Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 09:26 am BST

PDB ID	:	4AV6
Title	:	Crystal structure of Thermotoga maritima sodium pumping membrane integral pyrophosphatase at 4 A in complex with phosphate and magnesium
Authors	:	Kajander, T.; Kellosalo, J.; Kogan, K.; Pokharel, K.; Goldman, A.
Deposited on	:	2012-05-23
Resolution	:	4.00 Å(reported)

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

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	Percentile Ranks	Value
Rfree		0.357
Clashscore		80
Ramachandran outliers		3.5%
Sidechain outliers		10.9%
RSRZ outliers		4.5%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
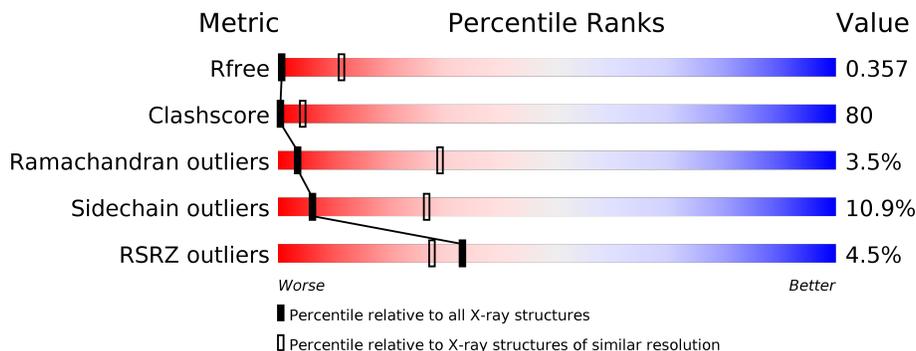
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	735	3% 26% 54% 8% · 11%
1	B	735	5% 28% 51% 8% · 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1728	-	-	X	-
2	PO4	B	1728	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9406 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 K(+)-STIMULATED PYROPHOSPHATE-ENERGIZED SODIUM PUMP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total 4771	C 3140	N 742	O 868	S 21	0	0	0
1	B	642	Total 4605	C 3025	N 718	O 842	S 20	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q9S5X0
A	-7	ARG	-	expression tag	UNP Q9S5X0
A	-6	GLY	-	expression tag	UNP Q9S5X0
A	-5	SER	-	expression tag	UNP Q9S5X0
A	-4	HIS	-	expression tag	UNP Q9S5X0
A	-3	HIS	-	expression tag	UNP Q9S5X0
A	-2	HIS	-	expression tag	UNP Q9S5X0
A	-1	HIS	-	expression tag	UNP Q9S5X0
A	0	HIS	-	expression tag	UNP Q9S5X0
A	1	HIS	-	expression tag	UNP Q9S5X0
A	353	LEU	VAL	engineered mutation	UNP Q9S5X0
A	395	GLY	SER	engineered mutation	UNP Q9S5X0
B	-8	MET	-	expression tag	UNP Q9S5X0
B	-7	ARG	-	expression tag	UNP Q9S5X0
B	-6	GLY	-	expression tag	UNP Q9S5X0
B	-5	SER	-	expression tag	UNP Q9S5X0
B	-4	HIS	-	expression tag	UNP Q9S5X0
B	-3	HIS	-	expression tag	UNP Q9S5X0
B	-2	HIS	-	expression tag	UNP Q9S5X0
B	-1	HIS	-	expression tag	UNP Q9S5X0
B	0	HIS	-	expression tag	UNP Q9S5X0
B	1	HIS	-	expression tag	UNP Q9S5X0
B	353	LEU	VAL	engineered mutation	UNP Q9S5X0
B	395	GLY	SER	engineered mutation	UNP Q9S5X0

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O$_4$P).
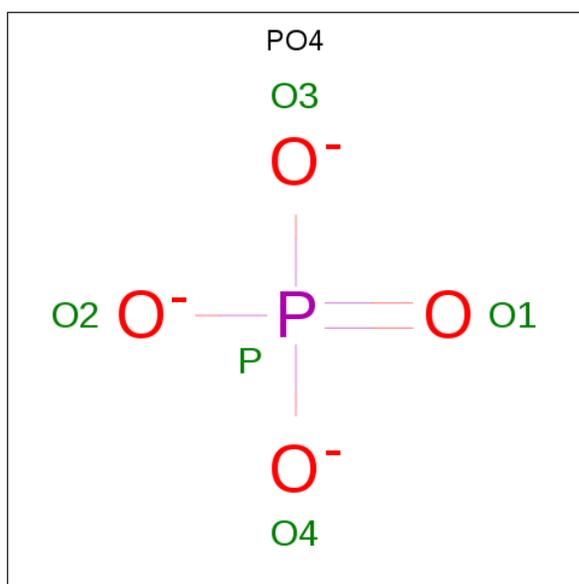
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	Mg 4	0	0
3	A	4	Total 4	Mg 4	0	0

• Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0

3 Residue-property plots (i)

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

• Molecule 1: K(+)-STIMULATED PYROPHOSPHATE-ENERGIZED SODIUM PUMP

L648 A649 I650 L651 T652 N654 S655 G656 G657 A658 W659 D660 N661 A662 K663 K664 Y665 L666 E667 A668 G669 N670 L671 E672 G673 Y674 G675 K676 G677 S678 E679 P680 H681 L684 V685 I686 G687 D688 T689 V690 G691 D692 P693 L694 K695 D696 T697 V698 G699 P700 S701 L702 D703 I704 L705 I706 K707 I708
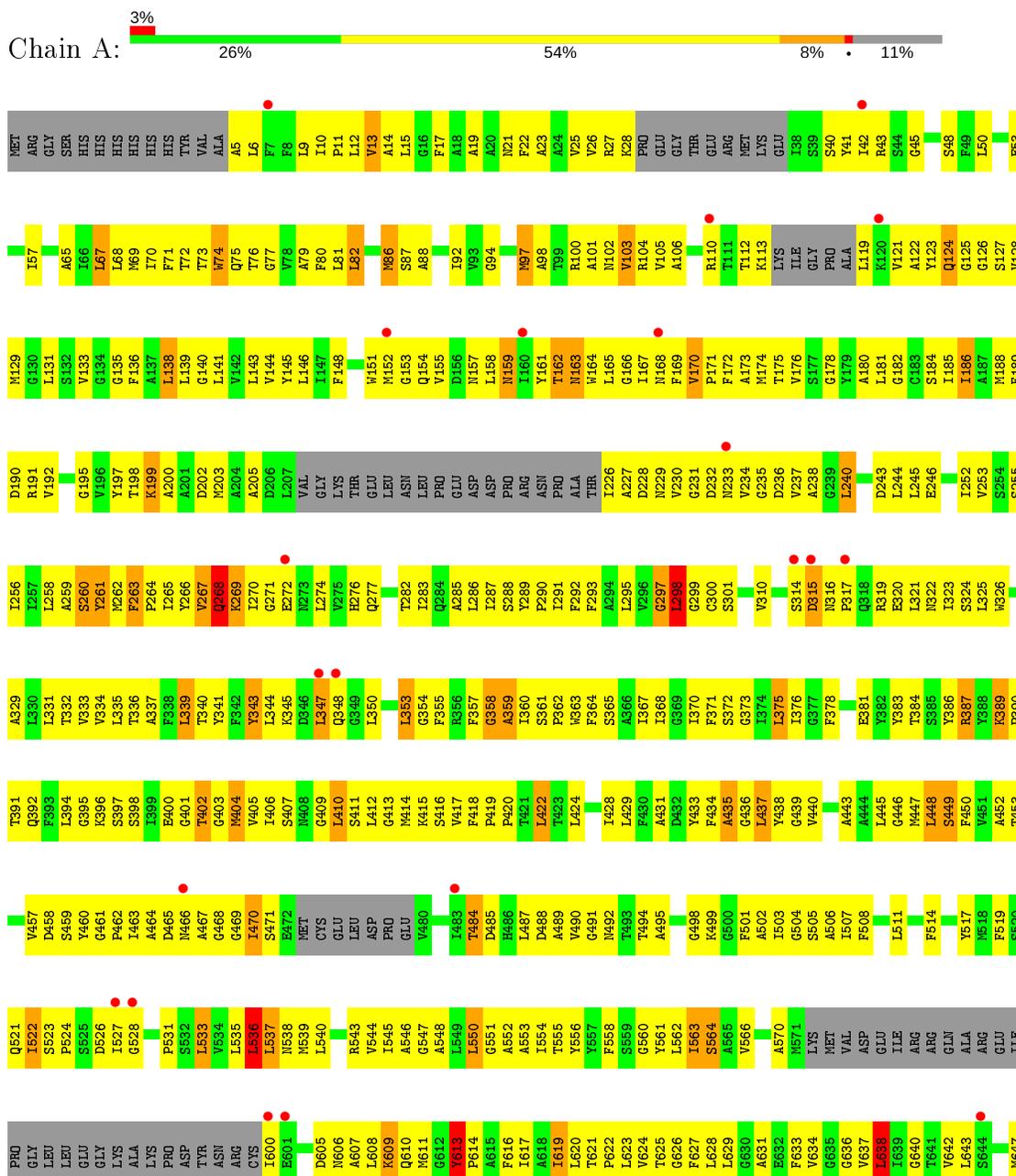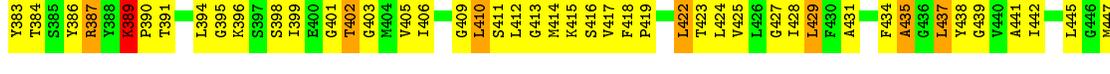
M709 S710 V711 V712 S713 V714 V717 S718 I719 F720 K721 H722 V723 H724 L725 F726

● Molecule 1: K(+)-STIMULATED PYROPHOSPHATE-ENERGIZED SODIUM PUMP

Chain B:

MET ARG GLY SER HIS HIS HIS HIS HIS TYR VAL ALA A5 L6 F7 F8 L9 I10 P11 L12 V13 A14 L15 G16 F17 A18 A19 A20 N21 F22 A23 A24 V25 V26 R27 K28 PRO GLU GLY THR GLU ARG MET LYS GLU I38 S39 S40 Y41 I42 R43 S44 G45 S48 F49 L50 E53

I57 I62 A65 I66 L67 L68 M69 I70 F71 T72 T73 W74 Q75 T76 G77 F80 L81 L82 M86 S87 A88 I92 V93 G94 M97 A98 T99 R100 A101 N102 V103 R104 A106 E107 A108 A109 R110 T111 T112 K113 LYS ILE GLY PRO ALA L119 K120 V121 A122 Y123 Q124 G125

G126 S127 V128 M129 G130 L131 S132 V133 G134 G135 F136 A137 L138 L139 G140 L141 V142 L143 V144 Y145 F148 GLY LYS TRP MET G153 Q154 V155 D156 N157 L158 N159 I160 Y161 T162 N163 W164 L165 G166 L167 N168 F169 V170 P171 F172 A173 M174 T175 V176 S177 G178 Y179 A180 L181 G182 C183 S184 I185 I186

A187 M188 F189 D190 R191 V192 G193 G194 G195 V196 Y197 T198 K199 A200 A201 D202 A205 D206 L207 VAL GLY LYS THR GLU LEU ASN LEU PRO GLU ASP PRO ARG ASN PRO ALA THR I226 A227 D228 N229 V230 G231 D232 N233 V234 G235 D236 V237 A238 G239 L240 G241 A242 D243 L244 L245 E246 S247

F248 I252 V253 I256 I257 L258 A259 S260 Y261 M262 F263 P264 L265 Y266 V267 Q268 K269 I270 G271 E272 N273 L274 V275 H276 Q277 V278 T282 I283 L286 I287 S288 P289 P290 I291 F292 P293 A294 L295 V296 G297 L298 G299 C300 C301 L306 L307 V308 Y307 V310 K311 P312 P313 S314 D315 N316

P317 Q318 B319 E320 L321 N322 I323 W326 L331 T332 V333 V334 L335 T336 A337 F338 L339 T340 Y341 F342 V343 L344 K345 D346 L347 Q348 GLY LEU ASP VAL LEU GLY PHE ARG PHE G358 A359 I360 S361 P362 W363 F364 S365 A366 I367 I368 G369 I370 F371 I374 L375 I376 F377 F378 E381 Y382

Y383 T384 S385 Y386 R387 V388 K389 P390 T391 L394 G395 K396 S397 S398 I399 E400 G401 T402 G403 M404 V405 I406 G409 L410 L412 G413 M414 K415 S416 V417 F418 P419 L422 T423 L424 V425 L426 G427 I428 F429 F430 A431 F434 A435 G436 L437 Y438 G439 V440 A441 I442 L445 G446 M447

L448 S449 A452 T453 V457 D458 S459 Y460 G461 P462 I463 A464 D465 N466 A467 G468 E472 MET CYS GLU LEU ASP PRO GLU V430 T484 D485 H486 L487 D488 A489 V490 G491 N492 T493 T494 A495 A496 I497 G498 K499 A502 I503 G504 S505 A506 I507 F508 L511 L513 F514 A515 S516

Y517 M518 F519 S520 Q521 I522 S523 P524 S525 D526 I527 G528 L533 V534 L535 I536 L537 N538 M539 L540 R543 V544 A546 G547 A548 L549 L550 G551 A552 A553 I554 T555 Y556 Y557 F558 S559 G560 Y561 L562 I563 S564 A565 V566 A570 M571 LYS MET VAL ASP ARG ILE ARG ARG GLN ALA ARG

GLU ILE PRO GLY LEU LEU GLU GLY LYS ALA LYS PRO ASP TYR ASN ARG CYS I600 T603 S604 D605 N606 A607 L608 K609 Q610 M611 G612 Y613 P614 A615 F616 I617 A618 I619 L620 T621 P622 L623 V624 T625 G626 F627 L628 L629 G630 A631 E632 F633 V634 V637 L638 V642 L643 A646 M647

L648 A649 I650 L651 N654 S655 G656 W659 D660 N661 A662 K663 K664 Y665 L666 E667 A668 G669 N670 L671 G675 K676 G677 S678 E679 P680 H681 L684 V685 I686 G687 D688 T689 V690 G691 D692 P693 L694 K695 D696 T697 V698 G699 P700 S701 L702 D703 I704 L705 I706 K707 I708 M709 S710 V711 V712

W O R L D W I D E
PDB
PROTEIN DATA BANK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.80Å 112.27Å 109.71Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	29.83 – 4.00 48.26 – 3.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.83-4.00) 98.3 (48.26-3.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.64 (at 4.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.295 , 0.365 0.294 , 0.357	Depositor DCC
R_{free} test set	866 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	178.0	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 187.2	EDS
L-test for twinning[2]	$<|L|> = 0.43, <L^2> = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9406	wwPDB-VP
Average B, all atoms (Å^2)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, K

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	0.53	0/4869	1.03	13/6629 (0.2%)
1	B	0.49	0/4692	1.00	17/6390 (0.3%)
All	All	0.51	0/9561	1.02	30/13019 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	LYS	N-CA-CB	14.91	137.44	110.60
1	B	261	TYR	CA-CB-CG	-10.41	93.62	113.40
1	A	536	LEU	CA-CB-CG	9.45	137.04	115.30
1	A	613	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	A	261	TYR	CA-CB-CG	-8.68	96.91	113.40
1	B	536	LEU	CA-CB-CG	8.09	133.91	115.30
1	A	613	TYR	CB-CG-CD1	7.97	125.78	121.00
1	A	261	TYR	CB-CG-CD1	-7.75	116.35	121.00
1	A	268	GLN	N-CA-C	7.54	131.34	111.00
1	B	261	TYR	CB-CG-CD1	-7.43	116.54	121.00
1	B	669	GLY	N-CA-C	-6.43	97.01	113.10
1	A	170	VAL	C-N-CD	6.16	141.33	128.40
1	A	272	GLU	N-CA-C	5.97	127.11	111.00
1	B	638	LEU	CA-CB-CG	5.87	128.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	343	TYR	CA-CB-CG	-5.82	102.34	113.40
1	A	638	LEU	CA-CB-CG	5.72	128.45	115.30
1	B	161	TYR	N-CA-C	-5.60	95.89	111.00
1	B	160	ILE	N-CA-C	-5.53	96.07	111.00
1	B	170	VAL	C-N-CD	5.46	139.87	128.40
1	A	261	TYR	CB-CG-CD2	5.43	124.25	121.00
1	B	519	PHE	CB-CG-CD2	-5.38	117.03	120.80
1	B	375	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	513	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	389	LYS	CB-CG-CD	5.25	125.25	111.60
1	B	272	GLU	N-CA-C	5.19	125.02	111.00
1	B	694	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	261	TYR	N-CA-C	5.11	124.79	111.00
1	B	261	TYR	N-CA-C	5.09	124.76	111.00
1	B	298	LEU	CA-CB-CG	5.01	126.82	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	268	GLN	CA

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	4771	0	4805	811	0
1	B	4605	0	4619	739	0
2	A	10	0	0	3	0
2	B	10	0	0	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9406	0	9424	1503	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 80.

