B:4:LEU:HA	1:B:485:LYS:O	2.15	0.46
1:C:224:ILE:HD11	1:C:237:LEU:HG	1.97	0.46
1:A:288:VAL:HG12	1:A:300:MET:HB3	1.98	0.46
1:C:187:LYS:HD3	1:C:197:LEU:CD1	2.34	0.46
1:D:344:VAL:CG1	1:D:345:GLU:H	2.28	0.46
1:B:18:PRO:N	1:B:417:THR:HG21	2.31	0.46
1:D:255:GLN:OE1	1:D:257:TYR:CE2	2.68	0.46
1:D:398:VAL:CB	1:D:669:ARG:NH1	2.55	0.46
1:C:293:LEU:HD13	1:C:297:LEU:HG	1.97	0.46
1:C:351:LEU:O	1:C:353:VAL:HG23	2.16	0.46
1:B:445:ASN:O	1:B:446:LEU:C	2.53	0.46
1:C:506:LEU:CD1	1:C:582:VAL:HG12	2.46	0.46
1:A:71:HIS:HE1	1:A:478:PRO:N	2.13	0.46
1:D:18:PRO:HB3	1:D:417:THR:HG22	1.97	0.46
1:C:650:HIS:O	1:C:653:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:O	1:B:573:GLU:HB2	2.15	0.46
1:C:552:ASP:C	1:C:552:ASP:OD1	2.54	0.46
1:B:157:ASP:C	1:B:159:THR:H	2.19	0.46
1:B:326:SER:O	1:B:327:ALA:HB3	2.15	0.46
1:D:363:LEU:HG	1:D:364:GLN:N	2.30	0.46
1:A:280:LEU:HD12	1:A:280:LEU:O	2.15	0.46
1:C:283:TYR:O	1:C:284:ASN:O	2.33	0.46
1:D:227:LYS:CG	1:D:282:LEU:HD22	2.45	0.46
1:D:227:LYS:HG3	1:D:282:LEU:HD22	1.98	0.46
1:A:187:LYS:HD3	1:A:197:LEU:CD1	2.34	0.46
1:D:58:ASN:HA	1:D:474:ASN:HD22	1.79	0.46
1:C:232:ARG:HD2	1:C:233:TYR:CE1	2.50	0.46
1:A:506:LEU:CD1	1:A:582:VAL:HG12	2.46	0.46
1:A:491:GLU:O	1:A:495:TYR:HD2	1.98	0.46
1:D:157:ASP:C	1:D:159:THR:H	2.19	0.46
1:B:326:SER:OG	1:B:328:ILE:HG13	2.16	0.46
1:B:265:SER:O	1:B:267:PRO:N	2.49	0.46
1:B:500:GLU:HG2	1:B:501:THR:O	2.16	0.46
1:B:341:GLU:HG3	1:B:341:GLU:O	2.16	0.46
1:B:427:LEU:HD21	1:B:449:ILE:HG13	1.98	0.46
1:D:185:GLY:C	1:D:186:LEU:HD12	2.36	0.46
1:C:619:LEU:HD11	1:C:623:LEU:HD11	1.97	0.46
1:A:445:ASN:O	1:A:446:LEU:C	2.54	0.46
1:C:525:LEU:O	1:C:526:ARG:C	2.54	0.46
1:A:232:ARG:HD2	1:A:233:TYR:CE1	2.50	0.46
1:C:233:TYR:O	1:C:235:ILE:HD12	2.16	0.46
1:D:427:LEU:HD21	1:D:449:ILE:HG13	1.97	0.46
1:D:506:LEU:CD1	1:D:582:VAL:HG12	2.45	0.46
1:A:650:HIS:O	1:A:653:THR:HB	2.16	0.46
1:D:113:VAL:CG2	1:D:118:LEU:HB2	2.46	0.46
1:C:280:LEU:O	1:C:280:LEU:HD12	2.15	0.46
1:C:137:PHE:O	1:C:137:PHE:CG	2.68	0.46
1:A:351:LEU:O	1:A:353:VAL:HG23	2.16	0.46
1:A:694:ASN:N	1:A:697:GLN:NE2	2.64	0.46
1:A:227:LYS:HG3	1:A:282:LEU:HD22	1.98	0.46
1:A:245:ILE:HG21	1:A:311:LEU:CD2	2.46	0.46
1:B:95:ILE:HG21	1:B:131:LEU:HD11	1.98	0.46
1:D:569:ILE:HG22	1:D:573:GLU:OE1	2.16	0.46
1:A:113:VAL:CG2	1:A:118:LEU:HB2	2.46	0.46
1:A:124:LYS:O	1:A:126:GLY:N	2.49	0.46
1:A:172:GLN:HA	1:A:188:LYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:HD22	1:B:297:LEU:CD1	2.44	0.46
1:C:288:VAL:HG12	1:C:300:MET:HB3	1.98	0.46
1:C:694:ASN:ND2	1:C:697:GLN:HG3	2.31	0.46
1:B:436:HIS:CD2	1:B:438:GLU:HB2	2.51	0.46
1:B:180:ASP:C	1:B:182:GLY:N	2.70	0.46
1:B:247:ASP:HB3	1:B:250:SER:HB2	1.98	0.46
1:D:245:ILE:HG21	1:D:311:LEU:HD22	1.97	0.46
1:A:534:ASP:HA	1:A:537:THR:OG1	2.15	0.46
1:C:534:ASP:HA	1:C:537:THR:OG1	2.15	0.46
1:C:128:PHE:HB3	1:C:153:GLN:HB3	1.97	0.45
1:D:293:LEU:HD22	1:D:297:LEU:CD1	2.44	0.45
1:B:351:LEU:O	1:B:353:VAL:HG23	2.16	0.45
1:D:351:LEU:O	1:D:353:VAL:HG23	2.15	0.45
1:A:283:TYR:O	1:A:284:ASN:O	2.33	0.45
1:A:101:SER:HB2	1:A:107:THR:HG1	1.78	0.45
1:A:340:LEU:O	1:A:341:GLU:HB3	2.15	0.45
1:C:310:ILE:O	1:C:310:ILE:CG2	2.64	0.45
1:A:552:ASP:C	1:A:552:ASP:OD1	2.54	0.45
1:B:255:GLN:OE1	1:B:257:TYR:CE2	2.69	0.45
1:A:240:ASN:O	1:A:242:HIS:N	2.50	0.45
1:A:128:PHE:HB3	1:A:153:GLN:HB3	1.97	0.45
1:B:293:LEU:HD13	1:B:297:LEU:HG	1.97	0.45
1:D:288:VAL:HG12	1:D:300:MET:HB3	1.97	0.45
1:A:341:GLU:O	1:A:341:GLU:HG3	2.16	0.45
1:C:403:ASP:HB3	1:C:406:ARG:CB	2.46	0.45
1:A:528:ILE:C	1:A:530:LYS:N	2.68	0.45
1:A:71:HIS:CE1	1:A:478:PRO:HB3	2.52	0.45
1:A:18:PRO:HB3	1:A:417:THR:CG2	2.46	0.45
1:C:569:ILE:HG22	1:C:573:GLU:OE1	2.17	0.45
1:C:28:VAL:HG13	1:C:150:PHE:CD1	2.51	0.45
1:B:14:TYR:CE2	1:B:613:ILE:HG22	2.50	0.45
1:D:428:SER:O	1:D:429:GLU:C	2.54	0.45
1:A:157:ASP:C	1:A:159:THR:H	2.19	0.45
1:D:326:SER:O	1:D:327:ALA:HB3	2.16	0.45
1:B:215:SER:HB3	1:B:216:SER:H	1.65	0.45
1:B:128:PHE:HB3	1:B:153:GLN:HB3	1.97	0.45
1:B:172:GLN:HA	1:B:188:LYS:HB3	1.97	0.45
1:B:192:VAL:O	1:B:193:HIS:ND1	2.49	0.45
1:B:288:VAL:HG12	1:B:300:MET:HB3	1.98	0.45
1:A:694:ASN:CG	1:A:697:GLN:HG3	2.36	0.45
1:A:103:ASN:H	1:A:107:THR:HG23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:GLU:HG3	1:D:341:GLU:O	2.16	0.45
1:C:71:HIS:CE1	1:C:478:PRO:HB3	2.51	0.45
1:C:707:SER:C	1:C:709:VAL:N	2.70	0.45
1:C:232:ARG:HG2	1:C:248:LEU:H	1.82	0.45
1:A:349:LEU:HB2	1:A:368:VAL:HG21	1.97	0.45
1:C:95:ILE:HG21	1:C:131:LEU:CD1	2.47	0.45
1:A:354:LEU:HD21	1:A:460:ALA:HB1	1.98	0.45
1:D:28:VAL:HG13	1:D:150:PHE:CD1	2.51	0.45
1:C:157:ASP:C	1:C:159:THR:H	2.19	0.45
1:D:293:LEU:HD13	1:D:297:LEU:HG	1.97	0.45
1:B:319:ILE:HG23	1:B:320:PRO:HD2	1.98	0.45
1:A:291:LEU:HA	1:A:292:PRO:HD3	1.80	0.45
1:D:351:LEU:HG	1:D:353:VAL:CG2	2.45	0.45
1:C:500:GLU:HG2	1:C:501:THR:O	2.16	0.45
1:B:651:ILE:O	1:B:654:LEU:N	2.49	0.45
1:B:491:GLU:O	1:B:495:TYR:HD2	1.98	0.45
1:B:28:VAL:HG13	1:B:150:PHE:CD1	2.51	0.45
1:C:14:TYR:CZ	1:C:613:ILE:HG22	2.51	0.45
1:C:326:SER:O	1:C:327:ALA:HB3	2.17	0.45
1:B:534:ASP:HA	1:B:537:THR:OG1	2.17	0.45
1:A:594:GLY:C	1:A:595:ILE:HD12	2.37	0.45
1:B:241:CYS:O	1:B:259:MET:CG	2.64	0.45
1:A:293:LEU:HD13	1:A:297:LEU:HG	1.98	0.45
1:A:227:LYS:CG	1:A:282:LEU:HD22	2.46	0.45
1:D:342:LEU:HD12	1:D:379:ILE:HD12	1.94	0.45
1:B:650:HIS:O	1:B:653:THR:HB	2.16	0.45
1:D:542:ASP:O	1:D:543:SER:C	2.55	0.45
1:C:180:ASP:O	1:C:182:GLY:N	2.50	0.45
1:D:172:GLN:NE2	1:D:172:GLN:H	2.15	0.45
1:A:500:GLU:HG2	1:A:501:THR:O	2.16	0.45
1:B:183:LEU:HD23	1:B:183:LEU:N	2.32	0.45
1:D:707:SER:C	1:D:709:VAL:N	2.70	0.45
1:B:629:ILE:O	1:B:630:THR:C	2.54	0.45
1:C:594:GLY:C	1:C:595:ILE:HD12	2.37	0.45
1:D:128:PHE:HB3	1:D:153:GLN:HB3	1.97	0.45
1:C:694:ASN:N	1:C:697:GLN:NE2	2.65	0.45
1:C:226:CYS:O	1:C:227:LYS:HG2	2.17	0.45
1:C:227:LYS:HG3	1:C:282:LEU:HD22	1.99	0.45
1:D:500:GLU:HG2	1:D:501:THR:O	2.17	0.45
1:D:340:LEU:O	1:D:341:GLU:HB3	2.17	0.45
1:A:323:LEU:HD11	1:A:355:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ASP:C	1:D:182:GLY:N	2.70	0.45
1:A:180:ASP:O	1:A:182:GLY:N	2.50	0.45
1:D:68:ILE:HD11	1:D:81:PHE:HD1	1.82	0.45
1:C:716:GLU:HG2	1:C:721:MET:C	2.37	0.45
1:A:28:VAL:HG13	1:A:150:PHE:CD1	2.52	0.45
1:A:306:ASP:OD1	1:A:307:SER:N	2.38	0.45
1:B:346:ALA:HB1	1:B:369:ASN:HB3	1.99	0.45
1:A:61:LEU:O	1:A:62:LEU:HD23	2.16	0.45
1:C:240:ASN:O	1:C:242:HIS:N	2.50	0.45
1:B:180:ASP:O	1:B:182:GLY:N	2.50	0.45
1:C:201:ASP:O	1:C:202:ASN:C	2.55	0.45
1:A:9:ALA:HA	1:A:613:ILE:HD11	1.99	0.45
1:C:14:TYR:OH	1:C:613:ILE:HA	2.16	0.45
1:B:594:GLY:C	1:B:595:ILE:HD12	2.37	0.45
1:A:144:THR:HG22	1:A:145:LEU:N	2.32	0.45
1:C:315:PHE:CD1	1:C:316:GLN:N	2.85	0.45
1:D:192:VAL:O	1:D:193:HIS:ND1	2.50	0.45
1:C:291:LEU:HA	1:C:292:PRO:HD3	1.81	0.45
1:C:694:ASN:CG	1:C:697:GLN:HG3	2.37	0.45
1:B:340:LEU:CD2	1:B:342:LEU:HD21	2.37	0.45
1:D:183:LEU:N	1:D:183:LEU:HD23	2.32	0.45
1:B:201:ASP:O	1:B:202:ASN:C	2.55	0.45
1:D:201:ASP:O	1:D:202:ASN:C	2.55	0.45
1:B:95:ILE:HG21	1:B:131:LEU:CD1	2.47	0.45
1:C:569:ILE:O	1:C:573:GLU:HB2	2.16	0.45
1:A:326:SER:O	1:A:327:ALA:HB3	2.17	0.45
1:B:240:ASN:O	1:B:242:HIS:N	2.50	0.45
1:C:180:ASP:C	1:C:182:GLY:N	2.69	0.45
1:C:244:LYS:HD3	1:C:253:LEU:CD2	2.47	0.45
1:D:319:ILE:HG23	1:D:320:PRO:HD2	1.99	0.45
1:D:337:THR:OG1	1:D:338:ARG:N	2.50	0.45
1:D:697:GLN:O	1:D:700:ALA:HB3	2.17	0.45
1:C:245:ILE:HG21	1:C:311:LEU:CD2	2.47	0.45
1:A:707:SER:C	1:A:709:VAL:N	2.70	0.45
1:B:528:ILE:O	1:B:531:LYS:N	2.50	0.45
1:A:95:ILE:HG21	1:A:131:LEU:HD11	1.98	0.45
1:C:651:ILE:O	1:C:654:LEU:N	2.49	0.45
1:D:552:ASP:C	1:D:552:ASP:OD1	2.55	0.45
1:A:14:TYR:CE2	1:A:613:ILE:HG22	2.52	0.45
1:B:428:SER:O	1:B:429:GLU:C	2.55	0.45
1:C:483:LEU:HD23	1:C:483:LEU:C	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:ASP:O	1:B:543:SER:C	2.56	0.45
1:A:137:PHE:O	1:A:137:PHE:CG	2.70	0.45
1:C:249:THR:HG22	1:C:249:THR:O	2.17	0.45
1:D:694:ASN:N	1:D:697:GLN:NE2	2.65	0.44
1:C:427:LEU:HD21	1:C:449:ILE:HG13	1.99	0.44
1:A:427:LEU:HD21	1:A:449:ILE:HG13	1.99	0.44
1:A:201:ASP:O	1:A:202:ASN:C	2.55	0.44
1:C:349:LEU:HB2	1:C:368:VAL:HG21	1.98	0.44
1:C:629:ILE:O	1:C:630:THR:C	2.54	0.44
1:A:95:ILE:HG21	1:A:131:LEU:CD1	2.47	0.44
1:D:95:ILE:HG21	1:D:131:LEU:CD1	2.47	0.44
1:B:111:GLN:HG3	1:B:168:TYR:CE2	2.52	0.44
1:A:637:PHE:CD2	1:A:651:ILE:HD11	2.50	0.44
1:B:716:GLU:HG2	1:B:721:MET:C	2.38	0.44
1:B:144:THR:HG22	1:B:145:LEU:N	2.32	0.44
1:C:244:LYS:HD3	1:C:253:LEU:HD22	1.97	0.44
1:D:172:GLN:HA	1:D:188:LYS:HB3	1.98	0.44
1:B:340:LEU:O	1:B:341:GLU:HB3	2.17	0.44
1:A:528:ILE:O	1:A:531:LYS:N	2.50	0.44
1:C:382:VAL:HG12	1:C:384:LYS:H	1.83	0.44
1:A:9:ALA:CA	1:A:613:ILE:HD11	2.47	0.44
1:D:594:GLY:C	1:D:595:ILE:HD12	2.38	0.44