All (1503) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:TYR:CD2	1:A:680:PRO:HG2	1.61	1.35
1:A:170:VAL:HG22	1:A:261:TYR:OH	1.32	1.28
1:B:326:TRP:NE1	1:B:378:PHE:HZ	1.38	1.21
1:A:674:TYR:CE2	1:A:680:PRO:HG2	1.75	1.19
1:B:170:VAL:HG22	1:B:261:TYR:OH	1.37	1.19
1:A:19:ALA:HA	1:A:22:PHE:CE1	1.79	1.17
1:B:19:ALA:HA	1:B:22:PHE:CE1	1.79	1.16
1:B:383:TYR:HA	1:B:390:PRO:HG2	1.22	1.15
1:A:263:PHE:HB3	1:A:283:ILE:CD1	1.75	1.14
1:A:158:LEU:O	1:A:263:PHE:CZ	2.01	1.14
1:A:326:TRP:NE1	1:A:378:PHE:HZ	1.48	1.12
1:A:717:VAL:O	1:A:721:LYS:HG3	1.50	1.12
1:B:521:GLN:HE22	1:B:631:ALA:HB1	1.13	1.12
1:A:321:LEU:HD23	1:A:457:VAL:HG13	1.13	1.11
1:A:383:TYR:HA	1:A:390:PRO:HG2	1.13	1.10
1:A:263:PHE:CD1	1:A:264:PRO:HD3	1.86	1.10
1:A:65:ALA:HB2	1:A:81:LEU:HD21	1.34	1.09
1:B:19:ALA:HA	1:B:22:PHE:HE1	1.07	1.09
1:A:170:VAL:HG22	1:A:261:TYR:CZ	1.86	1.09
1:B:561:TYR:HE2	1:B:614:PRO:HD3	1.18	1.09
1:B:717:VAL:O	1:B:721:LYS:HG3	1.53	1.08
1:B:321:LEU:HD23	1:B:457:VAL:HG13	1.29	1.07
1:B:337:ALA:HB2	1:B:363:TRP:CE2	1.90	1.07
1:A:19:ALA:HA	1:A:22:PHE:HE1	1.06	1.07
1:A:561:TYR:CE2	1:A:614:PRO:HD3	1.90	1.06
1:A:561:TYR:HE2	1:A:614:PRO:HD3	1.01	1.06
1:A:198:THR:HG21	1:A:235:GLY:N	1.71	1.05
1:A:263:PHE:CE1	1:A:264:PRO:HD3	1.91	1.05
1:B:461:GLY:CA	1:B:491:GLY:HA2	1.87	1.05
1:B:198:THR:HG21	1:B:235:GLY:N	1.71	1.05
1:B:65:ALA:HB2	1:B:81:LEU:HD21	1.36	1.05
1:A:619:ILE:HD11	1:A:708:ILE:HG12	1.39	1.04
1:B:233:ASN:O	1:B:237:VAL:HG22	1.57	1.04
1:B:246:GLU:OE1	1:B:704:ILE:HD12	1.57	1.04
1:A:655:SER:OG	1:A:659:TRP:CZ3	2.10	1.04
1:A:468:GLY:HA2	1:A:484:THR:HG23	1.39	1.03
1:B:468:GLY:CA	1:B:484:THR:HG23	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLY:HA2	1:A:484:THR:CG2	1.89	1.02
1:A:674:TYR:HD2	1:A:680:PRO:HG2	1.22	1.02
1:A:492:ASN:ND2	2:A:1728:PO4:O2	1.91	1.02
1:A:674:TYR:CE2	1:A:680:PRO:CG	2.42	1.02
1:A:65:ALA:CB	1:A:81:LEU:HD21	1.88	1.01
1:A:102:ASN:O	1:A:105:VAL:HG12	1.61	1.01
1:B:73:THR:HG21	1:B:169:PHE:CE2	1.96	1.00
1:B:468:GLY:HA2	1:B:484:THR:HG23	1.39	1.00
1:A:563:ILE:HG21	1:B:411:SER:HB2	1.44	1.00
1:A:536:LEU:HD21	1:B:536:LEU:HD21	1.42	1.00
1:A:332:THR:O	1:A:336:THR:OG1	1.79	1.00
1:A:674:TYR:CD2	1:A:680:PRO:CG	2.45	1.00
1:B:105:VAL:HG11	1:B:467:ALA:HB2	1.39	1.00
1:B:162:THR:HA	1:B:168:ASN:HA	1.42	1.00
1:A:357:PHE:CE2	1:A:361:SER:HA	1.96	0.99
1:A:514:PHE:HZ	1:A:537:LEU:HD12	1.23	0.99
1:B:188:MET:HB2	1:B:704:ILE:HG21	1.40	0.99
1:B:170:VAL:HG22	1:B:261:TYR:CZ	1.98	0.98
1:A:286:LEU:O	1:A:438:TYR:OH	1.79	0.98
1:A:563:ILE:CG2	1:B:411:SER:HB2	1.93	0.98
1:B:461:GLY:HA3	1:B:491:GLY:HA2	1.40	0.98
1:B:65:ALA:CB	1:B:81:LEU:HD21	1.94	0.97
1:B:185:ILE:HG12	1:B:708:ILE:HD11	1.44	0.97
1:A:73:THR:O	1:A:75:GLN:N	1.96	0.97
1:B:561:TYR:CE2	1:B:614:PRO:HD3	1.99	0.97
1:B:102:ASN:O	1:B:105:VAL:HG12	1.64	0.97
1:B:468:GLY:HA2	1:B:484:THR:CG2	1.94	0.97
1:B:543:ARG:NH1	1:B:629:LEU:O	1.98	0.96
1:B:73:THR:O	1:B:75:GLN:N	1.97	0.96
1:A:233:ASN:O	1:A:237:VAL:HG22	1.65	0.96
1:B:556:TYR:CE1	1:B:648:LEU:HD11	2.01	0.96
1:A:464:ALA:HB1	1:A:487:LEU:HB3	1.45	0.95
1:A:711:VAL:O	1:A:714:VAL:HG22	1.64	0.95
1:A:357:PHE:CE2	1:A:364:PHE:HD2	1.84	0.95
1:A:236:ASP:HB2	1:A:462:PRO:HG3	1.47	0.95
1:B:332:THR:O	1:B:336:THR:OG1	1.85	0.94
1:A:411:SER:HB2	1:B:563:ILE:CG2	1.96	0.94
1:A:514:PHE:CZ	1:A:537:LEU:HD12	2.03	0.94
1:A:105:VAL:HG11	1:A:467:ALA:HB2	1.48	0.94
1:A:634:VAL:HG21	1:A:720:PHE:HE1	1.32	0.94
1:B:10:ILE:O	1:B:13:VAL:HG13	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:O	1:A:299:GLY:N	2.01	0.93
1:B:677:GLY:O	1:B:678:SER:OG	1.87	0.93
1:A:246:GLU:OE1	1:A:704:ILE:HD12	1.69	0.93
1:A:188:MET:HB2	1:A:704:ILE:HG21	1.51	0.93
1:B:619:ILE:HD11	1:B:708:ILE:HG12	1.51	0.93
1:A:401:GLY:O	1:A:403:GLY:N	2.01	0.93
1:A:316:ASN:O	1:A:320:GLU:OE1	1.86	0.92
1:B:333:VAL:O	1:B:363:TRP:NE1	2.00	0.92
1:A:73:THR:HG21	1:A:169:PHE:CE2	2.04	0.92
1:A:411:SER:HB2	1:B:563:ILE:HG21	1.48	0.92
1:B:634:VAL:HG21	1:B:720:PHE:HE1	1.33	0.91
1:B:399:ILE:HA	1:B:680:PRO:HG3	1.50	0.91
1:A:72:THR:O	1:A:163:ASN:ND2	2.02	0.91
1:A:198:THR:HG21	1:A:235:GLY:H	1.32	0.91
1:B:326:TRP:NE1	1:B:378:PHE:CZ	2.26	0.90
1:A:169:PHE:HE1	1:A:171:PRO:HA	1.36	0.90
1:B:462:PRO:HA	1:B:465:ASP:HB3	1.54	0.90
1:B:409:GLY:HA3	1:B:659:TRP:CZ2	2.07	0.90
1:A:262:MET:HG2	1:A:353:LEU:HD22	1.52	0.90
1:A:720:PHE:HA	1:A:723:VAL:HG12	1.51	0.90
1:B:316:ASN:O	1:B:320:GLU:OE1	1.90	0.90
1:B:401:GLY:O	1:B:403:GLY:N	2.05	0.90
1:B:711:VAL:O	1:B:714:VAL:HG22	1.70	0.90
1:B:170:VAL:HG22	1:B:261:TYR:HH	1.32	0.90
1:B:170:VAL:HB	1:B:173:ALA:HB3	1.54	0.90
1:A:499:LYS:HE2	1:A:695:LYS:O	1.72	0.89
1:B:68:LEU:HD21	1:B:76:THR:HB	1.54	0.89
1:A:170:VAL:CG2	1:A:261:TYR:CE2	2.54	0.89
1:A:638:LEU:O	1:A:642:VAL:HG23	1.71	0.89
1:A:656:GLY:CA	1:A:695:LYS:HD3	2.02	0.89
1:A:263:PHE:CD1	1:A:264:PRO:CD	2.56	0.88
1:A:622:PRO:HB3	1:A:713:SER:OG	1.74	0.88
1:B:170:VAL:HG21	1:B:261:TYR:CE2	2.08	0.88
1:A:461:GLY:CA	1:A:491:GLY:HA2	2.04	0.88
1:B:414:MET:HG3	1:B:651:LEU:HD21	1.55	0.88
1:B:363:TRP:CZ2	1:B:367:ILE:HD11	2.08	0.87
1:A:666:LEU:C	1:A:666:LEU:HD13	1.95	0.87
1:A:468:GLY:CA	1:A:484:THR:HG23	2.05	0.86
1:B:622:PRO:HB3	1:B:713:SER:OG	1.76	0.86
1:A:10:ILE:O	1:A:13:VAL:HG13	1.75	0.86
1:A:333:VAL:HG13	1:A:367:ILE:HD11	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLY:O	1:B:299:GLY:N	2.08	0.86
1:A:666:LEU:HB3	1:A:684:LEU:HD23	1.56	0.86
1:B:720:PHE:HA	1:B:723:VAL:HG12	1.56	0.86
1:B:180:ALA:HB2	1:B:253:VAL:HG21	1.57	0.85
1:B:464:ALA:HB1	1:B:487:LEU:HB3	1.56	0.85
1:B:521:GLN:NE2	1:B:631:ALA:HB1	1.90	0.85
1:B:25:VAL:HG21	1:B:124:GLN:HB3	1.59	0.85
1:B:170:VAL:CG2	1:B:261:TYR:CE2	2.59	0.85
1:A:489:ALA:HA	1:A:661:ASN:HD21	1.42	0.85
1:A:68:LEU:HD21	1:A:76:THR:HB	1.57	0.85
1:B:169:PHE:HB2	1:B:174:MET:HE3	1.56	0.85
1:A:170:VAL:HG21	1:A:261:TYR:CE2	2.12	0.85
1:A:424:LEU:O	1:A:428:ILE:HD13	1.76	0.85
1:A:561:TYR:HE2	1:A:614:PRO:CD	1.89	0.85
1:A:656:GLY:HA3	1:A:695:LYS:CD	2.07	0.85
1:B:666:LEU:HD13	1:B:666:LEU:C	1.98	0.85
1:A:517:TYR:OH	1:A:634:VAL:HG23	1.77	0.84
1:B:161:TYR:CD2	1:B:169:PHE:CE2	2.65	0.84
1:A:503:ILE:O	1:A:507:ILE:HD12	1.77	0.84
1:A:161:TYR:CD2	1:A:169:PHE:CE2	2.65	0.84
1:B:169:PHE:HE1	1:B:171:PRO:HA	1.41	0.84
1:A:409:GLY:HA3	1:A:659:TRP:CZ2	2.13	0.84
1:B:492:ASN:ND2	2:B:1728:PO4:O2	2.11	0.84
1:A:227:ALA:O	1:A:230:VAL:HG22	1.76	0.83
1:A:263:PHE:HB3	1:A:283:ILE:HD11	1.59	0.83
1:A:326:TRP:HE1	1:A:378:PHE:HZ	0.98	0.83
1:B:268:GLN:CB	1:B:275:VAL:HB	2.07	0.83
1:A:169:PHE:HB2	1:A:174:MET:HE3	1.60	0.83
1:A:263:PHE:HB3	1:A:283:ILE:HD13	1.59	0.83
1:B:395:GLY:O	1:B:398:SER:OG	1.97	0.83
1:A:22:PHE:HA	1:A:97:MET:CE	2.07	0.82
1:A:503:ILE:HG12	1:A:703:ASP:OD1	1.78	0.82
1:A:545:ILE:HG13	1:B:511:LEU:HD21	1.59	0.82
1:B:663:LYS:HA	1:B:684:LEU:HB3	1.62	0.82
1:A:25:VAL:HG21	1:A:124:GLN:HB3	1.60	0.81
1:B:526:ASP:O	1:B:528:GLY:N	2.13	0.81
1:A:198:THR:HG22	1:A:231:GLY:HA2	1.62	0.81
1:A:536:LEU:CD2	1:B:536:LEU:HD21	2.10	0.81
1:B:105:VAL:HA	1:B:121:VAL:HG11	1.62	0.81
1:A:167:ILE:HG23	1:A:718:SER:HB3	1.62	0.81
1:A:263:PHE:CZ	1:A:264:PRO:HD3	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:HD21	1:B:164:TRP:HD1	1.26	0.81
1:A:355:PHE:CE2	1:A:362:PRO:HD3	2.16	0.81
1:A:656:GLY:CA	1:A:695:LYS:CD	2.59	0.81
1:B:321:LEU:CD2	1:B:457:VAL:HG13	2.08	0.81
1:B:506:ALA:HB1	1:B:706:ILE:HD11	1.60	0.81
1:A:167:ILE:HG23	1:A:718:SER:CB	2.11	0.80
1:A:205:ALA:HB2	1:A:228:ASP:HB2	1.64	0.80
1:A:42:ILE:HD12	1:A:43:ARG:N	1.96	0.80
1:A:656:GLY:HA3	1:A:695:LYS:HB3	1.61	0.80
1:B:666:LEU:HB3	1:B:684:LEU:HD23	1.63	0.80
1:A:170:VAL:HG11	1:A:173:ALA:CB	2.12	0.80
1:A:22:PHE:HA	1:A:97:MET:HE1	1.62	0.80
1:B:244:LEU:CD2	1:B:502:ALA:HB2	2.12	0.80
1:A:105:VAL:HA	1:A:121:VAL:HG11	1.62	0.80
1:B:608:LEU:HD23	1:B:611:MET:HE2	1.64	0.80
1:A:350:LEU:HD22	1:A:355:PHE:CD2	2.17	0.80
1:A:14:ALA:O	1:A:17:PHE:HB3	1.82	0.80
1:B:522:ILE:HG23	1:B:522:ILE:O	1.82	0.79
1:B:617:ILE:O	1:B:621:THR:OG1	2.00	0.79
1:A:162:THR:HA	1:A:168:ASN:HA	1.64	0.79
1:A:461:GLY:HA3	1:A:491:GLY:HA2	1.62	0.79
1:A:719:ILE:HG22	1:A:723:VAL:HG11	1.65	0.79
1:A:226:ILE:HG22	1:A:227:ALA:N	1.96	0.79
1:A:357:PHE:CZ	1:A:361:SER:HA	2.16	0.79
1:B:105:VAL:CG1	1:B:467:ALA:HB2	2.10	0.79
1:B:556:TYR:HE1	1:B:648:LEU:HD11	1.47	0.79
1:B:282:THR:HG23	1:B:347:LEU:HB3	1.64	0.79
1:A:321:LEU:CD2	1:A:457:VAL:HG13	2.06	0.79
1:A:414:MET:HG3	1:A:651:LEU:HD21	1.64	0.79
1:A:282:THR:HA	1:A:347:LEU:HD12	1.65	0.79
1:A:169:PHE:CE1	1:A:171:PRO:HA	2.17	0.79
1:B:42:ILE:HD12	1:B:43:ARG:N	1.98	0.79
1:A:550:LEU:HD13	1:A:554:ILE:HD11	1.66	0.78
1:A:73:THR:HG21	1:A:169:PHE:CD2	2.18	0.78
1:A:521:GLN:HE22	1:A:631:ALA:HB1	1.46	0.78
1:A:170:VAL:CG2	1:A:261:TYR:CZ	2.65	0.78
1:B:198:THR:HG21	1:B:235:GLY:CA	2.14	0.78
1:B:72:THR:O	1:B:163:ASN:ND2	2.16	0.78
1:B:127:SER:O	1:B:131:LEU:HD13	1.83	0.78
1:B:73:THR:HG21	1:B:169:PHE:CD2	2.18	0.78
1:B:634:VAL:HG21	1:B:720:PHE:CE1	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PHE:HA	1:B:97:MET:CE	2.14	0.77
1:A:357:PHE:HE2	1:A:360:ILE:HG23	1.49	0.77
1:A:333:VAL:O	1:A:363:TRP:NE1	2.16	0.77
1:A:521:GLN:NE2	1:A:631:ALA:HB1	2.00	0.77
1:A:663:LYS:HA	1:A:684:LEU:HB3	1.65	0.77
1:A:161:TYR:HD2	1:A:169:PHE:CE2	2.01	0.77
1:B:289:TYR:HB2	1:B:344:LEU:HD21	1.65	0.77
1:B:460:TYR:O	1:B:463:ILE:HG22	1.84	0.77
1:B:424:LEU:O	1:B:428:ILE:HD13	1.84	0.77
1:B:244:LEU:HD23	1:B:502:ALA:HB2	1.65	0.77
1:A:226:ILE:HG22	1:A:227:ALA:H	1.50	0.77
1:B:666:LEU:HD11	1:B:681:HIS:HB2	1.67	0.77
1:A:259:ALA:C	1:A:261:TYR:H	1.87	0.77
1:A:445:LEU:O	1:A:449:SER:N	2.18	0.77
1:B:170:VAL:CB	1:B:173:ALA:HB3	2.14	0.77
1:A:337:ALA:HB2	1:A:363:TRP:CE2	2.19	0.77
1:A:634:VAL:HG21	1:A:720:PHE:CE1	2.18	0.77
1:B:686:ILE:O	1:B:690:VAL:HG23	1.84	0.77
1:A:357:PHE:CE1	1:A:434:PHE:HB3	2.20	0.77
1:A:424:LEU:HD21	1:A:447:MET:HE1	1.66	0.77
1:A:170:VAL:O	1:A:171:PRO:C	2.22	0.76
1:A:263:PHE:CG	1:A:264:PRO:HD3	2.20	0.76
1:A:357:PHE:CZ	1:A:364:PHE:HD2	2.02	0.76
1:A:547:GLY:O	1:A:637:VAL:HA	1.85	0.76
1:B:14:ALA:O	1:B:17:PHE:HB3	1.83	0.76
1:A:21:ASN:HB3	1:A:124:GLN:OE1	1.86	0.76
1:A:666:LEU:HD11	1:A:681:HIS:HB2	1.68	0.76
1:B:317:PRO:O	1:B:321:LEU:HD13	1.85	0.76
1:B:521:GLN:HE22	1:B:631:ALA:CB	1.97	0.76
1:A:556:TYR:CE1	1:A:648:LEU:HD11	2.19	0.76
1:B:489:ALA:HA	1:B:661:ASN:HD21	1.50	0.76
1:A:237:VAL:HG23	1:A:238:ALA:N	1.99	0.76
1:A:289:TYR:HB2	1:A:344:LEU:HD21	1.66	0.76
1:A:236:ASP:HB2	1:A:462:PRO:CG	2.15	0.76
1:B:169:PHE:CE1	1:B:171:PRO:HA	2.21	0.75
1:B:301:SER:HB2	1:B:452:ALA:HB3	1.66	0.75
1:B:73:THR:HG21	1:B:169:PHE:CZ	2.21	0.75
1:A:298:LEU:HD12	1:A:299:GLY:N	2.01	0.75
1:A:357:PHE:CE2	1:A:360:ILE:HG23	2.22	0.75
1:B:396:LYS:HG2	1:B:671:LEU:CD2	2.16	0.75
1:A:259:ALA:O	1:A:261:TYR:N	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASP:HB2	1:B:462:PRO:CG	2.17	0.75
1:B:560:GLY:O	1:B:563:ILE:HG22	1.87	0.75
1:A:97:MET:CG	1:A:125:GLY:HA2	2.16	0.75
1:B:666:LEU:HD11	1:B:681:HIS:CB	2.17	0.75
1:A:288:SER:HA	1:A:291:ILE:HD12	1.67	0.75
1:A:394:LEU:HD21	1:A:659:TRP:CD1	2.22	0.75
1:B:170:VAL:O	1:B:171:PRO:C	2.21	0.75
1:B:237:VAL:HG23	1:B:238:ALA:N	2.02	0.75
1:B:719:ILE:HG22	1:B:723:VAL:HG11	1.67	0.75
1:A:127:SER:O	1:A:131:LEU:HD13	1.87	0.74
1:A:526:ASP:O	1:A:528:GLY:N	2.20	0.74
1:B:402:THR:O	1:B:405:VAL:HG22	1.86	0.74
1:B:236:ASP:HB2	1:B:462:PRO:HG3	1.67	0.74
1:A:326:TRP:NE1	1:A:378:PHE:CZ	2.33	0.74
1:A:464:ALA:O	1:A:467:ALA:HB3	1.87	0.74
1:A:121:VAL:HG13	1:A:122:ALA:H	1.53	0.74
1:B:161:TYR:HD2	1:B:169:PHE:CE2	2.04	0.74
1:B:358:GLY:N	1:B:361:SER:HG	1.85	0.74
1:B:561:TYR:HE2	1:B:614:PRO:CD	1.97	0.74
1:B:461:GLY:HA2	1:B:491:GLY:HA2	1.66	0.74
1:B:710:SER:O	1:B:714:VAL:HG13	1.86	0.74
1:B:76:THR:HG23	1:B:174:MET:O	1.88	0.74
1:B:268:GLN:O	1:B:269:LYS:CB	2.35	0.74
1:A:617:ILE:O	1:A:621:THR:OG1	2.04	0.74
1:B:22:PHE:HB3	1:B:128:VAL:HG21	1.69	0.74
1:B:97:MET:CG	1:B:125:GLY:HA2	2.17	0.74
1:B:247:SER:OG	1:B:707:LYS:NZ	2.16	0.73
1:A:22:PHE:HB3	1:A:128:VAL:HG21	1.69	0.73
1:A:357:PHE:CE2	1:A:364:PHE:CD2	2.73	0.73
1:A:386:TYR:O	1:A:387:ARG:CB	2.35	0.73
1:B:460:TYR:CE1	1:B:490:VAL:CG1	2.71	0.73
1:A:129:MET:HE1	1:A:237:VAL:HB	1.70	0.73
1:A:674:TYR:HE2	1:A:680:PRO:CG	1.94	0.73
1:A:460:TYR:O	1:A:463:ILE:HG22	1.88	0.73
1:A:710:SER:O	1:A:714:VAL:HG13	1.88	0.73
1:B:521:GLN:HG2	1:B:721:LYS:HG2	1.70	0.73
1:A:298:LEU:HD12	1:A:299:GLY:H	1.52	0.73
1:B:259:ALA:O	1:B:261:TYR:N	2.22	0.73
1:A:290:PRO:HD3	1:A:438:TYR:OH	1.88	0.73
1:B:429:LEU:HD23	1:B:429:LEU:N	2.03	0.73
1:A:297:GLY:O	1:A:300:CYS:N	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:VAL:CG2	1:B:261:TYR:CZ	2.70	0.73
1:B:170:VAL:HG21	1:B:261:TYR:HE2	1.51	0.73
1:B:461:GLY:CA	1:B:491:GLY:CA	2.66	0.73
1:B:233:ASN:HD21	1:B:466:ASN:HD22	1.37	0.72
1:A:666:LEU:HD11	1:A:681:HIS:CB	2.19	0.72
1:A:686:ILE:O	1:A:690:VAL:HG23	1.89	0.72
1:A:5:ALA:O	1:A:9:LEU:HD12	1.89	0.72
1:A:262:MET:HG3	1:A:266:TYR:CD2	2.25	0.72
1:A:102:ASN:HD21	1:A:466:ASN:ND2	1.87	0.72
1:A:700:PRO:O	1:A:703:ASP:HB2	1.90	0.72
1:B:514:PHE:HZ	1:B:537:LEU:HD12	1.53	0.72
1:A:522:ILE:O	1:A:522:ILE:HG23	1.89	0.72
1:A:489:ALA:HA	1:A:661:ASN:ND2	2.05	0.72
1:B:396:LYS:HG2	1:B:671:LEU:HD21	1.71	0.72
1:B:396:LYS:O	1:B:399:ILE:HG12	1.89	0.72
1:A:317:PRO:O	1:A:321:LEU:HD13	1.89	0.72
1:A:192:VAL:HG13	1:A:562:LEU:HD21	1.69	0.72
1:A:619:ILE:HG22	1:A:620:LEU:HD12	1.72	0.72
1:B:268:GLN:N	1:B:275:VAL:O	2.17	0.72
1:A:105:VAL:CG1	1:A:467:ALA:HB2	2.20	0.72
1:B:536:LEU:O	1:B:536:LEU:HD13	1.89	0.72
1:B:167:ILE:HG23	1:B:718:SER:CB	2.20	0.71
1:B:558:PHE:CE1	1:B:562:LEU:HD11	2.25	0.71
1:B:613:TYR:O	1:B:617:ILE:HG13	1.91	0.71
1:B:86:MET:HE2	1:B:140:GLY:H	1.55	0.71
1:A:19:ALA:CA	1:A:22:PHE:CE1	2.69	0.71
1:B:322:ASN:ND2	1:B:381:GLU:OE1	2.21	0.71
1:A:511:LEU:HD21	1:B:545:ILE:HG13	1.72	0.71
1:B:621:THR:O	1:B:625:THR:OG1	2.05	0.71
1:A:357:PHE:HE1	1:A:434:PHE:HB3	1.55	0.71
1:A:45:GLY:HA2	1:A:600:ILE:HD13	1.73	0.71
1:A:647:MET:CE	1:B:553:ALA:HA	2.20	0.71
1:B:386:TYR:HB3	1:B:391:THR:HG21	1.73	0.71
1:A:129:MET:SD	1:A:459:SER:HB2	2.30	0.71
1:B:198:THR:HG21	1:B:235:GLY:H	1.53	0.71
1:B:129:MET:SD	1:B:459:SER:HB2	2.30	0.71
1:A:236:ASP:CB	1:A:462:PRO:HG3	2.21	0.70
1:B:700:PRO:O	1:B:703:ASP:HB2	1.91	0.70
1:A:170:VAL:HG21	1:A:261:TYR:HE2	1.55	0.70
1:B:307:TYR:O	1:B:311:LYS:CB	2.38	0.70
1:B:191:ARG:O	1:B:195:GLY:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LEU:HD21	1:B:659:TRP:CD1	2.26	0.70
1:A:170:VAL:HG11	1:A:173:ALA:HB3	1.72	0.70
1:B:492:ASN:ND2	2:B:1728:PO4:O4	2.24	0.70
1:B:259:ALA:C	1:B:261:TYR:H	1.93	0.70
1:B:386:TYR:HB3	1:B:391:THR:CG2	2.22	0.70
1:B:97:MET:HG2	1:B:128:VAL:CG2	2.21	0.70
1:B:492:ASN:ND2	2:B:1728:PO4:P	2.64	0.70
1:A:461:GLY:HA2	1:A:491:GLY:HA2	1.72	0.70
1:B:448:LEU:HD22	1:B:505:SER:OG	1.92	0.70
1:B:188:MET:CB	1:B:704:ILE:HG21	2.17	0.70
1:A:185:ILE:HG12	1:A:708:ILE:HD11	1.74	0.70
1:A:68:LEU:HD23	1:A:72:THR:OG1	1.92	0.70
1:B:521:GLN:O	1:B:523:SER:N	2.19	0.70
1:B:383:TYR:CA	1:B:390:PRO:HG2	2.12	0.70
1:A:170:VAL:CG1	1:A:173:ALA:HB3	2.20	0.69
1:B:194:GLY:O	1:B:198:THR:HG23	1.91	0.69
1:A:162:THR:OG1	1:A:162:THR:O	2.05	0.69
1:A:191:ARG:HH22	1:A:240:LEU:HD23	1.57	0.69
1:A:158:LEU:O	1:A:263:PHE:CE2	2.44	0.69
1:A:170:VAL:CB	1:A:173:ALA:HB3	2.22	0.69
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.73	0.69
1:B:333:VAL:HG13	1:B:367:ILE:HD11	1.73	0.69
1:A:69:MET:HE2	1:A:74:TRP:HB2	1.73	0.69
1:B:21:ASN:HB3	1:B:124:GLN:OE1	1.93	0.69
1:B:290:PRO:HD3	1:B:438:TYR:OH	1.93	0.69
1:B:5:ALA:O	1:B:9:LEU:HD12	1.91	0.69
1:A:546:ALA:HB1	1:B:425:VAL:HG13	1.73	0.69
1:A:674:TYR:CE2	1:A:680:PRO:HG3	2.28	0.69
1:B:126:GLY:HA2	1:B:459:SER:OG	1.91	0.69
1:B:468:GLY:HA2	1:B:484:THR:OG1	1.92	0.69
1:B:521:GLN:HG2	1:B:721:LYS:CD	2.22	0.69
1:A:606:ASN:O	1:A:610:GLN:HB3	1.93	0.69
1:A:717:VAL:HG22	1:A:721:LYS:CG	2.22	0.69
1:B:550:LEU:O	1:B:554:ILE:HD12	1.93	0.69
1:A:334:VAL:HG13	1:A:335:LEU:N	2.07	0.69
1:B:86:MET:HE2	1:B:140:GLY:N	2.07	0.69
1:A:261:TYR:CD1	1:A:519:PHE:CE1	2.81	0.69
1:A:656:GLY:HA3	1:A:695:LYS:CB	2.23	0.69
1:B:383:TYR:HA	1:B:390:PRO:CG	2.12	0.69
1:B:514:PHE:CZ	1:B:537:LEU:HD12	2.28	0.69
1:B:562:LEU:O	1:B:566:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:HG12	1:B:708:ILE:CD1	2.23	0.68
1:A:619:ILE:CD1	1:A:708:ILE:HG12	2.21	0.68
1:B:341:TYR:O	1:B:345:LYS:N	2.27	0.68
1:B:45:GLY:HA2	1:B:600:ILE:HD13	1.74	0.68
1:B:717:VAL:HG22	1:B:721:LYS:CG	2.24	0.68
1:A:521:GLN:HG2	1:A:721:LYS:HG2	1.75	0.68
1:B:97:MET:HG3	1:B:125:GLY:HA2	1.74	0.68
1:B:19:ALA:CA	1:B:22:PHE:CE1	2.69	0.68
1:B:468:GLY:HA2	1:B:484:THR:CB	2.22	0.68
1:A:553:ALA:HA	1:B:647:MET:HE1	1.75	0.68
1:A:608:LEU:HD23	1:A:611:MET:HE2	1.75	0.68
1:B:167:ILE:HG23	1:B:718:SER:HB3	1.75	0.68
1:B:517:TYR:OH	1:B:634:VAL:HG23	1.93	0.68
1:B:666:LEU:HD12	1:B:681:HIS:HD2	1.59	0.68
1:B:705:LEU:HD21	1:B:709:MET:HE2	1.76	0.68
1:A:205:ALA:CB	1:A:228:ASP:HB2	2.24	0.68
1:B:148:PHE:HB3	1:B:175:THR:HG21	1.76	0.67
1:A:121:VAL:HG13	1:A:122:ALA:N	2.09	0.67
1:A:398:SER:HB3	1:A:684:LEU:HD13	1.76	0.67
1:B:12:LEU:HD11	1:B:139:LEU:HD13	1.76	0.67
1:B:261:TYR:CD1	1:B:519:PHE:HE2	2.11	0.67
1:A:262:MET:HG3	1:A:266:TYR:CE2	2.29	0.67
1:B:317:PRO:HA	1:B:320:GLU:CD	2.15	0.67
1:B:121:VAL:HG13	1:B:122:ALA:H	1.60	0.67
1:B:199:LYS:CG	1:B:696:ASP:HB2	2.24	0.67
1:A:86:MET:HE2	1:A:136:PHE:O	1.93	0.67
1:A:363:TRP:CZ2	1:A:367:ILE:HD11	2.30	0.67
1:B:414:MET:CG	1:B:651:LEU:HD21	2.25	0.67
1:A:545:ILE:HG13	1:B:511:LEU:CD2	2.25	0.66
1:A:100:ARG:O	1:A:103:VAL:HG23	1.96	0.66
1:A:355:PHE:HA	1:A:435:ALA:HA	1.77	0.66
1:A:86:MET:CE	1:A:139:LEU:HB3	2.25	0.66
1:A:263:PHE:CD1	1:A:264:PRO:N	2.64	0.66
1:B:368:ILE:HG21	1:B:431:ALA:N	2.11	0.66
1:B:261:TYR:CD1	1:B:519:PHE:CE2	2.84	0.66
1:B:22:PHE:HA	1:B:97:MET:HE1	1.77	0.66
1:A:198:THR:CG2	1:A:231:GLY:O	2.43	0.66
1:B:184:SER:OG	1:B:246:GLU:HG3	1.96	0.66
1:B:71:PHE:O	1:B:167:ILE:HD12	1.96	0.66
1:A:539:MET:HG2	1:B:539:MET:CG	2.25	0.66
1:A:666:LEU:HD12	1:A:681:HIS:HD2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ALA:O	1:B:230:VAL:HG22	1.96	0.66
1:A:406:ILE:HD11	1:A:686:ILE:HG22	1.78	0.66
1:A:119:LEU:N	1:A:121:VAL:HG12	2.11	0.65
1:A:259:ALA:HB3	1:A:287:ILE:HG12	1.76	0.65
1:A:354:GLY:HA3	1:A:436:GLY:CA	2.26	0.65
1:A:717:VAL:HG22	1:A:721:LYS:HG2	1.76	0.65
1:B:12:LEU:HD11	1:B:139:LEU:CD1	2.26	0.65
1:B:205:ALA:HB2	1:B:228:ASP:HB2	1.78	0.65
1:B:261:TYR:CG	1:B:519:PHE:CE2	2.84	0.65
1:B:521:GLN:HG2	1:B:721:LYS:HD3	1.77	0.65
1:A:88:ALA:O	1:A:92:ILE:HG13	1.96	0.65
1:B:68:LEU:HD23	1:B:72:THR:OG1	1.96	0.65
1:A:357:PHE:HE1	1:A:434:PHE:CB	2.10	0.65
1:A:616:PHE:CD2	1:A:620:LEU:HD22	2.31	0.65
1:B:556:TYR:CD1	1:B:648:LEU:HD11	2.31	0.65
1:A:263:PHE:CE1	1:A:264:PRO:CD	2.77	0.65
1:A:332:THR:HG21	1:A:449:SER:OG	1.96	0.65
1:A:102:ASN:ND2	1:A:466:ASN:HD22	1.94	0.65
1:A:666:LEU:HD23	1:A:671:LEU:HD12	1.78	0.65
1:A:691:GLY:O	1:A:695:LYS:HG2	1.96	0.65
1:A:198:THR:CG2	1:A:234:VAL:HB	2.27	0.65
1:A:65:ALA:HB2	1:A:81:LEU:CD2	2.21	0.65
1:A:417:VAL:HG22	1:A:650:ILE:HB	1.79	0.65
1:A:619:ILE:HD11	1:A:708:ILE:CG1	2.24	0.65
1:B:376:ILE:HD11	1:B:424:LEU:HG	1.79	0.65
1:A:200:ALA:HA	1:A:570:ALA:HB2	1.78	0.65
1:B:163:ASN:CG	1:B:164:TRP:N	2.50	0.65
1:B:22:PHE:HA	1:B:97:MET:HE2	1.78	0.65
1:B:317:PRO:HA	1:B:320:GLU:OE1	1.97	0.65
1:B:199:LYS:HG3	1:B:696:ASP:HB2	1.78	0.65
1:A:12:LEU:HD11	1:A:139:LEU:HD13	1.76	0.64
1:A:390:PRO:HB3	1:A:412:LEU:HG	1.78	0.64
1:B:386:TYR:O	1:B:387:ARG:CB	2.44	0.64
1:A:97:MET:HG3	1:A:125:GLY:HA2	1.79	0.64
1:A:154:GLN:HG2	1:A:171:PRO:HB3	1.78	0.64
1:A:199:LYS:HA	1:A:199:LYS:HE3	1.79	0.64
1:A:170:VAL:HB	1:A:173:ALA:HB3	1.78	0.64
1:A:198:THR:HG22	1:A:231:GLY:O	1.98	0.64
1:B:148:PHE:CB	1:B:175:THR:HG21	2.27	0.64
1:A:286:LEU:HD21	1:A:350:LEU:HD21	1.79	0.64
1:A:679:GLU:N	1:A:679:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:VAL:C	1:A:721:LYS:HE3	2.17	0.64
1:B:11:PRO:HG3	1:B:295:LEU:CD2	2.28	0.64
1:A:319:ARG:O	1:A:323:ILE:HD13	1.96	0.64
1:A:450:PHE:CZ	1:A:501:PHE:CE2	2.84	0.64
1:B:119:LEU:N	1:B:121:VAL:HG12	2.12	0.64
1:B:170:VAL:HG11	1:B:173:ALA:CB	2.28	0.64
1:B:298:LEU:HD12	1:B:299:GLY:N	2.12	0.64
1:B:261:TYR:HB3	1:B:519:PHE:CE2	2.32	0.64
1:A:202:ASP:HA	1:A:228:ASP:CG	2.18	0.64
1:A:341:TYR:O	1:A:345:LYS:N	2.30	0.64
1:B:365:SER:HB3	1:B:439:GLY:O	1.97	0.64
1:B:638:LEU:O	1:B:642:VAL:HG23	1.97	0.64
1:A:170:VAL:CG2	1:A:261:TYR:HE2	2.04	0.64
1:A:383:TYR:CA	1:A:390:PRO:HG2	2.08	0.64
1:A:550:LEU:HB3	1:A:637:VAL:HG22	1.79	0.64
1:B:11:PRO:HB3	1:B:138:LEU:HB3	1.80	0.64
1:B:121:VAL:HG13	1:B:122:ALA:N	2.13	0.64
1:B:719:ILE:O	1:B:723:VAL:HG12	1.98	0.64
1:B:158:LEU:HD23	1:B:158:LEU:O	1.98	0.64
1:A:237:VAL:CG2	1:A:238:ALA:N	2.61	0.64
1:A:705:LEU:HD22	1:A:705:LEU:O	1.97	0.64
1:B:521:GLN:HG2	1:B:721:LYS:CG	2.27	0.64
1:A:429:LEU:O	1:A:433:TYR:N	2.29	0.63
1:B:460:TYR:C	1:B:460:TYR:CD1	2.72	0.63
1:B:705:LEU:O	1:B:705:LEU:HD22	1.98	0.63
1:A:23:ALA:HA	1:A:26:VAL:HG22	1.80	0.63
1:B:383:TYR:CD1	1:B:416:SER:HB2	2.32	0.63
1:B:468:GLY:HA3	1:B:484:THR:HG23	1.78	0.63
1:A:488:ASP:OD2	1:A:664:LYS:HE3	1.98	0.63
1:A:647:MET:HE1	1:B:553:ALA:HA	1.79	0.63
1:A:521:GLN:HA	1:A:721:LYS:HD3	1.80	0.63
1:A:511:LEU:HD11	1:B:545:ILE:HG21	1.81	0.63
1:A:514:PHE:CE2	1:B:540:LEU:HD12	2.33	0.63
1:A:492:ASN:ND2	2:A:1728:PO4:P	2.72	0.63
1:B:402:THR:HG21	1:B:686:ILE:HD13	1.80	0.63
1:B:691:GLY:O	1:B:695:LYS:HG2	1.99	0.63
1:B:656:GLY:C	1:B:695:LYS:HD3	2.20	0.63
1:B:717:VAL:C	1:B:721:LYS:HE3	2.19	0.63
1:A:521:GLN:O	1:A:523:SER:N	2.22	0.63
1:B:104:ARG:C	1:B:121:VAL:HG21	2.19	0.63
1:B:521:GLN:NE2	1:B:631:ALA:CB	2.59	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:TYR:HD2	1:A:680:PRO:CG	2.00	0.62
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.80	0.62
1:A:198:THR:HG22	1:A:231:GLY:CA	2.29	0.62
1:A:237:VAL:HG23	1:A:238:ALA:H	1.64	0.62
1:A:11:PRO:HG3	1:A:295:LEU:CD2	2.29	0.62
1:A:717:VAL:O	1:A:721:LYS:HE3	1.99	0.62
1:B:205:ALA:CB	1:B:228:ASP:HB2	2.29	0.62
1:B:298:LEU:HD12	1:B:299:GLY:H	1.64	0.62
1:A:22:PHE:HA	1:A:97:MET:HE2	1.80	0.62
1:B:297:GLY:O	1:B:300:CYS:N	2.32	0.62
1:A:548:ALA:HB1	1:B:643:LEU:HD11	1.81	0.62
1:B:563:ILE:CG2	1:B:564:SER:N	2.63	0.62
1:A:192:VAL:HG13	1:A:562:LEU:CD2	2.29	0.62
1:B:521:GLN:HA	1:B:721:LYS:HD3	1.80	0.62
1:B:88:ALA:O	1:B:92:ILE:HG13	1.99	0.62
1:A:97:MET:HG2	1:A:128:VAL:CG2	2.29	0.62
1:B:429:LEU:HD23	1:B:429:LEU:H	1.64	0.62
1:B:68:LEU:HD22	1:B:77:GLY:N	2.14	0.62
1:A:226:ILE:CG2	1:A:227:ALA:H	2.09	0.62
1:A:237:VAL:CG2	1:A:238:ALA:H	2.13	0.62
1:A:270:ILE:CG2	1:A:270:ILE:O	2.47	0.62
1:B:102:ASN:ND2	1:B:466:ASN:HD22	1.98	0.62
1:B:73:THR:CG2	1:B:169:PHE:CE2	2.77	0.62
1:B:667:GLU:HG2	1:B:681:HIS:NE2	2.14	0.62
1:A:511:LEU:CD2	1:B:545:ILE:HG13	2.29	0.62
1:B:163:ASN:ND2	1:B:164:TRP:HD1	1.97	0.61
1:B:286:LEU:O	1:B:438:TYR:OH	2.05	0.61
1:A:411:SER:CB	1:B:563:ILE:HG21	2.27	0.61
1:A:402:THR:HG21	1:A:686:ILE:HD13	1.80	0.61
1:A:396:LYS:HG2	1:A:671:LEU:HD21	1.81	0.61
1:A:678:SER:OG	1:A:679:GLU:N	2.33	0.61
1:A:68:LEU:HD21	1:A:76:THR:CB	2.29	0.61
1:B:23:ALA:HA	1:B:26:VAL:HG22	1.82	0.61
1:B:717:VAL:HG22	1:B:721:LYS:HG2	1.83	0.61
1:A:203:MET:CE	1:A:693:PRO:HG3	2.30	0.61
1:A:511:LEU:HD21	1:B:545:ILE:HG21	1.81	0.61
1:A:556:TYR:HE1	1:A:648:LEU:HD11	1.65	0.61
1:B:226:ILE:HG22	1:B:227:ALA:N	2.16	0.61
1:B:334:VAL:HG13	1:B:335:LEU:N	2.15	0.61
1:B:506:ALA:CB	1:B:706:ILE:HD11	2.29	0.61
1:A:104:ARG:C	1:A:121:VAL:HG21	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:THR:O	1:A:701:SER:OG	2.09	0.61
1:A:719:ILE:O	1:A:723:VAL:HG12	2.00	0.61
1:B:453:THR:O	1:B:457:VAL:HG23	2.01	0.61
1:A:154:GLN:NE2	1:A:175:THR:OG1	2.26	0.61
1:B:489:ALA:HA	1:B:661:ASN:ND2	2.14	0.61
1:A:495:ALA:O	1:A:499:LYS:HG3	2.01	0.61
1:A:556:TYR:CD1	1:A:648:LEU:HD11	2.35	0.61
1:B:237:VAL:HG23	1:B:238:ALA:H	1.64	0.61
1:B:445:LEU:O	1:B:449:SER:N	2.34	0.61
1:B:358:GLY:N	1:B:361:SER:OG	2.32	0.61
1:A:357:PHE:CZ	1:A:364:PHE:CD2	2.88	0.61
1:A:543:ARG:NH1	1:A:629:LEU:O	2.33	0.61
1:B:100:ARG:O	1:B:103:VAL:HG23	2.00	0.60
1:B:550:LEU:HD13	1:B:554:ILE:HD11	1.83	0.60
1:B:717:VAL:O	1:B:721:LYS:HE3	2.01	0.60
1:A:563:ILE:HG22	1:A:564:SER:N	2.15	0.60
1:A:611:MET:O	1:A:614:PRO:HD2	2.01	0.60
1:B:340:THR:HG23	1:B:344:LEU:HD12	1.81	0.60
1:A:540:LEU:HD12	1:B:514:PHE:CE2	2.36	0.60
1:A:259:ALA:C	1:A:261:TYR:N	2.54	0.60
1:A:261:TYR:CD1	1:A:519:PHE:HE1	2.19	0.60
1:B:76:THR:HG22	1:B:178:GLY:HA3	1.83	0.60
1:B:333:VAL:HG22	1:B:367:ILE:HG12	1.83	0.60
1:A:129:MET:CE	1:A:237:VAL:HB	2.31	0.60
1:A:398:SER:HB3	1:A:684:LEU:CD1	2.30	0.60
1:A:434:PHE:O	1:A:435:ALA:HB2	2.00	0.60
1:A:265:ILE:CB	1:A:519:PHE:HE2	2.14	0.60
1:B:144:VAL:HG11	1:B:176:VAL:HG12	1.84	0.60
1:B:611:MET:O	1:B:614:PRO:HD2	2.01	0.60
1:A:12:LEU:HD11	1:A:139:LEU:CD1	2.30	0.60
1:A:396:LYS:HG2	1:A:671:LEU:CD2	2.32	0.60
1:A:677:GLY:O	1:A:678:SER:HB3	2.00	0.60
1:B:340:THR:HG22	1:B:359:ALA:O	2.01	0.60
1:B:608:LEU:HD23	1:B:611:MET:CE	2.32	0.60
1:B:68:LEU:CD2	1:B:76:THR:HB	2.29	0.60
1:B:705:LEU:HD21	1:B:709:MET:CE	2.31	0.60
1:A:261:TYR:HB3	1:A:519:PHE:CZ	2.36	0.60
1:B:102:ASN:HD21	1:B:466:ASN:ND2	1.98	0.60
1:B:499:LYS:HE2	1:B:695:LYS:O	2.02	0.60
1:A:539:MET:HG2	1:B:539:MET:HG3	1.83	0.60
1:B:68:LEU:HD21	1:B:76:THR:CB	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD22	1:A:77:GLY:N	2.17	0.60
1:B:468:GLY:CA	1:B:484:THR:CG2	2.66	0.60
1:A:553:ALA:HA	1:B:647:MET:CE	2.31	0.60
1:A:102:ASN:ND2	1:A:466:ASN:ND2	2.50	0.60
1:A:322:ASN:ND2	1:A:381:GLU:OE1	2.33	0.60
1:B:86:MET:CE	1:B:139:LEU:HB3	2.32	0.60
1:B:261:TYR:HE1	1:B:264:PRO:HG3	1.67	0.60
1:A:170:VAL:HG11	1:A:173:ALA:HB2	1.83	0.59
1:B:170:VAL:HG11	1:B:173:ALA:HB2	1.84	0.59
1:B:187:ALA:CB	1:B:242:ALA:HB1	2.31	0.59
1:A:539:MET:CG	1:B:539:MET:HG2	2.32	0.59
1:A:25:VAL:HG21	1:A:124:GLN:CB	2.30	0.59
1:B:26:VAL:HG11	1:B:100:ARG:HH11	1.67	0.59
1:B:237:VAL:CG2	1:B:238:ALA:H	2.15	0.59
1:B:170:VAL:CG2	1:B:261:TYR:HE2	2.09	0.59
1:A:199:LYS:CG	1:A:696:ASP:HB2	2.33	0.59
1:A:286:LEU:HD13	1:A:353:LEU:CD1	2.32	0.59
1:A:40:SER:O	1:A:42:ILE:N	2.35	0.59
1:B:460:TYR:CE1	1:B:490:VAL:HG12	2.38	0.59
1:B:384:THR:HG21	1:B:496:ALA:CB	2.32	0.59
1:B:619:ILE:HG22	1:B:620:LEU:HD12	1.84	0.59
1:B:666:LEU:HB3	1:B:684:LEU:CD2	2.33	0.59
1:A:70:ILE:O	1:A:164:TRP:NE1	2.35	0.59
1:A:368:ILE:HG21	1:A:431:ALA:N	2.18	0.59
1:A:367:ILE:HG23	1:A:371:PHE:CE2	2.37	0.59
1:B:237:VAL:CG2	1:B:238:ALA:N	2.64	0.59
1:A:233:ASN:HD21	1:A:466:ASN:HD22	1.51	0.59
1:A:548:ALA:O	1:A:640:GLY:HA3	2.01	0.59
1:B:246:GLU:OE2	1:B:704:ILE:HG23	2.03	0.59
1:B:492:ASN:HD21	2:B:1728:PO4:P	2.25	0.59
1:B:620:LEU:O	1:B:624:VAL:HG23	2.02	0.59
1:A:340:THR:HG22	1:A:359:ALA:O	2.01	0.59
1:A:681:HIS:O	1:A:685:VAL:HG23	2.02	0.59
1:B:198:THR:HG22	1:B:234:VAL:HB	1.83	0.59
1:B:263:PHE:CZ	1:B:276:HIS:CE1	2.91	0.59
1:B:536:LEU:O	1:B:536:LEU:CD1	2.51	0.59
1:B:429:LEU:CD2	1:B:429:LEU:N	2.65	0.59
1:A:371:PHE:O	1:A:375:LEU:HD13	2.02	0.59
1:A:679:GLU:N	1:A:680:PRO:CD	2.65	0.59
1:A:704:ILE:N	1:A:704:ILE:HD13	2.18	0.59
1:A:71:PHE:O	1:A:167:ILE:HD12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH2	1:B:700:PRO:HB3	2.18	0.59
1:B:167:ILE:O	1:B:168:ASN:C	2.41	0.59
1:B:70:ILE:O	1:B:164:TRP:NE1	2.35	0.59
1:A:519:PHE:O	1:A:522:ILE:HB	2.02	0.58
1:A:705:LEU:CD2	1:A:709:MET:HB2	2.33	0.58
1:B:457:VAL:O	1:B:460:TYR:HB3	2.03	0.58
1:B:606:ASN:O	1:B:610:GLN:CB	2.51	0.58
1:A:198:THR:HG21	1:A:235:GLY:CA	2.33	0.58
1:B:460:TYR:CE1	1:B:490:VAL:HG11	2.38	0.58
1:B:265:ILE:CB	1:B:519:PHE:HE1	2.15	0.58
1:B:199:LYS:HG3	1:B:692:ASP:O	2.02	0.58
1:B:191:ARG:CZ	1:B:700:PRO:HB3	2.33	0.58
1:A:717:VAL:O	1:A:721:LYS:CG	2.39	0.58
1:B:102:ASN:ND2	1:B:466:ASN:ND2	2.51	0.58
1:A:263:PHE:CG	1:A:264:PRO:CD	2.85	0.58
1:A:461:GLY:CA	1:A:491:GLY:CA	2.81	0.58
1:A:656:GLY:HA2	1:A:695:LYS:HD3	1.85	0.58
1:B:666:LEU:HD23	1:B:671:LEU:HD12	1.86	0.58
1:A:449:SER:O	1:A:449:SER:OG	2.19	0.58
1:B:129:MET:HE1	1:B:237:VAL:HB	1.85	0.58
1:A:126:GLY:HA2	1:A:459:SER:OG	2.01	0.58
1:A:533:LEU:O	1:A:533:LEU:HD23	2.02	0.58
1:A:667:GLU:HG2	1:A:681:HIS:NE2	2.19	0.58
1:B:666:LEU:CD1	1:B:666:LEU:C	2.72	0.58
1:A:170:VAL:HG22	1:A:261:TYR:HH	1.64	0.58
1:B:101:ALA:HB1	1:B:121:VAL:O	2.04	0.58
1:B:616:PHE:CD2	1:B:620:LEU:HD22	2.37	0.58
1:B:283:ILE:O	1:B:287:ILE:HG13	2.04	0.58
1:A:556:TYR:OH	1:B:556:TYR:OH	2.22	0.58
1:B:243:ASP:CG	1:B:704:ILE:HD11	2.24	0.58
1:A:263:PHE:CD2	1:A:264:PRO:HD3	2.39	0.58
1:A:65:ALA:CB	1:A:81:LEU:CD2	2.74	0.58
1:A:67:LEU:HD12	1:A:71:PHE:HE2	1.68	0.58
1:B:25:VAL:HG21	1:B:124:GLN:CB	2.32	0.58
1:B:461:GLY:HA3	1:B:491:GLY:CA	2.24	0.58
1:B:462:PRO:CA	1:B:465:ASP:HB3	2.31	0.58
1:B:563:ILE:HG22	1:B:564:SER:N	2.18	0.58
1:A:76:THR:HG22	1:A:178:GLY:HA3	1.86	0.57
1:A:298:LEU:CD1	1:A:299:GLY:N	2.67	0.57
1:A:285:ALA:HB3	1:A:347:LEU:HD11	1.85	0.57
1:A:457:VAL:HG12	1:A:494:THR:HB	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:MET:HE2	1:B:553:ALA:HA	1.87	0.57
1:B:717:VAL:HG22	1:B:721:LYS:HG3	1.87	0.57
1:A:620:LEU:O	1:A:624:VAL:N	2.23	0.57
1:A:97:MET:HE2	1:A:128:VAL:HG21	1.86	0.57
1:B:261:TYR:HB3	1:B:519:PHE:CZ	2.38	0.57
1:B:367:ILE:HG23	1:B:371:PHE:CE2	2.39	0.57
1:A:333:VAL:HG13	1:A:367:ILE:CD1	2.33	0.57
1:B:394:LEU:HD11	1:B:405:VAL:O	2.04	0.57
1:A:563:ILE:HG22	1:B:411:SER:HB2	1.83	0.57
1:A:288:SER:HG	1:A:292:PHE:HE2	1.50	0.57
1:A:410:LEU:O	1:A:414:MET:HB2	2.05	0.57
1:A:270:ILE:HG23	1:A:270:ILE:O	2.03	0.57
1:A:347:LEU:O	1:A:348:GLN:HB2	2.05	0.57
1:A:506:ALA:HB1	1:A:706:ILE:HD11	1.86	0.57
1:B:383:TYR:CZ	1:B:416:SER:HA	2.39	0.57
1:A:105:VAL:N	1:A:121:VAL:HG21	2.19	0.57
1:A:266:TYR:CE1	1:A:531:PRO:HG2	2.40	0.57
1:A:22:PHE:O	1:A:26:VAL:HG13	2.05	0.57
1:A:301:SER:HB2	1:A:452:ALA:HB3	1.87	0.57
1:B:200:ALA:HA	1:B:570:ALA:HB2	1.86	0.57
1:A:536:LEU:O	1:A:536:LEU:HD13	2.05	0.57
1:B:556:TYR:HE1	1:B:648:LEU:CD1	2.15	0.57
1:B:191:ARG:CZ	1:B:700:PRO:CB	2.83	0.57
1:A:550:LEU:HD13	1:A:554:ILE:CD1	2.34	0.57
1:B:634:VAL:CG2	1:B:720:PHE:HE1	2.12	0.57
1:A:263:PHE:CB	1:A:283:ILE:HD11	2.34	0.57
1:A:286:LEU:O	1:A:438:TYR:CZ	2.58	0.57
1:A:402:THR:O	1:A:405:VAL:HG22	2.04	0.57
1:A:606:ASN:O	1:A:610:GLN:CB	2.52	0.57
1:B:86:MET:HE3	1:B:139:LEU:HB3	1.86	0.57
1:A:448:LEU:HD22	1:A:505:SER:OG	2.05	0.56
1:A:68:LEU:CD2	1:A:76:THR:HB	2.31	0.56
1:B:258:LEU:HD23	1:B:516:SER:OG	2.05	0.56
1:A:263:PHE:CE2	1:A:264:PRO:HD3	2.40	0.56
1:A:293:PHE:CZ	1:A:336:THR:HG21	2.40	0.56
1:A:666:LEU:HD13	1:A:667:GLU:N	2.19	0.56
1:B:191:ARG:HH22	1:B:240:LEU:CD2	2.17	0.56
1:B:464:ALA:O	1:B:467:ALA:HB3	2.05	0.56
1:B:723:VAL:O	1:B:723:VAL:HG22	2.05	0.56
1:A:76:THR:HG23	1:A:174:MET:O	2.04	0.56
1:A:73:THR:HG21	1:A:169:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD12	1:A:71:PHE:CE2	2.40	0.56
1:B:73:THR:CG2	1:B:169:PHE:CD2	2.87	0.56
1:B:382:TYR:HE1	1:B:389:LYS:HB3	1.69	0.56
1:B:517:TYR:HE1	1:B:717:VAL:HB	1.69	0.56
1:B:188:MET:HB2	1:B:704:ILE:CG2	2.26	0.56
1:B:667:GLU:CG	1:B:681:HIS:NE2	2.67	0.56
1:A:11:PRO:HB3	1:A:138:LEU:HB3	1.87	0.56
1:A:184:SER:HA	1:A:246:GLU:HG3	1.88	0.56
1:A:82:LEU:O	1:A:86:MET:HB2	2.06	0.56
1:B:105:VAL:N	1:B:121:VAL:HG21	2.21	0.56
1:B:170:VAL:CG1	1:B:173:ALA:HB3	2.34	0.56
1:B:547:GLY:O	1:B:637:VAL:HA	2.05	0.56
1:A:340:THR:HG23	1:A:344:LEU:HD12	1.88	0.56
1:A:417:VAL:HG11	1:A:647:MET:HE3	1.88	0.56
1:B:105:VAL:CG1	1:B:467:ALA:CB	2.82	0.56
1:B:40:SER:O	1:B:42:ILE:N	2.38	0.56
1:B:441:ALA:HB2	1:B:512:SER:CB	2.36	0.56
1:B:622:PRO:HG3	1:B:709:MET:HG2	1.87	0.56
1:B:6:LEU:H	1:B:6:LEU:HD12	1.71	0.56
1:B:184:SER:HA	1:B:246:GLU:HG3	1.88	0.56
1:A:386:TYR:O	1:A:387:ARG:HB2	2.04	0.56
1:A:705:LEU:HD21	1:A:709:MET:CE	2.36	0.56
1:A:80:PHE:HD2	1:A:81:LEU:HD22	1.70	0.56
1:B:605:ASP:O	1:B:609:LYS:HB2	2.06	0.56
1:A:73:THR:CG2	1:A:169:PHE:CD2	2.88	0.55
1:A:73:THR:CG2	1:A:169:PHE:CE2	2.86	0.55
1:A:667:GLU:CG	1:A:681:HIS:NE2	2.69	0.55
1:A:560:GLY:HA3	1:B:415:LYS:HG3	1.89	0.55
1:A:268:GLN:HG3	1:A:277:GLN:OE1	2.06	0.55
1:A:343:TYR:N	1:A:343:TYR:CD1	2.74	0.55
1:A:622:PRO:HG3	1:A:709:MET:HG2	1.88	0.55
1:A:634:VAL:CG2	1:A:720:PHE:HE1	2.13	0.55
1:B:22:PHE:O	1:B:26:VAL:HG13	2.05	0.55
1:B:550:LEU:C	1:B:554:ILE:HD12	2.26	0.55
1:A:123:TYR:C	1:A:123:TYR:CD1	2.80	0.55
1:A:354:GLY:HA3	1:A:436:GLY:HA3	1.89	0.55
1:A:550:LEU:O	1:A:554:ILE:HD12	2.07	0.55
1:A:232:ASP:O	1:A:462:PRO:HB3	2.06	0.55
1:B:102:ASN:OD1	1:B:102:ASN:C	2.45	0.55
1:B:261:TYR:CG	1:B:519:PHE:HE2	2.24	0.55
1:A:556:TYR:CE2	1:B:647:MET:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:LEU:CD1	1:B:681:HIS:CD2	2.89	0.55
1:B:252:ILE:O	1:B:256:ILE:HD13	2.07	0.55
1:B:666:LEU:HD13	1:B:667:GLU:N	2.21	0.55
1:A:552:ALA:C	1:B:647:MET:HE2	2.26	0.55
1:A:554:ILE:HD13	1:A:621:THR:HG21	1.89	0.55
1:A:695:LYS:HE2	1:A:696:ASP:OD2	2.06	0.55
1:B:163:ASN:CG	1:B:164:TRP:H	2.09	0.55
1:B:358:GLY:O	1:B:359:ALA:HB3	2.06	0.55
1:B:460:TYR:HE1	1:B:490:VAL:CG1	2.19	0.55
1:B:318:GLN:OE1	1:B:490:VAL:HG22	2.07	0.55
1:A:415:LYS:HG3	1:B:560:GLY:HA3	1.88	0.55
1:A:392:GLN:NE2	1:A:665:TYR:CZ	2.75	0.55
1:A:607:ALA:O	1:A:611:MET:HB2	2.06	0.55
1:A:705:LEU:HD21	1:A:709:MET:HE2	1.89	0.55
1:B:334:VAL:HG13	1:B:335:LEU:H	1.72	0.55
1:B:629:LEU:HD13	1:B:633:PHE:CD2	2.42	0.55
1:A:315:ASP:OD1	1:A:315:ASP:N	2.40	0.55