1:B:61:LEU:O	1:B:62:LEU:HD23	2.17	0.44
1:C:192:VAL:O	1:C:193:HIS:ND1	2.50	0.44
1:B:694:ASN:N	1:B:697:GLN:NE2	2.65	0.44
1:A:103:ASN:O	1:A:106:TYR:HB2	2.17	0.44
1:A:180:ASP:C	1:A:182:GLY:N	2.70	0.44
1:B:707:SER:C	1:B:709:VAL:N	2.71	0.44
1:A:716:GLU:HG2	1:A:721:MET:C	2.38	0.44
1:D:95:ILE:HG21	1:D:131:LEU:HD11	1.99	0.44
1:D:651:ILE:O	1:D:654:LEU:N	2.50	0.44
1:D:569:ILE:O	1:D:573:GLU:HB2	2.17	0.44
1:B:496:ASN:HA	1:B:499:SER:HB3	1.99	0.44
1:B:552:ASP:C	1:B:552:ASP:OD1	2.55	0.44
1:D:61:LEU:O	1:D:62:LEU:HD23	2.17	0.44
1:D:346:ALA:HB1	1:D:369:ASN:HB3	1.99	0.44
1:C:346:ALA:HB1	1:C:369:ASN:HB3	1.98	0.44
1:A:172:GLN:H	1:A:172:GLN:NE2	2.14	0.44
1:D:335:VAL:HG13	1:D:335:VAL:O	2.17	0.44
1:A:694:ASN:ND2	1:A:697:GLN:HG3	2.32	0.44
1:A:697:GLN:O	1:A:700:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ASN:ND2	1:B:697:GLN:HG3	2.33	0.44
1:A:667:LEU:HD13	1:C:723:PHE:CD2	2.52	0.44
1:A:245:ILE:HG21	1:A:311:LEU:HD22	1.97	0.44
1:C:705:LEU:O	1:C:709:VAL:HG23	2.17	0.44
1:D:445:ASN:O	1:D:446:LEU:C	2.54	0.44
1:C:382:VAL:HG21	1:C:495:TYR:CD1	2.52	0.44
1:C:491:GLU:O	1:C:495:TYR:HD2	2.00	0.44
1:C:28:VAL:CB	1:C:98:PRO:HD3	2.47	0.44
1:D:14:TYR:OH	1:D:613:ILE:HA	2.17	0.44
1:C:61:LEU:O	1:C:62:LEU:HD23	2.16	0.44
1:D:564:ILE:HA	1:D:564:ILE:HD12	1.83	0.44
1:A:616:LEU:HD22	1:A:676:ALA:HB2	1.99	0.44
1:D:240:ASN:O	1:D:242:HIS:N	2.50	0.44
1:C:154:ASN:N	1:C:155:PRO:CD	2.79	0.44
1:D:694:ASN:ND2	1:D:697:GLN:HG3	2.33	0.44
1:A:705:LEU:O	1:A:706:ASN:C	2.56	0.44
1:A:719:PHE:CD1	1:A:720:PHE:N	2.86	0.44
1:A:569:ILE:O	1:A:573:GLU:HB2	2.17	0.44
1:C:428:SER:O	1:C:429:GLU:C	2.54	0.44
1:A:428:SER:O	1:A:429:GLU:C	2.54	0.44
1:D:483:LEU:C	1:D:483:LEU:HD23	2.38	0.44
1:B:100:ALA:O	1:B:124:LYS:HG3	2.18	0.44
1:D:144:THR:HG22	1:D:145:LEU:N	2.32	0.44
1:B:351:LEU:HG	1:B:353:VAL:CG2	2.46	0.44
1:C:227:LYS:CG	1:C:282:LEU:HD22	2.47	0.44
1:A:68:ILE:HD11	1:A:81:PHE:HD1	1.82	0.44
1:B:68:ILE:HD11	1:B:81:PHE:HD1	1.83	0.44
1:D:168:TYR:HA	1:D:174:SER:CB	2.47	0.44
1:A:18:PRO:HB3	1:A:417:THR:HG22	1.99	0.44
1:A:477:GLN:O	1:A:480:ASN:HB2	2.18	0.44
1:A:315:PHE:CD1	1:A:316:GLN:N	2.86	0.44
1:C:183:LEU:HD23	1:C:183:LEU:N	2.32	0.44
1:C:177:PHE:CZ	1:C:234:LEU:HD21	2.40	0.44
1:A:192:VAL:O	1:A:193:HIS:ND1	2.50	0.44
1:D:297:LEU:CD1	1:D:318:ASN:HD21	2.31	0.44
1:C:286:THR:CG2	1:C:287:LEU:H	2.30	0.44
1:C:340:LEU:O	1:C:341:GLU:HB3	2.17	0.44
1:C:341:GLU:HG3	1:C:341:GLU:O	2.17	0.44
1:B:199:PHE:HB3	1:B:251:PHE:O	2.18	0.44
1:D:528:ILE:O	1:D:531:LYS:N	2.51	0.44
1:B:168:TYR:HA	1:B:174:SER:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:HIS:O	1:D:653:THR:HB	2.18	0.44
1:C:457:PHE:CG	1:C:477:GLN:HG2	2.53	0.44
1:B:477:GLN:O	1:B:480:ASN:HB2	2.17	0.44
1:B:14:TYR:OH	1:B:613:ILE:HA	2.17	0.44
1:B:559:GLU:O	1:B:560:ASN:HB2	2.17	0.44
1:D:265:SER:O	1:D:267:PRO:CD	2.66	0.44
1:B:172:GLN:H	1:B:172:GLN:NE2	2.16	0.44
1:A:319:ILE:HG23	1:A:320:PRO:HD2	1.98	0.44
1:B:102:MET:CB	1:B:107:THR:HG21	2.35	0.44
1:A:183:LEU:N	1:A:183:LEU:HD23	2.32	0.44
1:D:233:TYR:O	1:D:235:ILE:HD12	2.18	0.44
1:A:629:ILE:O	1:A:630:THR:C	2.55	0.44
1:D:382:VAL:HG21	1:D:495:TYR:CD1	2.53	0.44
1:D:28:VAL:CB	1:D:98:PRO:HD3	2.48	0.44
1:D:265:SER:O	1:D:267:PRO:N	2.51	0.44
1:B:564:ILE:HD12	1:B:564:ILE:HA	1.84	0.44
1:C:128:PHE:HE2	1:C:194:TYR:CE2	2.36	0.44
1:B:337:THR:OG1	1:B:338:ARG:N	2.51	0.44
1:A:286:THR:CG2	1:A:287:LEU:H	2.30	0.44
1:A:335:VAL:HG13	1:A:335:VAL:O	2.18	0.44
1:A:351:LEU:HG	1:A:353:VAL:CG2	2.46	0.44
1:D:226:CYS:O	1:D:227:LYS:HG2	2.17	0.44
1:C:443:LEU:O	1:C:444:ALA:C	2.56	0.44
1:D:180:ASP:O	1:D:182:GLY:N	2.51	0.44
1:A:233:TYR:O	1:A:235:ILE:HD12	2.18	0.44
1:D:439:ASP:O	1:D:441:GLU:N	2.51	0.44
1:D:705:LEU:C	1:D:707:SER:N	2.70	0.44
1:C:95:ILE:HG21	1:C:131:LEU:HD11	1.98	0.44
1:B:528:ILE:C	1:B:530:LYS:N	2.68	0.44
1:C:719:PHE:CD1	1:C:720:PHE:N	2.86	0.44
1:D:306:ASP:OD1	1:D:307:SER:N	2.46	0.44
1:D:716:GLU:HG2	1:D:721:MET:C	2.39	0.44
1:B:719:PHE:CD1	1:B:720:PHE:N	2.86	0.44
1:A:69:CYS:SG	1:A:82:TYR:CE1	3.11	0.44
1:B:315:PHE:CD1	1:B:316:GLN:N	2.86	0.44
1:A:346:ALA:HB1	1:A:369:ASN:HB3	1.99	0.44
1:C:144:THR:HG22	1:C:145:LEU:N	2.33	0.44
1:D:260:VAL:O	1:D:261:SER:CB	2.65	0.44
1:D:128:PHE:HE2	1:D:194:TYR:CE2	2.36	0.43
1:C:478:PRO:O	1:C:479:TYR:HB2	2.18	0.43
1:B:478:PRO:O	1:B:479:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:GLN:HG3	1:D:168:TYR:CE2	2.52	0.43
1:D:305:VAL:HG23	1:D:306:ASP:H	1.83	0.43
1:C:528:ILE:C	1:C:530:LYS:N	2.69	0.43
1:D:719:PHE:CD1	1:D:720:PHE:N	2.86	0.43
1:B:28:VAL:CB	1:B:98:PRO:HD3	2.48	0.43
1:C:9:ALA:CA	1:C:613:ILE:HD11	2.48	0.43
1:D:468:ASP:HB2	1:D:469:GLU:OE2	2.18	0.43
1:B:128:PHE:HE2	1:B:194:TYR:CE2	2.36	0.43
1:C:293:LEU:HD22	1:C:297:LEU:CD1	2.45	0.43
1:C:319:ILE:HG23	1:C:320:PRO:HD2	1.99	0.43
1:A:694:ASN:OD1	1:A:697:GLN:HG3	2.19	0.43
1:B:233:TYR:O	1:B:235:ILE:HD12	2.18	0.43
1:A:707:SER:O	1:A:710:TYR:N	2.50	0.43
1:B:71:HIS:CE1	1:B:478:PRO:N	2.86	0.43
1:D:110:ILE:O	1:D:111:GLN:NE2	2.51	0.43
1:D:541:PRO:HD2	1:D:544:MET:HE1	2.00	0.43
1:C:496:ASN:HA	1:C:499:SER:HB3	1.99	0.43
1:D:382:VAL:HG12	1:D:384:LYS:H	1.83	0.43
1:A:154:ASN:N	1:A:155:PRO:CD	2.80	0.43
1:A:293:LEU:HD22	1:A:297:LEU:CD1	2.45	0.43
1:B:306:ASP:O	1:B:307:SER:CB	2.65	0.43
1:B:103:ASN:O	1:B:106:TYR:HB2	2.18	0.43
1:A:323:LEU:CD1	1:A:329:TRP:HB2	2.40	0.43
1:C:533:LEU:CD1	1:C:729:ILE:HD11	2.49	0.43
1:D:443:LEU:O	1:D:444:ALA:C	2.56	0.43
1:D:53:GLY:HA3	1:D:71:HIS:HB3	2.00	0.43
1:B:18:PRO:HB3	1:B:417:THR:HG22	2.00	0.43
1:B:541:PRO:HD2	1:B:544:MET:HE1	2.01	0.43
1:B:354:LEU:HD21	1:B:460:ALA:HB1	1.99	0.43
1:B:637:PHE:CD2	1:B:651:ILE:HD11	2.52	0.43
1:C:18:PRO:HB3	1:C:417:THR:CG2	2.48	0.43
1:A:559:GLU:O	1:A:560:ASN:HB2	2.17	0.43
1:C:448:THR:O	1:C:452:ASP:OD2	2.36	0.43
1:B:187:LYS:HE2	1:B:197:LEU:HD21	2.01	0.43
1:B:184:LEU:HD11	1:B:196:PRO:CB	2.49	0.43
1:A:402:GLY:O	1:A:403:ASP:O	2.36	0.43
1:A:443:LEU:O	1:A:444:ALA:C	2.56	0.43
1:B:630:THR:HG22	1:B:634:LEU:HD11	2.00	0.43
1:A:496:ASN:HA	1:A:499:SER:HB3	1.99	0.43
1:B:61:LEU:HD12	1:B:62:LEU:H	1.83	0.43
1:C:61:LEU:HD12	1:C:62:LEU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:GLU:O	1:D:560:ASN:HB2	2.18	0.43
1:C:665:LEU:O	1:C:668:TYR:HB3	2.17	0.43
1:D:102:MET:CB	1:D:107:THR:HG21	2.36	0.43
1:B:439:ASP:O	1:B:441:GLU:N	2.51	0.43
1:A:533:LEU:CD1	1:A:729:ILE:HD11	2.49	0.43
1:A:177:PHE:CZ	1:A:234:LEU:HD21	2.40	0.43
1:D:608:ASP:HB2	1:D:691:LYS:HZ3	1.81	0.43
1:C:245:ILE:HG21	1:C:311:LEU:HD22	1.98	0.43
1:D:707:SER:O	1:D:710:TYR:N	2.51	0.43
1:A:673:CYS:O	1:A:677:GLU:HG2	2.18	0.43
1:D:100:ALA:O	1:D:124:LYS:HG3	2.19	0.43
1:D:315:PHE:CD1	1:D:316:GLN:N	2.87	0.43
1:D:297:LEU:HD13	1:D:318:ASN:ND2	2.33	0.43
1:B:297:LEU:CD1	1:B:318:ASN:HD21	2.31	0.43
1:B:694:ASN:CG	1:B:697:GLN:HG3	2.38	0.43
1:B:697:GLN:O	1:B:700:ALA:HB3	2.19	0.43
1:A:104:GLN:C	1:A:106:TYR:N	2.71	0.43
1:C:103:ASN:O	1:C:106:TYR:HB2	2.19	0.43
1:B:430:ASN:O	1:B:432:ILE:HG13	2.18	0.43
1:C:111:GLN:HG3	1:C:168:TYR:CE2	2.53	0.43
1:A:28:VAL:CB	1:A:98:PRO:HD3	2.48	0.43
1:C:9:ALA:HA	1:C:613:ILE:HD11	2.00	0.43
1:D:9:ALA:CA	1:D:613:ILE:HD11	2.48	0.43
1:A:100:ALA:O	1:A:124:LYS:HG3	2.18	0.43
1:B:243:LEU:HD23	1:B:259:MET:HE3	2.01	0.43
1:A:128:PHE:HE2	1:A:194:TYR:CE2	2.37	0.43
1:D:103:ASN:O	1:D:106:TYR:HB2	2.19	0.43
1:C:439:ASP:O	1:C:441:GLU:N	2.51	0.43
1:A:667:LEU:HD22	1:C:723:PHE:HE2	1.75	0.43
1:B:228:LEU:HA	1:B:233:TYR:O	2.19	0.43
1:B:572:ASP:O	1:B:575:ASN:HB2	2.18	0.43
1:D:572:ASP:O	1:D:575:ASN:HB2	2.18	0.43
1:D:73:SER:CB	1:D:78:LEU:H	2.31	0.43
1:B:73:SER:HB3	1:B:78:LEU:N	2.30	0.43
1:B:719:PHE:O	1:B:722:THR:N	2.51	0.43
1:C:651:ILE:O	1:C:653:THR:N	2.52	0.43
1:B:448:THR:O	1:B:452:ASP:OD2	2.37	0.43
1:B:137:PHE:O	1:B:137:PHE:CG	2.71	0.43
1:C:547:VAL:HG22	1:C:644:THR:CG2	2.48	0.43
1:C:73:SER:O	1:C:76:SER:N	2.48	0.43
1:A:547:VAL:HG22	1:A:644:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:LEU:O	1:D:660:LYS:N	2.52	0.43
1:A:719:PHE:O	1:A:722:THR:N	2.51	0.43
1:C:477:GLN:O	1:C:480:ASN:HB2	2.19	0.43
1:D:457:PHE:CG	1:D:477:GLN:HG2	2.53	0.43
1:D:477:GLN:O	1:D:480:ASN:HB2	2.18	0.43
1:A:61:LEU:HD12	1:A:62:LEU:H	1.82	0.43
1:D:61:LEU:HD12	1:D:62:LEU:H	1.84	0.43
1:C:616:LEU:HD22	1:C:676:ALA:HB2	2.00	0.43
1:A:22:ASN:HD21	1:A:91:LYS:HD3	1.84	0.43
1:D:22:ASN:HD22	1:D:91:LYS:HB2	1.84	0.43
1:A:244:LYS:HD3	1:A:253:LEU:HD22	2.00	0.43
1:C:335:VAL:O	1:C:335:VAL:HG13	2.19	0.43
1:A:287:LEU:HD12	1:A:288:VAL:H	1.84	0.43
1:B:227:LYS:HG3	1:B:282:LEU:HD22	2.01	0.43
1:A:406:ARG:C	1:A:408:PHE:N	2.70	0.43
1:D:73:SER:HB3	1:D:78:LEU:N	2.30	0.43
1:A:457:PHE:CG	1:A:477:GLN:HG2	2.54	0.43
1:A:382:VAL:HG12	1:A:384:LYS:H	1.84	0.43
1:C:177:PHE:CD1	1:C:183:LEU:HB3	2.54	0.43