1:A:621:THR:O	1:A:625:THR:OG1	2.11	0.55
1:B:176:VAL:HG23	1:B:253:VAL:HG13	1.89	0.55
1:B:428:ILE:HD12	1:B:508:PHE:CE2	2.41	0.55
1:A:386:TYR:O	1:A:387:ARG:HB3	2.06	0.55
1:A:267:VAL:HG13	1:A:276:HIS:HA	1.89	0.55
1:A:450:PHE:CZ	1:A:501:PHE:HE2	2.24	0.55
1:A:321:LEU:HG	1:A:457:VAL:HG22	1.89	0.55
1:A:200:ALA:CA	1:A:570:ALA:HB2	2.36	0.55
1:A:626:GLY:HA2	1:A:634:VAL:HG13	1.88	0.55
1:B:243:ASP:O	1:B:246:GLU:HB3	2.07	0.55
1:B:263:PHE:HB3	1:B:264:PRO:CD	2.37	0.55
1:A:172:PHE:O	1:A:176:VAL:HG22	2.07	0.54
1:A:386:TYR:HB3	1:A:391:THR:CG2	2.37	0.54
1:A:417:VAL:O	1:A:420:PRO:HG2	2.06	0.54
1:A:98:ALA:HA	1:A:463:ILE:HD12	1.89	0.54
1:A:102:ASN:O	1:A:105:VAL:CG1	2.46	0.54
1:A:334:VAL:O	1:A:337:ALA:HB3	2.07	0.54
1:A:384:THR:HG22	1:A:657:GLY:HA3	1.90	0.54
1:B:289:TYR:HE1	1:B:339:LEU:HD12	1.72	0.54
1:B:434:PHE:O	1:B:435:ALA:HB2	2.08	0.54
1:B:82:LEU:CD1	1:B:144:VAL:HG23	2.36	0.54
1:B:261:TYR:CE1	1:B:264:PRO:HG3	2.43	0.54
1:B:126:GLY:O	1:B:129:MET:HG2	2.08	0.54
1:B:607:ALA:O	1:B:611:MET:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:LEU:O	1:B:624:VAL:N	2.25	0.54
1:A:129:MET:O	1:A:133:VAL:HG23	2.08	0.54
1:A:153:GLY:O	1:A:157:ASN:N	2.39	0.54
1:A:365:SER:HB3	1:A:439:GLY:O	2.08	0.54
1:B:287:ILE:O	1:B:291:ILE:HD12	2.07	0.54
1:B:390:PRO:HB3	1:B:412:LEU:HG	1.90	0.54
1:B:503:ILE:HG12	1:B:703:ASP:OD1	2.07	0.54
1:A:424:LEU:HD11	1:A:504:GLY:HA2	1.90	0.54
1:A:499:LYS:O	1:A:503:ILE:HG13	2.08	0.54
1:A:605:ASP:O	1:A:609:LYS:HB2	2.07	0.54
1:B:65:ALA:HB2	1:B:81:LEU:CD2	2.25	0.54
1:B:717:VAL:O	1:B:721:LYS:CG	2.41	0.54
1:A:334:VAL:HG13	1:A:335:LEU:H	1.71	0.54
1:A:188:MET:CB	1:A:704:ILE:HG21	2.33	0.54
1:A:717:VAL:HG22	1:A:721:LYS:HG3	1.90	0.54
1:A:65:ALA:HB1	1:A:81:LEU:HD21	1.81	0.54
1:A:546:ALA:HB2	1:B:429:LEU:HD21	1.89	0.54
1:B:704:ILE:N	1:B:704:ILE:HD13	2.23	0.54
1:B:321:LEU:HD23	1:B:457:VAL:CG1	2.20	0.54
1:B:326:TRP:CE2	1:B:378:PHE:HZ	2.18	0.54
1:B:416:SER:OG	1:B:654:ASN:ND2	2.39	0.54
1:B:718:SER:HA	1:B:721:LYS:HE3	1.89	0.54
1:B:97:MET:HG2	1:B:128:VAL:HG21	1.90	0.54
1:B:384:THR:HG21	1:B:496:ALA:HB1	1.89	0.54
1:A:539:MET:HG2	1:B:539:MET:HG2	1.88	0.54
1:A:170:VAL:CG1	1:A:173:ALA:CB	2.84	0.54
1:A:720:PHE:HA	1:A:723:VAL:CG1	2.32	0.54
1:B:123:TYR:CD1	1:B:123:TYR:C	2.81	0.54
1:B:198:THR:CG2	1:B:234:VAL:HB	2.38	0.54
1:B:67:LEU:HD12	1:B:71:PHE:HE2	1.72	0.54
1:B:159:ASN:HA	1:B:263:PHE:HE2	1.73	0.53
1:A:289:TYR:CD1	1:A:344:LEU:HD11	2.43	0.53
1:A:358:GLY:O	1:A:360:ILE:N	2.39	0.53
1:A:460:TYR:C	1:A:460:TYR:CD1	2.82	0.53
1:A:69:MET:CE	1:A:74:TRP:HB2	2.38	0.53
1:A:101:ALA:HB1	1:A:121:VAL:O	2.08	0.53
1:A:191:ARG:HH22	1:A:240:LEU:CD2	2.21	0.53
1:A:199:LYS:HG2	1:A:696:ASP:HB2	1.89	0.53
1:B:170:VAL:HG12	1:B:173:ALA:H	1.73	0.53
1:A:145:TYR:CE1	1:A:291:ILE:HD13	2.43	0.53
1:A:244:LEU:CD2	1:A:502:ALA:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:LEU:HD13	1:A:633:PHE:CD2	2.42	0.53
1:B:677:GLY:C	1:B:678:SER:HG	1.95	0.53
1:B:656:GLY:O	1:B:695:LYS:HD3	2.08	0.53
1:A:80:PHE:CE1	1:A:182:GLY:HA2	2.44	0.53
1:A:613:TYR:O	1:A:617:ILE:HG13	2.08	0.53
1:B:102:ASN:O	1:B:105:VAL:CG1	2.48	0.53
1:B:266:TYR:CB	1:B:278:VAL:HG23	2.38	0.53
1:B:337:ALA:HB2	1:B:363:TRP:CD2	2.43	0.53
1:B:495:ALA:O	1:B:499:LYS:HG3	2.09	0.53
1:A:608:LEU:HD23	1:A:611:MET:CE	2.39	0.53
1:B:337:ALA:HB2	1:B:363:TRP:CZ2	2.39	0.53
1:B:80:PHE:HD2	1:B:81:LEU:HD22	1.73	0.53
1:B:82:LEU:O	1:B:86:MET:HB2	2.09	0.53
1:A:286:LEU:HD13	1:A:353:LEU:HD11	1.91	0.53
1:A:468:GLY:HA2	1:A:484:THR:HG21	1.87	0.53
1:B:163:ASN:HB2	1:B:169:PHE:CD2	2.43	0.53
1:B:666:LEU:CD1	1:B:681:HIS:HD2	2.20	0.53
1:A:26:VAL:HG11	1:A:100:ARG:HH11	1.73	0.53
1:A:297:GLY:O	1:A:298:LEU:C	2.47	0.53
1:A:521:GLN:HA	1:A:721:LYS:CE	2.39	0.53
1:A:81:LEU:HD22	1:A:81:LEU:N	2.24	0.53
1:B:424:LEU:HD21	1:B:447:MET:HE1	1.91	0.53
1:A:395:GLY:O	1:A:398:SER:OG	2.07	0.53
1:A:674:TYR:HE2	1:A:680:PRO:HG3	1.65	0.53
1:B:464:ALA:HB1	1:B:487:LEU:CB	2.32	0.53
1:B:520:SER:O	1:B:721:LYS:NZ	2.36	0.53
1:B:81:LEU:HD22	1:B:81:LEU:N	2.24	0.53
1:A:679:GLU:CA	1:A:679:GLU:OE1	2.57	0.53
1:B:133:VAL:HG13	1:B:245:LEU:HD12	1.90	0.53
1:A:102:ASN:OD1	1:A:102:ASN:C	2.47	0.52
1:A:723:VAL:HG22	1:A:723:VAL:O	2.08	0.52
1:B:76:THR:CG2	1:B:174:MET:O	2.57	0.52
1:A:402:THR:O	1:A:406:ILE:HG12	2.09	0.52
1:A:412:LEU:C	1:A:412:LEU:HD23	2.29	0.52
1:B:461:GLY:HA2	1:B:491:GLY:CA	2.36	0.52
1:A:82:LEU:CD1	1:A:144:VAL:HG23	2.39	0.52
1:A:259:ALA:HB3	1:A:287:ILE:CG1	2.40	0.52
1:A:259:ALA:O	1:A:283:ILE:HG23	2.09	0.52
1:A:545:ILE:HG21	1:B:511:LEU:HD21	1.92	0.52
1:B:424:LEU:HD21	1:B:447:MET:CE	2.39	0.52
1:B:638:LEU:HD11	1:B:713:SER:OG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:C	1:A:299:GLY:N	2.62	0.52
1:B:460:TYR:OH	1:B:487:LEU:HD23	2.10	0.52
1:B:606:ASN:O	1:B:610:GLN:HB3	2.09	0.52
1:A:172:PHE:CE2	1:A:256:ILE:HG21	2.45	0.52
1:B:489:ALA:CA	1:B:661:ASN:HD21	2.20	0.52
1:B:718:SER:CA	1:B:721:LYS:HE3	2.38	0.52
1:A:321:LEU:HD12	1:A:321:LEU:N	2.25	0.52
1:A:718:SER:CA	1:A:721:LYS:HE3	2.40	0.52
1:B:382:TYR:HD1	1:B:382:TYR:O	1.91	0.52
1:B:233:ASN:ND2	1:B:466:ASN:HD22	2.05	0.52
1:B:25:VAL:HB	1:B:97:MET:HE1	1.90	0.52
1:A:252:ILE:O	1:A:256:ILE:HD13	2.09	0.52
1:A:563:ILE:CG2	1:A:564:SER:N	2.73	0.52
1:B:337:ALA:HB2	1:B:363:TRP:NE1	2.22	0.52
1:A:197:TYR:HE2	1:A:230:VAL:HG23	1.75	0.52
1:A:317:PRO:HA	1:A:320:GLU:OE1	2.10	0.52
1:B:184:SER:CB	1:B:246:GLU:HG3	2.40	0.52
1:B:191:ARG:HH22	1:B:240:LEU:HD23	1.74	0.52
1:B:507:ILE:HD11	1:B:646:ALA:CB	2.39	0.52
1:A:555:THR:HG23	1:A:702:LEU:HD11	1.92	0.52
1:A:718:SER:HA	1:A:721:LYS:HE3	1.91	0.52
1:B:97:MET:CB	1:B:128:VAL:HB	2.40	0.52
1:A:10:ILE:N	1:A:11:PRO:CD	2.72	0.51
1:A:203:MET:HE2	1:A:693:PRO:HG3	1.92	0.51
1:B:619:ILE:CD1	1:B:708:ILE:HG12	2.33	0.51
1:A:200:ALA:HB1	1:A:570:ALA:CA	2.41	0.51
1:B:129:MET:CE	1:B:237:VAL:HB	2.40	0.51
1:B:186:ILE:O	1:B:186:ILE:HG12	2.11	0.51
1:B:233:ASN:ND2	1:B:466:ASN:ND2	2.59	0.51
1:B:244:LEU:HD21	1:B:502:ALA:HB2	1.88	0.51
1:B:382:TYR:C	1:B:382:TYR:CD1	2.84	0.51
1:A:6:LEU:O	1:A:10:ILE:HD13	2.09	0.51
1:B:298:LEU:CD1	1:B:299:GLY:N	2.73	0.51
1:A:261:TYR:CG	1:A:519:PHE:CE1	2.98	0.51
1:A:334:VAL:CG1	1:A:335:LEU:N	2.71	0.51
1:B:705:LEU:CD2	1:B:709:MET:HB2	2.39	0.51
1:B:621:THR:HB	1:B:622:PRO:HD3	1.92	0.51
1:B:719:ILE:C	1:B:723:VAL:HG12	2.31	0.51
1:A:656:GLY:HA3	1:A:695:LYS:CG	2.40	0.51
1:A:666:LEU:CD1	1:A:681:HIS:CD2	2.93	0.51
1:B:158:LEU:O	1:B:263:PHE:CD2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HD12	1:B:71:PHE:CE2	2.46	0.51
1:A:154:GLN:HE21	1:A:172:PHE:HA	1.76	0.51
1:A:226:ILE:CG2	1:A:227:ALA:N	2.63	0.51
1:A:262:MET:O	1:A:266:TYR:HD2	1.94	0.51
1:A:562:LEU:O	1:A:566:VAL:HG23	2.11	0.51
1:B:243:ASP:OD1	1:B:704:ILE:CD1	2.59	0.51
1:B:442:ILE:O	1:B:445:LEU:HB3	2.10	0.51
1:A:126:GLY:O	1:A:129:MET:HG2	2.11	0.51
1:A:170:VAL:CG1	1:A:261:TYR:HE2	2.23	0.51
1:A:621:THR:HB	1:A:622:PRO:HD3	1.93	0.51
1:B:138:LEU:HD12	1:B:141:LEU:HD12	1.93	0.51
1:B:360:ILE:O	1:B:363:TRP:HB3	2.11	0.51
1:B:367:ILE:CG2	1:B:371:PHE:CE2	2.94	0.51
1:B:666:LEU:HD12	1:B:681:HIS:CD2	2.44	0.51
1:A:331:LEU:O	1:A:334:VAL:HG12	2.11	0.51
1:A:468:GLY:CA	1:A:484:THR:CG2	2.73	0.51
1:A:262:MET:HG2	1:A:353:LEU:CD2	2.33	0.51
1:B:53:GLU:OE2	1:B:190:ASP:OD1	2.29	0.51
1:B:370:ILE:O	1:B:374:ILE:HG13	2.11	0.51
1:A:154:GLN:NE2	1:A:171:PRO:O	2.45	0.50
1:A:286:LEU:CD1	1:A:353:LEU:HG	2.40	0.50
1:A:255:SER:HB3	1:A:290:PRO:HG3	1.93	0.50
1:A:536:LEU:O	1:A:536:LEU:CD1	2.59	0.50
1:B:97:MET:HG3	1:B:125:GLY:CA	2.41	0.50
1:A:321:LEU:HD23	1:A:457:VAL:CG1	2.08	0.50
1:A:623:LEU:HD13	1:A:712:VAL:CG1	2.42	0.50
1:B:261:TYR:CB	1:B:519:PHE:CE2	2.93	0.50
1:A:162:THR:O	1:A:163:ASN:O	2.28	0.50
1:A:186:ILE:HG12	1:A:186:ILE:O	2.11	0.50
1:B:297:GLY:O	1:B:298:LEU:C	2.49	0.50
1:B:343:TYR:CD1	1:B:343:TYR:N	2.80	0.50
1:B:718:SER:N	1:B:721:LYS:HE3	2.26	0.50
1:A:261:TYR:CE1	1:A:264:PRO:HG3	2.47	0.50
1:A:666:LEU:CD1	1:A:681:HIS:HA	2.42	0.50
1:B:112:THR:O	1:B:113:LYS:HG2	2.12	0.50
1:B:267:VAL:O	1:B:268:GLN:O	2.30	0.50
1:B:623:LEU:HD13	1:B:712:VAL:CG1	2.42	0.50
1:A:164:TRP:CH2	1:A:165:LEU:HD21	2.46	0.50
1:A:350:LEU:O	1:A:355:PHE:HB2	2.11	0.50
1:A:718:SER:N	1:A:721:LYS:HE3	2.26	0.50
1:A:123:TYR:O	1:A:123:TYR:CD1	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:O	1:A:168:ASN:C	2.50	0.50
1:B:462:PRO:HA	1:B:465:ASP:CB	2.35	0.50
1:B:236:ASP:HB2	1:B:462:PRO:HG2	1.91	0.50
1:A:15:LEU:HG	1:A:135:GLY:HA3	1.94	0.50
1:A:392:GLN:NE2	1:A:665:TYR:CE1	2.80	0.50
1:B:10:ILE:N	1:B:11:PRO:CD	2.74	0.50
1:B:144:VAL:HA	1:B:148:PHE:HD2	1.77	0.50
1:A:460:TYR:OH	1:A:487:LEU:CD2	2.60	0.50
1:A:638:LEU:HD11	1:A:713:SER:OG	2.12	0.50
1:A:719:ILE:C	1:A:723:VAL:HG12	2.31	0.50
1:B:123:TYR:CD1	1:B:123:TYR:O	2.65	0.50
1:A:167:ILE:HG22	1:A:167:ILE:O	2.12	0.50
1:A:260:SER:HA	1:A:287:ILE:HD11	1.93	0.50
1:B:424:LEU:HD11	1:B:504:GLY:HA2	1.94	0.50
1:B:666:LEU:HD11	1:B:681:HIS:HA	1.93	0.50
1:A:708:ILE:HA	1:A:711:VAL:HG22	1.94	0.49
1:B:170:VAL:CG1	1:B:173:ALA:CB	2.89	0.49
1:B:666:LEU:CD1	1:B:681:HIS:HA	2.42	0.49
1:A:236:ASP:CB	1:A:462:PRO:CG	2.86	0.49
1:A:288:SER:HB2	1:A:292:PHE:CE2	2.47	0.49
1:B:321:LEU:N	1:B:321:LEU:CD1	2.75	0.49
1:B:363:TRP:CE2	1:B:367:ILE:HD11	2.46	0.49
1:A:465:ASP:OD2	1:A:488:ASP:OD1	2.29	0.49
1:A:489:ALA:CA	1:A:661:ASN:HD21	2.20	0.49
1:B:289:TYR:CD1	1:B:344:LEU:HD11	2.47	0.49
1:B:94:GLY:HA3	1:B:129:MET:CB	2.42	0.49
1:A:97:MET:CB	1:A:128:VAL:HB	2.42	0.49
1:A:180:ALA:HB2	1:A:253:VAL:HG21	1.94	0.49
1:A:199:LYS:HG3	1:A:692:ASP:O	2.11	0.49
1:B:101:ALA:CB	1:B:125:GLY:HA3	2.43	0.49
1:B:321:LEU:HG	1:B:457:VAL:HG22	1.93	0.49
1:B:65:ALA:CB	1:B:81:LEU:CD2	2.80	0.49
1:A:163:ASN:HB2	1:A:169:PHE:HD2	1.76	0.49
1:A:357:PHE:CZ	1:A:434:PHE:HB3	2.48	0.49
1:A:185:ILE:CG1	1:A:708:ILE:HD11	2.42	0.49
1:B:11:PRO:HG3	1:B:295:LEU:HD21	1.93	0.49
1:B:464:ALA:CB	1:B:487:LEU:HB3	2.37	0.49
1:A:453:THR:O	1:A:457:VAL:HG23	2.13	0.49
1:A:97:MET:HG2	1:A:125:GLY:HA2	1.92	0.49
1:B:514:PHE:O	1:B:517:TYR:HB3	2.13	0.49
1:B:162:THR:O	1:B:163:ASN:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:O	1:B:343:TYR:HB2	2.13	0.49
1:B:697:THR:O	1:B:701:SER:OG	2.09	0.49
1:A:105:VAL:CG1	1:A:467:ALA:CB	2.90	0.49
1:A:461:GLY:HA2	1:A:491:GLY:CA	2.43	0.49
1:A:652:THR:HG22	1:A:694:LEU:HB3	1.95	0.49
1:A:674:TYR:CD2	1:A:680:PRO:CB	2.95	0.49
1:A:98:ALA:HA	1:A:463:ILE:CD1	2.43	0.49
1:B:423:THR:O	1:B:427:GLY:N	2.40	0.49
1:B:708:ILE:HA	1:B:711:VAL:HG22	1.94	0.49
1:B:97:MET:HE2	1:B:128:VAL:HG21	1.93	0.49
1:A:94:GLY:HA3	1:A:129:MET:CB	2.43	0.49
1:A:82:LEU:HD11	1:A:140:GLY:O	2.13	0.49
1:A:170:VAL:HG11	1:A:261:TYR:HE2	1.78	0.49
1:B:161:TYR:CD2	1:B:169:PHE:HE2	2.24	0.49
1:B:192:VAL:O	1:B:196:VAL:CG2	2.61	0.49
1:B:312:LYS:HA	1:B:313:PRO:HD3	1.63	0.49
1:B:341:TYR:O	1:B:345:LYS:CA	2.61	0.49
1:B:236:ASP:CB	1:B:462:PRO:HG3	2.40	0.49
1:B:526:ASP:C	1:B:528:GLY:H	2.16	0.49
1:B:626:GLY:HA2	1:B:634:VAL:HG13	1.95	0.49
1:A:121:VAL:CG1	1:A:122:ALA:H	2.24	0.48
1:B:15:LEU:HD11	1:B:136:PHE:HD1	1.78	0.48
1:B:198:THR:CG2	1:B:235:GLY:N	2.62	0.48
1:B:463:ILE:CG2	1:B:464:ALA:N	2.76	0.48
1:A:138:LEU:HD12	1:A:141:LEU:HD12	1.95	0.48
1:A:229:ASN:HD21	1:A:469:GLY:HA3	1.78	0.48
1:A:548:ALA:HA	1:A:636:GLY:O	2.13	0.48
1:A:643:LEU:HD12	1:B:643:LEU:HD12	1.95	0.48
1:A:202:ASP:OD2	1:A:692:ASP:OD2	2.31	0.48
1:A:354:GLY:O	1:A:435:ALA:C	2.51	0.48
1:A:97:MET:HG3	1:A:125:GLY:CA	2.44	0.48
1:A:158:LEU:O	1:A:263:PHE:HZ	1.84	0.48
1:A:170:VAL:CG1	1:A:261:TYR:CE2	2.96	0.48
1:A:170:VAL:HG22	1:A:261:TYR:CE2	2.20	0.48
1:A:158:LEU:HG	1:A:263:PHE:CE2	2.49	0.48
1:A:357:PHE:CD2	1:A:360:ILE:CG2	2.96	0.48
1:A:539:MET:CG	1:B:539:MET:CG	2.90	0.48
1:A:6:LEU:HD12	1:A:6:LEU:H	1.77	0.48
1:B:263:PHE:HB2	1:B:283:ILE:HD13	1.95	0.48
1:A:105:VAL:O	1:A:106:ALA:C	2.50	0.48
1:A:514:PHE:O	1:A:517:TYR:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:THR:HG23	1:B:662:ALA:CA	2.42	0.48
1:A:144:VAL:HA	1:A:148:PHE:HD2	1.79	0.48
1:A:470:ILE:O	1:A:471:SER:C	2.50	0.48
1:A:503:ILE:HD13	1:A:649:ALA:CB	2.43	0.48
1:A:97:MET:HE2	1:A:128:VAL:CG2	2.43	0.48
1:B:153:GLY:O	1:B:157:ASN:N	2.42	0.48
1:B:167:ILE:HG22	1:B:167:ILE:O	2.13	0.48
1:B:161:TYR:CE2	1:B:169:PHE:HE2	2.30	0.48
1:B:26:VAL:C	1:B:28:LYS:H	2.17	0.48
1:B:259:ALA:HB3	1:B:287:ILE:HG12	1.94	0.48
1:B:391:THR:HG23	1:B:662:ALA:HA	1.96	0.48
1:B:191:ARG:CZ	1:B:700:PRO:HB2	2.44	0.48
1:A:97:MET:HB2	1:A:128:VAL:HG11	1.96	0.48
1:A:11:PRO:HG3	1:A:295:LEU:HD22	1.93	0.48
1:A:666:LEU:CD1	1:A:681:HIS:HD2	2.25	0.48
1:A:139:LEU:O	1:A:143:LEU:HD12	2.13	0.48
1:A:164:TRP:CZ2	1:A:165:LEU:HD21	2.49	0.48
1:A:191:ARG:HH21	1:A:243:ASP:HB2	1.78	0.48
1:A:656:GLY:HA3	1:A:695:LYS:HD2	1.91	0.48
1:A:667:GLU:HG3	1:A:681:HIS:CD2	2.49	0.48
1:B:65:ALA:HB1	1:B:81:LEU:HD21	1.87	0.48
1:A:655:SER:OG	1:A:659:TRP:CE3	2.56	0.48
1:A:666:LEU:C	1:A:666:LEU:CD1	2.71	0.48
1:B:76:THR:CG2	1:B:178:GLY:HA3	2.43	0.48
1:B:263:PHE:HB3	1:B:264:PRO:HD3	1.95	0.48
1:B:368:ILE:HG21	1:B:431:ALA:H	1.77	0.48
1:B:98:ALA:HB2	1:B:129:MET:CE	2.43	0.48
1:A:76:THR:CG2	1:A:178:GLY:HA3	2.44	0.48
1:B:82:LEU:HD11	1:B:140:GLY:O	2.14	0.48
1:B:158:LEU:HD23	1:B:263:PHE:CD2	2.49	0.48
1:B:202:ASP:HA	1:B:228:ASP:CG	2.34	0.48
1:B:461:GLY:O	1:B:465:ASP:HB2	2.13	0.48
1:B:232:ASP:OD2	1:B:465:ASP:OD1	2.32	0.48
1:B:551:GLY:CA	1:B:637:VAL:HG13	2.43	0.48
1:A:264:PRO:O	1:A:267:VAL:HG23	2.14	0.47
1:A:402:THR:HG21	1:A:686:ILE:CD1	2.43	0.47
1:B:386:TYR:O	1:B:387:ARG:HB3	2.14	0.47
1:A:666:LEU:HD11	1:A:681:HIS:HA	1.96	0.47
1:A:656:GLY:C	1:A:695:LYS:HD2	2.35	0.47
1:A:97:MET:HG2	1:A:128:VAL:HG21	1.96	0.47
1:B:390:PRO:CB	1:B:412:LEU:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:CD2	1:B:516:SER:OG	2.61	0.47
1:A:620:LEU:O	1:A:624:VAL:HG23	2.14	0.47
1:B:144:VAL:HA	1:B:148:PHE:CD2	2.49	0.47
1:B:233:ASN:O	1:B:234:VAL:C	2.53	0.47
1:B:519:PHE:O	1:B:522:ILE:HB	2.15	0.47
1:A:262:MET:SD	1:A:266:TYR:HE2	2.38	0.47
1:A:26:VAL:C	1:A:28:LYS:H	2.16	0.47
1:A:521:GLN:HG2	1:A:721:LYS:CG	2.42	0.47
1:B:465:ASP:OD2	1:B:488:ASP:OD1	2.33	0.47
1:B:667:GLU:HG3	1:B:681:HIS:CD2	2.50	0.47
1:A:144:VAL:O	1:A:148:PHE:HB2	2.15	0.47
1:A:656:GLY:CA	1:A:695:LYS:HD2	2.42	0.47
1:B:321:LEU:N	1:B:321:LEU:HD12	2.29	0.47
1:A:15:LEU:HD11	1:A:136:PHE:HD1	1.79	0.47
1:A:245:LEU:C	1:A:245:LEU:HD23	2.34	0.47
1:A:334:VAL:CG1	1:A:335:LEU:H	2.27	0.47
1:B:158:LEU:C	1:B:159:ASN:O	2.53	0.47
1:B:667:GLU:CG	1:B:681:HIS:CD2	2.97	0.47
1:A:360:ILE:O	1:A:363:TRP:HB3	2.14	0.47
1:A:463:ILE:CG2	1:A:464:ALA:N	2.78	0.47
1:B:139:LEU:O	1:B:143:LEU:HD12	2.15	0.47
1:B:144:VAL:O	1:B:148:PHE:HB2	2.14	0.47
1:B:80:PHE:CE1	1:B:182:GLY:HA2	2.50	0.47
1:B:101:ALA:HB3	1:B:463:ILE:HD11	1.97	0.47
1:B:522:ILE:CG2	1:B:522:ILE:O	2.54	0.47
1:A:161:TYR:CD2	1:A:169:PHE:HE2	2.26	0.47
1:A:383:TYR:CD1	1:A:416:SER:HB2	2.50	0.47
1:B:686:ILE:HA	1:B:689:THR:HG22	1.97	0.47
1:A:434:PHE:O	1:A:435:ALA:CB	2.63	0.47
1:A:325:LEU:HD22	1:A:450:PHE:HE2	1.80	0.47
1:A:521:GLN:CB	1:A:721:LYS:HD3	2.44	0.47
1:B:675:GLY:O	1:B:676:LYS:CB	2.63	0.47
1:A:155:VAL:HA	1:A:158:LEU:HD13	1.97	0.47
1:A:244:LEU:HD23	1:A:502:ALA:HB2	1.97	0.47
1:A:521:GLN:HA	1:A:721:LYS:CD	2.43	0.47
1:A:97:MET:O	1:A:98:ALA:C	2.53	0.47
1:B:236:ASP:CB	1:B:462:PRO:CG	2.91	0.47
1:B:533:LEU:HD23	1:B:533:LEU:O	2.14	0.47
1:B:711:VAL:HG23	1:B:712:VAL:N	2.30	0.47
1:A:68:LEU:HD21	1:A:76:THR:CG2	2.44	0.47
1:B:169:PHE:HB2	1:B:174:MET:CE	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LEU:CG	1:B:457:VAL:HG13	2.44	0.47
1:B:619:ILE:HD11	1:B:708:ILE:CG1	2.33	0.47
1:B:488:ASP:OD2	1:B:664:LYS:HE3	2.14	0.47
1:B:720:PHE:HA	1:B:723:VAL:CG1	2.37	0.47
1:A:121:VAL:CG1	1:A:122:ALA:N	2.78	0.46
1:A:608:LEU:HA	1:A:611:MET:HB2	1.97	0.46
1:A:633:PHE:CE1	1:A:637:VAL:CG2	2.97	0.46
1:B:105:VAL:O	1:B:106:ALA:C	2.52	0.46
1:B:699:GLY:N	1:B:700:PRO:CD	2.78	0.46
1:A:144:VAL:HA	1:A:148:PHE:CD2	2.50	0.46
1:A:154:GLN:NE2	1:A:172:PHE:HA	2.30	0.46
1:A:288:SER:OG	1:A:292:PHE:HE2	1.98	0.46
1:A:503:ILE:CD1	1:A:649:ALA:HB1	2.44	0.46
1:B:164:TRP:CZ2	1:B:165:LEU:HD21	2.51	0.46
1:B:191:ARG:HH21	1:B:243:ASP:HB2	1.81	0.46
1:B:301:SER:CB	1:B:452:ALA:HB3	2.42	0.46
1:A:101:ALA:CB	1:A:125:GLY:HA3	2.46	0.46
1:A:98:ALA:HB2	1:A:129:MET:CE	2.45	0.46
1:A:154:GLN:CG	1:A:171:PRO:HB3	2.43	0.46
1:B:187:ALA:HB1	1:B:242:ALA:HB1	1.96	0.46
1:B:297:GLY:C	1:B:299:GLY:N	2.68	0.46
1:B:390:PRO:HB3	1:B:412:LEU:CG	2.45	0.46
1:A:129:MET:SD	1:A:459:SER:CB	3.01	0.46
1:A:170:VAL:HG12	1:A:173:ALA:H	1.79	0.46
1:A:26:VAL:C	1:A:28:LYS:N	2.69	0.46
1:A:462:PRO:HA	1:A:465:ASP:HB3	1.98	0.46
1:A:511:LEU:HD21	1:B:545:ILE:CG1	2.43	0.46
1:B:71:PHE:O	1:B:167:ILE:CD1	2.64	0.46
1:B:197:TYR:HE2	1:B:230:VAL:HG23	1.81	0.46
1:B:230:VAL:CG2	1:B:231:GLY:N	2.78	0.46
1:B:447:MET:SD	1:B:505:SER:N	2.89	0.46
1:A:188:MET:O	1:A:192:VAL:HG23	2.16	0.46
1:A:240:LEU:HD12	1:A:458:ASP:HB3	1.97	0.46
1:A:623:LEU:O	1:A:627:PHE:HD2	1.98	0.46
1:A:416:SER:OG	1:A:654:ASN:ND2	2.47	0.46
1:A:666:LEU:HD12	1:A:681:HIS:CD2	2.45	0.46
1:B:122:ALA:O	1:B:463:ILE:HD13	2.15	0.46
1:B:12:LEU:CD1	1:B:139:LEU:HD13	2.43	0.46
1:B:193:GLY:O	1:B:197:TYR:N	2.48	0.46
1:B:200:ALA:CA	1:B:570:ALA:HB2	2.46	0.46
1:B:441:ALA:HB2	1:B:512:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:C	1:A:159:ASN:H	2.18	0.46
1:A:458:ASP:OD2	1:A:498:GLY:HA3	2.16	0.46
1:A:53:GLU:HA	1:A:608:LEU:CD1	2.46	0.46
1:A:663:LYS:HD3	1:A:688:ASP:CB	2.44	0.46
1:A:172:PHE:CE2	1:A:256:ILE:CG2	2.98	0.46
1:A:176:VAL:HG23	1:A:253:VAL:HG13	1.98	0.46
1:B:386:TYR:O	1:B:387:ARG:HB2	2.14	0.46
1:B:619:ILE:HD12	1:B:712:VAL:HG21	1.98	0.46
1:A:368:ILE:HG21	1:A:431:ALA:H	1.81	0.46
1:B:396:LYS:HA	1:B:671:LEU:HD21	1.98	0.46
1:B:681:HIS:O	1:B:685:VAL:HG23	2.15	0.46
1:A:263:PHE:CD1	1:A:263:PHE:C	2.88	0.46
1:A:390:PRO:HB3	1:A:412:LEU:CG	2.46	0.46
1:A:400:GLU:HB2	1:A:404:MET:HE2	1.98	0.46
1:A:460:TYR:OH	1:A:487:LEU:HD23	2.16	0.46
1:A:517:TYR:OH	1:A:634:VAL:CG2	2.56	0.46
1:A:521:GLN:HG2	1:A:721:LYS:CD	2.46	0.46
1:A:372:SER:O	1:A:376:ILE:HG13	2.15	0.46
1:A:522:ILE:O	1:A:522:ILE:CG2	2.61	0.46
1:A:666:LEU:HD11	1:A:681:HIS:CA	2.46	0.46
1:B:202:ASP:OD2	1:B:692:ASP:OD2	2.34	0.46
1:B:298:LEU:HA	1:B:301:SER:OG	2.15	0.46
1:B:319:ARG:O	1:B:323:ILE:HD13	2.15	0.46
1:B:363:TRP:CZ2	1:B:367:ILE:CD1	2.92	0.46
1:A:138:LEU:HD22	1:A:298:LEU:HD23	1.97	0.45
1:A:12:LEU:CD1	1:A:139:LEU:HD13	2.43	0.45
1:A:261:TYR:HE1	1:A:264:PRO:HG3	1.81	0.45
1:A:263:PHE:O	1:A:267:VAL:HG22	2.16	0.45
1:A:357:PHE:CE2	1:A:360:ILE:CG2	2.97	0.45
1:A:383:TYR:CD1	1:A:390:PRO:HG3	2.51	0.45
1:A:656:GLY:C	1:A:695:LYS:CD	2.83	0.45
1:B:97:MET:HB2	1:B:128:VAL:HG11	1.98	0.45
1:B:406:ILE:HD11	1:B:686:ILE:HG22	1.98	0.45
1:A:256:ILE:HD12	1:A:290:PRO:HG2	1.97	0.45
1:A:357:PHE:CE2	1:A:361:SER:CA	2.84	0.45
1:A:431:ALA:HB1	1:A:443:ALA:HB2	1.98	0.45
1:A:705:LEU:C	1:A:705:LEU:HD22	2.36	0.45
1:B:170:VAL:HG11	1:B:261:TYR:HE2	1.81	0.45
1:B:383:TYR:CD1	1:B:390:PRO:HG3	2.50	0.45
1:B:503:ILE:CD1	1:B:649:ALA:HB1	2.46	0.45
1:B:447:MET:SD	1:B:504:GLY:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:O	1:A:290:PRO:HD2	2.16	0.45
1:A:424:LEU:HD23	1:A:424:LEU:HA	1.58	0.45
1:A:666:LEU:CB	1:A:684:LEU:HD23	2.38	0.45
1:A:705:LEU:HD22	1:A:709:MET:HB2	1.98	0.45
1:B:86:MET:CE	1:B:139:LEU:HD23	2.46	0.45
1:B:321:LEU:H	1:B:321:LEU:CD1	2.28	0.45
1:B:447:MET:HE3	1:B:508:PHE:CD2	2.51	0.45
1:B:484:THR:HG22	1:B:485:ASP:N	2.31	0.45
1:A:386:TYR:HB3	1:A:391:THR:HG22	1.98	0.45
1:A:460:TYR:CE1	1:A:490:VAL:CG1	2.99	0.45
1:A:663:LYS:HD3	1:A:688:ASP:HB3	1.98	0.45
1:B:289:TYR:CG	1:B:344:LEU:HD11	2.52	0.45
1:B:334:VAL:CG1	1:B:335:LEU:N	2.80	0.45
1:B:333:VAL:HG13	1:B:363:TRP:CZ2	2.51	0.45
1:B:666:LEU:HD11	1:B:681:HIS:CA	2.45	0.45
1:B:76:THR:OG1	1:B:174:MET:HG3	2.15	0.45
1:A:148:PHE:HB3	1:A:175:THR:HG21	1.97	0.45
1:A:233:ASN:O	1:A:234:VAL:C	2.53	0.45
1:A:465:ASP:OD2	2:A:1727:PO4:O1	2.35	0.45
1:B:25:VAL:O	1:B:28:LYS:CB	2.65	0.45
1:B:663:LYS:HZ3	1:B:664:LYS:HE2	1.81	0.45
1:A:519:PHE:C	1:A:519:PHE:CD1	2.90	0.45
1:A:266:TYR:CD1	1:A:531:PRO:HG2	2.52	0.45
1:A:626:GLY:CA	1:A:634:VAL:HG13	2.47	0.45
1:A:80:PHE:CD2	1:A:81:LEU:HD22	2.49	0.45
1:B:428:ILE:HD12	1:B:508:PHE:CZ	2.51	0.45
1:B:517:TYR:HB2	1:B:714:VAL:HG12	1.99	0.45
1:B:608:LEU:HA	1:B:611:MET:HB2	1.99	0.45
1:B:73:THR:O	1:B:73:THR:OG1	2.30	0.45
1:A:161:TYR:CE2	1:A:169:PHE:HE2	2.34	0.45
1:A:350:LEU:HD22	1:A:355:PHE:CE2	2.51	0.45
1:A:386:TYR:HB3	1:A:391:THR:HG21	1.97	0.45
1:B:145:TYR:CE1	1:B:291:ILE:HD13	2.52	0.45
1:B:157:ASN:O	1:B:159:ASN:N	2.50	0.45
1:B:164:TRP:CH2	1:B:165:LEU:HD21	2.52	0.45
1:B:198:THR:CG2	1:B:235:GLY:H	2.27	0.45
1:B:26:VAL:C	1:B:28:LYS:N	2.70	0.45
1:B:317:PRO:HA	1:B:320:GLU:OE2	2.16	0.45
1:B:606:ASN:O	1:B:610:GLN:HB2	2.17	0.45
1:A:357:PHE:CE1	1:A:434:PHE:CD1	3.04	0.45
1:A:667:GLU:CG	1:A:681:HIS:CD2	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:OE2	1:A:190:ASP:OD1	2.34	0.45
1:A:546:ALA:CB	1:B:429:LEU:HD21	2.47	0.45
1:A:192:VAL:CG1	1:A:562:LEU:HD21	2.44	0.45
1:A:610:GLN:O	1:A:610:GLN:HG3	2.16	0.45
1:B:15:LEU:HD11	1:B:136:PHE:CD1	2.52	0.45
1:A:112:THR:O	1:A:113:LYS:HG2	2.17	0.45
1:A:181:LEU:HD13	1:A:711:VAL:CG2	2.46	0.45
1:A:506:ALA:CB	1:A:706:ILE:HD11	2.46	0.45
1:B:97:MET:HE2	1:B:128:VAL:CG2	2.47	0.45
1:A:258:LEU:O	1:A:262:MET:HE2	2.16	0.44
1:A:466:ASN:O	1:A:467:ALA:C	2.54	0.44
1:A:470:ILE:HG22	1:A:471:SER:N	2.31	0.44
1:A:484:THR:HG22	1:A:485:ASP:N	2.31	0.44
1:A:507:ILE:HG21	1:B:549:LEU:HD11	1.99	0.44
1:A:686:ILE:HA	1:A:689:THR:HG22	1.99	0.44
1:A:711:VAL:HG23	1:A:712:VAL:N	2.32	0.44
1:B:205:ALA:C	1:B:207:LEU:H	2.21	0.44
1:B:623:LEU:O	1:B:627:PHE:HD2	2.00	0.44
1:A:535:LEU:HB3	1:B:540:LEU:HD23	2.00	0.44
1:B:395:GLY:O	1:B:398:SER:CB	2.65	0.44
1:B:708:ILE:HA	1:B:711:VAL:CG2	2.48	0.44
1:A:154:GLN:HB3	1:A:171:PRO:HB2	1.99	0.44
1:A:185:ILE:O	1:A:189:PHE:HD1	2.01	0.44
1:A:347:LEU:HD13	1:A:347:LEU:HA	1.80	0.44
1:A:397:SER:HB2	1:A:404:MET:CE	2.48	0.44
1:B:288:SER:O	1:B:291:ILE:HB	2.17	0.44
1:B:663:LYS:HD3	1:B:688:ASP:CB	2.48	0.44
1:B:666:LEU:O	1:B:669:GLY:N	2.48	0.44
1:B:705:LEU:HD22	1:B:705:LEU:C	2.36	0.44
1:B:80:PHE:CD2	1:B:81:LEU:HD22	2.52	0.44
1:A:419:PRO:N	1:A:420:PRO:HD2	2.32	0.44
1:B:181:LEU:HD13	1:B:711:VAL:CG2	2.48	0.44
1:A:167:ILE:CG2	1:A:167:ILE:O	2.65	0.44
1:A:25:VAL:O	1:A:28:LYS:CB	2.65	0.44
1:A:292:PHE:HB3	1:A:339:LEU:HD21	2.00	0.44
1:A:398:SER:HB2	1:A:680:PRO:O	2.18	0.44
1:B:138:LEU:HD22	1:B:298:LEU:HD23	1.99	0.44
1:B:163:ASN:HB2	1:B:169:PHE:HD2	1.81	0.44
1:B:341:TYR:O	1:B:345:LYS:CB	2.66	0.44
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.61	0.44
1:A:321:LEU:CD1	1:A:321:LEU:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:C	1:A:339:LEU:HD13	2.38	0.44
1:A:341:TYR:O	1:A:345:LYS:CA	2.65	0.44
1:A:424:LEU:O	1:A:428:ILE:CD1	2.59	0.44
1:A:558:PHE:HE1	1:A:701:SER:HB3	1.83	0.44
1:A:87:SER:O	1:A:88:ALA:C	2.56	0.44
1:B:233:ASN:C	1:B:237:VAL:HG22	2.33	0.44
1:B:262:MET:HE2	1:B:262:MET:N	2.33	0.44
1:B:307:TYR:O	1:B:311:LYS:N	2.49	0.44
1:B:62:ILE:O	1:B:65:ALA:HB3	2.17	0.44
1:B:662:ALA:O	1:B:684:LEU:HD23	2.18	0.44
1:B:94:GLY:CA	1:B:129:MET:HA	2.48	0.44
1:A:499:LYS:CE	1:A:695:LYS:O	2.57	0.44
1:A:719:ILE:HG22	1:A:723:VAL:CG1	2.42	0.44
1:A:521:GLN:CA	1:A:721:LYS:HD3	2.47	0.44
1:B:386:TYR:HB3	1:B:391:THR:HG22	1.97	0.44
1:A:545:ILE:CG1	1:B:511:LEU:HD21	2.39	0.44
1:B:261:TYR:CD1	1:B:264:PRO:CG	3.01	0.44
1:B:347:LEU:HD13	1:B:347:LEU:HA	1.77	0.44
1:B:559:SER:OG	1:B:702:LEU:HD21	2.17	0.44
1:A:25:VAL:HB	1:A:97:MET:HE1	1.98	0.44
1:B:129:MET:O	1:B:133:VAL:HG23	2.17	0.44
1:A:15:LEU:HD11	1:A:136:PHE:CD1	2.53	0.43
1:A:702:LEU:HA	1:A:702:LEU:HD12	1.69	0.43
1:A:22:PHE:CA	1:A:97:MET:HE1	2.39	0.43
1:B:82:LEU:HD21	1:B:140:GLY:HA2	1.99	0.43
1:B:185:ILE:O	1:B:189:PHE:HD1	2.01	0.43
1:B:184:SER:CA	1:B:246:GLU:HG3	2.47	0.43
1:B:263:PHE:CE1	1:B:276:HIS:CE1	3.06	0.43
1:B:288:SER:HG	1:B:292:PHE:HE2	1.63	0.43
1:A:169:PHE:HB2	1:A:174:MET:CE	2.42	0.43
1:A:623:LEU:O	1:A:627:PHE:CD2	2.71	0.43
1:B:633:PHE:CE1	1:B:637:VAL:CG2	3.02	0.43
1:A:82:LEU:HD21	1:A:140:GLY:HA2	2.00	0.43
1:A:270:ILE:O	1:A:271:GLY:C	2.57	0.43
1:A:285:ALA:CB	1:A:347:LEU:HD11	2.48	0.43
1:A:122:ALA:O	1:A:463:ILE:HG21	2.17	0.43
1:A:705:LEU:HD11	1:A:709:MET:HE3	2.00	0.43
1:A:708:ILE:HA	1:A:711:VAL:CG2	2.47	0.43
1:B:138:LEU:HA	1:B:138:LEU:HD12	1.68	0.43
1:A:411:SER:CB	1:B:563:ILE:CG2	2.83	0.43
1:A:295:LEU:O	1:A:298:LEU:HD12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLU:OE2	1:A:704:ILE:HG23	2.18	0.43
1:B:248:PHE:CE1	1:B:252:ILE:HD11	2.53	0.43
1:B:334:VAL:CG1	1:B:335:LEU:H	2.32	0.43
1:A:539:MET:HG3	1:B:539:MET:HG2	1.98	0.43
1:B:717:VAL:HG13	1:B:721:LYS:HE2	1.99	0.43
1:A:158:LEU:HD21	1:A:283:ILE:HG21	1.98	0.43
1:B:15:LEU:HG	1:B:135:GLY:HA3	2.00	0.43
1:B:382:TYR:CE1	1:B:389:LYS:HB3	2.52	0.43
1:A:398:SER:HA	1:A:405:VAL:CG1	2.48	0.43
1:A:417:VAL:HG11	1:A:647:MET:CE	2.48	0.43
1:A:325:LEU:HD22	1:A:450:PHE:CE2	2.53	0.43
1:B:72:THR:C	1:B:73:THR:HG23	2.38	0.43
1:B:68:LEU:HD22	1:B:77:GLY:CA	2.49	0.43
1:A:411:SER:HB2	1:B:563:ILE:HG23	1.94	0.43
1:A:551:GLY:HA2	1:A:637:VAL:HG13	2.01	0.43
1:B:158:LEU:C	1:B:158:LEU:HD23	2.39	0.43
1:B:167:ILE:CG2	1:B:167:ILE:O	2.67	0.43
1:B:199:LYS:CG	1:B:696:ASP:CB	2.96	0.43
1:B:337:ALA:N	1:B:363:TRP:CD1	2.87	0.43
1:B:437:LEU:HA	1:B:437:LEU:HD13	1.59	0.43
1:B:97:MET:O	1:B:98:ALA:C	2.55	0.43
1:A:145:TYR:CD1	1:A:291:ILE:HD13	2.54	0.43
1:A:373:GLY:HA3	1:A:447:MET:HG3	2.01	0.43
1:B:326:TRP:CE2	1:B:378:PHE:CZ	3.00	0.43
1:B:448:LEU:HA	1:B:448:LEU:HD12	1.81	0.43
1:A:101:ALA:HB3	1:A:125:GLY:HA3	2.00	0.43
1:A:264:PRO:HG2	1:A:519:PHE:HZ	1.84	0.43
1:B:197:TYR:HE2	1:B:230:VAL:CG2	2.30	0.43
1:B:664:LYS:HA	1:B:664:LYS:HD3	1.80	0.43
1:A:261:TYR:O	1:A:264:PRO:HD2	2.19	0.43
1:A:554:ILE:HG21	1:A:709:MET:HE1	2.00	0.43
1:B:121:VAL:CG1	1:B:122:ALA:H	2.31	0.43
1:B:170:VAL:CG1	1:B:261:TYR:HE2	2.32	0.43
1:B:69:MET:HE2	1:B:74:TRP:CB	2.49	0.43
1:A:191:ARG:O	1:A:195:GLY:N	2.47	0.42
1:A:457:VAL:O	1:A:460:TYR:HB3	2.19	0.42
1:A:65:ALA:HB1	1:A:81:LEU:CD2	2.47	0.42
1:A:720:PHE:CA	1:A:723:VAL:HG12	2.35	0.42
1:A:81:LEU:HA	1:A:81:LEU:HD13	1.72	0.42
1:B:144:VAL:CG1	1:B:176:VAL:HG12	2.49	0.42
1:B:289:TYR:CE1	1:B:339:LEU:HD12	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:OD1	1:B:316:ASN:C	2.57	0.42
1:B:331:LEU:O	1:B:334:VAL:HG12	2.19	0.42
1:B:562:LEU:HD13	1:B:701:SER:CB	2.49	0.42
1:A:148:PHE:CB	1:A:175:THR:HG21	2.49	0.42
1:A:200:ALA:HB1	1:A:570:ALA:HA	2.00	0.42
1:A:289:TYR:CE2	1:A:362:PRO:HB2	2.53	0.42
1:A:72:THR:C	1:A:73:THR:HG23	2.40	0.42
1:B:200:ALA:HB1	1:B:570:ALA:CA	2.48	0.42
1:A:22:PHE:O	1:A:26:VAL:N	2.40	0.42
1:A:301:SER:CB	1:A:452:ALA:HB3	2.50	0.42
1:A:684:LEU:HD12	1:A:684:LEU:HA	1.41	0.42
1:B:261:TYR:HD1	1:B:264:PRO:HD2	1.84	0.42
1:B:263:PHE:O	1:B:267:VAL:HG23	2.19	0.42
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.59	0.42
1:B:517:TYR:OH	1:B:634:VAL:CG2	2.62	0.42
1:B:684:LEU:HA	1:B:684:LEU:HD12	1.46	0.42
1:B:68:LEU:HD21	1:B:76:THR:CG2	2.49	0.42
1:B:77:GLY:O	1:B:80:PHE:HB3	2.20	0.42
1:A:138:LEU:HD23	1:A:298:LEU:CD2	2.50	0.42
1:A:261:TYR:CD1	1:A:519:PHE:CZ	3.07	0.42
1:B:623:LEU:O	1:B:627:PHE:CD2	2.72	0.42
1:A:322:ASN:O	1:A:326:TRP:CD1	2.73	0.42
1:B:101:ALA:HB3	1:B:125:GLY:HA3	2.01	0.42
1:A:540:LEU:HD23	1:B:535:LEU:HD23	2.01	0.42
1:B:558:PHE:O	1:B:562:LEU:HG	2.20	0.42
1:B:72:THR:O	1:B:73:THR:HG22	2.19	0.42
1:A:321:LEU:CD1	1:A:321:LEU:H	2.33	0.42
1:A:431:ALA:HB1	1:A:443:ALA:CB	2.49	0.42
1:B:261:TYR:CD1	1:B:264:PRO:HD2	2.54	0.42
1:A:10:ILE:N	1:A:11:PRO:HD3	2.34	0.42
1:A:343:TYR:O	1:A:344:LEU:HD23	2.20	0.42
1:A:699:GLY:N	1:A:700:PRO:CD	2.81	0.42
1:B:358:GLY:O	1:B:359:ALA:CB	2.67	0.42
1:B:417:VAL:HG22	1:B:650:ILE:HB	2.02	0.42
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.87	0.42
1:A:289:TYR:CG	1:A:344:LEU:HD11	2.54	0.42
1:A:666:LEU:O	1:A:669:GLY:N	2.50	0.42
1:A:669:GLY:O	1:A:670:ASN:HB2	2.19	0.42
1:B:263:PHE:HB2	1:B:283:ILE:CD1	2.49	0.42
1:B:339:LEU:C	1:B:339:LEU:CD1	2.88	0.42
1:B:461:GLY:O	1:B:465:ASP:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ILE:HG22	1:B:564:SER:H	1.85	0.42
1:B:667:GLU:HG2	1:B:681:HIS:CD2	2.55	0.42
1:B:677:GLY:O	1:B:678:SER:CB	2.66	0.42
1:A:282:THR:HA	1:A:347:LEU:CD1	2.45	0.42
1:A:337:ALA:HB2	1:A:363:TRP:NE1	2.34	0.42
1:A:422:LEU:O	1:A:422:LEU:HD22	2.20	0.42
1:A:616:PHE:C	1:A:616:PHE:CD1	2.93	0.42
1:A:6:LEU:O	1:A:10:ILE:CD1	2.68	0.42
1:B:15:LEU:CD2	1:B:135:GLY:HA3	2.49	0.42
1:B:398:SER:OG	1:B:684:LEU:CD2	2.68	0.42
1:B:422:LEU:O	1:B:422:LEU:HD22	2.20	0.42
1:B:7:PHE:HA	1:B:10:ILE:HD13	2.02	0.42
1:A:526:ASP:C	1:A:528:GLY:H	2.24	0.42
1:A:71:PHE:O	1:A:167:ILE:CD1	2.68	0.42
1:B:72:THR:C	1:B:73:THR:CG2	2.88	0.42
1:A:329:ALA:O	1:A:333:VAL:HG23	2.20	0.41
1:A:286:LEU:HD13	1:A:353:LEU:HG	2.01	0.41
1:A:705:LEU:CD2	1:A:705:LEU:O	2.68	0.41
1:B:189:PHE:CD2	1:B:611:MET:SD	3.13	0.41
1:B:266:TYR:O	1:B:267:VAL:C	2.57	0.41
1:B:616:PHE:CD1	1:B:616:PHE:C	2.93	0.41
1:B:72:THR:O	1:B:73:THR:CG2	2.68	0.41
1:A:192:VAL:HG11	1:A:614:PRO:HG2	2.00	0.41
1:A:200:ALA:CB	1:A:570:ALA:HB2	2.50	0.41
1:A:363:TRP:CZ2	1:A:367:ILE:CD1	3.02	0.41
1:A:370:ILE:HG12	1:A:446:GLY:O	2.21	0.41
1:B:366:ALA:O	1:B:370:ILE:HG13	2.20	0.41
1:A:259:ALA:CB	1:A:287:ILE:CG1	2.99	0.41
1:A:627:PHE:CD1	1:A:720:PHE:HB3	2.56	0.41
1:B:198:THR:O	1:B:201:ALA:HB3	2.20	0.41
1:B:663:LYS:HD3	1:B:688:ASP:HB3	2.02	0.41
1:A:151:TRP:CE3	1:A:152:MET:HG2	2.55	0.41
1:A:337:ALA:HA	1:A:363:TRP:CD1	2.56	0.41
1:A:79:ALA:O	1:A:82:LEU:HB3	2.20	0.41
1:B:140:GLY:O	1:B:143:LEU:HB2	2.21	0.41
1:B:261:TYR:CE1	1:B:264:PRO:CG	3.03	0.41
1:B:382:TYR:O	1:B:382:TYR:CD1	2.73	0.41
1:A:448:LEU:C	1:A:450:PHE:H	2.23	0.41
1:A:613:TYR:HB3	1:A:614:PRO:HD3	2.02	0.41
1:B:289:TYR:HH	1:B:293:PHE:HD2	1.67	0.41
1:B:282:THR:HA	1:B:347:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:HB3	1:B:390:PRO:HD3	2.03	0.41
1:A:300:CYS:SG	1:A:332:THR:HA	2.60	0.41
1:A:373:GLY:CA	1:A:447:MET:HG3	2.50	0.41
1:B:170:VAL:CG1	1:B:261:TYR:CE2	3.03	0.41
1:B:81:LEU:HA	1:B:81:LEU:HD13	1.65	0.41
1:A:86:MET:CE	1:A:139:LEU:HD23	2.50	0.41
1:A:185:ILE:HG23	1:A:189:PHE:CE1	2.55	0.41
1:A:259:ALA:HB1	1:A:287:ILE:HG13	2.01	0.41
1:A:413:GLY:O	1:A:416:SER:HB3	2.21	0.41
1:A:717:VAL:HG13	1:A:721:LYS:HE2	2.03	0.41
1:B:460:TYR:OH	1:B:487:LEU:HA	2.20	0.41
1:A:553:ALA:CA	1:B:647:MET:HE1	2.48	0.41
1:A:154:GLN:NE2	1:A:171:PRO:C	2.74	0.41
1:A:282:THR:O	1:A:286:LEU:HG	2.21	0.41
1:A:370:ILE:CG1	1:A:446:GLY:O	2.69	0.41
1:A:72:THR:O	1:A:73:THR:HG22	2.21	0.41
1:B:619:ILE:O	1:B:622:PRO:HD2	2.21	0.41
1:B:649:ALA:HA	1:B:699:GLY:CA	2.51	0.41
1:B:87:SER:O	1:B:88:ALA:C	2.58	0.41
1:A:138:LEU:CD2	1:A:298:LEU:HD23	2.51	0.41
1:A:198:THR:HG22	1:A:231:GLY:C	2.41	0.41
1:A:288:SER:CB	1:A:292:PHE:CE2	3.04	0.41
1:A:138:LEU:HD23	1:A:298:LEU:HD21	2.03	0.41
1:A:410:LEU:HD12	1:A:410:LEU:HA	1.81	0.41
1:A:538:ASN:O	1:A:544:VAL:HG21	2.20	0.41
1:A:67:LEU:CD1	1:A:71:PHE:HE2	2.32	0.41
1:A:72:THR:C	1:A:73:THR:CG2	2.89	0.41
1:A:72:THR:O	1:A:73:THR:CG2	2.69	0.41
1:A:77:GLY:O	1:A:80:PHE:HB3	2.21	0.41
1:B:413:GLY:O	1:B:417:VAL:HG23	2.21	0.41
1:B:494:THR:HA	1:B:497:ILE:HD12	2.03	0.41
1:A:317:PRO:HA	1:A:320:GLU:CD	2.41	0.41
1:A:341:TYR:O	1:A:345:LYS:CB	2.68	0.41
1:A:523:SER:HB3	1:A:524:PRO:HD2	2.03	0.41
1:A:561:TYR:CE2	1:A:613:TYR:HB3	2.56	0.41
1:A:605:ASP:OD1	1:A:609:LYS:HD2	2.21	0.41
1:A:619:ILE:HD12	1:A:712:VAL:HG21	2.03	0.41
1:A:652:THR:HB	1:A:694:LEU:C	2.42	0.41
1:A:68:LEU:HD22	1:A:77:GLY:CA	2.51	0.41
1:B:129:MET:SD	1:B:459:SER:CB	3.06	0.41
1:B:168:ASN:ND2	1:B:168:ASN:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:THR:O	1:B:336:THR:CB	2.69	0.41
1:B:651:LEU:O	1:B:655:SER:HB3	2.20	0.41
1:A:337:ALA:HB2	1:A:363:TRP:CZ2	2.55	0.40
1:A:357:PHE:CE1	1:A:434:PHE:HD1	2.39	0.40
1:A:448:LEU:HA	1:A:448:LEU:HD12	1.77	0.40
1:A:69:MET:HE3	1:A:74:TRP:O	2.20	0.40
1:B:163:ASN:ND2	1:B:164:TRP:H	2.19	0.40
1:A:563:ILE:HG21	1:A:563:ILE:HD13	1.91	0.40
1:A:53:GLU:HA	1:A:608:LEU:HD11	2.04	0.40
1:A:624:VAL:O	1:A:628:LEU:HD13	2.21	0.40
1:A:553:ALA:HB1	1:B:418:PHE:CD1	2.56	0.40
1:B:679:GLU:N	1:B:680:PRO:CD	2.84	0.40
1:A:310:VAL:CG1	1:A:310:VAL:O	2.69	0.40
1:A:339:LEU:O	1:A:343:TYR:HB2	2.21	0.40
1:A:357:PHE:HZ	1:A:364:PHE:HB2	1.85	0.40
1:A:386:TYR:C	1:A:386:TYR:CD1	2.93	0.40
1:A:437:LEU:O	1:A:440:VAL:HB	2.21	0.40
1:A:503:ILE:HD13	1:A:649:ALA:HB1	2.01	0.40
1:B:460:TYR:C	1:B:463:ILE:HG22	2.40	0.40
1:B:603:THR:HA	1:B:606:ASN:HB3	2.04	0.40
1:B:626:GLY:CA	1:B:634:VAL:HG13	2.51	0.40
1:B:719:ILE:HG22	1:B:723:VAL:CG1	2.45	0.40
1:B:87:SER:OG	1:B:186:ILE:HG21	2.21	0.40
1:B:50:LEU:HD13	1:B:50:LEU:HA	1.91	0.40
1:A:354:GLY:O	1:A:435:ALA:CA	2.69	0.40
1:A:450:PHE:HZ	1:A:501:PHE:CE2	2.35	0.40
1:B:122:ALA:O	1:B:463:ILE:HG21	2.21	0.40
1:B:523:SER:HB3	1:B:524:PRO:HD2	2.03	0.40
1:B:521:GLN:C	1:B:523:SER:N	2.73	0.40
1:B:622:PRO:HG3	1:B:709:MET:CG	2.51	0.40
1:B:517:TYR:CE1	1:B:717:VAL:HG11	2.56	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	643/735 (88%)	579 (90%)	42 (6%)	22 (3%)	3	30
1	B	626/735 (85%)	566 (90%)	37 (6%)	23 (4%)	3	28
All	All	1269/1470 (86%)	1145 (90%)	79 (6%)	45 (4%)	3	29