1:C:246:TRP:HA	1:C:253:LEU:HA	2.00	0.43
1:D:398:VAL:CG2	1:D:669:ARG:HH12	2.32	0.43
1:C:270:PHE:HE2	1:C:292:PRO:HG2	1.84	0.43
1:C:187:LYS:HE2	1:C:197:LEU:HD21	2.01	0.43
1:A:226:CYS:O	1:A:227:LYS:HG2	2.19	0.43
1:B:250:SER:O	1:B:251:PHE:HB2	2.18	0.43
1:A:199:PHE:HB3	1:A:251:PHE:O	2.19	0.43
1:A:439:ASP:O	1:A:441:GLU:N	2.51	0.43
1:B:602:ILE:O	1:B:602:ILE:HG22	2.18	0.43
1:D:402:GLY:O	1:D:403:ASP:O	2.37	0.43
1:B:705:LEU:C	1:B:707:SER:N	2.71	0.43
1:A:535:ILE:CG2	1:A:655:LEU:HD13	2.49	0.43
1:A:535:ILE:HG21	1:A:655:LEU:HD13	2.00	0.43
1:A:111:GLN:HG3	1:A:168:TYR:CE2	2.54	0.43
1:C:528:ILE:O	1:C:531:LYS:N	2.52	0.43
1:D:637:PHE:CD2	1:D:651:ILE:HD11	2.52	0.43
1:A:14:TYR:OH	1:A:613:ILE:HA	2.19	0.43
1:B:483:LEU:C	1:B:483:LEU:HD23	2.39	0.43
1:B:27:TYR:CD1	1:B:27:TYR:N	2.87	0.43
1:C:270:PHE:CD2	1:C:270:PHE:C	2.91	0.42
1:C:297:LEU:CD1	1:C:318:ASN:HD21	2.31	0.42
1:D:694:ASN:CG	1:D:697:GLN:HG3	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:LYS:HE2	1:D:197:LEU:HD21	2.01	0.42
1:C:402:GLY:O	1:C:403:ASP:O	2.37	0.42
1:B:443:LEU:O	1:B:444:ALA:C	2.57	0.42
1:C:727:TYR:HB3	1:C:728:ILE:H	1.70	0.42
1:B:185:GLY:O	1:B:196:PRO:HA	2.19	0.42
1:B:245:ILE:HG21	1:B:311:LEU:CD2	2.49	0.42
1:C:71:HIS:CE1	1:C:478:PRO:N	2.87	0.42
1:A:602:ILE:HG22	1:A:602:ILE:O	2.18	0.42
1:D:602:ILE:O	1:D:602:ILE:HG22	2.18	0.42
1:C:705:LEU:O	1:C:706:ASN:C	2.58	0.42
1:A:564:ILE:HD12	1:A:564:ILE:HA	1.84	0.42
1:B:348:TYR:HB3	1:B:368:VAL:HG23	2.01	0.42
1:C:630:THR:HG22	1:C:634:LEU:HD11	2.00	0.42
1:D:528:ILE:C	1:D:530:LYS:N	2.69	0.42
1:D:255:GLN:OE1	1:D:257:TYR:HE2	2.02	0.42
1:A:398:VAL:CG2	1:A:669:ARG:HH12	2.33	0.42
1:C:398:VAL:HG21	1:C:665:LEU:HD13	2.01	0.42
1:B:287:LEU:HD12	1:B:288:VAL:H	1.84	0.42
1:B:335:VAL:O	1:B:335:VAL:HG13	2.18	0.42
1:D:104:GLN:C	1:D:106:TYR:N	2.72	0.42
1:C:406:ARG:C	1:C:408:PHE:N	2.71	0.42
1:B:406:ARG:C	1:B:408:PHE:N	2.71	0.42
1:B:705:LEU:O	1:B:709:VAL:HG23	2.18	0.42
1:A:18:PRO:N	1:A:417:THR:HG21	2.33	0.42
1:B:468:ASP:HB2	1:B:469:GLU:OE2	2.19	0.42
1:B:665:LEU:O	1:B:668:TYR:HB3	2.18	0.42
1:B:398:VAL:CB	1:B:669:ARG:NH1	2.58	0.42
1:C:172:GLN:NE2	1:C:172:GLN:H	2.16	0.42
1:A:187:LYS:HE2	1:A:197:LEU:HD21	2.01	0.42
1:B:187:LYS:CE	1:B:197:LEU:HD21	2.49	0.42
1:B:104:GLN:C	1:B:106:TYR:N	2.71	0.42
1:B:226:CYS:O	1:B:227:LYS:HG2	2.19	0.42
1:C:104:GLN:C	1:C:106:TYR:N	2.72	0.42
1:C:441:GLU:O	1:C:445:ASN:ND2	2.52	0.42
1:B:436:HIS:C	1:B:438:GLU:H	2.22	0.42
1:D:176:VAL:CG1	1:D:177:PHE:N	2.78	0.42
1:D:184:LEU:HD11	1:D:196:PRO:CB	2.50	0.42
1:D:705:LEU:O	1:D:706:ASN:C	2.57	0.42
1:A:564:ILE:O	1:A:567:LEU:HB3	2.19	0.42
1:C:110:ILE:O	1:C:111:GLN:NE2	2.52	0.42
1:C:430:ASN:ND2	1:C:430:ASN:N	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:PHE:O	1:D:722:THR:N	2.52	0.42
1:C:12:LEU:HD13	1:C:18:PRO:O	2.18	0.42
1:A:12:LEU:HD13	1:A:18:PRO:O	2.18	0.42
1:B:616:LEU:HD22	1:B:676:ALA:HB2	2.00	0.42
1:D:367:ASN:HB3	1:D:377:GLU:O	2.20	0.42
1:B:297:LEU:HD13	1:B:318:ASN:ND2	2.34	0.42
1:C:287:LEU:HD12	1:C:288:VAL:H	1.85	0.42
1:C:187:LYS:CE	1:C:197:LEU:HD21	2.50	0.42
1:C:602:ILE:O	1:C:602:ILE:HG22	2.18	0.42
1:D:228:LEU:HA	1:D:233:TYR:O	2.20	0.42
1:B:73:SER:CB	1:B:78:LEU:H	2.32	0.42
1:C:430:ASN:O	1:C:432:ILE:HG13	2.19	0.42
1:D:354:LEU:HD21	1:D:460:ALA:HB1	2.00	0.42
1:C:64:ASN:N	1:C:64:ASN:OD1	2.48	0.42
1:D:137:PHE:CG	1:D:137:PHE:O	2.71	0.42
1:A:64:ASN:OD1	1:A:64:ASN:N	2.48	0.42
1:D:340:LEU:CD2	1:D:342:LEU:HD21	2.39	0.42
1:B:177:PHE:CD1	1:B:183:LEU:HB3	2.55	0.42
1:A:254:ILE:CB	1:A:311:LEU:HD12	2.49	0.42
1:A:53:GLY:HA3	1:A:71:HIS:HB3	2.02	0.42
1:B:651:ILE:O	1:B:653:THR:N	2.52	0.42
1:C:468:ASP:HB2	1:C:469:GLU:OE2	2.20	0.42
1:D:27:TYR:N	1:D:27:TYR:CD1	2.88	0.42
1:A:310:ILE:O	1:A:310:ILE:HG22	2.19	0.42
1:C:337:THR:OG1	1:C:338:ARG:N	2.51	0.42
1:C:187:LYS:HD3	1:C:197:LEU:HD21	2.02	0.42
1:C:323:LEU:CD1	1:C:329:TRP:HB2	2.41	0.42
1:A:619:LEU:HD11	1:A:623:LEU:HD11	2.01	0.42
1:B:245:ILE:HG21	1:B:311:LEU:HD22	2.01	0.42
1:B:707:SER:O	1:B:710:TYR:N	2.53	0.42
1:C:69:CYS:SG	1:C:82:TYR:CE1	3.12	0.42
1:D:466:TYR:O	1:D:470:ILE:HB	2.19	0.42
1:A:297:LEU:CD1	1:A:318:ASN:HD21	2.32	0.42
1:A:568:LYS:HZ2	1:D:210:ARG:NH2	2.15	0.42
1:A:337:THR:OG1	1:A:338:ARG:N	2.51	0.42
1:D:694:ASN:N	1:D:697:GLN:HE21	2.18	0.42
1:A:102:MET:CB	1:A:107:THR:HG21	2.36	0.42
1:D:342:LEU:N	1:D:342:LEU:HD23	2.35	0.42
1:D:177:PHE:CD1	1:D:183:LEU:HB3	2.55	0.42
1:A:441:GLU:O	1:A:445:ASN:ND2	2.53	0.42
1:B:705:LEU:O	1:B:706:ASN:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:TYR:HB3	1:D:368:VAL:HG23	2.01	0.42
1:B:53:GLY:HA3	1:B:71:HIS:HB3	2.02	0.42
1:B:430:ASN:N	1:B:430:ASN:ND2	2.66	0.42
1:D:630:THR:HG22	1:D:634:LEU:HD11	2.01	0.42
1:C:596:PHE:C	1:C:598:LYS:N	2.73	0.42
1:C:559:GLU:O	1:C:560:ASN:HB2	2.18	0.42
1:A:542:ASP:O	1:A:543:SER:C	2.57	0.42
1:B:367:ASN:HB3	1:B:377:GLU:O	2.20	0.42
1:C:367:ASN:HB3	1:C:377:GLU:O	2.19	0.42
1:B:466:TYR:O	1:B:470:ILE:HB	2.20	0.42
1:C:102:MET:CB	1:C:107:THR:HG21	2.36	0.42
1:B:441:GLU:O	1:B:445:ASN:ND2	2.53	0.42
1:D:185:GLY:O	1:D:196:PRO:HA	2.20	0.42
1:C:690:VAL:CG1	1:C:691:LYS:H	2.33	0.42
1:A:536:ILE:HD11	1:A:655:LEU:CB	2.49	0.42
1:A:73:SER:O	1:A:76:SER:N	2.49	0.42
1:A:110:ILE:O	1:A:111:GLN:NE2	2.53	0.42
1:A:430:ASN:ND2	1:A:430:ASN:N	2.66	0.42
1:D:651:ILE:O	1:D:653:THR:N	2.52	0.42
1:A:596:PHE:C	1:A:598:LYS:N	2.73	0.42
1:A:549:LYS:O	1:A:552:ASP:N	2.53	0.42
1:D:9:ALA:HA	1:D:613:ILE:HD11	2.00	0.42
1:D:665:LEU:O	1:D:668:TYR:HB3	2.19	0.42
1:D:550:PHE:CD2	1:D:638:VAL:HG12	2.55	0.42
1:C:466:TYR:O	1:C:470:ILE:HB	2.19	0.42
1:B:255:GLN:OE1	1:B:257:TYR:HE2	2.03	0.42
1:D:287:LEU:HD12	1:D:288:VAL:H	1.85	0.42
1:A:187:LYS:CE	1:A:197:LEU:HD21	2.50	0.42
1:A:187:LYS:HD3	1:A:197:LEU:HD21	2.02	0.42
1:C:323:LEU:HD11	1:C:355:TRP:CE3	2.55	0.42
1:A:670:GLN:HG3	1:C:727:TYR:CZ	2.55	0.42
1:B:176:VAL:CG1	1:B:177:PHE:N	2.79	0.42
1:A:250:SER:O	1:A:251:PHE:HB2	2.19	0.42
1:D:553:ILE:O	1:D:553:ILE:CG2	2.60	0.42
1:D:430:ASN:N	1:D:430:ASN:ND2	2.66	0.42
1:C:354:LEU:HD21	1:C:460:ALA:HB1	2.01	0.42
1:C:637:PHE:CD2	1:C:651:ILE:HG12	2.55	0.42
1:B:382:VAL:HG12	1:B:384:LYS:H	1.84	0.42
1:D:673:CYS:O	1:D:677:GLU:HG2	2.20	0.42
1:B:69:CYS:SG	1:B:82:TYR:CE1	3.13	0.42
1:C:346:ALA:HB3	1:C:369:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:CG2	1:A:93:ILE:HG12	2.50	0.42
1:C:237:LEU:CD1	1:C:241:CYS:HA	2.50	0.42
1:A:317:ASN:ND2	1:A:319:ILE:CG1	2.70	0.42
1:C:290:LEU:HD13	1:C:298:PHE:CE1	2.55	0.42
1:D:334:LEU:CD1	1:D:351:LEU:HD11	2.37	0.42
1:B:187:LYS:HD3	1:B:197:LEU:HD21	2.01	0.42
1:C:124:LYS:C	1:C:126:GLY:H	2.23	0.42
1:A:340:LEU:O	1:A:341:GLU:CB	2.68	0.42
1:C:436:HIS:CD2	1:C:438:GLU:HB2	2.55	0.42
1:A:228:LEU:HA	1:A:233:TYR:O	2.20	0.42
1:C:254:ILE:CG2	1:C:311:LEU:HB2	2.45	0.42
1:A:348:TYR:HB3	1:A:368:VAL:HG23	2.01	0.42
1:B:110:ILE:O	1:B:111:GLN:NE2	2.53	0.42
1:A:541:PRO:HD2	1:A:544:MET:HE1	2.01	0.42
1:B:637:PHE:CD2	1:B:651:ILE:HG12	2.55	0.42
1:D:566:ASN:HA	1:D:569:ILE:CD1	2.50	0.42
1:C:24:VAL:CG2	1:C:93:ILE:HG12	2.50	0.42
1:D:263:SER:O	1:D:264:ASP:C	2.57	0.42
1:C:564:ILE:O	1:C:567:LEU:HB3	2.20	0.42
1:B:103:ASN:H	1:B:107:THR:HG23	1.80	0.41
1:B:227:LYS:CG	1:B:282:LEU:HD22	2.49	0.41
1:B:323:LEU:HD11	1:B:355:TRP:CE3	2.55	0.41
1:C:53:GLY:HA3	1:C:71:HIS:HB3	2.02	0.41
1:A:423:ALA:HB2	1:A:453:VAL:HG21	2.02	0.41
1:C:541:PRO:HD2	1:C:544:MET:HE1	2.02	0.41
1:D:536:ILE:HD11	1:D:655:LEU:CB	2.50	0.41
1:A:637:PHE:CD2	1:A:651:ILE:HG12	2.55	0.41
1:D:12:LEU:HD13	1:D:18:PRO:O	2.19	0.41
1:C:18:PRO:HB3	1:C:417:THR:HG22	2.01	0.41
1:D:69:CYS:SG	1:D:82:TYR:CE1	3.13	0.41
1:A:411:LEU:O	1:A:415:TYR:HB2	2.20	0.41
1:A:367:ASN:HB3	1:A:377:GLU:O	2.20	0.41
1:D:237:LEU:CD1	1:D:241:CYS:HA	2.50	0.41
1:B:620:HIS:CD2	1:B:668:TYR:CD2	3.07	0.41
1:C:291:LEU:N	1:C:297:LEU:O	2.53	0.41
1:A:572:ASP:O	1:A:575:ASN:HB2	2.19	0.41
1:B:402:GLY:O	1:B:403:ASP:O	2.38	0.41
1:A:727:TYR:HB3	1:A:728:ILE:H	1.71	0.41
1:D:184:LEU:O	1:D:199:PHE:CE1	2.73	0.41
1:C:707:SER:O	1:C:710:TYR:N	2.52	0.41
1:C:348:TYR:HB3	1:C:368:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LYS:O	1:B:533:LEU:HB2	2.19	0.41
1:D:535:ILE:HG21	1:D:655:LEU:HD13	2.02	0.41
1:B:457:PHE:CG	1:B:477:GLN:HG2	2.55	0.41
1:A:124:LYS:C	1:A:126:GLY:H	2.23	0.41
1:C:542:ASP:O	1:C:543:SER:C	2.57	0.41
1:C:591:MET:HB3	1:C:591:MET:HE2	1.91	0.41
1:A:237:LEU:CD1	1:A:241:CYS:HA	2.50	0.41
1:A:244:LYS:HE2	1:A:256:ASP:OD1	2.19	0.41
1:C:182:GLY:C	1:C:183:LEU:HD23	2.41	0.41
1:A:290:LEU:HD13	1:A:298:PHE:CE1	2.56	0.41
1:C:297:LEU:HD13	1:C:318:ASN:ND2	2.34	0.41
1:A:694:ASN:N	1:A:697:GLN:HE21	2.18	0.41
1:B:694:ASN:N	1:B:697:GLN:HE21	2.18	0.41
1:D:187:LYS:CE	1:D:197:LEU:HD21	2.50	0.41
1:B:423:ALA:HB2	1:B:453:VAL:HG21	2.01	0.41
1:A:530:LYS:O	1:A:533:LEU:HB2	2.20	0.41
1:B:184:LEU:O	1:B:199:PHE:CE1	2.73	0.41
1:B:55:GLU:HB3	1:B:56:TYR:H	1.74	0.41
1:A:705:LEU:O	1:A:709:VAL:HG23	2.20	0.41
1:D:406:ARG:C	1:D:408:PHE:N	2.72	0.41
1:D:71:HIS:CE1	1:D:478:PRO:HB3	2.55	0.41
1:D:71:HIS:CE1	1:D:478:PRO:N	2.88	0.41
1:D:530:LYS:O	1:D:533:LEU:HB2	2.20	0.41
1:A:430:ASN:O	1:A:432:ILE:HG13	2.20	0.41
1:C:549:LYS:O	1:C:552:ASP:N	2.54	0.41
1:C:673:CYS:O	1:C:677:GLU:HG2	2.20	0.41
1:B:124:LYS:C	1:B:126:GLY:H	2.23	0.41
1:B:616:LEU:HD11	1:B:675:LEU:CD2	2.50	0.41
1:D:24:VAL:CG2	1:D:93:ILE:HG12	2.50	0.41
1:A:386:LEU:O	1:A:390:GLN:HG3	2.20	0.41
1:B:237:LEU:CD1	1:B:241:CYS:HA	2.50	0.41
1:A:255:GLN:OE1	1:A:257:TYR:HE2	2.03	0.41
1:A:291:LEU:N	1:A:297:LEU:O	2.53	0.41
1:C:697:GLN:O	1:C:700:ALA:HB3	2.20	0.41
1:C:99:ASN:O	1:C:100:ALA:O	2.39	0.41
1:A:177:PHE:CD1	1:A:183:LEU:HB3	2.55	0.41
1:A:184:LEU:O	1:A:199:PHE:CE1	2.73	0.41
1:A:184:LEU:HD11	1:A:196:PRO:CB	2.50	0.41
1:D:55:GLU:HB3	1:D:56:TYR:H	1.75	0.41
1:A:58:ASN:HA	1:A:474:ASN:HD22	1.81	0.41
1:B:553:ILE:CG2	1:B:553:ILE:O	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:HIS:C	1:D:438:GLU:H	2.24	0.41
1:B:535:ILE:HG21	1:B:655:LEU:HD13	2.02	0.41
1:B:73:SER:O	1:B:76:SER:N	2.50	0.41
1:A:651:ILE:O	1:A:654:LEU:N	2.52	0.41
1:B:22:ASN:HD21	1:B:91:LYS:HD3	1.86	0.41
1:C:22:ASN:HD21	1:C:91:LYS:HD3	1.86	0.41
1:B:550:PHE:CD2	1:B:638:VAL:HG12	2.56	0.41
1:D:268:SER:OG	1:D:269:HIS:N	2.54	0.41
1:C:262:GLN:OE1	1:C:315:PHE:HB2	2.21	0.41
1:D:291:LEU:N	1:D:297:LEU:O	2.53	0.41
1:A:667:LEU:HD22	1:C:723:PHE:CD2	2.54	0.41
1:B:199:PHE:HA	1:B:251:PHE:HB3	2.03	0.41
1:A:690:VAL:CG1	1:A:691:LYS:H	2.34	0.41
1:A:705:LEU:C	1:A:707:SER:N	2.69	0.41
1:A:630:THR:HG22	1:A:634:LEU:HD11	2.01	0.41
1:C:535:ILE:HG21	1:C:655:LEU:HD13	2.01	0.41
1:A:483:LEU:HD23	1:A:483:LEU:C	2.41	0.41
1:C:563:GLU:HB3	1:C:565:THR:HG22	2.02	0.41
1:B:22:ASN:HD22	1:B:91:LYS:HB2	1.86	0.41
1:C:22:ASN:HD22	1:C:91:LYS:HB2	1.84	0.41
1:B:77:THR:O	1:B:97:LEU:HB2	2.21	0.41
1:C:366:LEU:HD13	1:C:378:TRP:CE2	2.56	0.41
1:A:77:THR:O	1:A:97:LEU:HB2	2.20	0.41
1:C:317:ASN:ND2	1:C:319:ILE:CG1	2.71	0.41
1:C:694:ASN:OD1	1:C:697:GLN:HG3	2.21	0.41
1:B:605:ILE:CG1	1:B:606:LYS:H	2.19	0.41
1:B:342:LEU:N	1:B:342:LEU:HD23	2.36	0.41
1:D:323:LEU:HD11	1:D:355:TRP:CE3	2.55	0.41
1:C:228:LEU:HA	1:C:233:TYR:O	2.21	0.41
1:D:405:GLU:CD	1:D:437:ASN:ND2	2.74	0.41
1:D:73:SER:O	1:D:76:SER:N	2.50	0.41
1:C:535:ILE:CG2	1:C:655:LEU:HD13	2.51	0.41
1:C:719:PHE:O	1:C:722:THR:N	2.53	0.41
1:C:549:LYS:O	1:C:552:ASP:HB3	2.20	0.41
1:D:563:GLU:HB3	1:D:565:THR:HG22	2.02	0.41
1:A:22:ASN:ND2	1:A:91:LYS:HD3	2.35	0.41
1:B:24:VAL:CG2	1:B:93:ILE:HG12	2.50	0.41
1:A:466:TYR:O	1:A:470:ILE:HB	2.20	0.41
1:C:185:GLY:O	1:C:196:PRO:HA	2.21	0.41
1:C:184:LEU:HD11	1:C:196:PRO:CB	2.50	0.41
1:C:199:PHE:HA	1:C:251:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:C	1:A:183:LEU:HD23	2.41	0.41
1:C:55:GLU:HB3	1:C:56:TYR:H	1.75	0.41
1:C:396:ASP:OD2	1:C:399:THR:OG1	2.36	0.41
1:B:657:LEU:O	1:B:660:LYS:N	2.54	0.41
1:C:28:VAL:HG13	1:C:150:PHE:CE1	2.56	0.41
1:D:679:LEU:O	1:D:680:LEU:HD12	2.21	0.41
1:B:398:VAL:HG21	1:B:665:LEU:HD13	2.02	0.41
1:B:291:LEU:N	1:B:297:LEU:O	2.53	0.41
1:A:297:LEU:HD13	1:A:318:ASN:ND2	2.34	0.41
1:D:286:THR:CG2	1:D:287:LEU:H	2.30	0.41
1:C:124:LYS:C	1:C:126:GLY:N	2.74	0.41
1:B:165:PHE:HB3	1:B:177:PHE:HB2	2.03	0.41
1:A:73:SER:HB3	1:A:78:LEU:N	2.30	0.41
1:D:535:ILE:CG2	1:D:655:LEU:HD13	2.51	0.41
1:C:637:PHE:CD2	1:C:651:ILE:HD11	2.53	0.41
1:B:673:CYS:O	1:B:677:GLU:HG2	2.21	0.41
1:B:614:ILE:HA	1:B:614:ILE:HD13	1.89	0.41
1:A:468:ASP:HB2	1:A:469:GLU:OE2	2.21	0.41
1:A:27:TYR:N	1:A:27:TYR:CD1	2.87	0.41
1:C:322:ASN:N	1:C:322:ASN:OD1	2.50	0.41
1:A:270:PHE:C	1:A:270:PHE:CD2	2.94	0.41
1:C:184:LEU:O	1:C:199:PHE:CE1	2.73	0.41
1:C:620:HIS:CD2	1:C:668:TYR:CD2	3.09	0.41
1:D:283:TYR:N	1:D:336:LEU:HD23	2.36	0.41
1:C:283:TYR:N	1:C:336:LEU:HD23	2.36	0.41
1:B:307:SER:O	1:B:308:SER:C	2.58	0.41
1:D:187:LYS:HD3	1:D:197:LEU:HD21	2.02	0.41
1:C:340:LEU:O	1:C:341:GLU:CB	2.69	0.41
1:D:103:ASN:H	1:D:107:THR:HG23	1.81	0.41
1:C:100:ALA:O	1:C:124:LYS:HG3	2.20	0.41
1:C:423:ALA:HB2	1:C:453:VAL:HG21	2.03	0.41
1:A:185:GLY:O	1:A:196:PRO:HA	2.21	0.41
1:D:547:VAL:HG22	1:D:644:THR:CG2	2.48	0.41
1:C:58:ASN:HA	1:C:474:ASN:HD22	1.81	0.41
1:B:536:ILE:HD11	1:B:655:LEU:CB	2.51	0.41
1:B:71:HIS:CE1	1:B:478:PRO:HB3	2.56	0.41
1:A:71:HIS:CE1	1:A:478:PRO:N	2.89	0.41
1:A:133:LEU:HA	1:A:134:PRO:HD3	1.98	0.41
1:D:569:ILE:H	1:D:569:ILE:HG13	1.67	0.41
1:B:566:ASN:HA	1:B:569:ILE:CD1	2.51	0.41
1:B:596:PHE:C	1:B:598:LYS:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:LYS:O	1:B:552:ASP:HB3	2.21	0.41
1:D:11:LEU:HD23	1:D:11:LEU:HA	1.82	0.41
1:A:665:LEU:O	1:A:668:TYR:HB3	2.21	0.41
1:D:124:LYS:C	1:D:126:GLY:H	2.23	0.41
1:A:563:GLU:HB3	1:A:565:THR:HG22	2.03	0.41
1:B:563:GLU:HB3	1:B:565:THR:HG22	2.03	0.41
1:B:346:ALA:HB3	1:B:369:ASN:HD22	1.85	0.41
1:D:564:ILE:O	1:D:567:LEU:HB3	2.21	0.41
1:D:77:THR:O	1:D:97:LEU:HB2	2.21	0.41
1:C:25:ASP:OD1	1:C:94:ASN:HB2	2.21	0.41
1:B:679:LEU:O	1:B:680:LEU:HD12	2.21	0.41
1:C:398:VAL:CG2	1:C:669:ARG:HH12	2.34	0.41
1:B:398:VAL:CG2	1:B:669:ARG:HH12	2.34	0.41
1:B:283:TYR:N	1:B:336:LEU:HD23	2.36	0.41
1:C:352:ILE:HG22	1:C:463:ILE:CD1	2.51	0.41
1:D:340:LEU:O	1:D:341:GLU:CB	2.69	0.41
1:B:182:GLY:C	1:B:183:LEU:HD23	2.42	0.41
1:B:247:ASP:OD1	1:B:249:THR:HB	2.21	0.41
1:C:73:SER:O	1:C:74:SER:C	2.59	0.41
1:D:430:ASN:O	1:D:432:ILE:HG13	2.20	0.41
1:D:549:LYS:O	1:D:552:ASP:HB3	2.21	0.41
1:A:549:LYS:O	1:A:552:ASP:HB3	2.21	0.41
1:A:346:ALA:HB3	1:A:369:ASN:HD22	1.86	0.41
1:B:10:ASN:O	1:B:13:GLN:HB2	2.21	0.41
1:A:674:LEU:HB3	1:C:723:PHE:CE1	2.56	0.40
1:C:608:ASP:HB2	1:C:691:LYS:HZ3	1.84	0.40
1:D:423:ALA:HB2	1:D:453:VAL:HG21	2.02	0.40
1:A:478:PRO:O	1:A:479:TYR:HB2	2.21	0.40
1:D:534:ASP:C	1:D:536:ILE:N	2.75	0.40
1:D:663:LEU:HD12	1:D:729:ILE:HD12	2.03	0.40
1:D:596:PHE:C	1:D:598:LYS:N	2.74	0.40
1:C:82:TYR:CD1	1:C:82:TYR:C	2.95	0.40
1:D:22:ASN:HD21	1:D:91:LYS:HD3	1.87	0.40
1:D:620:HIS:CD2	1:D:668:TYR:CD2	3.08	0.40
1:B:91:LYS:HB3	1:B:91:LYS:HE2	1.94	0.40
1:C:22:ASN:ND2	1:C:91:LYS:HD3	2.36	0.40
1:B:386:LEU:O	1:B:390:GLN:HG3	2.20	0.40
1:C:260:VAL:O	1:C:261:SER:HB3	2.21	0.40
1:C:199:PHE:HD2	1:C:251:PHE:HA	1.86	0.40
1:A:161:ARG:NH2	1:A:178:LEU:HD12	2.36	0.40
1:B:694:ASN:OD1	1:B:697:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLY:C	1:D:183:LEU:HD23	2.42	0.40
1:C:73:SER:HB3	1:C:78:LEU:N	2.31	0.40
1:A:701:TYR:O	1:A:702:ILE:C	2.59	0.40
1:A:657:LEU:O	1:A:660:LYS:N	2.54	0.40
1:C:133:LEU:HA	1:C:134:PRO:HD3	1.98	0.40
1:A:124:LYS:C	1:A:126:GLY:N	2.75	0.40
1:C:165:PHE:CD2	1:C:177:PHE:CD2	3.05	0.40
1:D:290:LEU:HD13	1:D:298:PHE:CE1	2.56	0.40
1:A:283:TYR:N	1:A:336:LEU:HD23	2.36	0.40
1:B:693:PHE:CA	1:B:697:GLN:NE2	2.84	0.40
1:B:690:VAL:CG1	1:B:691:LYS:H	2.32	0.40
1:D:604:ALA:CB	1:D:691:LYS:HE2	2.50	0.40
1:D:632:GLN:O	1:D:635:LEU:HB3	2.21	0.40
1:D:441:GLU:O	1:D:445:ASN:ND2	2.55	0.40
1:B:663:LEU:HD12	1:B:729:ILE:HD12	2.03	0.40
1:D:540:LEU:HD23	1:D:544:MET:HE1	2.03	0.40
1:C:566:ASN:HA	1:C:569:ILE:CD1	2.51	0.40
1:B:124:LYS:C	1:B:126:GLY:N	2.74	0.40
1:B:265:SER:O	1:B:266:ASP:C	2.59	0.40
1:A:366:LEU:HD13	1:A:378:TRP:CE2	2.56	0.40
1:D:616:LEU:HD11	1:D:675:LEU:HD23	2.04	0.40
1:C:165:PHE:HB3	1:C:177:PHE:HB2	2.04	0.40
1:B:286:THR:CG2	1:B:287:LEU:H	2.31	0.40
1:C:161:ARG:NH2	1:C:178:LEU:HD12	2.37	0.40
1:A:723:PHE:CD2	1:C:667:LEU:HD22	2.55	0.40
1:A:723:PHE:HE2	1:C:667:LEU:HD22	1.78	0.40
1:C:663:LEU:HD12	1:C:729:ILE:HD12	2.03	0.40
1:C:657:LEU:O	1:C:660:LYS:N	2.55	0.40
1:B:530:LYS:CA	1:B:530:LYS:HE2	2.50	0.40
1:D:124:LYS:C	1:D:126:GLY:N	2.74	0.40
1:B:564:ILE:O	1:B:567:LEU:HB3	2.21	0.40
1:B:616:LEU:HD11	1:B:675:LEU:HD23	2.04	0.40
1:C:114:GLU:O	1:C:115:GLN:HB2	2.22	0.40
1:A:352:ILE:HG22	1:A:463:ILE:CD1	2.52	0.40
1:A:693:PHE:CA	1:A:697:GLN:NE2	2.85	0.40
1:A:663:LEU:HD12	1:A:729:ILE:HD12	2.03	0.40
1:A:727:TYR:CZ	1:C:670:GLN:HG3	2.57	0.40
1:B:184:LEU:HD11	1:B:196:PRO:HB3	2.03	0.40
1:A:165:PHE:CD2	1:A:177:PHE:CD2	3.06	0.40
1:C:572:ASP:O	1:C:575:ASN:HB2	2.20	0.40
1:B:12:LEU:HD13	1:B:18:PRO:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:LYS:O	1:B:552:ASP:N	2.54	0.40
1:A:614:ILE:HD13	1:A:614:ILE:HA	1.92	0.40
1:C:324:SER:O	1:C:325:ALA:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	702/729 (96%)	463 (66%)	169 (24%)	70 (10%)	1	3
1	B	702/729 (96%)	469 (67%)	159 (23%)	74 (10%)	1	3
1	C	702/729 (96%)	467 (66%)	165 (24%)	70 (10%)	1	3
1	D	702/729 (96%)	469 (67%)	165 (24%)	68 (10%)	1	3
All	All	2808/2916 (96%)	1868 (66%)	658 (23%)	282 (10%)	1	3