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	TYR
1	A	74	TRP
1	A	163	ASN
1	A	260	SER
1	A	269	LYS
1	A	298	LEU
1	A	359	ALA
1	A	402	THR
1	A	522	ILE
1	A	527	ILE
1	A	672	GLU
1	B	41	TYR
1	B	74	TRP
1	B	158	LEU
1	B	163	ASN
1	B	268	GLN
1	B	269	LYS
1	B	298	LEU
1	B	402	THR
1	B	522	ILE
1	B	527	ILE
1	A	159	ASN
1	A	297	GLY
1	A	358	GLY
1	A	387	ARG
1	A	435	ALA
1	B	159	ASN
1	B	260	SER
1	B	297	GLY
1	B	359	ALA
1	B	387	ARG
1	B	435	ALA
1	B	676	LYS

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Mol	Chain	Res	Type
1	A	449	SER
1	B	166	GLY
1	A	27	ARG
1	A	166	GLY
1	A	678	SER
1	B	168	ASN
1	A	389	LYS
1	A	470	ILE
1	B	27	ARG
1	B	389	LYS
1	B	523	SER
1	B	675	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	482/575 (84%)	428 (89%)	54 (11%)	6	25
1	B	460/575 (80%)	411 (89%)	49 (11%)	6	27
All	All	942/1150 (82%)	839 (89%)	103 (11%)	6	26