All (282) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ALA
1	A	104	GLN
1	A	113	VAL
1	A	214	ARG
1	A	241	CYS
1	A	256	ASP
1	A	261	SER
1	A	264	ASP
1	A	267	PRO
1	A	268	SER
1	A	284	ASN
1	A	307	SER

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Mol	Chain	Res	Type
1	A	324	SER
1	A	338	ARG
1	A	341	GLU
1	A	403	ASP
1	A	417	THR
1	A	435	ALA
1	A	576	SER
1	B	100	ALA
1	B	104	GLN
1	B	113	VAL
1	B	214	ARG
1	B	241	CYS
1	B	256	ASP
1	B	261	SER
1	B	284	ASN
1	B	307	SER
1	B	324	SER
1	B	338	ARG
1	B	341	GLU
1	B	403	ASP
1	B	417	THR
1	B	435	ALA
1	B	576	SER
1	B	651	ILE
1	C	100	ALA
1	C	113	VAL
1	C	214	ARG
1	C	241	CYS
1	C	256	ASP
1	C	261	SER
1	C	268	SER
1	C	284	ASN
1	C	324	SER
1	C	338	ARG
1	C	341	GLU
1	C	403	ASP
1	C	417	THR
1	C	435	ALA
1	C	576	SER
1	C	651	ILE
1	D	100	ALA
1	D	104	GLN

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Mol	Chain	Res	Type
1	D	113	VAL
1	D	214	ARG
1	D	241	CYS
1	D	256	ASP
1	D	261	SER
1	D	268	SER
1	D	284	ASN
1	D	307	SER
1	D	324	SER
1	D	341	GLU
1	D	403	ASP
1	D	417	THR
1	D	435	ALA
1	D	576	SER
1	D	651	ILE
1	A	105	ARG
1	A	202	ASN
1	A	231	GLU
1	A	265	SER
1	A	346	ALA
1	A	443	LEU
1	A	444	ALA
1	A	504	SER
1	A	541	PRO
1	A	553	ILE
1	A	600	ASP
1	A	651	ILE
1	A	684	SER
1	A	727	TYR
1	B	105	ARG
1	B	125	ASP
1	B	202	ASN
1	B	231	GLU
1	B	264	ASP
1	B	346	ALA
1	B	443	LEU
1	B	444	ALA
1	B	504	SER
1	B	541	PRO
1	B	553	ILE
1	B	600	ASP
1	B	684	SER

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Mol	Chain	Res	Type
1	B	727	TYR
1	C	104	GLN
1	C	105	ARG
1	C	202	ASN
1	C	231	GLU
1	C	264	ASP
1	C	267	PRO
1	C	307	SER
1	C	346	ALA
1	C	443	LEU
1	C	444	ALA
1	C	504	SER
1	C	541	PRO
1	C	553	ILE
1	C	600	ASP
1	C	684	SER
1	C	727	TYR
1	D	105	ARG
1	D	202	ASN
1	D	231	GLU
1	D	338	ARG
1	D	346	ALA
1	D	443	LEU
1	D	444	ALA
1	D	504	SER
1	D	541	PRO
1	D	553	ILE
1	D	600	ASP
1	D	684	SER
1	D	727	TYR
1	A	73	SER
1	A	125	ASP
1	A	212	PHE
1	A	333	ASP
1	A	440	GLU
1	A	461	SER
1	A	468	ASP
1	A	497	MET
1	A	544	MET
1	A	708	ASN
1	A	720	PHE
1	B	73	SER