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	48	SER
1	A	50	LEU
1	A	57	ILE
1	A	67	LEU
1	A	82	LEU
1	A	86	MET
1	A	97	MET
1	A	103	VAL
1	A	110	ARG
1	A	124	GLN

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Mol	Chain	Res	Type
1	A	138	LEU
1	A	162	THR
1	A	186	ILE
1	A	199	LYS
1	A	240	LEU
1	A	263	PHE
1	A	267	VAL
1	A	268	GLN
1	A	274	LEU
1	A	298	LEU
1	A	314	SER
1	A	315	ASP
1	A	324	SER
1	A	339	LEU
1	A	347	LEU
1	A	353	LEU
1	A	375	LEU
1	A	389	LYS
1	A	404	MET
1	A	407	SER
1	A	410	LEU
1	A	422	LEU
1	A	437	LEU
1	A	448	LEU
1	A	484	THR
1	A	508	PHE
1	A	533	LEU
1	A	536	LEU
1	A	537	LEU
1	A	550	LEU
1	A	563	ILE
1	A	564	SER
1	A	609	LYS
1	A	613	TYR
1	A	619	ILE
1	A	638	LEU
1	A	666	LEU
1	A	679	GLU
1	A	684	LEU
1	A	702	LEU
1	A	705	LEU
1	A	722	HIS

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Mol	Chain	Res	Type
1	A	725	LEU
1	B	13	VAL
1	B	48	SER
1	B	50	LEU
1	B	57	ILE
1	B	82	LEU
1	B	86	MET
1	B	97	MET
1	B	102	ASN
1	B	103	VAL
1	B	112	THR
1	B	124	GLN
1	B	138	LEU
1	B	143	LEU
1	B	158	LEU
1	B	162	THR
1	B	163	ASN
1	B	168	ASN
1	B	186	ILE
1	B	230	VAL
1	B	240	LEU
1	B	298	LEU
1	B	339	LEU
1	B	347	LEU
1	B	375	LEU
1	B	382	TYR
1	B	410	LEU
1	B	422	LEU
1	B	429	LEU
1	B	437	LEU
1	B	448	LEU
1	B	460	TYR
1	B	484	THR
1	B	508	PHE
1	B	533	LEU
1	B	536	LEU
1	B	537	LEU
1	B	539	MET
1	B	540	LEU
1	B	550	LEU
1	B	571	MET
1	B	609	LYS

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Mol	Chain	Res	Type
1	B	619	ILE
1	B	638	LEU
1	B	655	SER
1	B	666	LEU
1	B	684	LEU
1	B	702	LEU
1	B	705	LEU
1	B	722	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	229	ASN
1	A	233	ASN
1	A	408	ASN
1	A	466	ASN
1	A	521	GLN
1	A	661	ASN
1	B	233	ASN
1	B	466	ASN
1	B	521	GLN
1	B	661	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PO4	A	1727	3	4,4,4	0.92	0	6,6,6	0.40	0
2	PO4	B	1727	3	4,4,4	0.93	0	6,6,6	0.47	0
2	PO4	B	1728	3,4	4,4,4	0.93	0	6,6,6	0.40	0
2	PO4	A	1728	3,4	4,4,4	0.94	0	6,6,6	0.48	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1727	PO4	1	0
2	B	1728	PO4	4	0
2	A	1728	PO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	655/735 (89%)	0.00	23 (3%)	44	35	92, 214, 365, 540	0
1	B	642/735 (87%)	0.08	36 (5%)	24	21	77, 244, 418, 583	0
All	All	1297/1470 (88%)	0.04	59 (4%)	33	27	77, 228, 390, 583	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	SER	10.6
1	B	315	ASP	6.9
1	A	315	ASP	6.5
1	B	313	PRO	5.6
1	A	348	GLN	4.8
1	B	205	ALA	4.8
1	A	527	ILE	4.6
1	A	168	ASN	4.5
1	B	726	PHE	4.2
1	A	314	SER	4.1
1	B	570	ALA	4.0
1	A	528	GLY	3.9
1	B	528	GLY	3.9
1	A	601	GLU	3.7
1	A	42	ILE	3.6
1	B	309	ILE	3.5
1	A	152	MET	3.4
1	A	726	PHE	3.4
1	A	233	ASN	3.4
1	B	120	LYS	3.2
1	B	155	VAL	3.1
1	B	236	ASP	3.1
1	B	312	LYS	3.1
1	B	38	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	306	LEU	3.0
1	B	527	ILE	3.0
1	B	233	ASN	3.0
1	B	274	LEU	2.9
1	B	271	GLY	2.8
1	A	347	LEU	2.8
1	A	675	GLY	2.7
1	B	725	LEU	2.7
1	B	235	GLY	2.7
1	B	237	VAL	2.7
1	B	273	ASN	2.7
1	A	120	LYS	2.6
1	A	160	ILE	2.6
1	B	40	SER	2.6
1	B	310	VAL	2.5
1	B	111	THR	2.5
1	A	317	PRO	2.5
1	A	483	ILE	2.5
1	B	168	ASN	2.5
1	A	600	ILE	2.5
1	A	644	SER	2.5
1	B	109	ALA	2.5
1	A	7	PHE	2.4
1	B	39	SER	2.4
1	B	466	ASN	2.4
1	B	124	GLN	2.4
1	B	100	ARG	2.4
1	B	571	MET	2.3
1	B	108	ALA	2.3
1	A	466	ASN	2.2
1	B	166	GLY	2.1
1	A	272	GLU	2.1
1	A	110	ARG	2.1
1	B	42	ILE	2.1
1	B	272	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1732	1/1	0.37	0.13	220,220,220,220	0
3	MG	B	1731	1/1	0.63	0.22	269,269,269,269	0
3	MG	B	1732	1/1	0.73	0.09	184,184,184,184	0
3	MG	A	1730	1/1	0.78	0.15	194,194,194,194	0
2	PO4	A	1727	5/5	0.78	0.20	348,350,350,352	0
3	MG	B	1729	1/1	0.80	0.17	133,133,133,133	0
3	MG	B	1730	1/1	0.80	0.23	124,124,124,124	0
4	K	A	1733	1/1	0.82	0.36	151,151,151,151	0
2	PO4	B	1727	5/5	0.83	0.20	294,296,296,296	0
4	K	B	1733	1/1	0.84	0.22	151,151,151,151	0
2	PO4	B	1728	5/5	0.85	0.17	209,217,220,220	0
3	MG	A	1731	1/1	0.89	0.18	213,213,213,213	0
3	MG	A	1729	1/1	0.90	0.22	170,170,170,170	0
2	PO4	A	1728	5/5	0.91	0.15	184,205,210,217	0

6.5 Other polymers (i)

There are no such residues in this entry.