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Mol	Chain	Res	Type
1	B	333	ASP
1	B	440	GLU
1	B	461	SER
1	B	468	ASP
1	B	497	MET
1	B	544	MET
1	B	708	ASN
1	B	720	PHE
1	C	73	SER
1	C	125	ASP
1	C	212	PHE
1	C	333	ASP
1	C	439	ASP
1	C	440	GLU
1	C	461	SER
1	C	468	ASP
1	C	497	MET
1	C	544	MET
1	C	708	ASN
1	C	720	PHE
1	D	73	SER
1	D	125	ASP
1	D	212	PHE
1	D	333	ASP
1	D	440	GLU
1	D	461	SER
1	D	468	ASP
1	D	497	MET
1	D	544	MET
1	D	708	ASN
1	D	720	PHE
1	A	102	MET
1	A	192	VAL
1	A	215	SER
1	A	222	SER
1	A	263	SER
1	A	325	ALA
1	A	348	TYR
1	A	392	GLU
1	A	394	ASP
1	A	598	LYS
1	A	602	ILE

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Mol	Chain	Res	Type
1	B	102	MET
1	B	164	HIS
1	B	192	VAL
1	B	212	PHE
1	B	215	SER
1	B	222	SER
1	B	249	THR
1	B	268	SER
1	B	348	TYR
1	B	392	GLU
1	B	394	ASP
1	B	598	LYS
1	B	602	ILE
1	B	652	SER
1	C	102	MET
1	C	192	VAL
1	C	222	SER
1	C	325	ALA
1	C	348	TYR
1	C	392	GLU
1	C	394	ASP
1	C	410	ASN
1	C	598	LYS
1	C	602	ILE
1	D	102	MET
1	D	192	VAL
1	D	222	SER
1	D	267	PRO
1	D	348	TYR
1	D	392	GLU
1	D	394	ASP
1	D	598	LYS
1	D	602	ILE
1	D	652	SER
1	A	155	PRO
1	A	164	HIS
1	A	190	ASP
1	A	410	ASN
1	B	155	PRO
1	B	190	ASP
1	B	250	SER
1	B	267	PRO

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Mol	Chain	Res	Type
1	B	276	VAL
1	B	325	ALA
1	B	410	ASN
1	B	460	ALA
1	B	543	SER
1	C	155	PRO
1	C	164	HIS
1	C	190	ASP
1	C	215	SER
1	C	460	ALA
1	C	652	SER
1	D	155	PRO
1	D	164	HIS
1	D	190	ASP
1	D	215	SER
1	D	266	ASP
1	D	276	VAL
1	D	325	ALA
1	D	410	ASN
1	A	273	VAL
1	A	276	VAL
1	A	295	ASN
1	A	543	SER
1	B	266	ASP
1	B	273	VAL
1	B	295	ASN
1	B	439	ASP
1	C	273	VAL
1	C	276	VAL
1	C	295	ASN
1	D	273	VAL
1	D	295	ASN
1	D	543	SER
1	A	296	GLY
1	B	296	GLY
1	C	296	GLY
1	C	702	ILE
1	C	728	ILE
1	D	296	GLY
1	A	95	ILE
1	A	292	PRO
1	A	547	VAL

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Mol	Chain	Res	Type
1	A	702	ILE
1	A	728	ILE
1	B	95	ILE
1	B	292	PRO
1	B	547	VAL
1	B	702	ILE
1	C	95	ILE
1	C	292	PRO
1	C	547	VAL
1	D	95	ILE
1	D	292	PRO
1	D	547	VAL
1	D	702	ILE
1	D	728	ILE
1	A	416	GLY
1	B	728	ILE
1	C	416	GLY
1	B	416	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	661/682 (97%)	608 (92%)	53 (8%)	15	47
1	B	661/682 (97%)	607 (92%)	54 (8%)	14	46
1	C	661/682 (97%)	609 (92%)	52 (8%)	15	48
1	D	661/682 (97%)	610 (92%)	51 (8%)	16	50
All	All	2644/2728 (97%)	2434 (92%)	210 (8%)	15	48

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	PHE
1	A	92	THR
1	A	99	ASN

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Mol	Chain	Res	Type
1	A	150	PHE
1	A	151	HIS
1	A	164	HIS
1	A	172	GLN
1	A	180	ASP
1	A	183	LEU
1	A	211	PHE
1	A	236	VAL
1	A	270	PHE
1	A	280	LEU
1	A	294	GLU
1	A	297	LEU
1	A	312	THR
1	A	328	ILE
1	A	337	THR
1	A	338	ARG
1	A	349	LEU
1	A	363	LEU
1	A	375	ASN
1	A	377	GLU
1	A	385	SER
1	A	386	LEU
1	A	393	HIS
1	A	409	CYS
1	A	427	LEU
1	A	430	ASN
1	A	438	GLU
1	A	446	LEU
1	A	447	GLU
1	A	455	THR
1	A	464	THR
1	A	469	GLU
1	A	530	LYS
1	A	540	LEU
1	A	541	PRO
1	A	552	ASP
1	A	558	LEU
1	A	565	THR
1	A	583	LEU
1	A	590	GLN
1	A	596	PHE
1	A	597	TRP

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Mol	Chain	Res	Type
1	A	613	ILE
1	A	623	LEU
1	A	663	LEU
1	A	670	GLN
1	A	679	LEU
1	A	692	PHE
1	A	706	ASN
1	A	717	ASN
1	B	72	PHE
1	B	92	THR
1	B	99	ASN
1	B	150	PHE
1	B	151	HIS
1	B	164	HIS
1	B	172	GLN
1	B	180	ASP
1	B	183	LEU
1	B	211	PHE
1	B	236	VAL
1	B	270	PHE
1	B	280	LEU
1	B	294	GLU
1	B	297	LEU
1	B	312	THR
1	B	328	ILE
1	B	337	THR
1	B	338	ARG
1	B	349	LEU
1	B	363	LEU
1	B	375	ASN
1	B	377	GLU
1	B	385	SER
1	B	386	LEU
1	B	393	HIS
1	B	409	CYS
1	B	427	LEU
1	B	430	ASN
1	B	437	ASN
1	B	438	GLU
1	B	446	LEU
1	B	447	GLU
1	B	455	THR

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Mol	Chain	Res	Type
1	B	464	THR
1	B	469	GLU
1	B	530	LYS
1	B	540	LEU
1	B	541	PRO
1	B	552	ASP
1	B	558	LEU
1	B	565	THR
1	B	583	LEU
1	B	590	GLN
1	B	596	PHE
1	B	597	TRP
1	B	613	ILE
1	B	623	LEU
1	B	663	LEU
1	B	670	GLN
1	B	679	LEU
1	B	692	PHE
1	B	706	ASN
1	B	717	ASN
1	C	72	PHE
1	C	99	ASN
1	C	150	PHE
1	C	151	HIS
1	C	164	HIS
1	C	172	GLN
1	C	180	ASP
1	C	183	LEU
1	C	211	PHE
1	C	236	VAL
1	C	270	PHE
1	C	280	LEU
1	C	294	GLU
1	C	297	LEU
1	C	312	THR
1	C	328	ILE
1	C	337	THR
1	C	338	ARG
1	C	349	LEU
1	C	363	LEU
1	C	375	ASN
1	C	377	GLU

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Mol	Chain	Res	Type
1	C	385	SER
1	C	386	LEU
1	C	393	HIS
1	C	409	CYS
1	C	427	LEU
1	C	430	ASN
1	C	441	GLU
1	C	446	LEU
1	C	447	GLU
1	C	455	THR
1	C	464	THR
1	C	469	GLU
1	C	530	LYS
1	C	540	LEU
1	C	541	PRO
1	C	552	ASP
1	C	558	LEU
1	C	565	THR
1	C	583	LEU
1	C	590	GLN
1	C	596	PHE
1	C	597	TRP
1	C	613	ILE
1	C	623	LEU
1	C	663	LEU
1	C	670	GLN
1	C	679	LEU
1	C	692	PHE
1	C	706	ASN
1	C	717	ASN
1	D	72	PHE
1	D	99	ASN
1	D	150	PHE
1	D	151	HIS
1	D	164	HIS
1	D	172	GLN
1	D	180	ASP
1	D	183	LEU
1	D	211	PHE
1	D	236	VAL
1	D	280	LEU
1	D	294	GLU

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Mol	Chain	Res	Type
1	D	297	LEU
1	D	312	THR
1	D	328	ILE
1	D	337	THR
1	D	338	ARG
1	D	349	LEU
1	D	363	LEU
1	D	375	ASN
1	D	377	GLU
1	D	385	SER
1	D	386	LEU
1	D	393	HIS
1	D	409	CYS
1	D	427	LEU
1	D	430	ASN
1	D	438	GLU
1	D	446	LEU
1	D	447	GLU
1	D	455	THR
1	D	464	THR
1	D	469	GLU
1	D	530	LYS
1	D	540	LEU
1	D	541	PRO
1	D	552	ASP
1	D	558	LEU
1	D	565	THR
1	D	583	LEU
1	D	590	GLN
1	D	596	PHE
1	D	597	TRP
1	D	613	ILE
1	D	623	LEU
1	D	663	LEU
1	D	670	GLN
1	D	679	LEU
1	D	692	PHE
1	D	706	ASN
1	D	717	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	71	HIS
1	A	111	GLN
1	A	120	ASN
1	A	132	GLN
1	A	172	GLN
1	A	240	ASN
1	A	262	GLN
1	A	299	GLN
1	A	318	ASN
1	A	430	ASN
1	A	437	ASN
1	A	445	ASN
1	A	458	ASN
1	A	487	ASN
1	A	514	ASN
1	A	575	ASN
1	A	589	ASN
1	A	620	HIS
1	A	632	GLN
1	A	697	GLN
1	B	22	ASN
1	B	71	HIS
1	B	111	GLN
1	B	120	ASN
1	B	132	GLN
1	B	172	GLN
1	B	240	ASN
1	B	262	GLN
1	B	299	GLN
1	B	318	ASN
1	B	430	ASN
1	B	437	ASN
1	B	445	ASN
1	B	487	ASN
1	B	514	ASN
1	B	575	ASN
1	B	589	ASN
1	B	620	HIS
1	B	632	GLN
1	B	697	GLN
1	C	22	ASN
1	C	71	HIS

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Mol	Chain	Res	Type
1	C	111	GLN
1	C	120	ASN
1	C	132	GLN
1	C	172	GLN
1	C	240	ASN
1	C	242	HIS
1	C	262	GLN
1	C	299	GLN
1	C	318	ASN
1	C	430	ASN
1	C	445	ASN
1	C	458	ASN
1	C	487	ASN
1	C	514	ASN
1	C	575	ASN
1	C	589	ASN
1	C	620	HIS
1	C	632	GLN
1	C	697	GLN
1	D	22	ASN
1	D	71	HIS
1	D	111	GLN
1	D	120	ASN
1	D	132	GLN
1	D	172	GLN
1	D	240	ASN
1	D	262	GLN
1	D	299	GLN
1	D	318	ASN
1	D	430	ASN
1	D	445	ASN
1	D	487	ASN
1	D	514	ASN
1	D	575	ASN
1	D	589	ASN
1	D	620	HIS
1	D	632	GLN
1	D	697	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	706/729 (96%)	0.54	81 (11%)	6 2	51, 121, 174, 188	0
1	B	706/729 (96%)	0.55	75 (10%)	8 3	54, 121, 174, 188	0
1	C	706/729 (96%)	0.58	80 (11%)	7 2	52, 122, 174, 191	0
1	D	706/729 (96%)	0.52	71 (10%)	9 3	50, 121, 174, 186	0
All	All	2824/2916 (96%)	0.55	307 (10%)	7 3	50, 122, 174, 191	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	600	ASP	9.7
1	C	174	SER	9.7
1	B	244	LYS	9.6
1	C	186	LEU	8.8
1	B	194	TYR	8.2
1	D	558	LEU	8.1
1	C	185	GLY	7.9
1	C	184	LEU	7.8
1	B	197	LEU	7.8
1	A	600	ASP	7.8
1	C	175	VAL	7.6
1	A	183	LEU	7.2
1	A	313	TYR	7.0
1	D	237	LEU	6.9
1	B	166	LEU	6.7
1	C	313	TYR	6.7
1	D	186	LEU	6.6
1	C	176	VAL	6.4
1	B	155	PRO	6.2
1	B	198	LEU	5.9
1	A	184	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	186	LEU	5.8
1	C	601	PHE	5.7
1	B	288	VAL	5.5
1	D	270	PHE	5.4
1	C	215	SER	5.3
1	B	558	LEU	5.3
1	C	112	GLU	5.2
1	B	237	LEU	5.2
1	D	133	LEU	5.1
1	A	486	LEU	5.1
1	A	244	LYS	5.1
1	B	600	ASP	5.1
1	B	349	LEU	5.0
1	B	133	LEU	5.0
1	D	194	TYR	4.9
1	B	199	PHE	4.9
1	B	236	VAL	4.9
1	A	596	PHE	4.8
1	A	601	PHE	4.8
1	D	197	LEU	4.8
1	C	253	LEU	4.7
1	C	692	PHE	4.7
1	C	557	CYS	4.7
1	B	498	HIS	4.7
1	C	306	ASP	4.7
1	A	271	ARG	4.6
1	C	270	PHE	4.6
1	B	602	ILE	4.5
1	A	166	LEU	4.5
1	C	231	GLU	4.4
1	A	231	GLU	4.4
1	C	301	GLY	4.4
1	A	352	ILE	4.4
1	D	155	PRO	4.3
1	B	607	PHE	4.3
1	D	269	HIS	4.3
1	D	185	GLY	4.2
1	B	318	ASN	4.2
1	B	113	VAL	4.2
1	D	113	VAL	4.2
1	D	600	ASP	4.2
1	D	607	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	176	VAL	4.1
1	A	682	ASP	4.1
1	C	599	LYS	4.0
1	D	163	PRO	4.0
1	C	183	LEU	4.0
1	D	196	PRO	4.0
1	B	145	LEU	4.0
1	D	102	MET	4.0
1	A	692	PHE	3.9
1	B	287	LEU	3.9
1	A	287	LEU	3.9
1	D	112	GLU	3.9
1	B	550	PHE	3.9
1	B	601	PHE	3.9
1	A	353	VAL	3.9
1	A	365	ILE	3.9
1	C	607	PHE	3.8
1	D	14	TYR	3.8
1	A	113	VAL	3.8
1	A	174	SER	3.8
1	C	292	PRO	3.8
1	A	685	GLU	3.7
1	B	196	PRO	3.7
1	D	376	TYR	3.7
1	A	546	THR	3.7
1	B	183	LEU	3.7
1	C	259	MET	3.7
1	B	285	ASN	3.6
1	C	598	LYS	3.6
1	A	53	GLY	3.6
1	C	241	CYS	3.6
1	C	133	LEU	3.5
1	D	379	ILE	3.5
1	C	685	GLU	3.5
1	C	220	TYR	3.5
1	A	158	PHE	3.5
1	D	118	LEU	3.5
1	D	689	GLY	3.5
1	C	113	VAL	3.5
1	B	117	LEU	3.4
1	D	261	SER	3.4
1	C	246	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	302	THR	3.4
1	B	300	MET	3.4
1	B	603	SER	3.4
1	A	305	VAL	3.4
1	A	427	LEU	3.4
1	B	466	TYR	3.4
1	A	2	ALA	3.4
1	B	269	HIS	3.3
1	A	245	ILE	3.3
1	D	729	ILE	3.3
1	D	599	LYS	3.3
1	C	152	LEU	3.3
1	B	401	THR	3.3
1	B	242	HIS	3.2
1	C	2	ALA	3.2
1	A	119	VAL	3.2
1	B	379	ILE	3.2
1	C	53	GLY	3.2
1	D	691	LYS	3.2
1	C	158	PHE	3.2
1	A	498	HIS	3.2
1	A	189	VAL	3.2
1	C	606	LYS	3.2
1	A	695	TYR	3.2
1	A	243	LEU	3.2
1	A	163	PRO	3.2
1	A	607	PHE	3.2
1	A	241	CYS	3.1
1	D	692	PHE	3.1
1	D	378	TRP	3.1
1	D	119	VAL	3.1
1	C	118	LEU	3.1
1	A	684	SER	3.0
1	A	318	ASN	3.0
1	A	311	LEU	3.0
1	C	724	PHE	3.0
1	D	129	LEU	3.0
1	D	134	PRO	3.0
1	B	348	TYR	2.9
1	B	599	LYS	2.9
1	D	145	LEU	2.9
1	A	348	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	169	VAL	2.9
1	A	263	SER	2.9
1	C	311	LEU	2.9
1	D	248	LEU	2.9
1	A	300	MET	2.9
1	C	637	PHE	2.8
1	B	574	LEU	2.8
1	C	132	GLN	2.8
1	D	139	PHE	2.8
1	A	599	LYS	2.8
1	A	291	LEU	2.8
1	A	259	MET	2.8
1	D	640	PHE	2.8
1	B	153	GLN	2.8
1	C	682	ASP	2.8
1	A	297	LEU	2.8
1	D	727	TYR	2.8
1	A	175	VAL	2.8
1	A	185	GLY	2.8
1	A	558	LEU	2.8
1	B	365	ILE	2.8
1	C	166	LEU	2.8
1	A	606	LYS	2.8
1	D	131	LEU	2.7
1	B	192	VAL	2.7
1	D	166	LEU	2.7
1	D	381	SER	2.7
1	A	637	PHE	2.7
1	D	176	VAL	2.7
1	B	271	ARG	2.7
1	B	72	PHE	2.7
1	A	605	ILE	2.7
1	B	228	LEU	2.7
1	C	128	PHE	2.7
1	D	639	LEU	2.7
1	B	268	SER	2.7
1	A	272	LYS	2.7
1	C	19	GLU	2.7
1	C	596	PHE	2.7
1	C	117	LEU	2.6
1	B	378	TRP	2.6
1	A	501	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	2.6
1	D	590	GLN	2.6
1	B	295	ASN	2.6
1	A	591	MET	2.6
1	A	512	THR	2.6
1	B	270	PHE	2.6
1	D	9	ALA	2.6
1	A	198	LEU	2.6
1	C	197	LEU	2.6
1	D	158	PHE	2.6
1	D	650	HIS	2.6
1	A	709	VAL	2.6
1	C	299	GLN	2.5
1	D	463	ILE	2.5
1	B	596	PHE	2.5
1	C	129	LEU	2.5
1	C	639	LEU	2.5
1	B	186	LEU	2.5
1	D	285	ASN	2.5
1	A	246	TRP	2.5
1	C	177	PHE	2.5
1	C	427	LEU	2.5
1	D	298	PHE	2.5
1	B	342	LEU	2.5
1	D	359	THR	2.5
1	C	127	SER	2.5
1	C	222	SER	2.5
1	D	280	LEU	2.5
1	A	437	ASN	2.5
1	A	131	LEU	2.5
1	B	546	THR	2.4
1	C	310	ILE	2.4
1	A	117	LEU	2.4
1	D	164	HIS	2.4
1	A	431	LYS	2.4
1	C	349	LEU	2.4
1	A	319	ILE	2.4
1	A	81	PHE	2.4
1	B	245	ILE	2.4
1	B	376	TYR	2.4
1	B	685	GLU	2.4
1	C	263	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	493	TRP	2.4
1	D	355	TRP	2.4
1	A	299	GLN	2.4
1	A	514	ASN	2.3
1	C	271	ARG	2.3
1	C	18	PRO	2.3
1	B	367	ASN	2.3
1	A	118	LEU	2.3
1	D	303	LEU	2.3
1	D	618	SER	2.3
1	B	156	TYR	2.3
1	A	309	GLY	2.3
1	C	77	THR	2.3
1	A	577	PHE	2.3
1	B	375	ASN	2.3
1	D	184	LEU	2.3
1	D	288	VAL	2.3
1	A	683	SER	2.3
1	C	254	ILE	2.3
1	A	366	LEU	2.3
1	B	729	ILE	2.3
1	A	379	ILE	2.2
1	C	374	LYS	2.2
1	D	287	LEU	2.2
1	B	160	VAL	2.2
1	B	66	GLU	2.2
1	C	272	LYS	2.2
1	A	133	LEU	2.2
1	C	446	LEU	2.2
1	C	433	ILE	2.2
1	B	243	LEU	2.2
1	A	138	LEU	2.2
1	C	342	LEU	2.2
1	D	663	LEU	2.2
1	D	506	LEU	2.2
1	A	310	ILE	2.2
1	B	231	GLU	2.2
1	D	281	SER	2.2
1	D	333	ASP	2.2
1	B	355	TRP	2.2
1	D	321	THR	2.2
1	A	639	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	138	LEU	2.2
1	B	639	LEU	2.2
1	D	97	LEU	2.2
1	C	110	ILE	2.2
1	D	659	TYR	2.1
1	D	198	LEU	2.1
1	D	375	ASN	2.1
1	B	75	ARG	2.1
1	D	510	LEU	2.1
1	B	606	LYS	2.1
1	D	614	ILE	2.1
1	A	282	LEU	2.1
1	B	164	HIS	2.1
1	C	615	SER	2.1
1	C	223	VAL	2.1
1	C	558	LEU	2.1
1	B	486	LEU	2.1
1	B	532	PHE	2.1
1	C	198	LEU	2.1
1	C	437	ASN	2.1
1	C	119	VAL	2.1
1	B	158	PHE	2.0
1	D	334	LEU	2.0
1	C	300	MET	2.0
1	C	221	ASP	2.0
1	D	672	LYS	2.0
1	A	129	LEU	2.0
1	C	194	TYR	2.0
1	C	248	LEU	2.0
1	B	214	ARG	2.0
1	C	497	MET	2.0
1	B	131	LEU	2.0
1	B	184	LEU	2.0
1	D	4	LEU	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.